Spontaneous particle creation in time-dependent overcritical fields of QED

Dissertation
zur Erlangung des Doktorgrades
der Naturwissenschaften

vorgelegt beim Fachbereich Physik
der Johann Wolfgang Goethe – Universität
in Frankfurt am Main

von
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aus Bielsko-Biała, Polen

Frankfurt 2005

vom Fachbereich .....der

Johann Wolfgang Goethe – Universität als Dissertation angenommen.

Dekan: .....

Gutachter: .....

Datum der Disputation: .....

Abstract

In the classical Dirac equation with strong potentials, called overcritical, a bound state reaches the negative continuum. In QED the presence of a static overcritical external electric field leads to a charged vacuum and indicates spontaneous particle creation when the overcritical field is switched on. The goal of this work is to clarify whether this effect exists, i.e. if it can be uniquely defined and proved, in time-dependent physical processes. Starting from a fundamental level of the theory we check all mathematical and interpretational steps from the algebra of fields to the very effect.

In the first, theoretical part of this thesis we introduce the mathematical formulation of the classical and quantized Dirac theory with their most important results. Using this language we define rigorously the notion of spontaneous particle creation in overcritical fields. First, we give a rigorous definition of resonances as poles of the resolvent or the Green's function and show how eigenvalues become resonances under Hamiltonian perturbations. In particular, we consider essential for overcritical potentials perturbation of eigenvalues at the edge of the continuous spectrum. Next, we gather various adiabatic theorems and discuss well-posedness of the scattering in the adiabatic limit. Then, we construct Fock space representations of the field algebra, study their equivalence and give a unitary implementer of all Bogoliubov transformations induced by unitary transformations of the one-particle Hilbert space as well as by the projector (or vacuum vector) changes as long as they lead to unitarily equivalent Fock representations. We implement in Fock space self-adjoint and unitary operators from the one-particle space, discussing the charge, energy, evolution and scattering operators. Then we introduce the notion of particles and several particle interpretations for time-dependent processes with a different Fock space at every instant of time. We study how the charge, energy and number of particles change in consequence of a change of representation or in implemented evolution or scattering processes, what is especially interesting in presence of overcritical potentials. Using this language we define rigorously the notion of spontaneous particle creation. Then we look for physical processes which show the effect of vacuum decay and spontaneous particle creation exclusively due to the overcriticality of the potential. We consider several processes with static as well as suddenly switched on (and off) static overcritical potentials and conclude that they are unsatisfactory for observation of the spontaneous particle creation. Next, we consider properties of general time-dependent scattering processes with continuous switch on (and

off) of an overcritical potential and show that they also fail to produce stable signatures of the particle creation due to overcriticality. Further, we study and successfully define the spontaneous particle creation in adiabatic processes, where the spontaneous antiparticle is created as a result of a resonance (wave packet) decay in the negative continuum. Unfortunately, they lead to physically questionable pair production as the adiabatic limit is approached. Finally, we consider extension of these ideas to non-adiabatic processes involving overcritical potentials and argue that they are the best candidate for showing the spontaneous pair creation in physical processes. Demanding creation of the spontaneous antiparticle in the state corresponding to the overcritical resonance rather quick than slow processes should be considered, with a possibly long frozen overcritical period.

In the second part of this thesis we concentrate on a class of spherically symmetric square well potentials with a time-dependent depth. First, we solve the Dirac equation and analyze the structure and behaviour of bound states and appearance of overcriticality. Then, by analytic continuation we find and discuss the behaviour of resonances in overcritical potentials. Next, we derive and solve numerically (introducing a non-uniform continuum discretization for a consistent treatment of narrow peaks) a system of differential equations (coupled channel equations) to calculate particle and antiparticle production spectra for various time-dependent processes including sudden, quick, slow switch on and off of a sub- and overcritical potentials. We discuss in detail how and under which conditions an overcritical resonance decays during the evolution giving rise to the spontaneous production of an antiparticle. We compare the antiparticle production spectrum with the shape of the resonance in the overcritical potential. We study processes, where the overcritical potentials are switched on at different speed and are possibly frozen in the overcritical phase. We prove, in agreement with conclusions of the theoretical part, that the peak (wave packet) in the negative continuum representing a dived bound state partially follows the moving resonance and partially decays at every stage of its evolution. This continuous decay is more intensive in slow processes, while in quick processes the wave packet more precisely follows the resonance. In the adiabatic limit, the whole decay occurs already at the edge of the continuum, resulting in production of antiparticles with vanishing momentum. In contrast, in quick switch on processes with delay in the overcritical phase, the spectrum of the created antiparticles agrees best with the shape of the resonance. Finally, we address the question how much information about the time-dependent potential can be reconstructed from the scattering data, represented by the particle production spectrum. We propose a simple approximation method (master equation) basing on an exponential, decoherent decay of time-dependent resonances for prediction of particle creation spectra and obtain a good agreement with the results of full numerical calculations.

Additionally, we discuss various sources of errors introduced by the numerical discretization, find estimations for them and prove convergence of the numerical schemes.

"Everything should be made as simple as possible, but not simpler."
A. Einstein

Summary and Preface

The goal of this work is to clarify whether the effect of spontaneous particle creation exists in physical processes. More precisely, if it can be uniquely defined and proved. Since the considerations are made on the fundamental level, it is necessary to check all mathematical as well as interpretational steps in the construction of the theory from the algebra of fields to the very effect. We have observed in the literature that most of the discrepancies in opinions are due to the different frameworks chosen (e.g. Greiner, Scharf), like definition and measure of the effect, particle interpretation, and choice of the algebra representation (projectors).

In construction of the theory of a quantum Dirac field, describing electrons and positrons in an external electromagnetic field, one encounters the following questions and difficulties. Which of all possible representations of the canonical anticommutation relations (CAR) are physically plausible and which of them are unitarily equivalent? Representations via operators in a Hilbert space seem quite natural and the addition of a reference state (vacuum) makes them irreducible what is physically plausible. Despite these restrictions, there remains a freedom in the choice of a projector defining the distinction between particles and antiparticles. Although it can be chosen freely in the theory, not all choices lead to the same physics. Some choices keep the physical results untouched (unitarily equivalent representations) and some not (nonequivalent representations). It is the point – unfortunately very rarely discussed in the textbooks – where physical arguments must be used in order to guarantee the uniqueness of the constructed theory, e.g. that vacuum is chosen as an energetic ground state in Fock space. This definition is unique if the Hamiltonian, and thus the electromagnetic field, is static. If it is not, then there is no unique vacuum state and hence no unique particle interpretation. They can be restored asymptotically if the Hamiltonian is asymptotically (far past or future) static. Although the particle definition can then be extended to the whole time axis, it is a purely formal step and cannot serve as a real particle interpretation – this is possible only asymptotically ("in" and "out" interpretations).

Overcriticality in Fock space is a complex problem. Hamiltonians with potentials of different strength lead to different projectors and different vacua being always a ground state of the actual Hamiltonian. As long as potentials are weak, these vacua are similar. However, at some value of the strength of the potential, called critical, the corresponding

vacuum becomes charged with respect to the free vacuum. Consequently, the free vacuum becomes a one-antiparticle state with respect to the overcritical one. We call this phenomenon *weak overcriticality* since it appears as the lowest bound state of the potential crosses the line $E = 0$ and the corresponding eigenfunction changes subspace from particle to antiparticle. There appears a question, if this phenomenon corresponds to any physical (evolution, scattering) process, because, as described above, it concerns a purely static situation. Therefore, a description of time-dependent processes in Fock space is needed.

Time-evolution in Fock space is defined by implementation of the classical evolution operator as a unitary operator in Fock space. This is not a trivial operation and not always possible. It describes dynamical particle creation and annihilation processes, and problems occur when the production rate becomes too big. This happens for infinitely long lasting processes (e.g. scattering) in presence of potentials, which are supposed to produce particles continuously (Klein's paradox, Schwinger's effect). In such cases the external field approximation of QED breaks down and one has to use the full QED in order to include the backreaction effects on the quantum electromagnetic field. If the evolution or scattering process is implementable, the implementer (unitary operator in Fock space) carries the whole information about creation and annihilation of particles in this process. Its structure has two main parts. The first describes creation and annihilation of particle-antiparticle pairs and hence does not change the total charge of a state. The second describes creation and annihilation of single particles (as in the changeover from the free to the overcritical vacuum), called in this work *special*. It may change the total charge, when measured with respect to the final vacuum. Hence, a change from the initial to the final vacuum is necessary to see this effect, what is the case only when the initial and final potentials are different. Processes with equal initial and final value of the potential (e.g. asymptotic vanishing in scattering processes) cannot change the total charge, but still may create *special* particles and antiparticles in pairs. Therefore, creation of special (anti-)particles (in short: *special creation*) seems to be a candidate for the mathematical definition of *overcritical* or *spontaneous particle creation*. However, first, it turns out that special creation may occur independently of overcriticality of the potential, although in such cases it is very unstable under small variations of the potential (actually, an arbitrarily small change of the potential destroys such special creation). Second, even in presence of the overcritical potentials the special creation is unstable in the same way, independently of whether the potential is switched on and off or only on during the scattering process. The meaning of special creation can be rescued by considering adiabatic processes, which turn out to be free from the above instabilities. Moreover, in adiabatic scattering no special creation occurs until the energy of the lowest bound state reaches and dissolves in the negative continuum, what we call *strong overcriticality*. In the adiabatic situation special creation is equivalent to and can be used as a definition of the *spontaneous particle creation*. The special antiparticle is created as a result of a resonance (wave packet) decay in the negative continuum. Unfortunately, due to the slowness of the adiabatic processes, the

wave packet, which describes the dissolved bound state, decays fully already at the edge of the continuum, giving rise to production of antiparticles with vanishing momentum. This result is not quite satisfactory physically, but the adiabatic limit itself is not a physical situation, either. Therefore, there is a need to extend the definition of spontaneous particle creation beyond the adiabatic limit. It is not a simple task, because the key property, namely the special creation, usually gets lost. Yet, by continuity, slow processes do not differ much from the adiabatic limit and corresponding particles are still produced with big probabilities. Alternatively, one can try to specify the spontaneous particle creation by demanding creation of an antiparticle in the state corresponding to the resonance being a remnant of the dissolved bound state. Then, rather quick than slow processes should be considered, with a possibly long delayed overcritical period in the evolution.

We study numerically all these questions in the case of a time-dependent spherically symmetric square well potential with varying depth. On the one hand, it is the mathematically simplest potential for which the Dirac equation can be solved analytically. On the other hand, it shows overcriticality for depths beyond some threshold where bound states become resonances. We show existence of the resonances by analysis of the complex poles of the resolvent and the Green's function as well as by observation of peaks in the negative continuum giving rise to wave packets representing the dived bound states. In overcritical potentials the vacuum becomes charged with respect to the free vacuum, what we show both by calculating the expectation value of the charge operator and by study of the vacuum polarization charge density.

We implement scattering in several time-dependent processes in the Fock space and calculate numerically particle and antiparticle production spectra by solving the coupled channel equations. We compare the situations of subcritical, weakly and strongly overcritical potentials in sudden, quick, slow and adiabatic evolutions. In subcritical processes only dynamical particle production occurs, which vanishes in the adiabatic limit. In processes where a weakly overcritical potential is switched on, depending on the definition of the vacuum and particle interpretation, the vacuum may spontaneously get charged and there may appear a spontaneously created bound antiparticle, which together with the vacuum forms an electrically neutral state. After switching off the antiparticle disappears and the vacuum becomes neutral again. In contrary, after switching on a strongly overcritical potential the spontaneously charged vacuum gets accompanied by a spontaneously created antiparticle in a scattering state. If the overcritical phase persists for some time the antiparticle departs from the source (support of the potential) leaving the charged vacuum behind. Final switching off creates an additional particle, mostly in a bound state, thus giving rise to a *spontaneous pair creation*.

In very slow processes we observe the movement of the resonance peak in the negative continuum during the evolution. It partially decays at every stage. Approaching the adiabatic limit, the peak decays fully already near the continuum's edge. Observation of this effect presents a numerical challenge, because the peaks near the edge are extremely

narrow. In contrast, in quick processes the resonance peak moves in the continuum without much loss due to the own decay, but some part of its amplitude gets lost to the rest of the continuum causing dynamical creation of pairs. Comparing the two scenarios, our numerical evidence shows that quick switch on and off processes with a prolonged overcritical phase are more favorable for producing antiparticles with an energy spectrum corresponding to the resonance position in the prolonged (mostly deepest) potential.

Modeling in some approximation the process of decay of a resonance peak during the evolution we provide a method for inverse scattering, i.e. the time-dependence of the potential can be, via the time-dependence of the resonance position and width, read off from the antiparticle production spectrum. A simple model of an exponential, decoherent decay of peaks gives surprisingly good estimations for the antiparticle production spectrum.

Recommended literature

For the theory of the Dirac equation we refer to Thaller [Tha92]. For rigorous mathematical basis in functional analysis, operator analysis and scattering theory we refer to Reed and Simon I-IV [RS72, RS75, RS79, RS78] and in less extensive version to Richtmyer [Ric78]. In German we recommend also Weidmann [Wei03].

For an extensive survey on theory and experiments regarding QED in strong fields we refer to the monograph of Greiner, Müller and Rafelski [GMR85] and in case of relativistic atomic collisions to the monograph of Eichler and Meyerhof [EM95] as well as to the reviews of Reinhardt and Greiner [RG77], Rafelski, Fulcher and Klein [RFK78], and Müller-Nehler and Soff [MNS94]. For more detailed calculations regarding unstable vacuum in full QED we refer to [FGS91].

Other articles, single chapters of books and theses are referred to during the whole work and are listed at the end.

Acknowledgements

I want to express my thanks to my supervisor Prof. Walter Greiner for raising the problem of spontaneous particle creation and multiple support during my whole work at the Institute for Theoretical Physics of the University Frankfurt am Main. I am grateful to Dr. Joachim Reinhardt for various kinds of help and support and to Dr. Piotr Marecki for many fruitful discussions. Moreover, I want to thank to Dr. Dennis Dietrich for careful reading of the manuscript. Financial support of *Deutsche Forschungsgemeinschaft (Graduierter Kolleg)* and *Hessische Landesgraduiertenförderung* is also gratefully acknowledged. My thanks go also to the *Herrmann–Willkomm–Stiftung*, to *Vereinigung von Freunden und Förderern der JWG–Universität Frankfurt am Main* and to *WE–Heraeus–Förderprogramms der DPG* for their financial support allowing me participation in many conferences. Finally, I want to thank to my wife Ewa for her patience and support during my work on this thesis.

Frankfurt am Main, November 2005 *Nikodem Szpak*

Zusammenfassung

Das Ziel dieser Arbeit ist es zu klären, ob der Effekt der spontanen Teilchenerzeugung in physikalischen Prozessen existiert. Genauer, ob er eindeutig definiert und bewiesen werden kann. Da die Überlegungen auf einem fundamentalen Niveau gemacht werden, ist es notwendig, alle sowohl mathematischen als auch interpretationellen Schritte in der Konstruktion der Theorie zu prüfen, von der Algebra der Felder bis zu dem studierten Effekt selbst. Wir haben beobachtet, dass die meisten Meinungsverschiedenheiten in der Literatur (z.B. Greiner, Scharf) auf unterschiedlich gewählten Ansätzen beruhen, wie die Definition und das Maß des Effektes, Teilcheninterpretation und die Wahl der Darstellung der Algebra (Projektoren).

In der Konstruktion der Theorie des Dirac-Quantenfeldes, die Elektronen und Positronen in einem externen elektromagnetischen Potential beschreibt, stößt man auf folgende Fragen und Schwierigkeiten. Welche von allen möglichen Darstellungen der kanonischen Antikommutations-Relationen sind physikalisch plausibel und welche davon sind unitär äquivalent? Darstellungen durch Operatoren in einem Hilbert Raum scheinen ganz natürlich zu sein und die Einführung eines Bezugszustands (Vakuum) macht sie irreduzibel, was physikalisch plausibel ist. Trotz dieser Beschränkungen bleibt eine Freiheit in der Wahl des Projektors, der die Unterscheidung zwischen Teilchen und Antiteilchen definiert. Obwohl er in der Theorie frei gewählt werden kann, führen nicht alle Wahlen zu der gleichen Physik. Einige Wahlen lassen die physikalischen Ergebnisse unberührt (unitär äquivalente Darstellungen) und einige andere nicht (nicht äquivalente Darstellungen). Dies ist der Punkt – leider sehr selten diskutiert in den Lehrbüchern – wo physikalische Argumente müssen benutzt werden, um die Eindeutigkeit der konstruierten Theorie zu garantieren, z.B. dass das Vakuum als der energetische Grundzustand im Fock Raum gewählt wird. Diese Definition ist eindeutig wenn der Hamiltonian, und somit das elektromagnetische Feld, statisch ist. Wenn nicht, dann es gibt keinen eindeutigen Vakuumzustand und deswegen keine eindeutige Teilcheninterpretation. Diese können asymptotisch wiederhergestellt werden, wenn der Hamiltonian asymptotisch (weite Vergangenheit oder Zukunft) statisch ist. Obwohl die Teilcheninterpretation auf die ganze Zeitachse erweitert werden kann, ist es nur ein rein formaler Schritt und kann nicht als wirkliche Teilcheninterpretation dienen – das ist nur asymptotisch möglich ("in" und "out" Interpretationen).

Überkritikalität im Fock Raum ist ein komplexes Problem. Hamiltonians mit Poten-

tialen von verschiedenen Stärken führen zu verschiedenen Projektoren und verschiedenen Vakua, die immer Grundzustände der aktuellen Hamiltonians sind. Solange wie die Potentiale schwach sind, sind diese Vakua ähnlich. Bei einem, so genannten kritischen, Wert der Stärke des Potentials, wird das entsprechende Vakuum jedoch geladen gegenüber dem freien Vakuum. Entsprechend, wird das freie Vakuum ein Ein-Antiteilchen Zustand gegenüber dem überkritischen. Wir nennen dieses Phänomen *die schwache Überkritikalität*, denn es tritt auf, wenn der tiefstliegende gebundene Zustand in dem Potential die Linie $E = 0$ kreuzt und die entsprechende Eigenfunktion den Unterraum zwischen Teilchen und Antiteilchen wechselt. Es stellt sich die Frage, ob dieses Phänomen einem physikalischen Prozess entspricht (Evolution, Streuung), denn, wie es oben beschrieben ist, betrifft es nur eine rein statische Situation. Deswegen ist eine Beschreibung der zeitabhängigen Prozesse im Fock-Raum benötigt.

Die Zeit-Evolution im Fock Raum ist definiert durch Implementation des klassischen Evolutions-Operators als ein unitärer Operator im Fock-Raum. Das ist keine triviale Operation und sie ist nicht immer möglich. Sie beschreibt dynamische Teilchenerzeugungs- und Vernichtungs-Prozesse und Probleme treten auf, wenn die Produktionsrate zu gross wird. Das passiert für unendlich lang dauernde Prozesse (z.B. Streuung) bei Anwesenheit von Potentialen, die vermutlich Teilchen stetig produzieren (Klein's Paradoxon, Schwinger's Effekt). In solchen Fällen bricht die Näherung der QED in externen Feldern zusammen und es muss die volle QED benutzt werden, um die Rückkopplung-Effekte auf das Quanten-elektromagnetische Feld zu berücksichtigen. Wenn der Evolutions- oder Streuprozess implementierbar ist, trägt der Implementer (ein unitärer Operator im Fock Raum) die ganze Information über Erzeugung und Vernichtung von Teilchen in diesem Prozess. Seine Struktur hat zwei Hauptteile. Der erste beschreibt die Erzeugung und Vernichtung von Teilchen-Antiteilchen Paaren und ändert deshalb die Gesamtladung des Zustandes nicht. Der zweite beschreibt die Erzeugung und Vernichtung von einzelnen Teilchen (wie beim Übergang vom freien zum überkritischen Vakuum), die in dieser Arbeit *speziell* genannt werden. Er kann die Gesamtladung ändern, wenn gemessen bezüglich des End-Vakuums. Deshalb ein Übergang vom Anfangs- zum End-Vakuum notwendig ist, um diesen Effekt zu sehen, was nur dann der Fall ist, wenn die Anfang- und End-Potentiale unterschiedlich sind. Prozesse mit dem gleichen Anfangs- und End-Wert des Potentials (z.B. asymptotisches Verschwinden in Streuprozessen) können die Gesamtladung nicht ändern, können aber immerhin *spezielle* Teilchen und Antiteilchen in Paaren erzeugen. Deswegen scheint die Erzeugung von speziellen (Anti-)Teilchen (kurz: *spezielle Erzeugung*) ein Kandidat für eine mathematische Definition der *überkritischen* oder *spontanen Teilchenerzeugung* zu sein. Jedoch, es ergibt sich, erstens, dass die spezielle Erzeugung unabhängig von der Überkritikalität des Potentials auftreten kann, obwohl sie in solchen Fällen sehr instabil gegen kleine Variationen des Potentials ist (eine beliebig kleine Änderung des Potentials zerstört eine solche spezielle Erzeugung). Zweitens, sogar bei der Anwesenheit von überkritischen Potentialen ist die spezielle Erzeugung auf die gleiche Weise instabil, un-

abhängig davon, ob das Potential während des Streuprozesses ein- und ausgeschaltet oder nur eingeschaltet ist. Die Bedeutung der speziellen Erzeugung kann durch Betrachtung der adiabatischen Prozesse gerettet werden, die frei von den obigen Instabilitäten zu sein scheinen. Außerdem, kommt in adiabatischen Prozessen keine spezielle Erzeugung vor, bis die Energie des niedrigsten gebundenen Zustandes das negative Kontinuum erreicht und dort verschwindet, was wir als *starke Überkritikalität* bezeichnen. In der adiabatischen Situation ist die spezielle Erzeugung äquivalent zur *spontanen Teilchenerzeugung* und kann als Definition gebraucht werden. Das spezielle Antiteilchen wird erzeugt als Folge eines Resonanz-Zerfalls (Wellenpaket) im negativen Kontinuum. Wegen der Langsamkeit des adiabatischen Prozesses, zerfällt das Wellenpaket, das einen aufgelösten gebundenen Zustand beschreibt, schon am Rande des Kontinuums völlig, was zu Produktion von Antiteilchen mit verschwindendem Impuls führt. Dieses Ergebnis ist physikalisch nicht zufrieden stellend, aber der adiabatische Limes selbst ist auch keine physikalische Situation. Deswegen gibt es einen Bedarf, die Definition der spontanen Teilchenerzeugung über den adiabatischen Limes auszuweiten. Es ist keine einfache Aufgabe, denn die Schlüssel-Eigenschaft, nämlich die spezielle Erzeugung, geht meistens verloren. Durch Kontinuität, unterscheiden sich langsame Prozesse jedoch nicht viel vom adiabatischen Limes und die entsprechenden Teilchen werden immer noch mit großen Wahrscheinlichkeiten erzeugt. Alternativ kann man versuchen, die spontane Teilchenerzeugung zu bestimmen indem man die Erzeugung eines Antiteilchens in dem Zustand fordert, der einer Resonanz nach einem aufgelösten gebundenen Zustand entspricht. Dann sollen eher schnelle als langsame Prozesse berücksichtigt werden, mit einer möglichst langen verzögerten überkritischen Phase in der Evolution.

Wir studieren numerisch alle diesen Fragen im Falle eines zeitabhängigen sphärisch symmetrischen Potentialtopf mit sich ändernder Tiefe. Einerseits ist es mathematisch das einfachste Potential, für das die Dirac Gleichung analytisch gelöst werden kann. Anderseits zeigt es Überkritikalität wenn die Potentialtiefe einen Grenzwert überschreitet wo gebundene Zustände in Resonanzen übergehen. Wir zeigen die Existenz der Resonanzen durch eine Analyse der komplexen Pole der Resolvente und der Greenschen Funktion, ebenso auch durch Beobachtung von Peaks im negativen Kontinuum, die den durch Wellenpakete dargestellten aufgelösten gebundenen Zuständen entsprechen. In überkritischen Potentialen wird das Vakuum gegenüber dem freien Vakuum geladen sein, was wir sowohl durch eine Berechnung des Erwartungswertes des Ladung-Operators zeigen als auch durch das Studieren der Ladungsdichte der Vakuumspolarisation.

Wir implementieren die Streuung in verschiedenen zeitabhängigen Prozessen im Fock Raum und berechnen numerisch die Teilchen und Antiteilchen Produktionsspektren durch Lösung der gekoppelten Kanal-Gleichungen. Wir vergleichen die Situationen von unterkritischen, schwach und stark überkritischen Potentialen in plötzlichen, schnellen, langsamen und adiabatischen Evolutionsprozessen. In unterkritischen Prozessen kommt nur dynamische Teilchenproduktion vor, die im adiabatischen Limes verschwindet. In Prozessen, wo

ein schwach überkritisches Potential eingeschaltet wird, kann das Vakuum, abhängig von der Definition des Vakuums und der Teilcheninterpretation, spontan geladen werden und es kann ein spontan erzeugtes Antiteilchen erscheinen, das zusammen mit dem Vakuum einen elektrisch neutralen Zustand bildet. Nach dem Ausschalten verschwindet das Antiteilchen und das Vakuum wird wieder neutral. Dagegen wird nach Einschalten eines stark überkritischen Potentials das spontan geladenes Vakuum von einem spontan erzeugten Antiteilchen in einem Streuzustand begleitet. Wenn die überkritische Phase einige Zeit dauert, entfernt sich das Antiteilchen von der "Quelle" (Träger der Potentials) und lässt das geladene Vakuum hinter sich. Endgültiges Ausschalten des Potentials erzeugt ein zusätzliches Teilchen, meistens in einem gebundenen Zustand, was zu einer *spontanen Paarerzeugung* führt.

In sehr langsamen Prozessen beobachten wir die Bewegung des Resonanz-Peaks im negativen Kontinuum während der Evolution. Er zerfällt teilweise in jeder Phase. Beim Erreichen des adiabatischen Limes zerfällt der Peak schon am Rande des Kontinuums vollständig. Die Beobachtung dieses Effektes stellt eine numerische Herausforderung dar, weil die Peaks in der Nähe des Randes extrem schmal sind. Dagegen bewegt sich in schnellen Prozessen der Resonanz-Peak im Kontinuum ohne viel Verlust wegen des eigenen Zerfalls, geht aber ein Teil seiner Amplitude in den Rest des Kontinuums verloren, was zu einer dynamischen Paarerzeugung beiträgt. Im Vergleich der beiden Situationen zeigt unseres numerische Beweismaterial, dass schnelle Ein- und Ausschalt-Prozesse mit einer verzögerten überkritischen Phase günstiger für die Produktion der Antiteilchen mit einem der Position des Resonanzen im verzögerten Potential entsprechenden Energiespektrum sind.

Durch das Modellieren einer Näherung des Zerfallsprozesses eines Resonanz-Peaks während der Evolution wird eine Methode für die inverse Streuung entwickelt, d.h. die Zeitabhängigkeit des Potentials kann durch die Zeitabhängigkeit der Resonanz-Position und -Breite, vom Antiteilchen-Produktionsspektrum abgelesen werden. Das einfache Model eines exponentiellen, dekohärenten Zerfalls des Peaks gibt überraschend gute Abschätzungen für das Antiteilchen-Produktionsspektrum.

Contents

Overview of chapters

I Theory

In the first, theoretical part of this thesis we introduce the mathematical formulation of the classical and quantized Dirac theory with their most important results. Using this language we define rigorously the notion of spontaneous particle creation in overcritical fields.

1 Introduction

In this chapter we give a short introduction to the problem of spontaneous particle creation. We introduce the notion of overcritical potentials on the level of classical Dirac equation, show how bound states become resonances and discuss briefly the expectation regarding a spontaneous creation of particles and antiparticles in such situations. Since the classical Dirac theory is unable to offer a precise picture of particle production phenomena and a quantized theory is needed, we briefly mention the QED and its external field approximation. We introduce the notion of overcritical fields and spontaneous particle creation. Then we briefly describe the main discrepancies in approaches present in the literature and explain how we will clarify them. Finally, we comment on the existence and observability of spontaneous particle creation in various processes.

2 Fock space representation of CAR – particle interpretation

In this chapter we construct the theory of a quantized Dirac field, the so-called QED in external fields. We start from the construction of the representation of the canonical anticommutation relations (CAR), the Fock space consisting of the vacuum and many-particle states. Then we discuss its uniqueness as well as equivalence of representations based on different projectors. Next, we show how unitary transformations of the classical one-particle Hilbert space cause a rearrangement of the particle and antiparticle creation and annihilation operators, i.e. the Bogoliubov transformations. Analogously, we show how the change of representation, projectors and the definition of vacuum, when leading to a unitarily equivalent theory, implies a Bogoliubov transformation, for which we provide a unitary implementer in Fock space. Subsequently we give a prescription for implementing operators from the one-particle Hilbert space to many particle Fock space introducing the

notion of normal ordering. We discuss the physical meaning of the vacuum state being the ground state of the implemented Hamiltonian and simultaneously a no-particle state with respect to the particle number operator. Then we define the charge operator in Fock space and vacuum polarization charge density. Next, we define a time evolution in Fock space generalizing that of a one-particle Hilbert space. We calculate the change of the particle number and charge during the evolution. Further, we introduce the notion of particles and construct several particle interpretations for time-dependent processes. Then we define scattering processes in Fock space leading to particle production and we consider conditions under which QED in external fields provides consistent results.

3 Evolution and scattering in the classical Dirac equation

In this chapter we give the most important results from the theory of the classical Dirac equation. We start with the question about the self-adjointness of the Dirac Hamiltonian with a given potential and state an important fact that the strength of the potential itself does not play any role as long as the potential is locally regular (more than the Coulomb potential). Then, we study the spectrum of the Dirac Hamiltonian and cite the stability condition for its continuous part as well as the fact that there are no eigenvalues embedded in the continuum. We define critical and overcritical potentials in terms of spectral properties of the Hamiltonian. Next, we cite the spectral theorem introducing spectral measures, which will be essential in the transition to the discrete (numerical) approximation. Further, we give a rigorous definition of resonances as poles of the resolvent, Green's function or the scattering operator and discuss how eigenvalues become resonances under Hamiltonian perturbations. In particular, we consider a rarely discussed in the literature, but essential for overcritical potentials perturbation of eigenvalues at the edge of the continuous spectrum. As next, we state the most important results concerning existence of a unitary evolution, wave operators and the scattering operator in the case of static as well as time-dependent Hamiltonians. We cite various versions of the adiabatic theorem and discuss well-posedness of the scattering in the adiabatic limit.

4 Overcritical fields and spontaneous particle creation

In this chapter we define within the quantized Dirac theory the evolution and scattering processes in presence of overcritical potentials. We look for physical processes which show the effect of vacuum decay and spontaneous particle creation exclusively due to overcriticality of the potential. First, we analyze how the structure of the ground (vacuum) state changes from neutral to charged in presence of an overcritical potential. Then, we consider several processes with static as well as suddenly switched on (and off) static overcritical potentials and conclude that they are unsatisfactory for observation of the spontaneous particle creation. Next, we consider properties of general time-dependent scattering processes with continuous switch on (and off) of an overcritical potential and

show that they also fail to produce stable signatures of the particle creation due to overcriticality. Further, we study and successfully define the spontaneous particle creation in adiabatic processes, yet they lead to physically questionable pair production as the adiabatic limit is approached. Finally, we consider extension of these ideas to non-adiabatic processes involving overcritical potentials, speculate about the dynamical behaviour of time-dependent resonances (to be confirmed later numerically) and argue that they are the best candidate for showing the spontaneous pair creation in physical processes.

II Examples and numerical study

In the second part of this thesis we concentrate on an a class of spherically symmetric square well potentials with a time-dependent depth. First, we analyze in more details overcriticality and appearance of resonances. Then, we calculate numerically particle and antiparticle production spectra for various sub- and overcritical time-dependent processes. We show precisely how and under which conditions an overcritical resonance decays during the evolution giving rise to the spontaneous production of an antiparticle.

5 Dirac equation with a spherically symmetric square well potential

In this chapter we construct solutions to the Dirac equation in presence of a spherically symmetric potential well, which will be used in the next chapter, where we are going to study (numerically) the particle production in time-dependent overcritical potentials. We choose a two-parameter class of spherically symmetric square potential wells, which is sufficient to cover all cases of our interest. First, we give an introduction to the Dirac equation in presence of spherically symmetric potentials and construct the partial wave decomposition based on algebraic properties of the Dirac operator. Then we solve the Dirac equation with the spherically symmetric potential well, giving orthogonal and normalized complete set of wave functions, which we later use as a basis in the Hilbert space. Further, we analyze the structure and behaviour of bound states and appearance of overcriticality. Finally, by analytic continuation we find and discuss the behaviour of resonances in the overcritical potentials.

6 Particle production in a time-dependent overcritical potential

In this chapter we want to study these details of the spontaneous particle creation, discussed in part I, which could not be decided analytically on a purely theoretical level. Here, we construct a series of examples of time-dependent processes (sudden, quick, slow switch on and off of a sub- and overcritical potentials) by using always the same spatial potential and considering only various time-dependent amplitudes, what is sufficient to cover all cases of our interest. We derive a system of differential equations (coupled channel equations) to be implemented numerically for calculation of the scattering operator,

introduce non-uniform continuum discretization for consistent treatment of narrow peaks, discuss various sources of errors introduced by the numerical discretization and try to find estimations for them.

First, we consider sudden switch on and next switch on and off of an overcritical potential and calculate the spectrum of produced particles and antiparticles. We observe that for sufficiently long overcritical periods a peak forms in the antiparticle spectrum and we compare it with the shape of the resonance in the overcritical potential. Later, we consider continuous switch on and off processes, explaining how difficult the treatment of extremely narrow resonance peaks at the edge of the negative continuum is. We consider subcritical potentials in order to show an adiabatic limit in which no particles are created. Then we compare processes, where the overcritical potentials are switched on at different speed and are possibly frozen in the overcritical phase.

We prove, in agreement with the conclusions of the theoretical part, that the peak (wave packet) in the negative continuum representing a dived bound state partially follows the moving resonance and partially decays at every stage of its evolution. This continuous decay is more intensive in slow processes, while in quick processes the wave packet more precisely follows the resonance. In the adiabatic limit, the whole decay occurs already at the edge of continuum, resulting in production of antiparticles with vanishing momentum. In contrast, in quick switch on processes with delay in the overcritical phase, the spectrum of the created antiparticles agrees best with the shape of the resonance.

7 The inverse problem

In this chapter we want to ask the question how much information about the time-dependent potential can be reconstructed from the scattering data, represented by the scattering operator or the particle production spectrum. Being aware that such procedure is far from being unique, we consider several simplified cases, where only few degrees of freedom of the potential are to be guessed. Using results from the previous chapter we give some answers to what extent information about the potential's strength can be successfully obtained. Finally, we propose a simple approximation method (master equation) basing on exponential, decoherent decay of time-dependent resonances for prediction of particle creation spectra. Despite its simplicity we obtain relatively good agreement with the results of full numerical calculations from the previous chapter. This method can be relatively easily applied to the inverse problem.

Part I

Theory

Chapter 1

Introduction

1.1 The classical Dirac theory

Classical Dirac equation

Dirac [Dir28a, Dir28b] introduced the relativistic wave equation in order to improve the quantum mechanical description of an electron in a given electromagnetic field. It was a generalization of the Schrödinger equation, where the $\mathbb{C}$-number wave function became a spinor valued wave function $\psi_\alpha(t, \mathbf{x})$. In the explicitly relativistic form the Dirac equation with an external electromagnetic potential $A_\mu(x)$ reads

$$\gamma^\mu \left(i\hbar \, \partial_\mu - \frac{e}{c} A_\mu(x) \right) \Psi(x) - mc \, \Psi(x) = 0, \tag{1.1.1}$$

where x stands for 4-coordinates in Minkowski space and $x = (x^0, x^1, x^2, x^3) \equiv (t, \mathbf{x})$. It can be rewritten to the evolution (Hamiltonian) form

$$i\hbar \frac{\partial}{\partial t} \Psi(t, \mathbf{x}) = H(t) \Psi(t, \mathbf{x}) \tag{1.1.2}$$

with the full Hamiltonian

$$H(t) \equiv H_0 + V(t), \tag{1.1.3}$$

the free Hamiltonian

$$H_0 = c\alpha^i p_i + mc^2 \beta = -i\hbar c \alpha^i \frac{\partial}{\partial x^i} + mc^2 \beta, \tag{1.1.4}$$

and the time-dependent external potential

$$V(t) = eA_0 + e\alpha^i A_i. \tag{1.1.5}$$

If V is time-independent then there exists a set of stationary solutions

$$\psi_n(t, \mathbf{x}) = e^{-iE_n t} \phi_n(\mathbf{x}) \quad \text{with} \quad H\phi_n(\mathbf{x}) = E_n \phi_n(\mathbf{x}), \tag{1.1.6}$$

with $\phi_n(\mathbf{x})$ being eigenvectors or generalized eigenvectors of H. All $\phi_n(\mathbf{x})$ form a complete and orthonormal set in Hilbert space $\mathcal{H}$ of square integrable functions, i.e. $\mathcal{H} = L^2(\mathbb{R}^3)^4$ (4, because of four components of the bispinors). They will describe particle states with given energy.

The Spectrum

Spectrum of H consists of two separate continuous parts $(-\infty, -mc^2] \cup [mc^2, \infty)$ and a possible discrete (finite or countable) part $\{E_n \in (-mc^2, mc^2)\}$. The generalized eigenvectors $\psi_n(t, \mathbf{x})$, called wave functions, describe: electron scattering states for $E > mc^2$, bound states for $-mc^2 < E < mc^2$ and positron scattering states for $E < mc^2$. It is assumed that all states in the negative continuum are occupied by electrons (*Dirac sea*).

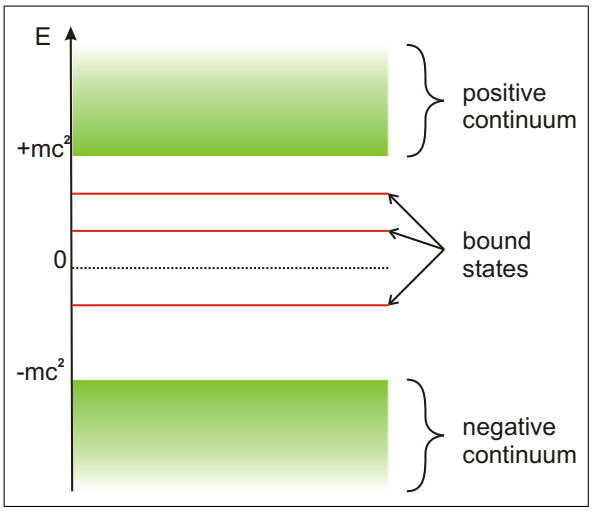


Figure 1.1: Typical spectrum of the Dirac Hamiltonian.

Overcriticality on the classical level

Consider purely electric potentials (no magnetic field present), i.e. $A_i = 0$. If one parameterizes the potential's strength with λ: $V_\lambda(\vec{x}) \equiv \lambda V(\vec{x})$ then energies $E_n(\lambda)$ of the bound states depend continuously on λ. Assume $V(\vec{x})$ is negative. Then the bigger λ is (deeper negative potential) the lower (towards $-mc^2$) lie the bound states $E_n(\lambda)$. Let's enumerate the bound states: $E_0(\lambda) < E_1(\lambda) < E_2(\lambda) < ...$ There are potentials $V(\vec{x})$ for which $E_0(\lambda)$ reaches the boundary of the negative continuum at $-mc^2$ for a finite value of $\lambda = \lambda_{cr}$, called *critical*. For $\lambda > \lambda_{cr}$ the state E_0 disappears from the spectrum. Such potentials V_λ are called *overcritical*. Further, the next bound states E_1, E_2, etc. disappear as λ grows (see figure 1.2). The effect of diving of the discrete energy levels into the negative continuum in strong potentials is called *overcriticality*.

Resonances as complex poles of the Green's function

Bound states of $H_\lambda = H_0 + \lambda V$ are poles of the resolvent $(H_\lambda - E)^{-1}$ at $E = E(\lambda)$ with $-mc^2 \leq E(\lambda) \leq mc^2$. They move continuously to the left as λ grows (and $V \leq 0$). At $\lambda = \lambda_{cr}$ the pole $E(\lambda)$ reaches $-mc^2$. As λ increases further, $E(\lambda)$ becomes a complex pole with $E_R(\lambda) \equiv \mathrm{Re}E(\lambda) < -mc^2$ and $\Gamma(\lambda) \equiv -\mathrm{Im}E(\lambda) > 0$ (on the second Riemann sheet

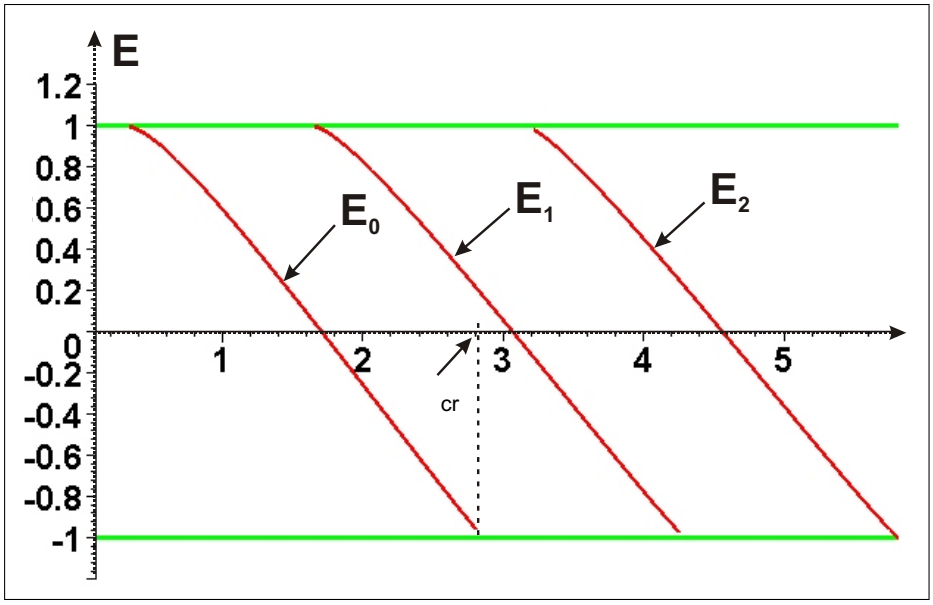


Figure 1.2: Dependence of the bound state energy levels on the potential's strength.

of the analytic continuation of the resolvent). It is called *resonance* and is (usually) equal to a pole of the Laplace- (or Fourier-) transformed Green's function. The wave function of the bound state turns into a wave packet localized spectrally in the negative continuum around $E = E_R(\lambda)$ and having width $\Gamma(\lambda)$. During evolution it decays exponentially like $e^{-\Gamma(\lambda)t}$.

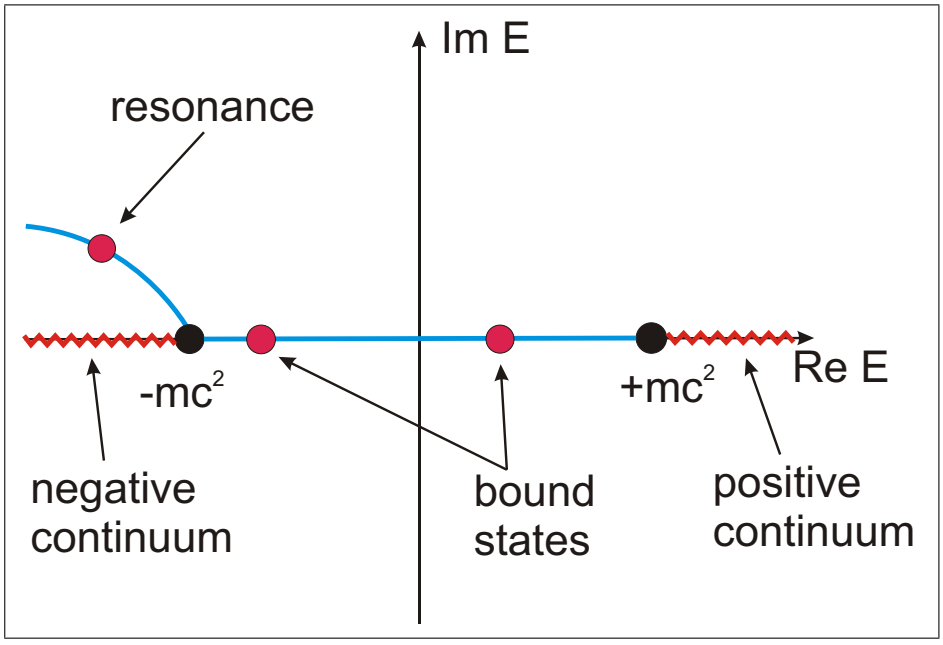


Figure 1.3: Resonances as poles of the resolvent or the Green's function.

By the technique of the Laplace (or Fourier) transform and the Green's function one can solve the evolution of a wave function in a static potential V_λ. The solution can be written as a sum over residua at poles E_k of the Laplace-transformed Green's function, which represent bound states (real) or resonances (complex) plus two integrals along the branch cuts, which represent the continua

$$\Psi(t,\mathbf{x}) = \sum_k e^{-iE_k t}\ \phi_k(\mathbf{x}) + \left(\int_{-\infty}^{-mc^2} + \int_{mc^2}^{\infty}\right) e^{-iEt}\ \phi_E(\mathbf{x})\ dE. \tag{1.1.7}$$

So the bound state and continuum wave functions oscillate in time ($E \in \mathbb{R}$) while resonances decay like $e^{-\Gamma(\lambda)t}$, because $E = E_R - i\Gamma$.

What can be expected by overcriticality ? (Intuitive answers.)

In static potentials V particles occupy stationary states. In time-dependent potentials $V(t)$ stationary states don't exist and particles "jump" between states (i.e. instantaneous eigenstates of the Hamiltonian $H(t)$). However, if $V(t)$ changes adiabatically, states change slowly and particles "follow" the states. If $V(t)$ can be slowly changed between the sub- and overcritical regimes, particles may be "transported" to or from the negative continuum. Dived electron states become resonances and decay in time. In the opposite direction, electrons may be "pulled" adiabatically from the Dirac sea and kept in a bound state, while the remaining holes correspond to the scattered positrons.

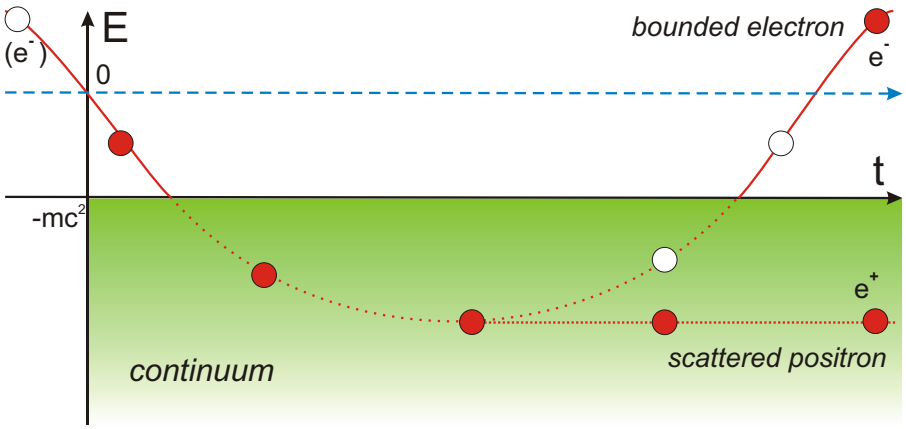


Figure 1.4: Electron bound state diving into the negative continuum.

The classical Dirac equation describes single electrons (fermions) and does not handle particle or antiparticle creation and annihilation processes. For that the *Quantum Electrodynamics (QED)*, a many-particle quantum theory of electrons and positrons is needed.

1.2 The quantized Dirac theory

"Second quantization"

The negative energy problem forced Dirac later to modify the meaning of the equation. This resulted in the "hole theory" [Dir30], very successful as a theory, but at the same time highly intuitive and difficult to formulate in a precise mathematical way. Later, the idea of "second quantization" has been developed, in which the wave function became an operator-field acting in a many-particle space of particles and anti-particles, the Fock-Hilbert space. All known operators acting in one-particle space had to be implemented in the many-particle space, what caused several difficulties.

QED

The full *Quantum Electrodynamics (QED)* is a theory of quantized Dirac and quantized electromagnetic field, i.e. describes electrons, positrons, photons and their interaction. It is very difficult to solve in particular situations, so one has to use approximations.

External field approximation

The external field approximation of QED treats the Dirac field as quantized while the electromagnetic field as classical. Therefore it describes electrons and positrons interacting with an external, classical electromagnetic field. Electrons and positrons don't interact with each other and do not influence the electromagnetic field. Therefore, the approximation is good when the number of electrons and positrons is small and the classical field is strong and dominates over quantum corrections. The approximation breaks down when the backreaction of the electrons and positrons on the electromagnetic field becomes important, what can lead to non-implementability of the evolution or scattering operator in Fock space since it produces too many particles. This unlimited particle creation would be suppressed in the full QED, since a big number of charged particles would modify the electromagnetic field and influence (prohibit) further particle production.

We choose the external field approximation of QED because we deal with strong electric fields and a small number of particles. The corrections of full QED are expected to be negligible, e.g. the self-energy correction for an electron in a nearly critical (Coulomb) potential almost cancels with the vacuum polarization effect and is negligible [SSMG82].

Overcritical fields in QED (of external fields)

There is an old observation [MRG72] that the vacuum structure changes from neutral to charged and an accompanying spontaneous particle creation occurs when a static external field exceeds some critical strength [RMG74]. This statement is unambiguous in the static situation because there exists a unique particle interpretation, the Furry picture [Fur51]. Unfortunately, this phenomenon does not happen in QED with external fields,

since scattering processes in static external fields either do not produce particles when the external field is regular [Bon70] or cannot be described within the external field approximation at all when the field is not regular and the notion of particles cannot be defined successfully. Therefore, it seems natural to look for this effect in time-dependent strong fields. Then, however, the meaning of a vacuum state and of particles becomes unclear. Fierz and Scharf [FS79] analyze the problem of particle interpretation in time-dependent external fields rigorously and conclude that the only consistent pictures are the in- and out-representations, so the particles can have only an asymptotic meaning[1].

Vacuum decay and spontaneous particle creation

There is a long debate in the literature between Greiner *et al.* [MRG72, RMG74, RG77] and Scharf *et al.* [KS77b, SS82], whether overcriticality causing the vacuum decay and spontaneous particle creation should be defined by the property of the classical Dirac Hamiltonian having an eigenvalue "dived" in the negative continuum (Greiner) or by change in the structure of the scattering operator implemented in Fock space (Scharf). While the first definition leads to overcriticality when a bound state reaches energy $E \leq -mc^2$, which we call *strong overcriticality*, the second one leads to overcriticality already for $E \leq 0$, which we call *weak overcriticality*. We show (chapter 2) that mathematically the difference is in the choice of the projector defining the Fock representation of the field algebra (CAR). It leads to different vacuum and particle definitions. Yet, because these representations are unitarily equivalent, all their physical results must be equivalent. We solve this puzzle (chapter 4) by showing that by weak overcriticality the corresponding choice of vacuum and particles leads to a charged vacuum and a spontaneous antiparticle creation, but this antiparticle is in a bound state and is localized spatially exactly there where the vacuum charge density is. Therefore the composite antiparticle-charged-vacuum is neutral and probably cannot be observed physically. At the same time in the Greiner-representation there are no particles and the vacuum stays neutral. So both pictures seem to be equivalent. First by the strong overcriticality the Greiner-representation predicts a vacuum decay to a charged state and an antiparticle creation, while in the Scharf-representation an important change happens, namely the spontaneously created antiparticle goes from a bound state to a scattering state and escapes to spatial infinity in evolution leaving a charged vacuum behind. This agrees with the spirit of Nenciu's conjecture [Nen80a, Nen87] formulated in the adiabatic limit and proved recently by Pickl [Pic05].

Concluding, we in principle agree with Scharf that the definition of the effect should be formulated in Fock space as well as that the information on particle creation is contained in the structure of the implemented scattering operator. Hence, we treat it as a part of the definition and a necessary condition, but we are aware that the change in the structure

[1] We want to mention that in $1+1$ dimensions the model can be solved analytically [FG88, CW91] and can serve as an illustrative example.

does not have to lead to observable effects. On the other hand, it is the Greiner's condition of a bound state diving into the continuum which decides about the existence of physically observable spontaneous particle creation. Hence we treat it as a (necessary and sufficient) criterion.

Spontaneous particle creation in time-dependent processes

Unfortunately it is not easy to find a time-dependent process during which an overcritical external field is switched on (or on and off) to observe purely and uniquely the effect of spontaneous particle creation. In quick processes there are many dynamical particle-antiparticle pairs produced from vacuum what can make the spontaneously created antiparticle difficult to distinguish. In slow (adiabatic) processes the production of dynamical pairs is suppressed but the spontaneous antiparticle is created with vanishing momentum, what can lead to serious difficulties of experimental nature. We study several time-dependent scenarios (chapter 6) from sudden discontinuous changes in the strength of the external field to very slow ones near the adiabatic limit and compare the observable effects in form of antiparticle production spectra with other fundamental predictions. For simplicity we choose the potential to be a time-dependent spherically symmetric square well. A similar calculation has been performed in [MDI93], but only in $1+1$ dimensions with a time-periodic potential. In [GG96] and [SSW93] potentials depending only on time are considered, but they have no bound states and hence no overcriticality. The richest bibliography concerns the experimentally motivated situation of atomic collisions [MRG72, RMGS79, Rei79, RMG81, RMMG81, MdRR$^+$88], etc. Pair production in strong laser fields has been calculated in [Mül03, MVG03].

We show that the spontaneous particle creation exists only in the weaker sense (defined in section 4.5), i.e. overcritical fields lead to a vacuum decay and spontaneous particle creation, but there are no processes in which one can observe exclusively the spontaneous antiparticle with the energy corresponding to the resonance position in the overcritical field. Either there are other particles confusing the picture (dynamical pairs in quick processes) or the spontaneous antiparticle has a vanishing momentum and kinetic energy, independent on the strength of the overcritical field and position of the resonance (adiabatic limit).

The inverse problem

It is an interesting question, whether the scattering information, i.e. the particle and antiparticle production spectra, is sufficient to reproduce the time-dependent potential. Although the answer is generally negative, restricting the set of all considered potentials to a small class, parameterized with a few parameters, can lead to a positive answer. We propose a simple approximative model of the influence of a decaying resonance on the final particle production spectrum, which can be inverted without much numerical effort,

i.e. the position of complex resonance during the evolution can be estimated from the scattering data. This, under restriction of the time-dependent potentials to a one time-dependent parameter (e.g. constant spatial shape with varying amplitude or two Coulomb centers with varying distance), gives a unique solution, i.e. a time-dependent potential leading to a required particle production spectrum.

Chapter 2

Fock space representation of CAR – projector choice, particle interpretation

2.1 The CAR algebra and its representations

2.1.1 "Smeared" field operators

An abstract $C*$-algebra of the fields $\hat{\Psi}(f), \hat{\Psi}^*(f)$ "smeared" by the test functions f is defined by the so called *canonical anticommutation relations* (CAR)

$$\{\hat{\Psi}(f), \hat{\Psi}^*(g)\}_+ = (f, g) \tag{2.1.1}$$

$$\{\hat{\Psi}(f), \hat{\Psi}(g)\}_+ = \{\hat{\Psi}^*(f), \hat{\Psi}^*(g)\}_+ = 0 \tag{2.1.2}$$

where f, g are complex-valued bi-spinor functions belonging to a Hilbert space $\mathcal{H}$ equipped with a scalar product

$$(f, g) = \int \sum_{s=1}^{4} \overline{f(x, s)}\, g(x, s)\, d^3x. \tag{2.1.3}$$

with $f(\cdot, s)$ being $\mathbb{C}$-number functions, components of the bi-spinors. We want to find a representation of this algebra in order to construct a physical interpretation and be able to perform more explicit calculations than those on the level of an abstract algebra. The situation is analogous to the search of representations of a well known algebra $[s_i, s_j] = i\epsilon_{ijk}s_k$. It may be represented by spin operators (2x2 Pauli matrices) on a Hilbert space, e.g. $[L^2(\mathbb{R}^n)]^2$, as well as by generators of rotations in 3 dimensions (3x3 matrices) acting on $\mathbb{R}^3$.

Among possible realizations of the CAR algebra there are anti-linear mappings $f \to \hat{\Psi}(f)$ from $\mathcal{H}$ into the bounded operators acting in a Hilbert space $\mathcal{F}$. Special realizations are realizations with a vacuum vector $\Omega \in \mathcal{F}$ (reference state). Their construction bases on the introduction of two elements: a projector P_+ (and $P_- \equiv 1 - P_+$), which splits the

Hilbert space into two orthogonal subspaces

$$P_+ : \mathcal{H} \to \mathcal{H}_+, \qquad P_- : \mathcal{H} \to \mathcal{H}_-, \qquad \mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-, \tag{2.1.4}$$

and a reference state, a vector $\Omega \in \mathcal{F}$, called vacuum, so that the following holds

$$\hat{\Psi}(P_+ f)\,\Omega = 0, \qquad \hat{\Psi}^*(P_- f)\,\Omega = 0 \qquad \forall f \in \mathcal{H}. \tag{2.1.5}$$

It is convenient to define a pair of operators

$$\hat{b}(f) \equiv \hat{\Psi}(P_+ f), \qquad \hat{d}(g) \equiv \hat{\Psi}^*(P_- g), \tag{2.1.6}$$

which are called particle and antiparticle annihilation operators, respectively. Then the field $\hat{\Psi}(f)$ becomes an operator in $\mathcal{F}$ and can be expressed as

$$\hat{\Psi}(f) = \hat{b}(P_+ f) + \hat{d}^*(P_- f), \qquad \hat{\Psi}^*(f) = \hat{b}^*(P_+ f) + \hat{d}(P_- f). \tag{2.1.7}$$

Creation and annihilation operators satisfy corresponding anticommutation relations

$$\{\hat{b}(f), \hat{b}^*(g)\}_+ = (P_+ f, P_+ g) \tag{2.1.8}$$
$$\{\hat{b}(f), \hat{b}(g)\}_+ = \{\hat{b}^*(f), \hat{b}^*(g)\}_+ = 0 \tag{2.1.9}$$
$$\{\hat{d}^*(f), \hat{d}(g)\}_+ = (P_- f, P_- g) \tag{2.1.10}$$
$$\{\hat{d}(f), \hat{d}(g)\}_+ = \{\hat{d}^*(f), \hat{d}^*(g)\}_+ = 0 \tag{2.1.11}$$

for every $f, g \in \mathcal{H}$.

A special representation with a vacuum vector, having the property of being irreducible, is the Fock representation introduced below according to the so-called GNS–construction (due to Gelfand, Naimark, and Segal). The idea of GNS is that the products of the creation operators $\hat{b}^*(f), \hat{d}^*(g)$ applied to the reference vector Ω may be used for construction of the basis of $\mathcal{F}$, by which the whole Fock space $\mathcal{F}$ can be spanned.

2.1.2 Distributional ("singular") field operators

Beside the smeared operators $\hat{\Psi}(f)$ there exist in the literature "singular" bispinor field operators $\Psi(\mathbf{x})$, being operator valued distributions, which depend on the space-point $\mathbf{x}$ and fulfill the corresponding canonical anticommutation relations (CAR)

$$\{\hat{\Psi}_\alpha(\mathbf{x}), \hat{\Psi}^*{}_\beta(\mathbf{y})\}_+ = \delta(\mathbf{x}-\mathbf{y})\,\delta_{\alpha\beta} \tag{2.1.12}$$
$$\{\hat{\Psi}_\alpha(\mathbf{x}), \hat{\Psi}_\beta(\mathbf{y})\}_+ = \{\hat{\Psi}^*{}_\alpha(\mathbf{x}), \hat{\Psi}^*{}_\beta(\mathbf{y})\}_+ = 0. \tag{2.1.13}$$

Both kinds of the field operators are connected by the relations

$$\hat{\Psi}(f) = \sum_{\alpha=1}^{4} \int \overline{f(\mathbf{x},\alpha)}\;\hat{\Psi}_\alpha(\mathbf{x})\;d^3x \tag{2.1.14}$$

and

$$\hat{\Psi}_\alpha(\mathbf{x}) = \sum_k f_k(\mathbf{x}, \alpha)\ \hat{\Psi}(f_k), \tag{2.1.15}$$

where $f_k(\mathbf{x}, \alpha)$ is an orthonormal basis in $\mathcal{H}$. In the following, we always assume that $\mathcal{H}$ is separable and therefore there always exists a countable set of orthonormal vectors forming a basis in $\mathcal{H}$. We rather choose this general kind of representation of vectors than a Fourier transform, which would be only of advantage in the free case where no x-dependent fields are present.

With these relations the CAR (2.1.12)-(2.1.13) are equivalent to (2.1.1)-(2.1.2).

2.2 Fock construction and implementation of operators

2.2.1 Fock space

Problem of negative energies

The spectrum of the classical Hamiltonian $\mathcal{H}$ is unbounded from below. It leads to infinitely many states with negative energy. Dirac recognized the problem as an energetic instability, because in such system there exists no ground state, and proposed the *Dirac sea* interpretation in which all states with negative energy are occupied. Mathematically, the operation is equivalent to an exchange of the roles of the antiparticle creation and annihilation operators: $\hat{d}(g), \hat{d}^*(g)$ relative to the particle operators $\hat{b}(f), \hat{b}^*(f)$ in the decomposition of the field operator

$$\hat{\Psi}(f) = \hat{b}(P_+ f) + \hat{d}^*(P_- f), \qquad \hat{\Psi}^*(f) = \hat{b}^*(P_+ f) + \hat{d}(P_- f) \tag{2.2.1}$$

together with the definition of the vacuum

$$\hat{b}(P_+ f)\ \Omega = 0, \qquad \hat{d}(P_- f)\ \Omega = 0 \qquad \forall f \in \mathcal{H}. \tag{2.2.2}$$

In consequence all particle as well as antiparticle energies can be made positive, what will become transparent in the following. We adopt the notation from [Tha92] and refer the reader to it for more details concerning the definitions.

Many-particle subspaces

Let $H(e)$ be the Hamiltonian defined in (1.1.3)-(1.1.5) which depends explicitly on e via V. Assume, we have chosen the projectors $P_\pm$ so that $H(e)$ restricted to $\mathcal{H}_+ = P_+\mathcal{H}$ is bounded from below and restricted to $\mathcal{H}_- = P_-\mathcal{H}$ is bounded from above. Assume, there exists an antiunitary map C called *charge conjugation* such that

$$CH(e)C^{-1} = -H(-e). \tag{2.2.3}$$

It converts eigenstates of $H(e)$ with negative energy and negative charge ψ_- (electrons) to eigenstates of $H(-e)$ with positive energy and positive charge $C\psi_-$ (positrons). Of

course, the overall sign of all charges is a convention, only the fact that electron and positron charges are opposite has physical consequences.

Define one-particle subspaces as

$$\mathcal{F}_+^{(1)} = \mathcal{H}_+, \qquad \mathcal{F}_-^{(1)} = C\mathcal{H}_-. \tag{2.2.4}$$

The n-particle-subspaces $\mathcal{F}_\pm^{(n)}$ are defined as an antisymmetrized tensor product of n copies of $\mathcal{F}_\pm^{(1)}$ with the (orthonormal) basis vectors

$$\begin{aligned}&\left(\frac{1}{\sqrt{n!}}\sum_{\text{permutations }\sigma}\text{sign}(\sigma)\; f_{\sigma(j_1)}\otimes f_{\sigma(j_2)}\otimes ...\otimes f_{\sigma(j_n)}\right)(x_1,s_1;x_2,s_2;...;x_n,s_n)\\ &\equiv\frac{1}{\sqrt{n!}}\sum_{\text{permutations }\sigma}\text{sign}(\sigma)\; f_{\sigma(j_1)}(x_1,s_1)\; f_{\sigma(j_2)}(x_2,s_2)\;...\; f_{\sigma(j_n)}(x_n,s_n),\end{aligned} \tag{2.2.5}$$

where $f_j(x,s)$ are (orthonormal) basis vectors in $\mathcal{H}_\pm$. Therefore any $\psi_\pm^{(n)} \in \mathcal{F}_\pm^{(n)}$ is antisymmetric in all its arguments. The scalar product in $\mathcal{F}_\pm^{(n)}$ has the form

$$\left(\psi_\pm^{(n)},\chi_\pm^{(n)}\right)_n = \sum_{s_1,...,s_n=1}^{4}\int_{\mathbb{R}^{3n}} d^3x_1...d^3x_n\;\overline{\psi_\pm^{(n)}(x_1,s_1;...;x_n,s_n)}\;\chi_\pm^{(n)}(x_1,s_1;...;x_n,s_n). \tag{2.2.6}$$

Fock space

In every many-particle subspace the number of particles is given. To be able to describe any number of particles as well as creation and annihilation processes define the Fock space as a direct sum of all subspaces constructed above

$$\mathcal{F} \equiv \bigoplus_{n,m=0}^{\infty}\mathcal{F}^{(n,m)}, \qquad \mathcal{F}^{(n,m)} \equiv \mathcal{F}_+^{(n)}\otimes\mathcal{F}_-^{(m)}, \tag{2.2.7}$$

where $\mathcal{F}_\pm^{(0)} = \mathbb{C}$. It consists of vectors $\Psi \in \mathcal{F}$ having components

$$\Psi \equiv (\psi^{(n,m)})_{n,m=0,1,2,...}, \tag{2.2.8}$$

where $\psi^{(n,m)} \in \mathcal{F}^{(n,m)}$. The scalar product in $\mathcal{F}$ is then a sum

$$(\Psi,\Phi)_{\mathcal{F}} \equiv \sum_{n,m=0}^{\infty}\left(\psi^{(n,m)},\phi^{(n,m)}\right)_{(n,m)} \tag{2.2.9}$$

with

$$\begin{aligned}&\left(\psi^{(n,m)},\phi^{(n,m)}\right)_{(n,m)} =\\ &\sum_{\substack{s_1,...,s_n,\\ z_1,...,z_m=1}}^{4}\int_{\mathbb{R}^{3(n+m)}} d^3x_1...d^3x_n\;d^3y_1...d^3y_m\;\overline{\psi^{(n,m)}(x_1,s_1;...;x_n,s_n;y_1,z_1;...;y_m,z_m)}\\ &\qquad\cdot\chi^{(n)}(x_1,s_1;...;x_n,s_n;y_1,z_1;...;y_m,z_m).\end{aligned} \tag{2.2.10}$$

Accordingly, the norm is defined by

$$||\Psi||^2_{\mathcal{F}} \equiv \sum_{n,m=0}^{\infty} ||\psi^{(n,m)}||^2_{(n,m)} = \sum_{n,m=0}^{\infty} \left(\psi^{(n,m)}, \psi^{(n,m)}\right)_{(n,m)}. \tag{2.2.11}$$

2.2.2 Creation and annihilation operators

In this construction creation $\hat{b}^*(f), \hat{d}^*(g)$ and annihilation $\hat{b}(f), \hat{d}(g)$ operators map subspaces with given number of particles into the "neighbouring" ones with one (anti)particle more or less, respectively.

- Particle annihilation: $\hat{b}(f) : \mathcal{F}^{(n+1,m)} \to \mathcal{F}^{(n,m)}$ for $f \in \mathcal{H}_+$

$$\left(\hat{b}(f)\psi\right)^{(n,m)}(x_1, s_1; ...; x_n, s_n; y_1, z_1; ...; y_m, z_m) =$$
$$\sqrt{n+1}\sum_{s=1}^{4}\int_{\mathbb{R}^3} d^3x\ \overline{f(x,s)}\ \psi^{(n+1,m)}(x, s; x_1, s_1; ...; x_n, s_n; y_1, z_1; ...; y_m, z_m). \tag{2.2.12}$$

- Particle creation: $\hat{b}^*(f) : \mathcal{F}^{(n,m)} \to \mathcal{F}^{(n+1,m)}$ for $f \in \mathcal{H}_+$

$$\left(\hat{b}^*(f)\psi\right)^{(n,m)}(x_1, s_1; ...; x_n, s_n; y_1, z_1; ...; y_m, z_m) =$$
$$\frac{1}{\sqrt{n}}\sum_{j=1}^{n}(-1)^{j+1} f(x_j, s_j)\ \psi^{(n-1,m)}(x_1, s_1; ...; \not{x}_j, \not{s}_j; ...; x_n, s_n; y_1, z_1; ...; y_m, z_m). \tag{2.2.13}$$

- Antiparticle annihilation: $\hat{d}(g) : \mathcal{F}^{(n,m+1)} \to \mathcal{F}^{(n,m)}$ for $g \in \mathcal{H}_-$

$$\left(\hat{d}(g)\psi\right)^{(n,m)}(x_1, s_1; ...; x_n, s_n; y_1, z_1; ...; y_m, z_m) =$$
$$(-1)^n\sqrt{m+1}\sum_{z=1}^{4}\int_{\mathbb{R}^3} d^3y\ \overline{Cg(y,z)}\ \psi^{(n,m+1)}(x_1, s_1; ...; x_n, s_n; y, z; y_1, z_1; ...; y_m, z_m). \tag{2.2.14}$$

- Antiparticle creation: $\hat{d}^*(g) : \mathcal{F}^{(n,m)} \to \mathcal{F}^{(n,m+1)}$ for $g \in \mathcal{H}_-$

$$\left(\hat{d}^*(g)\psi\right)^{(n,m)}(x_1, s_1; ...; x_n, s_n; y_1, z_1; ...; y_m, z_m) =$$
$$\frac{(-1)^n}{\sqrt{m}}\sum_{j=1}^{m}(-1)^{j+1} Cg(y_j, z_j)\ \psi^{(n,m-1)}(x_1, s_1; ...; x_n, s_n; y_1, z_1; ...; \not{y}_j, \not{z}_j; ...; y_m, z_m). \tag{2.2.15}$$

The creation and annihilation operators defined above satisfy the anticommutation relations (2.1.8)-(2.1.11) and annihilate the vacuum vector

$$\Omega \equiv (e^{i\lambda}, 0, 0, ...) \in \mathcal{F}, \qquad \lambda \in \mathbb{R} \tag{2.2.16}$$

according to (2.2.2).

2.2.3 Implementation of operators

Operators in $\mathcal{H}$ induce operators in $\mathcal{F}$.

Self-adjoint operators

A self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$ induces a self-adjoint operator $\hat{A} : \mathcal{F} \to \mathcal{F}$, which is defined by its action on the basis vectors

$$\begin{aligned}
&\hat{A}\left[\frac{1}{\sqrt{n!}} \sum_{\text{permutations } \sigma} \text{sign}(\sigma)\ f_{\sigma(j_1)} \otimes f_{\sigma(j_2)} \otimes ... \otimes f_{\sigma(j_n)}\right] \\
&= \frac{1}{\sqrt{n!}} \sum_{\text{permutations } \sigma} \text{sign}(\sigma)\ \left[A f_{\sigma(j_1)}\right] \otimes f_{\sigma(j_2)} \otimes ... \otimes f_{\sigma(j_n)} \\
&+ \frac{1}{\sqrt{n!}} \sum_{\text{permutations } \sigma} \text{sign}(\sigma)\ f_{\sigma(j_1)} \otimes \left[A f_{\sigma(j_2)}\right] \otimes ... \otimes f_{\sigma(j_n)} + ... \\
&+ \frac{1}{\sqrt{n!}} \sum_{\text{permutations } \sigma} \text{sign}(\sigma)\ f_{\sigma(j_1)} \otimes f_{\sigma(j_2)} \otimes ... \otimes \left[A f_{\sigma(j_n)}\right]
\end{aligned} \tag{2.2.17}$$

and

$$\hat{A}\Omega = 0. \tag{2.2.18}$$

Unitary operators

A unitary operator $U : \mathcal{H} \to \mathcal{H}$ induces a unitary operator $\hat{U} : \mathcal{F} \to \mathcal{F}$, which is defined by its action on the basis vectors

$$\begin{aligned}
&\hat{U}\left[\frac{1}{\sqrt{n!}} \sum_{\text{permutations } \sigma} \text{sign}(\sigma)\ f_{\sigma(j_1)} \otimes f_{\sigma(j_2)} \otimes ... \otimes f_{\sigma(j_n)}\right] \\
&= \frac{1}{\sqrt{n!}} \sum_{\text{permutations } \sigma} \text{sign}(\sigma)\ \left[U f_{\sigma(j_1)}\right] \otimes \left[U f_{\sigma(j_2)}\right] \otimes ... \otimes \left[U f_{\sigma(j_n)}\right]
\end{aligned} \tag{2.2.19}$$

and

$$\hat{U}\Omega = \Omega. \tag{2.2.20}$$

2.3 Choice of the projector

2.3.1 Fock representation

Irreducibility

Now, we give reasons why the Fock space is important and distinguished among all representations. First, the Fock representation $\mathcal{F}$, as constructed above, is an irreducible realization of CAR, i.e. there is no proper subspace of $\mathcal{F}$ invariant under all $\hat{\Psi}(f)$ and $\hat{\Psi}^*(f)$ [Tha92, Th. 10.2]. Second, any irreducible representation $\hat{\Phi}(f)$ of CAR on $\mathcal{G}$ with

a vacuum vector is unitarily equivalent to the Fock representation $\hat{\Psi}(f)$ on $\mathcal{F}$, i.e. there exists a unitary operator (isomorphism) $\hat{U} : \mathcal{F} \to \mathcal{G}$ such that $\hat{\Phi}(f) = \hat{U}\hat{\Psi}(f)\hat{U}^*$ [Tha92, Th. 10.3]. In this sense we can treat the Fock representation as unique (up to a unitary equivalence).

Projector uniquely defines representation

The above is true as long as the projector P_+ remains unchanged. While a given projector leads to a unique Fock representation, different choices of projectors may lead to different and nonequivalent representations. Therefore the choice of projectors is essential in the construction of a physical theory.

We want to note that the operator P_+ does not necessarily have to be a projector. It may be a more general self-adjoint bounded operator satisfying $0 \leq P_+ \leq 1$[1] and further conditions [Ara71]. Although we restrict ourselves here only to projectors, we cite a more general theorem [Ara71, Th. 1] which states that the choice of P_+ on $\mathcal{H}$ uniquely defines the (Fock) representation $\mathcal{F}$.

There appears a natural question: Which choices of the projector P_+ lead to the same physical interpretation (equivalent representations) and which not? Which choice or choices are then the correct ones from the physical point of view? The answer regarding equivalence is given by the theorem [KS77a, Ara71] cited in section 2.3.3. The answer concerning the physical interpretation bases on the notion of energy of the vacuum state, which will be discussed in section 2.4. First, we define some basic transformations in the Fock space.

2.3.2 Bogoliubov transformations

General definition

Introduce a basis $\{\phi_n^\pm\}$ in $\mathcal{H}_\pm$ (it is countable since we always assume $\mathcal{H}$ is separable, what is true e.g. for $\mathcal{H} = L^2(\mathbb{R}^3)^4$). Define

$$\hat{b}_n \equiv \hat{b}(\phi_n^+) \quad \text{and} \quad \hat{d}_n = \hat{d}(\phi_n^-). \tag{2.3.1}$$

Then $\hat{b}_n$, $\hat{b}_n^*$ annihilate and create particle in the state ϕ_n^+ and $\hat{d}_n$, $\hat{d}_n^*$ annihilate and create antiparticle in the state ϕ_n^-. In the following we will skip the sign $\pm$ in $\phi_n^\pm$ in order not to complicate the notation and assuming that the numbering of the basis vectors ϕ_n by n is unique.

Define *Bogoliubov transformation* as any transformation relating one set of such oper-

[1] where the positivity $A \geq 0$ is defined by $(Af, f) \geq 0 \; \forall f \in \mathcal{H}$ and $A \geq B \Leftrightarrow A - B \geq 0$.

ators to some other one via linear combinations

$$\hat{b}_n{}' = \sum_k W^{++}_{nk}\ \hat{b}_k + \sum_k W^{+-}_{nk}\ \hat{d}^*_k \tag{2.3.2}$$

$$\hat{d}^{*\prime}_n = \sum_k W^{-+}_{nk}\ \hat{b}_k + \sum_k W^{--}_{nk}\ \hat{d}^*_k \tag{2.3.3}$$

where $W^{\pm\pm}_{nk} \equiv (\phi_n, W\ \phi_k)$ are matrix elements of a unitary operator W in $\mathcal{H}$

$$W = \begin{pmatrix} W^{++} & W^{+-} \\ W^{-+} & W^{--} \end{pmatrix} \tag{2.3.4}$$

split so that $W^{\pm\pm'} : \mathcal{H}_\pm \to \mathcal{H}_{\pm'}$ (note the corresponding pairs of signs $\pm$ and $\pm'$).

$\hat{b}'$ and $\hat{d}'$ can be new annihilation operators in $\mathcal{F}$ representing the same CAR if and only if there exists a corresponding vacuum vector $\Omega' \in \mathcal{F}$ such that

$$\hat{b}'(P_+ f)\ \Omega' = 0 \quad \text{and} \quad \hat{d}'(P_- f)\ \Omega' = 0 \qquad \forall f \in \mathcal{H}. \tag{2.3.5}$$

If this is the case, the representation is unitarily equivalent to the original one and there exists a unitary operator $\hat{U} : \mathcal{F} \to \mathcal{F}$ such that

$$\hat{\Psi}'(f) = \hat{U}\Psi(f)\hat{U}^* \quad \text{and} \quad \Omega' = \hat{U}\Omega. \tag{2.3.6}$$

Then the Bogoliubov transformation is called *unitarily implementable*. A criterion for this is formulated in the Shale-Stinespring theorem [Tha92, Th. 10.7]

Theorem 1 *The unitary transformation U in $\mathcal{H}$ is unitarily implementable in $\mathcal{F}$ if and only if U^{+-} and U^{-+} are Hilbert-Schmidt operators.*

The Hilbert-Schmidt norm is defined as

$$||W^{+-}||^2_{HS} \equiv \mathrm{Tr}\ \left[(W^{+-})^*\ W^{+-}\right] = \sum_n ||W^{+-}\phi_n||^2 = \sum_{n,k} |(\phi_k, W^{+-}\phi_n)|^2 \tag{2.3.7}$$

and it must be finite for the operator W^{+-} to be Hilbert-Schmidt. In some sense

$$||W^{+-}||^2_{HS} = \sum_{n,k} |(\phi_k, W^{+-}\phi_n)|^2 = \sum_{n,k} |(P_+\phi_k, W P_-\phi_n)|^2 \tag{2.3.8}$$

measures the "number" of vectors mapped from $\mathcal{H}_-$ to $\mathcal{H}_+$ by W and $||W^{-+}||^2_{HS}$ measures the "number" of vectors mapped from $\mathcal{H}_+$ to $\mathcal{H}_-$. These "numbers" must be finite to allow and guarantee implementability of the transformation in Fock space. Otherwise no new vacuum vector Ω' satisfying (2.3.5) exists in $\mathcal{F}$.

The explicit form of the implemented transformation $\hat{U}$ will be given in section 2.3.4

Unitary transformation

The simplest situation where such transformations appear is a unitary transformation $U : \mathcal{H} \to \mathcal{H}$, which induces a transformation of the field operators

$$\hat{\Psi}(f) \to \hat{\Psi}'(f) = \hat{\Psi}(Uf). \tag{2.3.9}$$

It is easy to show that $\hat{\Psi}'(f)$ also satisfies the CAR algebra (2.1.1)-(2.1.2). Rewriting it by means of the creation and annihilation operators we find

$$\hat{b}'(P_+f) + \hat{d}^{*\prime}(P_-f) = \hat{b}(P_+Uf) + \hat{d}^*(P_-Uf). \tag{2.3.10}$$

Choosing once $f \in \mathcal{H}_+$ and once $f \in \mathcal{H}_-$ we find two relations

$$\hat{b}'(P_+f) = \hat{b}(P_+UP_+f) + \hat{d}^*(P_-UP_+f) \tag{2.3.11}$$
$$\hat{d}^{*\prime}(P_-f) = \hat{b}(P_+UP_-f) + \hat{d}^*(P_-UP_-f), \tag{2.3.12}$$

which represent a Bogoliubov transformation in a basis-independent formulation. Expressing them in a basis of $\mathcal{H}$ and introducing $U^{\pm\pm'}_{kn} = (\phi_k, P_\pm U P_{\pm'}\phi_n)$ we obtain

$$\hat{b}_n{}' = \hat{b}\left(P_+ \textstyle\sum_k U^{++}_{kn}\phi_k\right) + \hat{d}^*\left(P_- \sum_k U^{-+}_{kn}\phi_k\right) \tag{2.3.13}$$
$$\hat{d}^{*\prime}_n = \hat{b}\left(P_+ \textstyle\sum_k U^{+-}_{kn}\phi_k\right) + \hat{d}^*\left(P_- \sum_k U^{--}_{kn}\phi_k\right) \tag{2.3.14}$$

Using the antilinearity of $\hat{b}$ and $\hat{d}^*$

$$\hat{b}_n{}' = \textstyle\sum_k \overline{U^{++}_{kn}}\ \hat{b}\,(P_+\phi_k) + \sum_k \overline{U^{-+}_{kn}}\ \hat{d}^*\,(P_-\phi_k) \tag{2.3.15}$$
$$\hat{d}^{*\prime}_n = \textstyle\sum_k \overline{U^{+-}_{kn}}\ \hat{b}\,(P_+\phi_k) + \sum_k \overline{U^{--}_{kn}}\ \hat{d}^*\,(P_-\phi_k) \tag{2.3.16}$$

A short calculation shows

$$\begin{aligned}\overline{U^{AB}_{kn}} &= (U^{AB})^*_{nk} = (P_AUP_B)^*_{nk} = (P_BU^*P_A)_{nk}\\ &= (U^*)^{BA}_{nk} = (W)^{BA}_{nk},\end{aligned} \tag{2.3.17}$$

where $A, B = \pm$ and $W \equiv U^*$ is unitary in $\mathcal{H}$, too. Finally

$$\hat{b}_n{}' = \textstyle\sum_k W^{++}_{nk}\ \hat{b}_k + \sum_k W^{-+}_{nk}\ \hat{d}^*_k \tag{2.3.18}$$
$$\hat{d}^{*\prime}_n = \textstyle\sum_k W^{+-}_{nk}\ \hat{b}_k + \sum_k W^{--}_{nk}\ \hat{d}^*_k \tag{2.3.19}$$

what is a Bogoliubov transformation. It is implementable (theorem 1) if and only if U^{+-} and U^{-+} are Hilbert-Schmidt operators. This is equivalent to the same condition on $W^{\pm\mp}$, because

Lemma 1 *For $W = U^*$*

$$||U^{+-}||_{HS} = ||W^{-+}||_{HS} \quad \textit{and} \quad ||U^{-+}||_{HS} = ||W^{+-}||_{HS}. \tag{2.3.20}$$

Proof:

$$||U^{+-}||^2_{HS} = \sum_{n,k} |(\phi_n, U^{+-}\phi_k)|^2 = \sum_{n,k} |(\phi_n, P_+ U P_- \phi_k)|^2 = \sum_{n,k} |(P_- U^* P_+ \phi_n, \phi_k)|^2$$
$$= \sum_{n,k} |((U^*)^{-+}\phi_n, \phi_k)|^2 = \sum_{n,k} |(\phi_k, W^{-+}\phi_n)|^2 = ||W^{-+}||^2_{HS}. \square \quad (2.3.21)$$

The unitary transformation in (2.3.9) may also be understood as a one inducing a change of projectors, namely if we introduce

$$P'_\pm \equiv U\ P_\pm\ U^* \quad (2.3.22)$$

and substitute $f \to U^* f$ in (2.3.10) then we obtain

$$\hat{b}'(U^*\ P'_+ f) + \hat{d}^{*\prime}(U^*\ P'_- f) = \hat{b}(P_+ f) + \hat{d}^*(P_- f). \quad (2.3.23)$$

The operators on the left-hand side can be renamed

$$\hat{b}'(U^*\ P'_+ f) \equiv \hat{b}''(P'_+ f), \quad \hat{d}'(U^*\ P'_- f) \equiv \hat{d}''(P'_- f), \quad (2.3.24)$$

so that the new $\hat{b}'', \hat{d}''$ are connected with the new projectors $P'_\pm$. Finally, introducing

$$\hat{\Psi}''(f) \equiv \hat{b}''(P'_+ f) + \hat{d}^{*\prime\prime}(P'_- f) \quad (2.3.25)$$

we find the relation

$$\hat{\Psi}''(f) = \hat{\Psi}(f), \quad (2.3.26)$$

which is not trivial, because both operators decompose into creation and annihilation operators defined by different projectors. In such case implementability is decided by theorem 2 (see section 2.3.3).

Change of a basis

Another situation where Bogoliubov transformations appear is the change of the basis. Consider a unitary transformation $W : \mathcal{H} \to \mathcal{H}$, which maps $W\phi_n = \phi'_n$ and $W : \mathcal{H}_\pm \to \mathcal{H}'_\pm$. Since the new subspaces $\mathcal{H}'_\pm$ are, in general, different from the original, new projectors are induced

$$P'_\pm = W P_\pm W^*. \quad (2.3.27)$$

New creation and annihilation operators can be obtained starting from the relation

$$\hat{\Psi}'(f) = \hat{\Psi}(f), \quad (2.3.28)$$

which can be expressed as

$$\hat{b}'(P'_+ f) + \hat{d}^{*\prime}(P'_- f) = \hat{b}(P_+ f) + \hat{d}^*(P_- f). \quad (2.3.29)$$

Choose first $f = P'_+\phi'_n \in \mathcal{H}'_+$ so that $P'_-f = 0$. Then

$$\begin{aligned}\hat{b}_n{}' \equiv \hat{b}'(P'_+\phi'_n) &= \hat{b}(P_+P'_+\phi'_n) + \hat{d}^*(P_-P'_+\phi'_n)\\ &= \hat{b}(P_+P'_+W\phi_n) + \hat{d}^*(P_-P'_+W\phi_n)\\ &= \hat{b}(P_+WP_+\phi_n) + \hat{d}^*(P_-WP_+\phi_n).\end{aligned} \tag{2.3.30}$$

Now, introduce the matrix elements $W_{kn} \equiv (\phi_k, W\phi_n) = (\phi_k, \phi'_n)$ for W and analogously $W^{\pm\pm'}_{kn}$ for $P_\pm W P_{\pm'}$. Then (using the antilinearity of $\hat{b}$ and $\hat{d}^*$)

$$\begin{aligned}\hat{b}_n{}' &= \hat{b}\left(P_+\sum_k W^{++}_{kn}\phi_k\right) + \hat{d}^*\left(P_-\sum_k W^{-+}_{kn}\phi_k\right)\\ &= \sum_k \overline{W^{++}_{kn}}\,\hat{b}(P_+\phi_k) + \sum_k \overline{W^{-+}_{kn}}\,\hat{d}^*(P_-\phi_k)\\ &= \sum_k \overline{W^{++}_{kn}}\,\hat{b}_k + \sum_k \overline{W^{-+}_{kn}}\,\hat{d}^*_k.\end{aligned} \tag{2.3.31}$$

The complex conjugated matrix elements $\overline{W^{\pm\pm'}_{kn}}$ can be expressed as (for instance for $\overline{W^{-+}_{kn}}$)

$$\begin{aligned}\overline{W^{-+}_{kn}} &= (W^{-+})^*_{nk} = (P_-WP_+)^*_{nk} = (P_+W^*P_-)_{nk}\\ &= (W^*)^{+-}_{nk} = (V)^{+-}_{nk},\end{aligned} \tag{2.3.32}$$

where we have introduced $V \equiv W^*$, also unitary on $\mathcal{H}$, satisfying $V\phi'_n = \phi_n$. Finally, the transformation of the annihilation operators takes the form

$$\hat{b}_n{}' = \sum_k V^{++}_{nk}\,\hat{b}_k + \sum_k V^{+-}_{nk}\,\hat{d}^*_k, \tag{2.3.33}$$

which is a Bogoliubov transformation. The relations for $\hat{d}^{*\prime}_n$ can be found analogously.

According to theorem 1, the transformation is implementable if and only if W^{+-} and W^{-+} (or V^{-+} and V^{+-}) are Hilbert-Schmidt operators.

The same condition can be found by considering the transformation as a change of the projector $P_\pm \to P'_\pm = WP_\pm W^*$ and by applying theorem 2 (see next section). It gives

$$\infty > ||P_+P'_-||_{HS} \qquad = \qquad ||P_+WP_-W^*||_{HS} = ||W^{+-}||_{HS} \tag{2.3.34}$$

$$\infty > ||P'_+P_-||_{HS} \quad = ||P_-P'_+||_{HS} = \quad ||P_-WP_+W^*||_{HS} = ||W^{-+}||_{HS}. \tag{2.3.35}$$

2.3.3 Change of projectors – equivalence of representations

A change of projectors from $P_\pm$ to $P'_\pm$ defines automatically a different representation $\hat{\Psi}'(f)$ of CAR in a different Fock space $\mathcal{F}'$ which contains its vacuum vector Ω' such that

$$\hat{\Psi}'(f) = \hat{b}'(f) + \hat{d}^{*\prime}(f) \qquad \forall f \in \mathcal{H}, \tag{2.3.36}$$

$$\hat{b}'(P_+f)\,\Omega' = 0 \quad \text{and} \quad \hat{d}'(P_-f)\,\Omega' = 0 \qquad \forall f \in \mathcal{H}. \tag{2.3.37}$$

The two representations are unitarily equivalent if there exists a unitary mapping $\hat{U} : \mathcal{F}' \to \mathcal{F}$ such that

$$\hat{\Psi}(f) = \hat{U}\ \hat{\Psi}'(f)\ \hat{U}^* \qquad \forall f \in \mathcal{H}, \tag{2.3.38}$$

that is

$$\hat{b}(P_+ f) + \hat{d}^*(P_- f) = \hat{U}\ \hat{b}'(P'_+ f)\ \hat{U}^* + \hat{U}\ \hat{d}^{*\prime}(P'_- f)\ \hat{U}^* \qquad \forall f \in \mathcal{H}. \tag{2.3.39}$$

Choosing once $f \in \mathcal{H}'_+ \equiv P'_+ \mathcal{H}$ and once $f \in \mathcal{H}'_- \equiv P'_- \mathcal{H}$ we obtain two relations

$$\hat{b}(P_+ P'_+ f) + \hat{d}^*(P_- P'_+ f) = \hat{U}\ \hat{b}'(P'_+ f)\ \hat{U}^* \equiv \hat{b}''(P'_+ f) \tag{2.3.40}$$

$$\hat{b}(P_+ P'_- f) + \hat{d}^*(P_- P'_- f) = \hat{U}\ \hat{d}^{*\prime}(P'_- f)\ \hat{U}^* \equiv \hat{d}^{*\prime\prime}(P'_+ f), \tag{2.3.41}$$

with $\hat{b}''(f), \hat{d}''(f)$ annihilation operators in $\mathcal{F}$, unitarily equivalent to $\hat{b}'(f), \hat{d}'(f)$ in $\mathcal{F}'$. The equations present a Bogoliubov transformation for the operators $\hat{b}(f), \hat{d}(f)$ and $\hat{b}''(f), \hat{d}''(f)$. This transformation is implementable if there exists a vacuum vector $\Omega'' \in \mathcal{F}$ such that

$$\hat{b}''(P'_+ f)\ \Omega'' = 0 \quad \text{and} \quad \hat{d}''(P'_- f)\ \Omega'' = 0 \qquad \forall f \in \mathcal{H}. \tag{2.3.42}$$

Then there exists the unitary transformation $\hat{U}$ connecting $\mathcal{F}$ with $\mathcal{F}'$ via $\Omega'' = \hat{U}\Omega'$.

Analogously as in the Shale-Stinespring theorem, essential for implementation is the "number" of vectors appearing in the "mixing" terms $\hat{d}^*(P_- P'_+ f)$ in (2.3.40) and $\hat{b}(P_+ P'_- f)$ in (2.3.41) which is measured by the Hilbert-Schmidt norm. The corresponding general theorem [KS77a, Ara71] states

Theorem 2 *The choice of two different projectors P_+ and P'_+ leads to unitarily equivalent representations if and only if*

$$||P_+ P'_-||_{H.S.} < \infty \quad \textit{and} \quad ||P'_+ P_-||_{H.S.} < \infty. \tag{2.3.43}$$

or, what is equivalent,

$$||P_+ - P'_+||_{H.S.} < \infty \tag{2.3.44}$$

The equivalence of both criteria can be shown by a direct calculation

$$||P_+ P'_-||^2_{H.S.} + ||P'_+ P_-||^2_{H.S.} = ||P_+ - P'_+||^2_{H.S.}. \tag{2.3.45}$$

2.3.4 Explicit form of the implemented Bogoliubov transformation

Consider the Bogoliubov transformation

$$\hat{b}_n{}' = \textstyle\sum_k U^{++}_{nk}\ \hat{b}_k + \sum_k U^{+-}_{nk}\ \hat{d}^*_k \tag{2.3.46}$$

$$\hat{d}^*_n{}' = \textstyle\sum_k U^{-+}_{nk}\ \hat{b}_k + \sum_k U^{--}_{nk}\ \hat{d}^*_k, \tag{2.3.47}$$

induced in one of the two ways:

A) by a unitary transformation $S : \mathcal{H} \to \mathcal{H}$

$$\hat{\Psi}'_P(f) = \hat{\Psi}_P(S^* f) \qquad \forall f \in \mathcal{H}, \tag{2.3.48}$$

B) or by a change of projectors $P_\pm \to P'_\pm$

$$\hat{\Psi}'_{P'}(f) = \hat{\Psi}_P(f) \qquad \forall f \in \mathcal{H}. \tag{2.3.49}$$

The cases A and B were studied in the literature separately by [Rui77, Sei82] (case A) and [KS77a] (case B). Below we cite and extend both results[2] to a generalized form including both transformations simultaneously.

Here we have indicated explicitly to which projector the field operator corresponds

$$\hat{\Psi}_P(f) = \hat{b}(P_+ f) + \hat{d}^*(P_- f) \quad \text{and} \quad \hat{\Psi}_{P'}(f) = \hat{b}(P'_+ f) + \hat{d}^*(P'_- f). \tag{2.3.50}$$

The particle and antiparticle operators are defined with respect to the bases $\phi_n^\pm \in \mathcal{H}_\pm \equiv P_\pm \mathcal{H}$ and $\chi_n^\pm \in \mathcal{H}'_\pm \equiv P'_\pm \mathcal{H}$ as follows

$$\hat{b}_n \equiv \hat{b}(\phi_n^+), \qquad \hat{d}_n \equiv \hat{d}(\phi_n^-), \tag{2.3.51}$$

$$\hat{b}_n{}' \equiv \hat{b}'(\chi_n^+), \qquad \hat{d}_n{}' \equiv \hat{d}'(\chi_n^-), \tag{2.3.52}$$

where in case A we assume $\chi_n^\pm = \phi_n^\pm$. Case B contains also the situation where the projectors remain unchanged, i.e. $P'_\pm = P_\pm$, but the basis which defines particle states changes from $\phi_n^\pm$ to $\chi_n^\pm$.

In both cases, we look for the unitary implementer $\hat{U} : \mathcal{F} \to \mathcal{F}$ such that

$$\hat{U}^*\, \hat{b}_n\, \hat{U} = \hat{b}_n{}', \qquad \hat{U}^*\, \hat{d}_n\, \hat{U} = \hat{d}_n{}', \tag{2.3.53}$$

what corresponds to

$$\hat{U}^*\, \hat{\Psi}(f)\, \hat{U} = \begin{cases} \Psi(S^* f) & \text{in case A,} \\ \Psi(V^* f) & \text{in case B,} \end{cases} \tag{2.3.54}$$

where the unitary operator V is defined by the property that it maps the two bases onto each other (cf. (2.3.33))

$$V^* \phi_n^\pm = \chi_n^\pm, \tag{2.3.55}$$

$$V_{pq} \equiv (\phi_p, V\phi_r) = (V^*\phi_p, \phi_r) = (\chi_p, \phi_r). \tag{2.3.56}$$

Such V maps the two projectors onto each other

$$V^* P_\pm = P'_\pm V^*, \qquad P'_\pm = V^* P_\pm V. \tag{2.3.57}$$

[2] correcting several misprints in [KS77a]

Since in case A we have $V = \mathbf{1}$ and in case B we can assume $S = \mathbf{1}$, both cases can be generalized now to a universal form containing both of them

$$\hat{U}^* \, \hat{\Psi}(f) \, \hat{U} = \Psi(S^* V^* f) \equiv \Psi(U^* f), \tag{2.3.58}$$

with $U = VS$ and

$$\begin{aligned} U_{pq} \equiv (\phi_p, U\phi_q) = (\phi_p, VS\phi_q) &= \sum_r (\phi_p, V\phi_r)(\phi_r, S\phi_q) \equiv \sum_r V_{pr} S_{rq} \\ &= \sum_r (\chi_p, \phi_r)(\phi_r, S\phi_q) = (\chi_p, S\phi_q) \equiv \widetilde{S}_{pq}, \end{aligned} \tag{2.3.59}$$

Now both cases follow from the general form

$$\chi_n^{\pm} = \phi_n^{\pm} \Rightarrow \quad V = \mathbf{1} \quad \Rightarrow U^* = S^* \qquad \text{(case A)} \tag{2.3.60}$$

$$S = \mathbf{1} \quad \Rightarrow U^* = V^* \qquad \text{(case B)} \tag{2.3.61}$$

(Because

$$\begin{aligned} (V_{-+})_{pq} = (\phi_p^-, P_- V P_+ \phi_q^+) = (V^* \phi_p^-, \phi_q^+) &= (\chi_p^-, \phi_q^+) \\ = (\chi_p^-, P'_- P_+ \phi_q^+) \equiv (\chi_p^-, W\phi_q^+) &\equiv (\widetilde{W}_{-+})_{pq} \end{aligned} \tag{2.3.62}$$

with $P'_{\pm'} P_{\pm} \equiv W_{\pm'\pm}$, in [KS77a] actually implementation of W has been studied, but it is fully equivalent to our case B.)

If $\hat{U}$ exists it maps the vacuum vector Ω for $\hat{b}_n$ and $\hat{d}_n$

$$\hat{b}_n \Omega = \hat{d}_n \Omega = 0 \tag{2.3.63}$$

onto the vacuum vector Ω' for $\hat{b}_n{}'$ and $\hat{d}_n{}'$

$$\hat{b}_n{}' \Omega' = \hat{d}_n{}' \Omega' = 0, \tag{2.3.64}$$

which is given by

$$\Omega' = \hat{U}^* \, \Omega. \tag{2.3.65}$$

Before we construct $\hat{U}$ we need some definitions. Define subspaces

$$\mathcal{R}_+ \equiv \ker(U_{++}), \qquad n_+ \equiv \dim \mathcal{R}_+ \tag{2.3.66}$$

$$\mathcal{R}_- \equiv \ker(U_{--}), \qquad n_- \equiv \dim \mathcal{R}_-. \tag{2.3.67}$$

$\mathcal{R}_\pm$ are finite dimensional, what follows from the finiteness of the Hilbert-Schmidt norms of $U_{\pm\mp}$. It holds

$$\ker(U_{++}) = \ker((U_{++})^* U_{++}) = \ker(1 - (U_{-+})^* U_{-+}) \tag{2.3.68}$$

and it follows

$$f \in \mathcal{R}_+ \Leftrightarrow f \in \ker(1 - (U_{-+})^* U_{-+}) \Leftrightarrow (U_{-+})^* U_{-+} f = f, \tag{2.3.69}$$

i.e. f is an eigenvector to the eigenvalue 1 of $(U_{-+})^* U_{-+} = P_+ U^* P_- U P_+$ and $f \in \mathcal{H}_+$. Since $||(U_{-+})^*|| = ||U_{-+}|| = 1$, there exists $g \in \mathcal{H}_-$ such that

$$U_{-+} f = g, \qquad (U_{-+})^* g = f. \tag{2.3.70}$$

That means $\hat{b}^*(f) = \hat{d}'(g)$. In case B, in a suitable basis (defined below in the theorem) it means that there exists n for which

$$\phi_n^+ = \chi_n^- \qquad \left(= V^* \phi_n^- = P_+ V^* P_- \phi_n^- = (P_- V P_+)^* \phi_n^- = (V_{-+})^* \phi_n^- \right). \tag{2.3.71}$$

The analogous holds for $f \in \mathcal{R}_-$. Operators U with $n_+ + n_- > 0$ will be called *strong*[3], otherwise $(n_+ = n_- = 0)$ *weak*.

Now, we state the theorem constructing $\hat{U}^*$, which maps Ω on Ω'. It is straightforward to obtain $\hat{U}$ by taking the adjoint. The proof is almost identical to the proofs published in [Sei82] and [KS77a], but out notation is more general and includes both cases, what does not influence the way of the proof.

Theorem 3 *Define operators*

$$A \equiv -U_{++}^{-1} U_{+-}, \qquad B \equiv \pm U_{++}^{-1} \tag{2.3.72}$$

$$C \equiv \pm \overline{(U_{--}^{-1})} \qquad D \equiv \pm (U_{-+}\, U_{++}^{-1})^T, \tag{2.3.73}$$

where the upper sign is to be chosen if $(n_+ + n_-)$ is even and the lower if $(n_+ + n_-)$ is odd (here and in the following). The inverse operators are defined on the orthogonal complements $\mathcal{R}'_\pm$ (such that $\mathcal{R}_\pm \oplus \mathcal{R}'_\pm = \mathcal{H}$). Introduce a suitable basis

$$\varphi_1^+, ..., \varphi_{n_+}^+ \in \mathcal{R}_+ \tag{2.3.74}$$

$$\varphi_{n_+ +1}^+, ..., \varphi_\infty^+ \in \mathcal{R}'_+ \tag{2.3.75}$$

$$\varphi_1^-, ..., \varphi_{n_-}^- \in \mathcal{R}_- \tag{2.3.76}$$

$$\varphi_{n_- +1}^-, ..., \varphi_\infty^- \in \mathcal{R}'_-. \tag{2.3.77}$$

Define operators

$$\hat{b}_k \equiv \hat{b}(\varphi_k^+), \qquad \hat{d}_k \equiv \hat{d}(\varphi_k^-) \quad for \quad k = 1, ..., \infty \tag{2.3.78}$$

and

$$A_{kl} \equiv (\varphi_k^+, A\, \varphi_l^-), \qquad B_{kl} \equiv (\varphi_k^+, B\, \varphi_l^+), \tag{2.3.79}$$

$$C_{kl} \equiv (\varphi_k^-, C\, \varphi_l^-), \qquad D_{kl} \equiv (\varphi_k^+, D\, \varphi_l^-) \tag{2.3.80}$$

$$for \quad k = n_+ + 1, ..., \infty;\ l = n_- + 1, ..., \infty \tag{2.3.81}$$

Then

$$\hat{U}^* = C_0 \ : \hat{U}_0^*\ \widetilde{U}^* : \tag{2.3.82}$$

[3] In [Sei82] they are called *singular*, but we want to avoid confusion with the notion of a singular operator or a singular potential.

with

$$C_0 \equiv [\det(1 + A^*A)]^{-1/2}, \tag{2.3.83}$$

$$\begin{aligned} \widetilde{U}^* =: &\exp\left(\sum_{k,l} A_{kl}\hat{b}^*{}_k\hat{d}^*{}_l\right)\exp\left(\sum_{k,l}(B_{kl}-\delta_{kl})\hat{b}^*{}_k\hat{b}_l\right) \\ &\exp\left(\sum_{k,l}(C_{kl}-\delta_{kl})\hat{d}^*{}_k\hat{d}_l\right)\exp\left(\sum_{k,l} D_{kl}\hat{b}_k\hat{d}_l\right): \\ &k = n_+ + 1, ..., \infty;\ l = n_- + 1, ..., \infty \end{aligned} \tag{2.3.84}$$

$$\begin{aligned} \hat{U}_0^* \equiv &: \left(\hat{b}^*(\varphi_1^+) \mp \hat{d}(U\varphi_1^+)\right) ... \left(\hat{b}^*(\varphi_{n_+}^+) \mp \hat{d}(U\varphi_{n_+}^+)\right) \\ &\left(\hat{d}^*(\varphi_1^-) \mp \hat{b}(U\varphi_1^-)\right) ... \left(\hat{d}^*(\varphi_{n_-}^-) \mp \hat{b}(U\varphi_{n_+}^+)\right): \\ =: &\left(\hat{b}^*{}_1 \mp \sum_{k=1}^{n_+}(U_{-+})_{k1}\hat{d}_k\right) ... \left(\hat{b}^*{}_{n_+} \mp \sum_{k=1}^{n_+}(U_{-+})_{kn_+}\hat{d}_k\right) \\ &\left(\hat{d}^*{}_1 \mp \sum_{k=1}^{n_-}\overline{(U_{+-})_{k1}}\hat{b}_k\right) ... \left(\hat{d}^*{}_{n_-} \mp \sum_{k=1}^{n_-}\overline{(U_{+-})_{kn_-}}\hat{b}_k\right): \end{aligned} \tag{2.3.85}$$

The ": ... :" means normal ordering and is defined in section 2.4.2.

The existence of $\hat{U}$ allows for calculation of any expectation value of any operator $\hat{A}$ (build of $\hat{\Psi}, \hat{\Psi}^*$) in both representations

$$(\Phi_1', \hat{A}'\Phi_2') = (\hat{U}^*\Phi_1, \hat{U}^*\hat{A}\hat{U}\ \hat{U}^*\Phi_2) = (\Phi_1, \hat{A}\Phi_2) \tag{2.3.86}$$

or switching between the Heisenberg and Schrödinger pictures

$$(\Phi_1, \hat{A}'\Phi_2) = (\Phi_1, \hat{U}^*\hat{A}\hat{U}\ \Phi_2) = (\hat{U}\Phi_1, \hat{A}\ \hat{U}\Phi_2) = (\Phi_1'', \hat{A}\Phi_2''). \tag{2.3.87}$$

Consequences of Theorem 3

The Bogoliubov transformation considered in the above theorem has the form

$$\hat{b}_j' = \hat{d}_j^* \quad \text{for} \quad j = 1, ..., n_- \tag{2.3.88}$$

$$\hat{b}_j' = \sum_{k=n_++1}^{\infty}(U_{++})_{jk}\hat{b}_k + \sum_{k=n_-+1}^{\infty}(U_{+-})_{jk}\hat{d}_k^* \quad \text{for} \quad j = n_- + 1, ..., \infty \tag{2.3.89}$$

$$\hat{d}_j'^* = \hat{b}_j \quad \text{for} \quad j = 1, ..., n_+ \tag{2.3.90}$$

$$\hat{d}_j'^* = \sum_{k=n_++1}^{\infty}(U_{-+})_{jk}\hat{b}_k + \sum_{k=n_-+1}^{\infty}(U_{--})_{jk}\hat{d}_k^* \quad \text{for} \quad j = n_+ + 1, ..., \infty \tag{2.3.91}$$

and is assumed to be implementable (U_{+-} and U_{-+} are Hilbert-Schmidt).

The full operator $\hat{U}^*$, when transforming the vacua, can be simplified to

$$\Omega' = \hat{U}^*\Omega = C_0\ \hat{U}_0^*\ \exp\left(\sum_{\substack{k=n_++1\\ l=n_-+1}}^{\infty} A_{kl}\hat{b}^*{}_k\hat{d}^*{}_l\right)\Omega. \tag{2.3.92}$$

Ω' exists if it has finite norm. Here, the normalization is fixed by multiplication by C_0, which must be non-zero, that is, the (Fredholm) determinant

$$\det(1+A^*A) \equiv 1 + \sum_n \sum_{k_1<\ldots<k_n} \det(A^*A)_{k_ik_j} \tag{2.3.93}$$

must be finite, what is the case when A^*A is trace-class ($\sum_n (f_n, A^*Af_n) < \infty$). This can be traced back to the fact that U_{+-}, U_{-+} must be Hilbert-Schmidt, what has been assumed.

Moreover, $\hat{U}^*$ transforms any basis vector from $\mathcal{F}$ into a "basis vector" defined by means of the new vacuum Ω' and new creation operators $\hat{b}^{*\prime}{}_n, \hat{d}^{*\prime}{}_n$

$$\hat{U}^*\left(\hat{b}^*_{i_1}\ldots\hat{b}^*_{i_n}\hat{d}^*_{j_1}\ldots\hat{d}^*_{j_m}\Omega\right) = \hat{b}'^*_{i_1}\ldots\hat{b}'^*_{i_n}\hat{d}'^*_{j_1}\ldots\hat{d}'^*_{j_m}\Omega'. \tag{2.3.94}$$

It can be interpreted as a transformation of the creation operators writing

$$\begin{aligned}\hat{U}^*\left(\hat{b}^*_{i_1}\ldots\hat{b}^*_{i_n}\hat{d}^*_{j_1}\ldots\hat{d}^*_{j_m}\Omega\right) &= \left(\hat{U}^*\hat{b}^*_{i_1}\hat{U}\right)\ldots\left(\hat{U}^*\hat{b}^*_{i_n}\hat{U}\right)\left(\hat{U}^*\hat{d}^*_{j_1}\hat{U}\right)\ldots\left(\hat{U}^*\hat{d}^*_{j_m}\hat{U}\right)\hat{U}^*\Omega\\ &= \hat{b}'^*_{i_1}\ldots\hat{b}'^*_{i_n}\hat{d}'^*_{j_1}\ldots\hat{d}'^*_{j_m}\Omega',\end{aligned} \tag{2.3.95}$$

what gives the following relations

$$\hat{U}^*\hat{b}^*_i\hat{U} = \hat{b}'^*_i \quad \text{and} \quad \hat{U}^*\hat{d}^*_j\hat{U} = \hat{d}'^*_j. \tag{2.3.96}$$

The operators $\hat{b}^*_i$ with $i = 1, ..., n_+$ and $\hat{d}^*_j$ with $j = 1, ..., n_-$ correspond to the states ϕ^+_i, which are mapped from $\mathcal{H}_+ = P_+\mathcal{H}$ to $\mathcal{H}'_- = P'_-\mathcal{H}$ and to ϕ^-_j, which are mapped from $\mathcal{H}_- = P_-\mathcal{H}$ to $\mathcal{H}'_+ = P'_+\mathcal{H}$. They play a special role in the $\hat{U}^*_0$ part of the operator $\hat{U}^*$ and create particles and antiparticles from vacuum

$$\Omega' = \hat{U}^*\Omega = C_0\ \hat{d}^*_{n_-}\ldots\hat{d}^*_1\hat{b}^*_{n_+}\ldots\hat{b}^*_1\ \exp\left(\sum_{k,l} A_{kl}\hat{b}^*{}_k\hat{d}^*{}_l\right)\Omega, \tag{2.3.97}$$

what presents a charged vacuum in case $n_+ \neq n_-$. Operators $\hat{b}(U\varphi^-_s)$ and $\hat{d}(U\varphi^+_s)$ in (2.3.85) annihilate particles and antiparticles in states that are also mapped between $\mathcal{H}_+$ and $\mathcal{H}_-$. The role of the terms $\hat{b}^*(\varphi^+_s) \mp \hat{d}(U\varphi^+_s)$ in (2.3.85) is to either create a particle in state φ^+_s if there was no antiparticle in state $U\varphi^+_s$, or to annihilate the antiparticle φ^+_s if it was present. In the first case $\hat{b}^*(\varphi^+_s) \mp \hat{d}(U\varphi^+_s)$ acts on vector Φ which does not contain $\hat{d}^*(U\varphi^+_s)$ and the result is $\hat{b}^*(\varphi^+_s)\Phi$ (because $\hat{d}(U\varphi^+_s)\Phi = 0$). In the second case

$\Phi = \hat{d}^*(U\varphi_s^+)\widetilde{\Phi}$ and the second term gives $\hat{d}(U\varphi_s^+)\Phi = \widetilde{\Phi}$, while the first must give zero. It is possible because in between the operator $\widetilde{U}^*$ (2.3.84) there comes into play (which always stands to the left of $\hat{d}(U\varphi_s^+)$ due to normal ordering, but to the right of $\hat{b}^*(\varphi_s^+)$) and one gets $\hat{b}^*(\varphi_s^+)\widetilde{U}^*\hat{d}^*(U\varphi_s^+)\widetilde{\Phi}$ which turns out to be zero. To understand this we first must observe that the exponents in $\widetilde{U}^*$ can be written as

$$\begin{aligned}
:\exp\left((B-1)\hat{b}^*\hat{b}\right):&\equiv :\exp\left(\sum_{p,q}(B_{pq}-\delta_{pq})\hat{b}_p^*\hat{b}_q\right):\\
&=:\exp\left(\sum_{p,q}B_{pq}\hat{b}_p^*\hat{b}_q-\sum_q\hat{b}_q^*\hat{b}_q\right):\\
&=:\exp\left(\sum_{p,q}B_{pq}\hat{b}_p^*\hat{b}_q\right)\ \exp\left(-\sum_q\hat{b}_q^*\hat{b}_q\right):\\
&=:\prod_{p,q}\exp\left(B_{pq}\hat{b}_p^*\hat{b}_q\right)\ \prod_q\exp\left(-\hat{b}_q^*\hat{b}_q\right):\\
&=:\prod_{p,q}\left(1+B_{pq}\hat{b}_p^*\hat{b}_q\right)\ \prod_q\left(1-\hat{b}_q^*\hat{b}_q\right):\\
&=:\prod_q\left(1+\sum_pB_{pq}\hat{b}_p^*\hat{b}_q\right)\ \prod_q\left(1-\hat{b}_q^*\hat{b}_q\right):\\
&=:\prod_q\left[\left(1+\sum_pB_{pq}\hat{b}_p^*\hat{b}_q\right)\ \left(1-\hat{b}_q^*\hat{b}_q\right)\right]:\\
&=:\prod_q\left[\left(1+\sum_pB_{pq}\hat{b}_p^*\hat{b}_q-\hat{b}_q^*\hat{b}_q\right)\right]:
\end{aligned}\tag{2.3.98}$$

and analogously

$$:\exp\left((C-1)\hat{d}^*\hat{d}\right):=:\prod_q\left[\left(1+\sum_pC_{pq}\hat{d}_p^*\hat{d}_q-\hat{d}_q^*\hat{d}_q\right)\right]:\ .\tag{2.3.99}$$

Then it is simple to calculate the commutations

$$\begin{aligned}
:\exp\left((B-1)\hat{b}^*\hat{b}\right):\hat{b}_s^*&=\left(1+\sum_pB_{ps}\hat{b}_p^*\hat{b}_s-\hat{b}_s^*\hat{b}_s\right)\hat{b}_s^*:\exp\left((B-1)\hat{b}^*\hat{b}\right):\\
&=\left(\hat{b}_s^*+\sum_pB_{ps}\hat{b}_p^*-\hat{b}_s^*\right):\exp\left((B-1)\hat{b}^*\hat{b}\right):=\left(\sum_pB_{ps}\hat{b}_p^*\right):\exp\left((B-1)\hat{b}^*\hat{b}\right):
\end{aligned}\tag{2.3.100}$$

and analogously

$$:\exp\left((C-1)\hat{d}^*\hat{d}\right):\hat{d}_s^*=\left(\sum_pC_{ps}\hat{d}_p^*\right):\exp\left((C-1)\hat{d}^*\hat{d}\right):\ .\tag{2.3.101}$$

Or, using

$$\sum_p B_{ps}\hat{b}^*_p = \sum_p (\varphi_p, B\varphi_s)\hat{b}^*(\varphi_p) = \hat{b}^*\left(\sum_p (\varphi_p, B\varphi_s)\varphi_p\right) = \hat{b}^*(B\varphi_s) \tag{2.3.102}$$

we can write in short

$$:\exp\left((B-1)\hat{b}^*\hat{b}\right): \hat{b}^*(f) = \hat{b}^*(Bf) :\exp\left((B-1)\hat{b}^*\hat{b}\right): \tag{2.3.103}$$

and

$$:\exp\left((C-1)\hat{d}^*\hat{d}\right): \hat{d}^*(f) = \hat{d}^*(\overline{C}f) :\exp\left((C-1)\hat{d}^*\hat{d}\right): \ . \tag{2.3.104}$$

Now, we observe that for $s \leq n_-$, with $\varphi^-_s \in \mathcal{R}_-$ and $U\varphi^-_s \in \mathcal{H}_+$, it holds

$$:\exp\left((B-1)\hat{b}^*\hat{b}\right): \hat{b}^*(U\varphi^-_s) = \hat{b}^*(BU\varphi^-_s) :\exp\left((B-1)\hat{b}^*\hat{b}\right) := 0, \tag{2.3.105}$$

because

$$BU\varphi^-_s = (U^{-1})_{++}U\varphi^-_s = P_+U^*P_+U\varphi^-_s = P_+\varphi^-_s = 0. \tag{2.3.106}$$

For the last step see (2.3.69) and (2.3.70) or observe that $\varphi^-_s \in \ker(U_{--}) \Rightarrow U\varphi^-_s \in \ker(U^*_{++})$, i.e. $U^*_{++}(U\varphi^-_s) = 0$. Analogously for $s \leq n_+$ and $\varphi^+_s \in \mathcal{R}_+$ with $U\varphi^+_s \in \mathcal{H}_-$

$$:\exp\left((C-1)\hat{d}^*\hat{d}\right): \hat{d}^*(U\varphi^+_s) = \hat{d}^*(\overline{C}U\varphi^+_s) :\exp\left((C-1)\hat{d}^*\hat{d}\right) := 0, \tag{2.3.107}$$

because

$$\overline{C}U\varphi^+_s = (U^{-1})_{--}U\varphi^+_s = P_-U^*P_-U\varphi^+_s = 0 \tag{2.3.108}$$

since $\varphi^+_s \in \ker(U_{++}) \Rightarrow U\varphi^+_s \in \ker(U^*_{--})$, i.e. $U^*_{--}(U\varphi^+_s) = 0$.

Relations (2.3.105) and (2.3.107) show that

$$\widetilde{U}^*\hat{d}^*(U\varphi^+_s) = 0, \quad \text{and} \quad \widetilde{U}^*\hat{b}^*(U\varphi^-_s) = 0. \tag{2.3.109}$$

Finally, we can see how $\hat{U}^*$ acts on particles and antiparticles in the special states, for instance

$$\hat{U}^*\ \hat{d}^*(U\varphi^+_r)\ \hat{b}^*(U\varphi^-_s)\ \Omega = C_0\ \hat{d}^*_{n_-}\dots\not{\hat{d}}^*_r\dots\hat{d}^*_1\ \hat{b}^*_{n_+}\dots\not{\hat{b}}^*_r\dots\hat{b}^*_1\ \exp\left(\sum_{k,l} A_{kl}\hat{b}^*{}_k\hat{d}^*{}_l\right)\Omega. \tag{2.3.110}$$

Example

Consider a very simple, but illustrative example, which will be a basis for the analysis of overcritical fields studied in the next chapter. Let $\mathcal{R}_+$ be one-dimensional, i.e. $n_+ = 1$, and $n_- = \dim\mathcal{R}_- = 0$. Let the Bogoliubov transformation be of the form

$$\hat{d}'^*_1 = \hat{b}_1 \tag{2.3.111}$$

$$\hat{b}'_j = \hat{b}_{j+1} \quad \text{for} \quad j = 1, ..., \infty \tag{2.3.112}$$

$$\hat{d}'^*_{j+1} = \hat{d}^*_j \quad \text{for} \quad j = 1, ..., \infty. \tag{2.3.113}$$

It is implementable because $||U_{-+}||_{HS} = 1$ and $||U_{+-}||_{HS} = 0$. The explicit form of U is

$$(U_{++})_{ik} = \delta_{i+1,k} \qquad (U_{--})_{ik} = \delta_{i,k+1} \tag{2.3.114}$$

$$(U_{-+})_{ik} = \delta_{i,1} \cdot \delta_{k,1} \qquad (U_{+-})_{ik} = 0 \qquad \text{for} \quad i,k = 1,...,\infty \tag{2.3.115}$$

and the auxiliary operators are

$$B_{ik} = -\delta_{i,k+1} \qquad C_{ik} = -\delta_{i+1,k} \tag{2.3.116}$$

$$A_{ik} = 0 \qquad D_{ik} = 0. \tag{2.3.117}$$

The role of B and C is to shift the indices of $\hat{b}_j$ and $\hat{d}_j$ according to (2.3.112)-(2.3.113) and guarantee the appearance of additional minus signs in the following commutations, which will cancel in commutation with $\hat{U}_0^*$,

$$: \exp\left((B-1)\hat{b}^*\hat{b}\right) : \hat{b}_n^* = -\hat{b}_{n+1}^* : \exp\left((B-1)\hat{b}^*\hat{b}\right) : \quad \text{for} \quad n \geq 1 \tag{2.3.118}$$

$$: \exp\left((C-1)\hat{d}^*\hat{d}\right) : \hat{d}_n^* = \begin{cases} -\hat{d}_{n-1}^* : \exp\left((C-1)\hat{d}^*\hat{d}\right) : & \text{for} \quad n \geq 2 \\ 0 & \text{for} \quad n = 1. \end{cases} \tag{2.3.119}$$

The Bogoliubov transformation is implemented by the unitary operator

$$\hat{U}^* = C_0\, \hat{U}_0^* \exp\left(A\hat{b}^*\hat{d}^*\right) : \exp\left((B-1)\hat{b}^*\hat{b}\right) :: \exp\left((C-1)\hat{d}^*\hat{d}\right) : \exp\left(D\hat{b}\hat{d}\right) \tag{2.3.120}$$

where $A = 0$, $D = 0$, $C_0 = 1$, and

$$\hat{U}_0^* = \hat{b}_1^* + \hat{d}_1. \tag{2.3.121}$$

Therefore it reduces to

$$\hat{U}^* =: \left(\hat{b}_1^* + \hat{d}_1\right) \exp\left((B-1)\hat{b}^*\hat{b}\right) \exp\left((C-1)\hat{d}^*\hat{d}\right) : \tag{2.3.122}$$

$\hat{U}_0^*$ anti-commutes with all $\hat{b}_n^*$ and $\hat{d}_n^*$ except $\hat{b}_1^*$ with which it commutes

$$\hat{U}_0^*\, \hat{b}_n^*\, \hat{U}_0 = -\hat{b}_n^* \quad \text{for} \quad n \geq 2 \qquad \text{and} \qquad \hat{U}_0^*\, \hat{d}_n^*\, \hat{U}_0 = -\hat{d}_n^* \quad \text{for} \quad n \geq 1, \tag{2.3.123}$$

$$\hat{U}_0^*\, \hat{b}_1^*\, \hat{U}_0 = \hat{b}_1^*. \tag{2.3.124}$$

These additional minus signs cancel with those produced in (2.3.118) and (2.3.119). Finally, we obtain the required transformations

$$\hat{U}^*\, \hat{b}_n^*\, \hat{U} = \hat{b}_n'^* = \hat{b}_{n+1}^* \tag{2.3.125}$$

$$\hat{U}^*\, \hat{d}_n^*\, \hat{U} = \hat{d}_n'^* = \begin{cases} \hat{d}_{n-1}^* & \text{for} \quad n \geq 2 \\ \hat{b}_1 & \text{for} \quad n = 1. \end{cases} \tag{2.3.126}$$

The vacuum vector Ω with respect to the operators $\hat{b}_n$ and $\hat{d}_n$ transforms to the vacuum vector Ω' with respect to $\hat{b}'_n$ and $\hat{d}'_n$ and equals

$$\Omega' = \hat{U}^* \, \Omega = \left(\hat{b}_1^* + \hat{d}_1\right) \Omega = \hat{b}_1^* \, \Omega. \tag{2.3.127}$$

The inverse operator $\hat{U}$ is given by

$$\hat{U} =: \left(\hat{d}_1^* + \hat{b}_1\right) \exp\left((B^* - 1)\hat{b}^*\hat{b}\right) \exp\left((C^* - 1)\hat{d}^*\hat{d}\right) : \tag{2.3.128}$$

It connects the two vacua in the opposite way

$$\begin{aligned} \hat{U} \, \Omega' &= : \left(\hat{d}_1^* + \hat{b}_1\right) \exp\left((B^* - 1)\hat{b}^*\hat{b}\right) : \Omega' = \\ &= \left(\hat{d}_1^* : \exp\left((B^* - 1)\hat{b}^*\hat{b}\right) : + : \exp\left((B^* - 1)\hat{b}^*\hat{b}\right) : \hat{b}_1\right) \hat{b}_1^* \Omega = \\ &= 0 + : \exp\left((B^* - 1)\hat{b}^*\hat{b}\right) : \Omega = \Omega, \end{aligned} \tag{2.3.129}$$

where $: \exp\left((B^* - 1)\hat{b}^*\hat{b}\right) : \hat{b}_1^* = 0$ has been used, what is an analogue of (2.3.118)-(2.3.119) with B^* instead of B. On the other hand, we can calculate

$$\begin{aligned} \hat{d}_1{}'^* \Omega' &= (\hat{U}^* \hat{d}_1 \hat{U})(\hat{U}^* \Omega) = \hat{U}^* \hat{d}_1 \Omega \\ &= : \left(\hat{b}_1^* + \hat{d}_1\right) \exp\left((B - 1)\hat{b}^*\hat{b}\right) \exp\left((C - 1)\hat{d}^*\hat{d}\right) : \hat{d}_1 \Omega \\ &= \left(\hat{b}_1^* : \exp\left((C - 1)\hat{d}^*\hat{d}\right) : + : \exp\left((C - 1)\hat{d}^*\hat{d}\right) : \hat{d}_1\right) \hat{d}_1 \Omega \\ &= 0 + : \exp\left((C - 1)\hat{d}^*\hat{d}\right) : \Omega = \Omega, \end{aligned} \tag{2.3.130}$$

where we have used (2.3.119) in the last line.

Therefore for both reference systems the own vacuum is always a no particle state and the other vacuum seems to be a one particle (2.3.127), respectively a one anti-particle state (2.3.130).

We will come back to the results of this example in chapter 4, where overcritical potentials will be discussed.

2.4 Vacuum state and energy in Fock space

2.4.1 Energy operator

The notion of energy in Fock space is based on the *second quantized Dirac operator* $\hat{H} : \mathcal{F} \to \mathcal{F}$ which is an implemented version of the classical Hamilton operator $H : \mathcal{H} \to \mathcal{H}$. The prescription in section 2.2.3 is sufficient and unique, but practically rather complicated. It is of advantage to express the action of the implemented operator in terms of the field operator or of the creation and annihilation operators. It can be shown that

$$\hat{H} = \sum_k \left[\hat{b}^*(H f_k) \; \hat{b}(f_k) - \hat{d}^*(H g_k) \; \hat{d}(g_k)\right]. \tag{2.4.1}$$

It can be checked in every subspace of $\mathcal{F}$ separately. Choose for example $\Phi^{(1,1)} \in \mathcal{F}^{(1,1)}$. According to the definitions introduced in sections 2.2.1 and 2.2.2 it has the form

$$\Phi^{(1,1)} = f \otimes Cg = \hat{b}^*(f)\hat{d}^*(g)\Omega, \tag{2.4.2}$$

where $f \in \mathcal{H}_+$ and $g \in \mathcal{H}_-$. Directly from the definition formula for implementation of the self-adjoined operators (2.2.17) we get

$$\begin{aligned}
\hat{H}\Phi^{(1,1)} =& Hf \otimes Cg + f \otimes H(Cg) = Hf \otimes Cg + f \otimes (-CHg) \\
=& \hat{b}^*(Hf)\ \hat{d}^*(g)\ \Omega - \hat{b}^*(f)\ \hat{d}^*(Hg)\ \Omega \\
=& \hat{b}^* \left(\sum_k (f_k, Hf) f_k \right) \hat{d}^*(g)\ \Omega - \hat{b}^*(f)\ \hat{d}^* \left(\sum_k (g_k, Hg) g_k \right) \Omega \\
=& \sum_k \hat{b}^*(f_k)\ (f_k, Hf)\ \hat{d}^*(g)\ \Omega - \sum_k \hat{b}^*(f)\ \hat{d}^*(g_k)\ (Hg, g_k)\ \Omega \\
=& \sum_k \hat{b}^*(f_k)\ (Hf_k, f)\ \hat{d}^*(g)\ \Omega - \sum_k \hat{b}^*(f)\ \hat{d}^*(g_k)\ (g, Hg_k)\ \Omega \\
=& \sum_k \hat{b}^*(f_k) \left[\hat{b}(Hf_k)\ \hat{b}^*(f) + \hat{b}^*(f)\ \hat{b}(Hf_k) \right] \hat{d}^*(g)\ \Omega \\
& - \sum_k \hat{b}^*(f)\ \hat{d}^*(g_k) \left[\hat{d}^*(g)\ \hat{d}(Hg_k) + \hat{d}(Hg_k)\ \hat{d}^*(g) \right] \Omega \\
=& \sum_k \hat{b}^*(f_k)\ \hat{b}(Hf_k)\ \hat{b}^*(f)\ \hat{d}^*(g)\ \Omega - \sum_k \hat{d}^*(g_k)\ \hat{d}(Hg_k)\ \hat{b}^*(f)\ \hat{d}^*(g)\ \Omega \\
=& \sum_k \left[\hat{b}^*(f_k)\ \hat{b}(Hf_k) - \hat{d}^*(g_k)\ \hat{d}(Hg_k) \right] \hat{b}^*(f)\ \hat{d}^*(g)\ \Omega \\
=& \sum_k \left[\hat{b}^*(f_k)\ \hat{b}(Hf_k) - \hat{d}^*(g_k)\ \hat{d}(Hg_k) \right] \Phi^{(1,1)}.
\end{aligned} \tag{2.4.3}$$

The last step is to show

$$\begin{aligned}
\sum_k \hat{b}^*(f_k)\ \hat{b}(Hf_k) &= \sum_{k,l} \hat{b}^*(f_k)\ \hat{b}\left((f_l, Hf_k)\ f_l\right) = \sum_{k,l} \hat{b}^*(f_k)\ (Hf_k, f_l)\ \hat{b}(f_l) \\
&= \sum_{k,l} \hat{b}^*(f_k)\ (f_k, Hf_l)\ \hat{b}(f_l) = \sum_{k,l} \hat{b}^*\left((f_k, Hf_l)\ f_k\right)\ \hat{b}(f_l) \\
&= \sum_l \hat{b}^*(Hf_l)\ \hat{b}(f_l)
\end{aligned} \tag{2.4.4}$$

and analogously

$$\sum_k \hat{d}^*(g_k)\ \hat{d}(Hg_k) = \sum_l \hat{d}^*(Hg_l)\ \hat{d}(g_l). \tag{2.4.5}$$

Formula (2.4.1) can be rewritten as

$$\hat{H} = \sum_{k,l} \left[(f_k, Hf_l)\ \hat{b}^*(f_k)\ \hat{b}(f_l) - (g_l, Hg_k)\ \hat{d}^*(g_k)\ \hat{d}(g_l) \right] \tag{2.4.6}$$

and shows clearly that the energy is always positive if f_i belong to the positive and g_i to the negative spectral subspace of H. It can be made even more explicit by choosing a

spectral representation (defined in section 3.2.2) of H using generalized eigenfunctions f_E

$$\begin{aligned}\hat{H} &= \int_0^\infty E\ \hat{b}^*(f_E)\ \hat{b}(f_E)\ d\mu(E) - \int_{-\infty}^0 E\ \hat{d}^*(f_E)\ \hat{d}(f_E)\ d\mu(E) \\ &= \int_0^\infty |E|\ \hat{b}_E^*\ \hat{b}_E\ d\mu(E) + \int_{-\infty}^0 |E|\ \hat{d}_E^*\ \hat{d}_E\ d\mu(E) \geq 0\end{aligned} \tag{2.4.7}$$

and hence

$$(\Phi, \hat{H}\Phi) \geq 0 \qquad \forall\ \Phi \in \mathcal{F}. \tag{2.4.8}$$

With other words, it holds if the projectors $P_\pm$ are chosen to project onto the positive and negative spectral subspaces of H[4]

$$P_\pm = \frac{1 \pm \mathrm{sgn}(H)}{2}. \tag{2.4.9}$$

2.4.2 Normal ordering

It would be of advantage to have a general formula for the implementation of self-adjoint operators expressed via the field operators $\hat{\Psi}(f), \hat{\Psi}^*(f)$, similar to (2.4.1). First use the anticommutation relation for $\hat{d}$ and $\hat{d}^*$ (the reason for this operation will become clear later)

$$\hat{H} = \sum_k \left[\hat{b}^*(Hf_k)\ \hat{b}(f_k) + \hat{d}(g_k)\ \hat{d}^*(Hg_k) - (P_-Hg_k, P_-g_k)\right]. \tag{2.4.10}$$

Then substitute $\hat{b}(f) = \hat{\Psi}(P_+f)$ and $\hat{d}(g) = \hat{\Psi}^*(g)$

$$\hat{H} = \sum_k \left[\hat{\Psi}^*(P_+Hf_k)\ \hat{\Psi}(P_+f_k) + \hat{\Psi}^*(P_-g_k)\ \hat{\Psi}(P_-Hg_k) - (P_-Hg_k, P_-g_k)\right]. \tag{2.4.11}$$

The same trick as in (2.4.4) allows us to rewrite it as

$$\hat{H} = \sum_k \left[\hat{\Psi}^*(P_+Hf_k)\ \hat{\Psi}(P_+f_k) + \hat{\Psi}^*(P_-Hg_k)\ \hat{\Psi}(P_-g_k) - (P_-Hg_k, P_-g_k)\right]. \tag{2.4.12}$$

Since $P_\pm$ commute with H ($P_\pm$ are spectral projections of H) the first two terms can be combined together to give

$$\hat{H} = \sum_k \left[\hat{\Psi}^*(Hf_k)\ \hat{\Psi}(f_k) - (P_-Hg_k, P_-g_k)\right]. \tag{2.4.13}$$

The first term turns out to be universal (what can be observed by studying further examples). The second term appears due to the anticommutation of $\hat{d}$ and $\hat{d}^*$ while bringing them to the order $\hat{d}^*\hat{d}$ which has this significance that it guarantees finiteness of the expectation value of the infinite sum $\sum_k \hat{d}^*(Hg_k)\ \hat{d}(g_k)$ on any vector in the Fock space. This is a general feature of the sums of products of $\hat{b}, \hat{b}^*, \hat{d}, \hat{d}^*$ ordered so that the creation

[4] $\mathrm{sgn}(H)$ is well-defined by $H/|H|$ if 0 does not lie in the spectrum of H.

operators $\hat{b}^*, \hat{d}^*$ are placed to the left of the annihilation operators $\hat{b}, \hat{d}$. Their expectation values on all vectors in the Fock space are finite. The reason is that the creation operators on the left, like for instance in

$$\left(\Phi, \sum_k \hat{b}^*(f_k)\ \hat{d}^*(g_k)\ \hat{b}(f_k)\ \hat{d}(g_k)\ \Phi\right), \qquad f_k \in \mathcal{H}_+, \quad g_k \in \mathcal{H}_-, \tag{2.4.14}$$

can be transformed into annihilation operators acting on the vector Φ on the left

$$\left(\hat{d}(g_k)\ \hat{b}(f_k)\ \Phi, \sum_k \hat{b}(f_k)\ \hat{d}(g_k)\ \Phi\right). \tag{2.4.15}$$

Since Φ can be expressed as a sum over a finite number of creation operators acting on the vacuum

$$\Phi = \sum_{n,m=0}^{\infty} \sum_{\substack{i_1 \ldots i_n \\ j_1 \ldots j_m}} a_{i_1 \ldots i_n j_1 \ldots j_m} \hat{b}^*(f_{i_1}) \ldots \hat{b}^*(f_{i_n}) \hat{d}^*(g_{j_1}) \ldots \hat{d}^*(g_{j_m}) \Omega, \quad \text{with} \quad a_{i_1 \ldots i_n j_1 \ldots j_m} \in \mathbb{C} \tag{2.4.16}$$

only a finite number of terms remains after carrying out all anticommutations of the annihilation operators to move them from left to right to act directly on Ω and annihilate it. The only nonzero terms come from anticommutation of $\hat{b}(f_k)$ with $\hat{b}^*(f_{i_p})$ for $k = i_p$. The number of such terms is finite.

The special ordering of products of operators – creation on the left and annihilation on the right – has some significance and is called *normal ordering*. The price for carrying out the anticommutations to reach the normal ordered form is that there appear $\mathbb{C}$-number terms in form of scalar products of functions from $\mathcal{H}_-$. In order to simplify the notation and be able to deliver a simple formula for implementation of self-adjoint operators in $\mathcal{F}$ by means of the field operators, we introduce a new notation for the procedure transforming an expression to the normal ordered form with skipping all $\mathbb{C}$-number terms which appear. It is denoted by a pair of colons (like quotation marks), for example

$$: \hat{b}\hat{b}^* + \hat{d}^*\hat{d} := -\hat{b}^*\hat{b} + \hat{d}^*\hat{d} \tag{2.4.17}$$

and

$$: \hat{\Psi}^*\hat{\Psi} :=: (\hat{b}^* + \hat{d})(\hat{b} + \hat{d}^*) :=: \hat{b}^*\hat{b} + \hat{b}^*\hat{d}^* + \hat{d}\hat{b} + \hat{d}\hat{d}^* := \hat{b}^*\hat{b} + \hat{b}^*\hat{d}^* + \hat{d}\hat{b} - \hat{d}^*\hat{d}. \tag{2.4.18}$$

Now, the implementation of H can be expressed as

$$\hat{H} = \sum_k : \hat{\Psi}^*(Hf_k)\ \hat{\Psi}(f_k) : . \tag{2.4.19}$$

After expanding it like in (2.4.18) and carrying out the necessary anticommutations it becomes identical to (2.4.13).

2.4.3 Number of particles operator

Define the number-of-particles operator as an implementation of the operator $N \equiv P_+ - P_-$ (if $P_\pm = \frac{1}{2}[1 \pm \mathrm{sgn}(H)]$ then $N = \mathrm{sgn}(H)$). Analogously to the formula (2.4.19) we can write

$$\hat{N} \equiv \sum_k : \hat{\Psi}^*(N f_k)\hat{\Psi}(f_k) := \sum_k : \hat{\Psi}^*((P_+ - P_-)f_k)\hat{\Psi}(f_k) : . \tag{2.4.20}$$

It can be rewritten in terms of the creation and annihilation operators

$$\begin{aligned}
\hat{N} &= \sum_k : \left[\hat{b}^*(P_+(P_+ - P_-)f_k) + \hat{d}(P_-(P_+ - P_-)f_k)\right] \left[\hat{b}(P_+ f_k) + \hat{d}^*(P_- f_k)\right] : \\
&= \sum_k : \left[\hat{b}^*(P_+ f_k) - \hat{d}(P_- f_k)\right] \left[\hat{b}(P_+ f_k) + \hat{d}^*(P_- f_k)\right] : \\
&= \sum_k : \hat{b}^*(P_+ f_k)\, \hat{b}(P_+ f_k) - \hat{d}(P_- f_k)\, \hat{d}^*(P_- f_k) : \\
&= \sum_k \hat{b}^*(P_+ f_k)\, \hat{b}(P_+ f_k) + \hat{d}^*(P_- f_k)\, \hat{d}(P_- f_k)
\end{aligned} \tag{2.4.21}$$

Its eigenvalues are all natural numbers including zero and its eigenvectors are all states in $\mathcal{F}$ with a definite number of particles M, i.e. they consist of a sum of vectors from the subspaces $\mathcal{F}^{(n,m)}$ such that $n + m = M$.

2.4.4 Implementation of self-adjoint operators

Extending the analogy to the formulas (2.4.19) and (2.4.20) we can define a general implementation procedure for self-adjoint operators in $\mathcal{H}$, which bases on the normal ordering. For every bounded and self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$ with $A_{\pm\mp}$ being Hilbert-Schmidt, the operator

$$\begin{aligned}
\tilde{A} &\equiv \sum_{i,k} : (f_i, A f_k)\hat{\Psi}^*(f_i)\hat{\Psi}(f_k) : = \sum_k : \hat{\Psi}^*(A f_k)\hat{\Psi}(f_k) : \\
&= \sum_k \left[\hat{\Psi}^*(A f_k)\hat{\Psi}(f_k) - (P_- A f_k, P_- f_k)\right]
\end{aligned} \tag{2.4.22}$$

is essentially self-adjoint on the domain $\mathcal{D}(\hat{N})$ of the particle number operator and hence there exists its unique self-adjoint extension $\hat{A}$ to the whole $\mathcal{F}$ [Tha92, Th. 10.9].

2.4.5 Vacuum as a ground state

Among all choices of the vacuum vector Ω in $\mathcal{F}$, the one defined as the lowest energy state seems to be the most obvious from a physical point of view. The choice of Ω is equivalent to the choice of $P_\pm$ or $\mathcal{H}_\pm$, which is easier to characterize. As long as the Hamiltonian has no bound-states, its spectrum consists of two continuous parts separated by the gap

$(-1,1)$ (in units $mc^2 = 1$). Then the choice[5] $\mathcal{H}_+ = P_{[1,\infty)}(H)\mathcal{H}$ and $\mathcal{H}_- = P_{[-\infty,-1)}(H)\mathcal{H}$ specifies a vacuum vector Ω having the least energy equal to zero.

If bound-states are present the situation becomes more complicated. Still, splitting into two spectral subspaces of the Hamiltonian is physically plausible. A simple requirement that every particle state should have higher energy (with respect to the classical Hamiltonian) than any antiparticle, implies that the spectrum must be cut into two intervals

$$\mathcal{H}_+ = P_{[E_0,\infty)}(H)\mathcal{H} \quad \text{and} \quad \mathcal{H}_- = P_{[-\infty,E_0)}(H)\mathcal{H}. \tag{2.4.23}$$

The only remaining freedom is the choice of E_0. Different choices can be found in the literature, what is briefly but sufficiently discussed by Scharf and Seipp in [SS82]. One frequent choice, especially in the literature concerning overcritical fields, is $E_0 = -1$ ($-mc^2$ in dimensional units). It defines all bound-states in the gap $(-1,1)$ as particles. It has the advantage that it avoids complications appearing when during the time evolution a particle bound state crosses the level E_0 and suddenly turns into an antiparticle bound-state or vice versa. Then the number of particles as well as the total charge undergo a discontinuous change. The disadvantage is that the choice is not symmetric with respect to the exchange of particles and antiparticles. The same arguments which lead to the choice $E_0 = -mc^2$, studying positive potentials which bind electrons, can be applied to negative potentials (e.g. anti-nuclei) which bind positrons and would imply $E_0 = +mc^2$. Only the choice $E_0 = 0$ is symmetric and equal for both kinds of particles. In this case the charge conjugation symmetry is manifested by

$$\hat{C}\,\hat{H}\,\hat{C}^{-1} = \hat{H}, \tag{2.4.24}$$

where $\hat{C}$ is an implemented unitary charge conjugation operator

$$\hat{C}\,\hat{\Psi}(f)\,\hat{C}^{-1} = \hat{\Psi}^*(Cf) \tag{2.4.25}$$

and C is the antiunitary classical charge conjugation operator from section 2.2.1.

Equivalence of the projector choices

Considering various choices of the projectors there appears a problem of equivalence of the induced representations. Different choices of the vacuum vector (in the same Fock space $\mathcal{F}$) give rise to unitarily equivalent representations of CAR and correspond to different projectors $P_\pm$. On the other hand, not all choices of projectors $P_\pm$ give unitarily equivalent representations. In our context, we can use an immediate consequence of the theorem 2, that two projectors which differ only by a finite number of states (i.e. the subspaces $P_+P'_-\mathcal{H}$ and $P'_+P_-\mathcal{H}$ are finite dimensional) lead to unitarily equivalent representations.

[5] Notation $P_A(H)$ means a spectral projection with respect to the operator H on its spectral subspace A.

This is the case when we define two pairs of projectors

$$P_+ = P_{[E_0,\infty)}(H), \qquad P_- = P_{(-\infty,E_0]}(H), \qquad E_0 \in [-1,1], \tag{2.4.26}$$

$$P'_+ = P_{[E'_0,\infty)}(H), \qquad P'_- = P_{(-\infty,E'_0]}(H), \qquad E'_0 \in [-1,1] \tag{2.4.27}$$

and the number of eigenstates of the Hamiltonian H in the spectral gap between E_0 and E'_0 is finite, i.e. $\dim P_{[E_0,E'_0]}(H)\mathcal{H} < \infty$, where we have assumed $E_0 \leq E'_0$ for simplicity, but without restriction of generality. The only way how this condition can be violated is that the point spectrum of H contains infinitely many states, and hence possesses an accumulation point in the interval $[E_0, E'_0]$. For the Dirac Hamiltonians H accumulation points appear only at $E = \pm 1$ [ST04], so if E_0, E'_0 are chosen within the interval $(-1,1)$ the two projectors may differ only by a finite number of states. A serious problem appears when one of the cuts E_0, E'_0 is chosen at the accumulation point. As an example, consider a Dirac Hamiltonian with a Coulomb field of a positive charge Z (like nucleus). Its point spectrum is known to be

$$\sigma_p(H) = \left\{ E_{n,\kappa} \equiv \sqrt{1 + \frac{Z^2\alpha^2}{(n + \sqrt{\kappa^2 - Z^2\alpha^2})^2}}^{-1} ; n = 1,2,3,...; \kappa = \pm 1, \pm 2, ... \right\} \tag{2.4.28}$$

(assume $|Z\alpha| < 1$) and has an accumulation point at $+1$. Choose $E'_0 = +1$ and E_0 in $[-1,1)$ so that $E_0 < E'_0$. Then for every κ there exists a smallest $n_0(\kappa)$ such that

$$E'_0 > E_{n,\kappa} > E_0 \qquad \forall\, n \geq n_0(\kappa) \tag{2.4.29}$$

and

$$\lim_{n\to\infty} E_{n,\kappa} = E'_0 = 1. \tag{2.4.30}$$

The projectors are defined by (2.4.26) and (2.4.27) and give rise to different representations. We can now check the conditions of the theorem 2 for their unitary equivalence

$$\begin{aligned} ||P_+P'_-||^2_{H.S.} &= \sum_i ||P_{[E_0,\infty)}(H)\ P_{[-\infty,E'_0)}(H) f_i||^2 = \sum_i ||P_{(-\infty,E'_0]\cap[E_0,\infty)}(H) f_i||^2 \\ &= \sum_i ||P_{[E_0,E'_0]}(H) f_i||^2 = \sum_{\substack{\kappa=-\infty \\ \kappa\neq 0}}^{\infty} \sum_{n=n_0(\kappa)}^{\infty} ||\psi_{n,\kappa}||^2 = \sum_{\substack{\kappa=-\infty \\ \kappa\neq 0}}^{\infty} \sum_{n=n_0(\kappa)}^{\infty} 1 = \infty, \end{aligned} \tag{2.4.31}$$

where f_i is an orthonormal basis in $\mathcal{H}$ and $\psi_{n,\kappa}$ denote the bound-state wave functions. The second condition is fulfilled

$$\begin{aligned} ||P'_+P_-||^2_{H.S.} &= \sum_k ||P_{[E'_0,\infty)}(H)\ P_{[-\infty,E_0)}(H) f_k||^2 = \sum_k ||P_{(-\infty,E_0]\cap[E'_0,\infty)}(H) f_k||^2 \\ &= \sum_k ||P_\emptyset(H) f_k||^2 = 0, \end{aligned} \tag{2.4.32}$$

but the first is not, so we conclude

Corollary 1 *When two representations of CAR are constructed from projectors $P_\pm$ and $P'_\pm$ which differ by a spectral subspace of H (which can be any self-adjoint operator) corresponding to an interval I (open or closed, or a sum of intervals) in the point spectrum $\sigma_p(H)$, i.e. has the form $P_I(H)$, and such that the interval I contains an accumulation point of $\sigma_p(H)$, then they are unitarily non-equivalent.*

On the contrary, if I contains only a finite number of states, i.e. $\dim P_I(H)\mathcal{H} < \infty$, *then the two representations are unitarily equivalent.*

After it has been clarified which changes in the projectors (of those of interest) are allowed, the next point is to analyze their influence on the total number of particles and the total energy of a given state. Keeping the state unchanged during this procedure is justified because all considered induced representations (unitarily equivalent) are defined in the same Fock space. On the other hand, creation and annihilation operators change and so does the vacuum vector, with respect to which the number of particles in a given state is calculated.

Lowest energy condition

Another argument leading to the splitting at $E_0 = 0$ is a natural requirement of the vacuum being a state of the lowest energy, i.e. a ground state. Creation of any number of particles or antiparticles should increase and not decrease the total energy. The form of $\hat{H}$ in (2.4.6) makes clear that $f_n \in P_+\mathcal{H}$ must be contained in the positive and $g_n \in P_-\mathcal{H}$ in the negative spectral subspace of H. Only then the energy of Ω is minimal, namely $\hat{H}\Omega = 0$, and any creation process makes the total energy strictly positive.

So assume the vacuum Ω is defined in the Fock space $\mathcal{F}$ by means of $P_\pm$ which is chosen to be

$$P_\pm = \frac{1 \pm \mathrm{sgn}(H)}{2} \tag{2.4.33}$$

or, in other words, with a spectral cut in $\sigma(H)$ at $E_0 = 0$. Obviously, $(\Omega, \hat{N}\Omega) = 0$ and $(\Omega, \hat{H}\Omega) = 0$. Then choose another projector like in (2.4.27) with $E'_0 \neq E_0$, say $E'_0 < E_0 = 0$, without loss of generality. Assume, the representation based on $P'_\pm$ is unitarily equivalent to $\mathcal{F}$, so there exists in $\mathcal{F}$ a new vacuum vector Ω' for creation and annihilation operators $\hat{b}', \hat{b}^{*\prime}, \hat{d}', \hat{d}^{*\prime}$ defined with respect to $P'_\pm$. The two projectors may differ only by a finite dimensional subspace: $\dim P'_+P_-\mathcal{H} = \dim P_{[E'_0,E_0]}(H)\mathcal{H} < \infty$ (while $P_+P'_-\mathcal{H} = \emptyset$ because $P_+ \leq P'_+$ and $P_- \geq P'_-$ for $E_0 > E'_0$). Therefore the corresponding Bogoliubov transformation takes a special "triangular" form

$$\hat{b}'(P'_+f) = \hat{b}(P_+P'_+f) + \hat{d}^*(P_-P'_+f) \qquad \forall f \in \mathcal{H} \tag{2.4.34}$$

$$\hat{d}^{*\prime}(P'_+f) = \hat{d}^*(P_-P'_-f) \tag{2.4.35}$$

which gets especially simple in the basis f_n diagonalizing H with $\hat{b}_n \equiv \hat{b}(P_+f_n)$ and

$\hat{d}_n \equiv \hat{d}(P_- f_n)$

$$\begin{aligned}
\hat{b}_n{}' &= \hat{b}_n \quad \text{for} \quad f_n \in P_+ P'_+ \mathcal{H} \quad \text{- define} \quad n \in \mathbb{I}^{++} && (2.4.36)\\
\hat{b}_n{}' &= \hat{d}^*_n \quad \text{for} \quad f_n \in P_- P'_+ \mathcal{H} \quad \text{- define} \quad n \in \mathbb{I}^{-+} && (2.4.37)\\
\hat{d}^{*}_n{}' &= \hat{d}^*_n \quad \text{for} \quad f_n \in P_- P'_- \mathcal{H} \quad \text{- define} \quad n \in \mathbb{I}^{--}. && (2.4.38)
\end{aligned}$$

Then $\#\mathbb{I}^{++} = \#\mathbb{I}^{--} = \infty$ and $\#\mathbb{I}^{-+} < \infty$. The new particle number operator $\hat{N}'$, counting particles with respect to Ω', is

$$\begin{aligned}
\hat{N}' &= \sum_k \hat{b}^{*\prime}(P'_+ f_k)\, \hat{b}'(P'_+ f_k) + \hat{d}^{*\prime}(P'_- f_k)\, \hat{d}'(P'_- f_k) \\
&= \sum_k \hat{b}^{*}_k{}'\, \hat{b}_k{}' + \hat{d}^{*}_k{}'\, \hat{d}_k{}'
\end{aligned} \tag{2.4.39}$$

and it satisfies $(\Omega', \hat{N}'\,\Omega') = 0$. Analogously, the new Hamiltonian has the form

$$\begin{aligned}
\hat{H}' &= \sum_k E_k\, \hat{b}^{*\prime}(P'_+ f_k)\, \hat{b}'(P'_+ f_k) - E_k\, \hat{d}^{*\prime}(P'_- f_k)\, \hat{d}'(P'_- f_k) \\
&= \sum_k E_k\, \hat{b}_k{}'^{*}\, \hat{b}_k{}' - E_k\, \hat{d}_k{}'^{*}\, \hat{d}_k{}'.
\end{aligned} \tag{2.4.40}$$

Now, we are ready to check, which consequences the change of projectors has. First, consider the total energy. Obviously

$$(\Omega, \hat{H}\Omega) = 0 \quad \text{and} \quad (\Omega', \hat{H}'\Omega') = 0, \tag{2.4.41}$$

but

$$\begin{aligned}
(\Omega, \hat{H}'\Omega) &= \left(\Omega, \left[\sum_{k\in\mathbb{I}^{++}\cup\mathbb{I}^{-+}} E_k\, \hat{b}^{*}_k{}'\, \hat{b}_k{}' - \sum_{k\in\mathbb{I}^{--}} E_k\, \hat{d}^{*}_k{}'\, \hat{d}_k{}'\right]\Omega\right) \\
&= \left(\Omega, \left[\sum_{k\in\mathbb{I}^{++}} E_k\, \hat{b}^*_k\, \hat{b}_k + \sum_{k\in\mathbb{I}^{-+}} E_k\, \hat{d}_k\, \hat{d}^*_k - \sum_{k\in\mathbb{I}^{--}} E_k\, \hat{d}^*_k\, \hat{d}_k\right]\Omega\right) \\
&= \sum_{k\in\mathbb{I}^{-+}} E_k\, \underbrace{(\Omega, \hat{d}_k\, \hat{d}^*_k\, \Omega)}_{=1} = \sum_{k\in\mathbb{I}^{-+}} E_k < 0
\end{aligned} \tag{2.4.42}$$

what shows that in the new representation based on $P'_\pm$ the vacuum Ω' is not a ground state, because there exists another vector (Ω) which has a lower energy! Moreover, Ω has the lowest possible energy with respect to $\hat{H}'$ and hence remains a ground state. On the contrary

$$\begin{aligned}
(\Omega', \hat{H}\Omega') &= \left(\Omega', \left[\sum_{k\in\mathbb{I}^{++}} E_k\, \hat{b}^*_k\, \hat{b}_k - \sum_{k\in\mathbb{I}^{-+}\cup\mathbb{I}^{--}} E_k\, \hat{d}^*_k\, \hat{d}_k\right]\Omega'\right) \\
&= \left(\Omega', \left[\sum_{k\in\mathbb{I}^{++}} E_k\, \hat{b}^{*}_k{}'\, \hat{b}_k{}' - \sum_{k\in\mathbb{I}^{-+}} E_k\, \hat{b}_k{}'\, \hat{b}^{*}_k{}' - \sum_{k\in\mathbb{I}^{--}} E_k\, \hat{d}^{*}_k{}'\, \hat{d}_k{}'\right]\Omega'\right) \\
&= -\sum_{k\in\mathbb{I}^{-+}} E_k\, \underbrace{(\Omega', \hat{d}_k{}'\, \hat{d}^{*}_k{}'\, \Omega')}_{=1} = -\sum_{k\in\mathbb{I}^{-+}} E_k > 0
\end{aligned} \tag{2.4.43}$$

shows that in the representation based on $P_\pm$ the vector Ω' has higher energy than the ground state Ω. Therefore, this representation is distinguished by the condition of the vacuum being the ground state. For completeness, we observe how the number of particles changes. We have trivially

$$(\Omega, \hat{N}\Omega) = 0 \quad \text{and} \quad (\Omega', \hat{N}'\Omega') = 0, \tag{2.4.44}$$

but

$$\begin{aligned}(\Omega, \hat{N}'\Omega) &= \left(\Omega, \left[\sum_{k\in\mathbb{I}^{++}\cup\mathbb{I}^{-+}} \hat{b}_k^{*\prime}\, \hat{b}_k{}' + \sum_{k\in\mathbb{I}^{--}} \hat{d}_k^{*\prime}\, \hat{d}_k{}'\right]\Omega\right) \\ &= \left(\Omega, \left[\sum_{k\in\mathbb{I}^{++}} \hat{b}_k^{*}\, \hat{b}_k + \sum_{k\in\mathbb{I}^{-+}} \hat{d}_k\, \hat{d}_k^{*} + \sum_{k\in\mathbb{I}^{--}} \hat{d}_k^{*}\, \hat{d}_k\right]\Omega\right) \\ &= \sum_{k\in\mathbb{I}^{-+}} \underbrace{(\Omega, \hat{d}_k\, \hat{d}_k^{*}\, \Omega)}_{=1} = \sum_{k\in\mathbb{I}^{-+}} 1 = \#\mathbb{I}^{-+} > 0\end{aligned} \tag{2.4.45}$$

and

$$\begin{aligned}(\Omega', \hat{N}\Omega') &= \left(\Omega', \left[\sum_{k\in\mathbb{I}^{++}} \hat{b}_k^{*}\, \hat{b}_k + \sum_{k\in\mathbb{I}^{-+}\cup\mathbb{I}^{--}} \hat{d}_k^{*}\, \hat{d}_k\right]\Omega'\right) \\ &= \left(\Omega', \left[\sum_{k\in\mathbb{I}^{++}} \hat{b}_k^{*\prime}\, \hat{b}_k{}' + \sum_{k\in\mathbb{I}^{-+}} \hat{b}_k{}'\, \hat{b}_k^{*\prime} + \sum_{k\in\mathbb{I}^{--}} \hat{d}_k^{*\prime}\, \hat{d}_k{}'\right]\Omega'\right) \\ &= \sum_{k\in\mathbb{I}^{-+}} \underbrace{(\Omega', \hat{d}_k{}'\, \hat{d}_k^{*\prime}\, \Omega')}_{=1} = \sum_{k\in\mathbb{I}^{-+}} 1 > \#\mathbb{I}^{-+} > 0.\end{aligned} \tag{2.4.46}$$

The number of particles in the vacuum state in both representations is zero and in the "other vacuum" positive, equal to the number of states by which the two projectors differ. So the number-of-particles operator does not and cannot be used to distinguish any representation.

We conclude that the notion of the ground state is independent of the projector (as long as the representations are unitarily equivalent), i.e. a ground state with respect to one projector remains ground state with respect to all other projectors. However, in only one representation (unique choice of $P_\pm$) it is identical with the vacuum state. Therefore, the physically plausible condition of a vacuum state to be a ground state leads to a mathematically unique representation of CAR.

2.5 Charge in Fock space

Define the charge operator in Fock space $\mathcal{F}$ as an implementation of $Q \equiv 1$ on $\mathcal{H}$

$$\hat{Q} \equiv \sum_k : \hat{\Psi}^*(Qf_k)\hat{\Psi}(f_k) := \sum_k : \hat{\Psi}^*(f_k)\hat{\Psi}(f_k) : . \tag{2.5.1}$$

It can be rewritten in terms of the creation and annihilation operators

$$\begin{aligned}\hat{Q} &= \sum_k :\left[\hat{b}^*(P_+f_k) + \hat{d}(P_-f_k)\right]\left[\hat{b}(P_+f_k) + \hat{d}^*(P_-f_k)\right]: \\ &= \sum_k :\hat{b}^*(P_+f_k)\,\hat{b}(P_+f_k) + \hat{d}(P_-f_k)\,\hat{d}^*(P_-f_k):\\ &= \sum_k \hat{b}^*(P_+f_k)\,\hat{b}(P_+f_k) - \hat{d}^*(P_-f_k)\,\hat{d}(P_-f_k).\end{aligned} \tag{2.5.2}$$

Its eigenvalues are all integer numbers and its eigenvectors are all states in $\mathcal{F}$ with a definite charge q, i.e. consist of a sum of vectors from the subspaces $\mathcal{F}^{(n,m)}$ such that $n-m=q$. Obviously

$$(\Omega, \hat{Q}\,\Omega) = 0. \tag{2.5.3}$$

2.5.1 Consequence of the projector change

Similarly to the previous section, let us consider the consequence of the change of projectors and hence the vacuum vector on the expectation value of the charge in both vacua. Assume there are two pairs of projectors $P_\pm$ and $P'_\pm$ whose differences are Hilbert-Schmidt so that both induced representations of CAR are unitarily equivalent and can be realized in the same Fock space $\mathcal{F}$ (cf. theorem 2). They give rise to the corresponding vacuum vectors $\Omega, \Omega' \in \mathcal{F}$. While it is trivial that

$$(\Omega, \hat{Q}\,\Omega) = 0 \quad \text{and} \quad (\Omega', \hat{Q}'\,\Omega') = 0, \tag{2.5.4}$$

we are interested in the charges of both vacua with respect to the other representations, i.e. $(\Omega, \hat{Q}'\,\Omega)$ and $(\Omega', \hat{Q}'\,\Omega')$. With $\{f_n\}$ building an orthonormal basis in $\mathcal{H}$ we have

$$\hat{Q} \equiv \sum_n :\hat{\Psi}^*(f_n)\hat{\Psi}(f_n):_{P_-} = \sum_n \left[\hat{\Psi}^*(f_n)\hat{\Psi}(f_n) - (f_n, P_-f_n)\right], \tag{2.5.5}$$

$$\hat{Q}' \equiv \sum_n :\hat{\Psi}^*(f_n)\hat{\Psi}(f_n):_{P'_-} = \sum_n \left[\hat{\Psi}^*(f_n)\hat{\Psi}(f_n) - (f_n, P'_-f_n)\right], \tag{2.5.6}$$

where the notation $:(...):_{P_-}$ reflects the dependence of the normal ordering procedure on the projector P_-, i.e.

$$:\hat{\Psi}^*(f)\hat{\Psi}(g):_{P_-} \equiv \hat{\Psi}^*(f)\hat{\Psi}(g) - (g, P_-f). \tag{2.5.7}$$

Observe that the definitions of both charge operators differ only by the subtraction terms including different projectors. Therefore

$$\hat{Q} - \hat{Q}' = -\sum_n \left[(f_n, P_-f_n) - (f_n, P'_-f_n)\right] = -\mathrm{Tr}(P_- - P'_-) \tag{2.5.8}$$

or, using $-(P_- - P'_-) = -[(1-P_+) - (1-P'_+)] = P_+ - P'_+$,

$$\boxed{\hat{Q} - \hat{Q}' = \mathrm{Tr}(P_+ - P'_+)}. \tag{2.5.9}$$

The trace is to be calculated in $\mathcal{H}$, what means that the operator on the right-hand side is a $\mathbb{C}$-number times $\mathbf{1}$ in $\mathcal{F}$. This trace is well-defined and finite for this pair of projectors, because according to theorem 4 the trace of $P_+ - P'_+$ is a difference of two Hilbert-Schmidt norms, which are finite. Finally, we can calculate the charges of the vacua

$$(\Omega, \hat{Q}'\ \Omega) = (\Omega, (\hat{Q}' - \hat{Q})\ \Omega) + \underbrace{(\Omega, \hat{Q}\ \Omega)}_{0} = \mathrm{Tr}(P'_+ - P_+), \tag{2.5.10}$$

$$(\Omega', \hat{Q}\ \Omega') = (\Omega', (\hat{Q} - \hat{Q}')\ \Omega') + \underbrace{(\Omega', \hat{Q}'\ \Omega')}_{0} = \mathrm{Tr}(P_+ - P'_+). \tag{2.5.11}$$

2.5.2 Vacuum polarization

After defining the charge operator describing the total charge in a given state, one wants to find an expression for the charge density $\rho(\mathbf{x})$, or more generally, a charge density operator $\hat{\rho}(\mathbf{x})$ such that its expectation value in a given state will give $\rho(\mathbf{x})$. The classical property

$$\int \rho(\mathbf{x})\ d^3x = Q \tag{2.5.12}$$

is by correspondence required also in the operator version

$$\int \hat{\rho}(\mathbf{x})\ d^3x = \hat{Q}. \tag{2.5.13}$$

Consider two Hamiltonians H_0 and $H = H_0 + V$ and corresponding projectors $P^0_\pm$, $P_\pm$. Assume that they give equivalent representations with charge operators $\hat{Q}_0$ and $\hat{Q}$, respectively. Let Ω be the vacuum vector with respect to $P_\pm$. Then the charge of the (new) vacuum with respect to the free representation based on H_0 and $P^0_\pm$ is (2.5.9)

$$Q_{vac} = (\Omega, \hat{Q}_0\ \Omega) = -\mathrm{Tr}(P_+ - P^0_+). \tag{2.5.14}$$

This trace is well-defined and finite for regular potentials (in the sense of theorem 6), because according to theorem 4 it is a difference of two Hilbert-Schmidt norms, which are finite[6] Since the total charge appears to be a trace of an operator in $\mathcal{H}$ we can construct the charge density $\rho(\mathbf{x})$ starting from a smeared density (with test functions $f, g \in \mathcal{H}$)

$$\rho(f, g) \equiv -(f, (P_+ - P^0_+)g). \tag{2.5.15}$$

This expression can be viewed as a bilinear functional for which there exists a tempered kernel distribution $\rho(\mathbf{x}, \mathbf{y})$[KS77b, sec. 2] such that

$$\rho(f, g) \equiv \int d^3x\ d^3y\ \overline{f(x)}\ \rho(\mathbf{x}, \mathbf{y})\ g(y). \tag{2.5.16}$$

Then we can define the charge density as

$$\rho(\mathbf{x}) = \lim_{y \to x} \rho(\mathbf{x}, \mathbf{y}). \tag{2.5.17}$$

[6] For not regular potentials it requires renormalization [Hai04].

Finally, we must check if the required relation (2.5.12) holds.

$$\begin{aligned} Q_{vac} &= -\sum_n (f_n, (P_+ - P_+^0) f_n) = \sum_n \rho(f_n, f_n) \\ &= \sum_n \int d^3x \; d^3y \; \overline{f_n(x)} \; \rho(\mathbf{x}, \mathbf{y}) \; f_n(y) \\ &= \int d^3x \; d^3y \; \rho(\mathbf{x}, \mathbf{y}) \underbrace{\sum_n \overline{f_n(x)} \; f_n(y)}_{\delta(\mathbf{x}-\mathbf{y})} \\ &= \int d^3x \; d^3y \; \rho(\mathbf{x}, \mathbf{y}) \; \delta(\mathbf{x} - \mathbf{y}) \\ &= \int d^3x \; \rho(\mathbf{x}). \end{aligned} \tag{2.5.18}$$

In this way we have defined the expectation value of the charge density $\rho(\mathbf{x})$. Now, we should find the operator $\hat{\rho}(\mathbf{x})$ giving this expectation value. Unfortunately, it is not such an easy task, as it might be expected and there still exist differences in the literature concerning its form. The problem is the following. The usually defined smeared charge density operator [KS77b, sec. 2]

$$\hat{\rho}(f, g) \equiv -\frac{1}{2} \left[\hat{\Psi}(f) \hat{\Psi}^*(g) - \hat{\Psi}^*(g) \hat{\Psi}(f) \right] \tag{2.5.19}$$

gives

$$(\Omega, \hat{\rho}(f, g) \; \Omega) = -\frac{1}{2} (f, (P_+ - P_-) g), \tag{2.5.20}$$

where we have used

$$\frac{1}{2} (f, (P_+ - P_-) g) = : \hat{\Psi}^*(g) \hat{\Psi}(f) :_{P_-} + \frac{1}{2} \left[\hat{\Psi}(f) \hat{\Psi}^*(g) - \hat{\Psi}^*(g) \hat{\Psi}(f) \right]. \tag{2.5.21}$$

Connecting the smeared density $\hat{\rho}(f, g)$ with the total charge $\hat{Q}_0$ we obtain

$$Q_{vac} = (\Omega, \hat{Q}_0 \; \Omega) = \left(\Omega, \sum_n \hat{\rho}(f_n, f_n) \; \Omega \right) = -\sum_n \frac{1}{2} (f_n, (P_+ - P_-) f_n), \tag{2.5.22}$$

what is wrong because it disagrees with (2.5.14) and is, in general, divergent ($P_+ - P_-$ is not trace-class). The obtained $-\frac{1}{2}\mathrm{Tr}(P_+ - P_-)$ differs from the required $-\mathrm{Tr}(P_+ - P_+^0)$ by $\frac{1}{2}\mathrm{Tr}(P_+^0 - P_-^0)$. Some authors [Hai04, rem. 2], [GR95, eq. 7.25] argue that it is formally zero and so both results agree, but this trace is ill-defined because $P_+^0 - P_-^0$, in general, does not belong to the trace-class. Trying to define an operator valued charge density from such $\hat{\rho}(f, g)$ one rewrites it as

$$\hat{\rho}(f, g) = -\int d^3x \; d^3y \; \overline{f(\mathbf{x})} \; g(\mathbf{x}) \frac{1}{2} \left[\hat{\Psi}(\mathbf{x}) \hat{\Psi}^*(\mathbf{y}) - \hat{\Psi}^*(\mathbf{y}) \hat{\Psi}(\mathbf{x}) \right] \tag{2.5.23}$$

(where we have skipped the bispinorial indices for simplicity) and can conclude that

$$\hat{\rho}(\mathbf{x}, \mathbf{y}) = -\frac{1}{2} \left[\hat{\Psi}(\mathbf{x}) \hat{\Psi}^*(\mathbf{y}) - \hat{\Psi}^*(\mathbf{y}) \hat{\Psi}(\mathbf{x}) \right]. \tag{2.5.24}$$

Unfortunately, it is impossible to calculate the limit

$$\hat{\rho}(\mathbf{x}) = \lim_{y \to x} \hat{\rho}(\mathbf{x}, \mathbf{y}), \tag{2.5.25}$$

because it is singular and some renormalization procedure (in form of subtractions) must be carried out in order to obtain a well-defined expression [KS77b, sec. 2]. In our opinion the expression

$$\hat{\rho}(f, g) \equiv : \hat{\Psi}^*(f)\hat{\Psi}(g) :_{P^0_-} = \hat{\Psi}^*(f)\hat{\Psi}(g) - (g, P^0_- f) \tag{2.5.26}$$

is the correct smeared operator-valued charge density. The normal ordering, the so-called Wick product, with the subtraction term $(g, P^0_- f)$ guarantees well-posedness of this object[7]. This definition allows for an obvious connection to the definition of the total charge

$$\hat{Q}_0 = \sum_n \hat{\rho}(f_n, f_n) = \sum_n : \hat{\Psi}^*(f_n)\hat{\Psi}(f_n) :_{P^0_-} . \tag{2.5.27}$$

The expectation value in the (new) vacuum is

$$\begin{aligned} (\Omega, \hat{\rho}(f, g)\ \Omega) &= (\Omega, [\hat{\Psi}^*(f)\hat{\Psi}(g) - (g, P^0_- f)]\ \Omega) \\ &= (\Omega, [\, : \hat{\Psi}^*(f)\hat{\Psi}(g) :_{P_-} + (g, P_- f) - (g, P^0_- f)]\ \Omega) \\ &= (g, P_- f) - (g, P^0_- f) = (g, (P_- - P^0_-)f) = -(g, (P_+ - P^0_+)f), \end{aligned} \tag{2.5.28}$$

what, in contrary to the previous definition, agrees with (2.5.15). Finally, the corresponding charge distribution is given by [Mar03, sec. VI.7]

$$\hat{\rho}(\mathbf{x}) \equiv \lim_{y \to x} \hat{\rho}(\mathbf{x}, \mathbf{y}) \quad \text{with} \quad \hat{\rho}(\mathbf{x}, \mathbf{y}) \equiv : \hat{\Psi}^*(\mathbf{x})\hat{\Psi}(\mathbf{y}) :_{P^0_-} \tag{2.5.29}$$

and

$$\hat{\rho}(f, g) \equiv \int d^3x\ d^3y\ \overline{f(x)}\ \hat{\rho}(\mathbf{x}, \mathbf{y})\ g(y). \tag{2.5.30}$$

2.6 Time evolution in Fock space

In order to be able to describe time-dependent processes in Fock space we choose a "Heisenberg" picture in which the field operator evolves and the states remain constant in time. Assume, there exists a classical evolution operator $U(t_2, t_1)$ in $\mathcal{H}$ solving the classical Dirac equation

$$i\frac{d}{dt}\psi(t) = H\psi(t) \quad \text{with} \quad \psi(t) = U(t, t_0)\ \psi(t_0). \tag{2.6.1}$$

(Here and in the rest of this chapter we set $\hbar = 1$.) It has the following properties

- $U(t_1, t_2)$ is unitary in $\mathcal{H}$,
- $U(t_2, t_1) = U^*(t_1, t_2)$ and $U(t, t) = 1$,

[7] We refer to [Mar03, sec. VI.2] for more information on the Wick products and discussion of problems arising by multiplication of operator valued distributions.

- $U(t_1,t_2)U(t_2,t_3) = U(t_1,t_3)$.

Then the time evolution in $\mathcal{F}$ is induced by

$$\hat{\Psi}_t(f) \equiv \hat{\Psi}(U_t^* f), \quad \text{where} \quad U_t \equiv U(t,0). \tag{2.6.2}$$

If U_t is implementable (i.e. $P_\pm U_t P_\mp \in H.S.$) then there exists unitary $\hat{U}_t : \mathcal{F} \to \mathcal{F}$ such that

$$\hat{\Psi}_t(f) = \hat{\Psi}(U_t^* f) = \hat{U}_t\ \hat{\Psi}(f)\ \hat{U}_t^*. \tag{2.6.3}$$

If the Hamiltonian $\mathcal{H}$ is time-independent, then there exists a self-adjoint $\hat{H} : \mathcal{F} \to \mathcal{F}$ and $U_t = \exp(-iHt)$ is implemented by $\hat{U}_t = \exp(-i\hat{H}t)$ [Bon70]. The field operator $\hat{\Psi}_t(f)$ satisfies a Heisenberg evolution equation

$$i\frac{\partial}{\partial t}\hat{\Psi}_t(f) = [\hat{\Psi}_t(f), \hat{H}]. \tag{2.6.4}$$

All operators with the same time dependence will get an index t, like $\hat{A}_t$. It can be easily shown that the Heisenberg picture is equivalent to the Schrödinger picture

$$(\Phi, \hat{A}_t\ \Phi) = (\Phi, \hat{U}_t^*\ \hat{A}\ \hat{U}_t\ \Phi) = (\hat{U}_t\ \Phi, \hat{A}\ \hat{U}_t\ \Phi), \tag{2.6.5}$$

where the state evolves $\Phi \to \hat{U}_t\ \Phi$ and the operator $\hat{A}$ remains constant.

It follows the evolution of the particle and antiparticle creation and annihilation operators

$$\hat{\Psi}_t(f) \equiv \hat{b}_t(P_+ f) + \hat{d}_t^*(P_- f) = \hat{b}(P_+ U_t^* f) + \hat{d}^*(P_- U_t^* f) \tag{2.6.6}$$

and

$$\hat{b}_t(P_+ f) = \hat{U}_t\ \hat{b}(P_+ f)\ \hat{U}_t^*, \qquad \hat{d}_t^*(P_- f) = \hat{U}_t\ \hat{d}^*(P_- f)\ \hat{U}_t^* \tag{2.6.7}$$

if U is implementable in $\mathcal{F}$. Relation (2.6.6) defines a Bogoliubov transformation of the form

$$\hat{b}_t(P_+ f) = \hat{b}(P_+ U^* P_+ f) + \hat{d}^*(P_- U^* P_+ f) \tag{2.6.8}$$

$$\hat{d}_t^*(P_- f) = \hat{b}(P_+ U^* P_- f) + \hat{d}^*(P_- U^* P_- f), \tag{2.6.9}$$

which is implementable if and only if U_{+-}^* and U_{-+}^* are Hilbert-Schmidt operators.

2.6.1 Evolution of charge

Now, we can calculate how operators change under the time evolution implemented in $\mathcal{F}$ by $\hat{U}$. First, let us concentrate on the charge operator. Its expectation value in the state Φ is

$$\begin{aligned}
\hat{Q}_t = \hat{U}_t^* \hat{Q} \hat{U}_t &= \hat{U}_t^* \sum_n : \hat{\Psi}^*(f_n)\ \hat{\Psi}(f_n) : \hat{U}_t \\
&= \hat{U}_t^* \sum_n \Big[\hat{\Psi}^*(f_n)\ \hat{\Psi}(f_n) - (P_- f_n, P_- f_n)\Big]\ \hat{U}_t \\
&= \sum_n \Big[\hat{U}_t^*\ \hat{\Psi}^*(f_n)\ \hat{U}_t\ \hat{U}_t^*\ \hat{\Psi}(f_n)\ \hat{U}_t - \hat{U}_t^*\ (P_- f_n, P_- f_n)\ \hat{U}_t\Big] \\
&= \sum_n \Big[\hat{\Psi}^*(U_t^* f_n)\ \hat{\Psi}(U_t^* f_n) - (P_- f_n, P_- f_n)\Big].
\end{aligned} \tag{2.6.10}$$

Since the sum goes over all vectors in $\mathcal{H}$, the orthonormal basis can be chosen freely for convenience. Let us change it by $f_n \to f'_n = U_t f_n$, which gives also an orthonormal basis. Both terms under the sum must be kept and summed together and cannot be divided into two sums, because they separately are divergent. Therefore, the change of the basis cannot be performed separately on each term and influences both of them simultaneously

$$\begin{aligned}\hat{Q}_t &= \sum_n \left[\hat{\Psi}^*(f_n)\ \hat{\Psi}(f_n) - (P_- U_t f_n, P_- U_t f_n)\right] \\ &= \sum_n \left[\hat{\Psi}^*(f_n)\ \hat{\Psi}(f_n) - (P_- f_n, P_- f_n) + (P_- f_n, P_- f_n) - (P_- U_t f_n, P_- U_t f_n)\right].\end{aligned} \tag{2.6.11}$$

Here, the first two and the last two terms can be separated into independent sums, because both these sums are finite. To see it, we transform

$$\begin{aligned}&(P_- f_n, P_- f_n) - (P_- U_t f_n, P_- U_t f_n) = (U_t P_- f_n, U_t P_- f_n) - (P_- U_t f_n, P_- U_t f_n) \\ &= ((P_+ + P_-)U_t P_- f_n, (P_+ + P_-)U_t P_- f_n) - (P_- U_t (P_+ + P_-) f_n, P_- U_t (P_+ + P_-) f_n) \\ &= (P_+ U_t P_- f_n, P_+ U_t P_- f_n) + (P_- U_t P_- f_n, P_- U_t P_- f_n) \\ &- (P_- U_t P_+ f_n, P_- U_t P_+ f_n) - (P_- U_t P_- f_n, P_- U_t P_- f_n) \\ &= ||P_+ U_t P_- f_n||^2 - ||P_- U_t P_+ f_n||^2.\end{aligned} \tag{2.6.12}$$

Then the sum takes the form

$$\begin{aligned}\hat{Q}_t &= \sum_n \left[: \hat{\Psi}^*(f_n)\ \hat{\Psi}(f_n) : + ||P_+ U_t P_- f_n||^2 - ||P_- U_t P_+ f_n||^2\right] \\ &= \hat{Q} + ||(U_t)_{+-}||^2_{HS} - ||(U_t)_{-+}||^2_{HS},\end{aligned} \tag{2.6.13}$$

where the last two terms are finite for every implementable unitary transformation U. This is a very important result. It shows that the total charge changes in time exactly by the number of states which moved between the particle and antiparticle subspaces $\mathcal{H}_\pm$, namely it increases by one when a state moves from $\mathcal{H}_+$ to $\mathcal{H}_-$ and decreases by one when a state moves from $\mathcal{H}_-$ to $\mathcal{H}_+$. It is independent of the fact whether these states are occupied or not(!), and therefore can be written as

$$\boxed{\Delta Q \equiv \hat{Q}_t - \hat{Q} = ||(U_t)_{+-}||^2_{HS} - ||(U_t)_{-+}||^2_{HS}} \tag{2.6.14}$$

In the case when the evolution reduces to a simple change of projectors from $P_\pm$ to $P^t_\pm$ and $(U_t)_{\pm'\pm} = P^t_\pm P_\pm$ one can easily find

$$\Delta Q \equiv \hat{Q}_t - \hat{Q} = ||(U_t)_{+-}||^2_{HS} - ||(U_t)_{-+}||^2_{HS} = \mathrm{Tr}(P^t_+ - P_+), \tag{2.6.15}$$

what agrees with (2.5.9). It is a consequence of a more general very useful relation

Theorem 4 *For a unitary U and two pairs of projectors $P_\pm, P'_\pm$ it holds*

$$||P'_+ U P_-||^2_{HS} - ||P'_- U P_+||^2_{HS} = \mathrm{Tr}(U^* P'_+ U - P_+) \tag{2.6.16}$$

whenever this expression is finite.

Proof:

$$\begin{aligned}||P'_+UP_-||^2_{HS} - ||P'_-UP_+||^2_{HS} &= \mathrm{Tr}(P_-U^*P'_+UP_-) - \mathrm{Tr}(P_+U^*P'_-UP_+) \\ &= \mathrm{Tr}(U^*P'_+UP_-) - \mathrm{Tr}(U^*P'_-UP_+) + \mathrm{Tr}(\underbrace{U^*P'_+UP_+ - U^*P'_+UP_+}_{=0}) \\ &= \mathrm{Tr}(U^*P'_+U(P_- + P_+) - U^*(P'_- + P'_+)UP_+) \\ &= \mathrm{Tr}(U^*P'_+U - P_+). \quad \square\end{aligned} \tag{2.6.17}$$

Charge creation as an index

Formula (2.6.13) has an algebraic background. The difference $\Delta Q \equiv \hat{Q}_t - \hat{Q}$, which is a $\mathbb{C}$-number, is equal to the Fredholm index of a part of the classical evolution operator U_t, as states the following (cf. [Tha92, Th. 10.9])

Theorem 5 *If U is an implementable unitary evolution operator in $\mathcal{H}$ then its implementer $\hat{U}$, unitary in $\mathcal{F}$, maps each charge sector $\mathcal{F}_k$ onto $\mathcal{F}_{k-\Delta Q}$, where*

$$\Delta Q = -\mathrm{ind}\,[U_{++}] = \mathrm{ind}\,[U_{--}]\,. \tag{2.6.18}$$

Proof:
With the definition of the Fredholm index

$$\mathrm{ind}\,[W] \equiv \dim\ker W - \dim\ker W^*, \tag{2.6.19}$$

assuming that $U_{\pm\pm}$ is restricted to mapping $\mathcal{H}_\pm$ onto $\mathcal{H}_\pm$, we find by direct calculation

$$\begin{aligned}-\Delta Q = ||U_{-+}||^2_{HS} - ||U_{+-}||^2_{HS} &\overset{(Lem.1)}{=} ||U_{-+}||^2_{HS} - ||U^*_{-+}||^2_{HS} \\ = ||U_{-+}||^2_{HS} - ||(U_{+-})^*||^2_{HS} &= \sum_{f_n\in\mathcal{H}_+} ||U_{-+}f_n||^2 - \sum_{g_n\in\mathcal{H}_+} ||(U_{+-})^*g_n||^2.\end{aligned} \tag{2.6.20}$$

$\mathcal{H}_+$ can be decomposed as $(\ker U_{++})\oplus\mathrm{Range}(U_{++})^*$ and an orthonormal basis $\{f_n\}$ can be introduced such that every f_n belongs either to $\ker U_{++}$ or to $\mathrm{Range}(U_{++})^*$. Analogous, $\mathcal{H}_+$ can be decomposed as $(\ker(U_{++})^*) \oplus \mathrm{Range}U_{++}$ with a respective basis $\{g_n\}$. Then

$$\begin{aligned}-\Delta Q = &\sum_{f_n\in\ker U_{++}} \underbrace{||P_-UP_+f_n||}_{=1}^2 + \sum_{f_n\in\mathrm{Range}(U_{++})^*} ||P_-UP_+f_n||^2 \\ &- \sum_{g_n\in\ker(U_{++})^*} \underbrace{||P_-U^*P_+g_n||}_{=1}^2 - \sum_{g_n\in\mathrm{Range}U_{++}} ||P_-U^*P_+g_n||^2 \\ &= \dim\ker U_{++} - \dim\ker U^*_{++} \\ &+ \operatorname*{Tr}_{\mathrm{Range}U^*_{++}}[(U_{-+})^*U_{-+}] - \operatorname*{Tr}_{\mathrm{Range}U_{++}}[U_{+-}(U_{+-})^*].\end{aligned} \tag{2.6.21}$$

The first line in the last expression is the required $\mathrm{ind}\,[U_{++}]$. It remains to show that the second line is zero. Indeed, both traces are equal and cancel, what can be shown by the

following identity

$$\begin{aligned} U_{++}(U_{-+})^*U_{-+} &= U_{++}P_+U^* \underbrace{P_-}_{1-P_+} UP_+ = U_{++}(P_+ \underbrace{U^*U}_{=1} P_+ - P_+U^*P_+UP_+) \\ &= P_+UP_+(P_+ - (U_{++})^*U_{++}) = (P_+ - U_{++}(U_{++})^*)U_{++} \\ &= (P_+ \underbrace{UU^*}_{=1} P_+ - P_+UP_+U^*P_+)U_{++} = (P_+U \underbrace{(1-P_+)}_{P_-} U^*P_+)U_{++} \\ &= U_{+-}(U_{+-})^*U_{++}. \end{aligned} \tag{2.6.22}$$

Since $U_{++} : (\ker U_{++})^\perp \to \mathrm{Range}U_{++}$ and $(\ker U_{++})^\perp = \mathrm{Range}U_{++}^*$ it is invertible on $\mathrm{Range}U_{++}$ with the inverse $(U_{++})^{-1} : \mathrm{Range}U_{++} \to \mathrm{Range}U_{++}^*$. Hence, on $\mathrm{Range}U_{++}$ it holds

$$U_{++}[(U_{-+})^*U_{-+}](U_{++})^{-1} = U_{+-}(U_{+-})^*. \tag{2.6.23}$$

Using this relation we can transform the last trace term in the previous expression

$$\operatorname*{Tr}_{\mathrm{Range}U_{++}}[U_{+-}(U_{+-})^*] = \operatorname*{Tr}_{\mathrm{Range}U_{++}}[U_{++}[(U_{-+})^*U_{-+}](U_{++})^{-1}] = \operatorname*{Tr}_{\mathrm{Range}U_{++}^*}[(U_{-+})^*U_{-+}] \tag{2.6.24}$$

so that both traces cancel. Finally,

$$-\Delta Q = ||U_{-+}||_{HS}^2 - ||U_{+-}||_{HS}^2 = \dim\ker U_{++} - \dim\ker U_{++}^* = \mathrm{ind}\,[U_{++}]\,. \quad \square \tag{2.6.25}$$

Corollary 2 *For a unitary U and two pairs of projectors $P_\pm, P'_\pm$ it holds*

$$-\mathrm{ind}\,(P'_+UP_+) = \mathrm{Tr}(U^*P'_+U - P_+) \tag{2.6.26}$$

whenever this expression is finite.

Proof: Theorem 5 can be easily generalized to the case of different projectors

$$-\mathrm{ind}\,(P'_+UP_+) = ||P'_+UP_-||_{HS}^2 - ||P'_-UP_+||_{HS}^2. \tag{2.6.27}$$

On the other hand, from theorem 4 we have

$$||P'_+UP_-||_{HS}^2 - ||P'_-UP_+||_{HS}^2 = \mathrm{Tr}(U^*P'_+U - P_+). \quad \square \tag{2.6.28}$$

2.6.2 Evolution of the particle number

To find out how the occupation of the states changes, we must study the evolution of the particle number operator

$$\begin{aligned}\hat{N}_t &= \hat{U}_t^*\ \hat{N}\ \hat{U}_t = \hat{U}_t^* \sum_n \left[\hat{\Psi}^*(P_+f_n)\ \hat{\Psi}(P_+f_n) + \hat{\Psi}(P_-f_n)\ \hat{\Psi}^*(P_-f_n)\right] \hat{U}_t \\ &= \sum_n \left[\hat{\Psi}^*(U_t^*P_+f_n)\ \hat{\Psi}(U_t^*P_+f_n) + \hat{\Psi}(U_t^*P_-f_n)\ \hat{\Psi}^*(U_t^*P_-f_n)\right] \\ &= \sum_n \left\{ \begin{array}{l} \left[\hat{b}^*(P_+U_t^*P_+f_n) + \hat{d}(P_-U_t^*P_+f_n)\right]\left[\hat{b}(P_+U_t^*P_+f_n) + \hat{d}^*(P_-U_t^*P_+f_n)\right] \\ + \left[\hat{b}(P_+U_t^*P_-f_n) + \hat{d}^*(P_-U_t^*P_-f_n)\right]\left[\hat{b}^*(P_+U_t^*P_-f_n) + \hat{d}(P_-U_t^*P_-f_n)\right] \end{array} \right\}.\end{aligned} \tag{2.6.29}$$

Unfortunately, this operator has a much more complicated structure than the charge operator has. Therefore, in the following we restrict ourselves to the analysis of the expectation values of $\hat{N}_t$ in states Φ which have a simple form

$$\Phi = \hat{b}^*(P_+f_{i_1})...\hat{b}^*(P_+f_{i_n})\hat{d}^*(P_-f_{j_1})...\hat{d}^*(P_-f_{j_m})\Omega, \tag{2.6.30}$$

i.e. contain no superpositions. Then the terms containing $\hat{b}^*\hat{d}^*, \hat{b}\hat{d}, \hat{d}^*\hat{b}^*$ and $\hat{d}\hat{b}$ vanish.

$$\begin{aligned}&(\Phi, \hat{N}_t\Phi) = \\ &= \left(\Phi, \sum_n \begin{bmatrix} \hat{b}^*(P_+U_t^*P_+f_n)\ \hat{b}(P_+U_t^*P_+f_n) + \hat{d}(P_-U_t^*P_+f_n)\ \hat{d}^*(P_-U_t^*P_+f_n) \\ +\hat{b}(P_+U_t^*P_-f_n)\ \hat{b}^*(P_+U_t^*P_-f_n) + \hat{d}^*(P_-U_t^*P_-f_n)\ \hat{d}(P_-U_t^*P_-f_n) \end{bmatrix} \Phi\right) \\ &= \left(\Phi, \sum_n \begin{bmatrix} \hat{b}^*(P_+U_t^*P_+f_n)\ \hat{b}(P_+U_t^*P_+f_n) - \hat{b}^*(P_+U_t^*P_-f_n)\ \hat{b}(P_+U_t^*P_-f_n) \\ +\hat{d}^*(P_-U_t^*P_-f_n)\ \hat{d}(P_-U_t^*P_-f_n) - \hat{d}^*(P_-U_t^*P_+f_n)\ \hat{d}(P_-U_t^*P_+f_n) \\ +(P_+U_t^*P_-f_n, P_+U_t^*P_-f_n) + (P_-U_t^*P_+f_n, P_-U_t^*P_+f_n) \end{bmatrix} \Phi\right) \\ &= \left(\Phi, \sum_n \begin{bmatrix} \hat{b}^*(P_+U_t^*P_+f_n)\ \hat{b}(P_+U_t^*P_+f_n) + \hat{b}^*(P_+U_t^*P_-f_n)\ \hat{b}(P_+U_t^*P_-f_n) \\ +\hat{d}^*(P_-U_t^*P_-f_n)\ \hat{d}(P_-U_t^*P_-f_n) + \hat{d}^*(P_-U_t^*P_+f_n)\ \hat{d}(P_-U_t^*P_+f_n) \\ -2\hat{b}^*(P_+U_t^*P_-f_n)\ \hat{b}(P_+U_t^*P_-f_n) - 2\hat{d}^*(P_-U_t^*P_+f_n)\ \hat{d}(P_-U_t^*P_+f_n) \\ +(P_+U_t^*P_-f_n, P_+U_t^*P_-f_n) + (P_-U_t^*P_+f_n, P_-U_t^*P_+f_n) \end{bmatrix} \Phi\right) \\ &= \left(\Phi, \sum_n \begin{bmatrix} \hat{b}^*(P_+U_t^*f_n)\ \hat{b}(P_+U_t^*f_n) + \hat{d}^*(P_-U_t^*f_n)\ \hat{d}(P_-U_t^*f_n) \\ -2\ \hat{b}^*(P_+U_t^*P_-f_n)\ \hat{b}(P_+U_t^*P_-f_n) - 2\ \hat{d}^*(P_-U_t^*P_+f_n)\ \hat{d}(P_-U_t^*P_+f_n) \\ +(P_+U_t^*P_-f_n, P_+U_t^*P_-f_n) + (P_-U_t^*P_+f_n, P_-U_t^*P_+f_n) \end{bmatrix} \Phi\right).\end{aligned} \tag{2.6.31}$$

This sum can be split into four sums, every of which is finite

$$
\begin{aligned}
&(\Phi, \hat{N}_t \Phi) = \\
&= \left(\Phi, \sum_n \left[\hat{b}^*(P_+ U_t^* f_n)\, \hat{b}(P_+ U_t^* f_n) + \hat{d}^*(P_- U_t^* f_n)\, \hat{d}(P_- U_t^* f_n) \right] \Phi \right) \\
&- 2 \left(\Phi, \sum_n \hat{b}^*(P_+ U_t^* P_- f_n)\, \hat{b}(P_+ U_t^* P_- f_n) \Phi \right) \\
&- 2 \left(\Phi, \sum_n \hat{d}^*(P_- U_t^* P_+ f_n)\, \hat{d}(P_- U_t^* P_+ f_n) \Phi \right) \\
&+ \left(\Phi, \sum_n \left[(P_+ U_t^* P_- f_n, P_+ U_t^* P_- f_n) + (P_- U_t^* P_+ f_n, P_- U_t^* P_+ f_n) \right] \Phi \right) \\
&= \left(\Phi, \hat{N} \Phi \right) - 2 \left(\Phi, \hat{N}_{+-} \Phi \right) - 2 \left(\Phi, \hat{N}_{-+} \Phi \right) + ||U_{+-}^*||_{HS}^2 + ||U_{-+}^*||_{HS}^2 \\
&= \left(\Phi, \hat{N} - 2\hat{N}_{+-} - 2\hat{N}_{-+} \Phi \right) + ||U_{-+}||_{HS}^2 + ||U_{+-}||_{HS}^2,
\end{aligned}
\tag{2.6.32}
$$

where we have introduced new operators

$$
\hat{N}_{+-} \equiv \sum_n \hat{b}^*(P_+ U_t^* P_- f_n)\, \hat{b}(P_+ U_t^* P_- f_n) \tag{2.6.33}
$$

$$
\hat{N}_{-+} \equiv \sum_n \hat{d}^*(P_- U_t^* P_+ f_n)\, \hat{d}(P_- U_t^* P_+ f_n), \tag{2.6.34}
$$

counting the number of occupied states which moved from $\mathcal{H}_-$ to $\mathcal{H}_+$ and from $\mathcal{H}_+$ to $\mathcal{H}_-$, respectively. On the contrary, the expressions $||U_{-+}||_{HS}^2, ||U_{+-}||_{HS}^2$ make the same, but independently of the occupation.

If one empty state moves from the particle to the antiparticle subspace then the number of particles increases due to the term $||U_{-+}||_{HS}^2 = 1$, but if the state was initially occupied, then the number of particles changes by

$$
\left(\Phi, \left[||U_{-+}||_{HS}^2 - 2\hat{N}_{-+} \right] \Phi \right) = 1 - 2 = -1, \tag{2.6.35}
$$

i.e. decreases by one! The same happens in the opposite direction: from the antiparticle to the particle subspace. **We conclude that crossing the border between particle and antiparticle subspaces, an empty state becomes occupied and an occupied becomes empty.**

For the initial vacuum state, $\Phi = \Omega$, the result reduces to

$$
\boxed{\Delta N \equiv (\Omega, (\hat{N}_t - \hat{N})\, \Omega) = ||U_{-+}||_{HS}^2 + ||U_{+-}||_{HS}^2} \tag{2.6.36}
$$

2.6.3 Examples – single processes

Now, we are ready to summarize the consequences of the fact that under evolution (or any implementable unitary transformation) some states move between particle and antiparticle

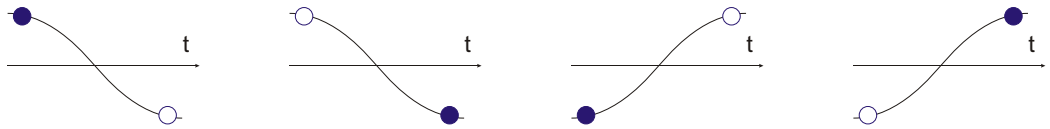


Figure 2.1: a) particle → vacuum, b) vacuum → antiparticle, c) antiparticle → vacuum, d) vacuum → particle.

subspaces, i.e. for some states $\mathcal{H}_{\pm} \ni \psi \to U\psi \in \mathcal{H}_{\mp}$. The most interesting four cases are sketched on the figures 2.1. Consider the following setting: in the Schrödinger picture we start with an initial state Φ with charge Q_0 and particle number N_0 which goes over into $\Phi_t = \hat{U}_t\,\Phi$. The final charge Q_t and particle number N_t are measured as expectation values of $\hat{Q}$ and $\hat{N}$, respectively. It is equivalent to $Q_t = (\Phi, \hat{Q}_t\Phi)$ and $N_t = (\Phi, \hat{N}_t\Phi)$ in the Heisenberg picture. Consider a single particle state $f_p \in \mathcal{H}_+$ and a single antiparticle state $f_a \in \mathcal{H}_-$ which are transformed one into the other under evolution U_t in $\mathcal{H}$.

a) An occupied particle state goes over into an empty antiparticle state:

$$U f_p = f_a, \qquad ||U_{-+}||^2_{HS} = 1, \qquad ||U_{+-}||^2_{HS} = 0, \tag{2.6.37}$$

$$\mathbf{\Phi} = \hat{\mathbf{b}}^*(\mathbf{P}_+\mathbf{f_p})\,\mathbf{\Omega}, \qquad Q_0 = 1, \qquad N_0 = 1, \tag{2.6.38}$$

$$\begin{aligned} Q_t &= Q_0 + ||U_{+-}||^2_{HS} - ||U_{-+}||^2_{HS} = 1 + 0 - 1 = 0, && (2.6.39)\\ N_t &= N_0 + ||U_{-+}||^2_{HS} - 2\,(\Phi, \hat{N}_{-+}\Phi) + ||U_{+-}||^2_{HS} - 2\,(\Phi, \hat{N}_{+-}\Phi) \\ &= 1 + 1 - 2 + 0 - 0 = 0, && (2.6.40) \end{aligned}$$

$$\mathbf{\Phi_t} = \mathbf{\Omega}. \tag{2.6.41}$$

b) An empty particle state goes over into an occupied antiparticle state:

$$U f_p = f_a, \qquad ||U_{-+}||^2_{HS} = 1, \qquad ||U_{+-}||^2_{HS} = 0, \tag{2.6.42}$$

$$\mathbf{\Phi} = \mathbf{\Omega}, \qquad Q_0 = 0, \qquad N_0 = 0, \tag{2.6.43}$$

$$\begin{aligned} Q_t &= Q_0 + ||U_{+-}||^2_{HS} - ||U_{-+}||^2_{HS} = 0 + 0 - 1 = -1, && (2.6.44)\\ N_t &= N_0 + ||U_{-+}||^2_{HS} - 2\,(\Phi, \hat{N}_{-+}\Phi) + ||U_{+-}||^2_{HS} - 2\,(\Phi, \hat{N}_{+-}\Phi) \\ &= 0 + 1 - 0 + 0 - 0 = 1, && (2.6.45) \end{aligned}$$

$$\mathbf{\Phi_t} = \hat{\mathbf{d}}^*(\mathbf{P}_-\mathbf{f_a})\,\mathbf{\Omega}. \tag{2.6.46}$$

c) An occupied antiparticle state goes over into an empty particle state:

$$Uf_a = f_f, \qquad ||U_{-+}||^2_{HS} = 0, \qquad ||U_{+-}||^2_{HS} = 1, \tag{2.6.47}$$

$$\mathbf{\Phi} = \hat{\mathbf{d}}^*(\mathbf{P}_-\mathbf{f_a})\,\mathbf{\Omega}, \qquad Q_0 = -1, \qquad N_0 = 1, \tag{2.6.48}$$

$$\begin{aligned} Q_t &= Q_0 + ||U_{+-}||^2_{HS} - ||U_{-+}||^2_{HS} = -1 + 1 - 0 = 0, && (2.6.49)\\ N_t &= N_0 + ||U_{-+}||^2_{HS} - 2\,(\Phi, \hat{N}_{-+}\Phi) + ||U_{+-}||^2_{HS} - 2\,(\Phi, \hat{N}_{+-}\Phi) \\ &= 1 + 0 - 0 + 1 - 2 = 0, && (2.6.50) \end{aligned}$$

$$\mathbf{\Phi_t} = \mathbf{\Omega}. \tag{2.6.51}$$

d) An empty antiparticle state goes over into an occupied particle state:

$$Uf_a = f_f, \qquad ||U_{-+}||^2_{HS} = 0, \qquad ||U_{+-}||^2_{HS} = 1, \tag{2.6.52}$$

$$\mathbf{\Phi} = \mathbf{\Omega}, \qquad Q_0 = 0, \qquad N_0 = 0, \tag{2.6.53}$$

$$\begin{aligned} Q_t &= Q_0 + ||U_{+-}||^2_{HS} - ||U_{-+}||^2_{HS} = 0 + 1 - 0 = 1, && (2.6.54)\\ N_t &= N_0 + ||U_{-+}||^2_{HS} - 2\,(\Phi, \hat{N}_{-+}\Phi) + ||U_{+-}||^2_{HS} - 2\,(\Phi, \hat{N}_{+-}\Phi) \\ &= 0 + 0 - 0 + 1 - 0 = 1, && (2.6.55) \end{aligned}$$

$$\mathbf{\Phi_t} = \hat{\mathbf{b}}^*(\mathbf{P}_+\mathbf{f_p})\,\mathbf{\Omega}. \tag{2.6.56}$$

These are consequences of the processes where states move between particle $\mathcal{H}_+$ and antiparticle $\mathcal{H}_-$ subspaces. Since the choice of these subspaces corresponds to the choice of the projectors $P_\pm$, in these examples it can be seen which meaning the choice of the projector on the observables has. To be allowed to form statements about the creation of particles and charge from vacuum in physical processes we need "physical" definitions of particles.

2.7 Particle interpretation

Particles and antiparticles are defined by the corresponding creation operators

$$\hat{b}^*_n \equiv \hat{b}^*(P_+\varphi_n) \quad \text{and} \quad \hat{d}^*_n \equiv \hat{d}^*(P_-\varphi_n), \tag{2.7.1}$$

where φ_n is an orthonormal basis in $\mathcal{H}$ and describes their single-particle wave functions. In the theory, the choice of the basis φ_n is arbitrary, but there appears a question which states describe physical particles. These can be characterized by additional conditions regarding their time evolution, namely particles should be states which remain essentially unchanged and evolve freely when there is no interaction. Therefore consider first the case of a

2.7.1 Free Hamiltonian

The unitary evolution operator $U_0(t_2, t_1)$ corresponding to the evolution generator, the free Dirac Hamiltonian H_0 is defined by

$$U_0(t_2, t_1) = e^{-iH_0(t_2-t_1)} \tag{2.7.2}$$

and the projectors are for all times t

$$P^0_+ \equiv P_{[1,\infty)}(H_0), \qquad P^0_- \equiv P_{(-\infty,-1]}(H_0) \tag{2.7.3}$$

having obviously the property $P_+ + P_- = 1$. Then, the field operator is defined at every time t as

$$\hat{\Psi}_t(f) = \hat{b}_t(P^0_+ f) + \hat{d}^*_t(P^0_- f) \tag{2.7.4}$$

and evolves according to

$$\hat{\Psi}_t(f) = \hat{\Psi}_{t_0}(U^*_0(t, t_0)f). \tag{2.7.5}$$

The particle's identity is independent of time when $\hat{b}^*_n(t) = \hat{b}^*_n(t_0)$ for all t, t_0, that is

$$\hat{b}^*_n(t) \equiv \hat{b}^*_t(P^0_+\varphi_n(t)) = \hat{b}^*_{t_0}(P^0_+\varphi_n(t_0)) \equiv \hat{b}^*_n(t_0). \tag{2.7.6}$$

The corresponding wave functions $\varphi_n(t)$ must be found, which satisfy this relation. Therefore we transform

$$\begin{aligned} \hat{b}^*_t(P^0_+\varphi_n(t)) &= \hat{\Psi}^*_t(P^0_+\varphi_n(t)) = \hat{\Psi}^*_{t_0}(U^*_0(t, t_0)P^0_+\varphi_n(t)) \\ &= \hat{\Psi}^*_{t_0}(P^0_+U^*_0(t, t_0)\varphi_n(t)) = \hat{b}^*_{t_0}(P^0_+U^*_0(t, t_0)\varphi_n(t)) \stackrel{!}{=} \hat{b}^*_{t_0}(P^0_+\varphi_n(t_0)), \end{aligned} \tag{2.7.7}$$

where in the step between the first and second line we have used the fact that $P^0_\pm$ and $U_0(t_2, t_1)$ commute, because $P^0_\pm$ are spectral projections of the evolution generator H_0. The last equation can be only fulfilled if

$$\varphi_n(t) = U_0(t, t_0)\varphi_n(t_0), \tag{2.7.8}$$

that is if the single-particle wave functions satisfy the single-particle evolution equation, which is the Dirac equation. If we add a further condition that particles must have definite energy, i.e. be generalized eigenvectors[8] of the Hamiltonian satisfying $H_0\ \varphi_n(t) = E_n\ \varphi_n(t)$, then they get the form

$$\varphi_n(t) \equiv e^{-iE_n t}\phi_n \quad \text{with} \quad H_0\ \phi_n = E_n\ \phi_n. \tag{2.7.9}$$

As we see, the notion of particles evolving due to the free Hamiltonian is relatively simple. So let's proceed with general

[8] eigenvectors or continuum wave functions

2.7.2 Static Hamiltonians

Here, the situation is similar to the previous, except that the evolution operator is now denoted as

$$U(t_2, t_1) = e^{-iH(t_2-t_1)} \tag{2.7.10}$$

and the projectors are defined with respect to the spectrum of H, which is, in general, richer than that of H_0, and usually possesses a discrete part contained in the interval $(-1, 1)$. Different choices of projectors in such a case and their consequences have been discussed in section 2.4.5. Here, we assume the projectors $P_\pm$ are given and have the form

$$P_+ \equiv P_{[E_0,\infty)}(H), \qquad P_-^0 \equiv P_{(-\infty,E_0)}(H). \tag{2.7.11}$$

The field operator is defined as

$$\hat{\Psi}_t(f) = \hat{b}_t(P_+ f) + \hat{d}_t^*(P_- f) \tag{2.7.12}$$

and evolves

$$\hat{\Psi}_t(f) = \hat{\Psi}_{t_0}(U^*(t, t_0)f). \tag{2.7.13}$$

The particles

$$\hat{b}_n^*(t) \equiv \hat{b}_t^*(P_+\varphi_n(t)) \tag{2.7.14}$$

are well defined, analogously like in the previous section, when the single-particle wave functions fulfill

$$\varphi_n(t) = U_0(t, t_0)\varphi_n(t_0). \tag{2.7.15}$$

If they are to have definite energy, they must take the form

$$\varphi_n(t) \equiv e^{-iE_n t}\phi_n \quad \text{with} \quad H\phi_n = E_n\phi_n. \tag{2.7.16}$$

This representation, where the particle states are defined with respect to the full Hamiltonian, is called Furry picture [Fur51]. There are situations where we have to compare this $(\mathcal{F})$ with the free representation $\mathcal{F}_0$, for example when the Hamiltonian changes in time from an initially free to a finally different one with a static external field present. Then there appears a question about the equivalence of both representations, since $\mathcal{F}$ and $\mathcal{F}_0$ are essentially different and unrelated. In the conventional formulation of the theory it is usually overlooked and one forces implicitly both representations in one Fock space. This problem is discussed in detail by Bongaarts [Bon70] and by Klaus and Scharf in [KS77a]. The results interesting for our context can be formulated in the following theorem.

Theorem 6 *Let the projectors $P_\pm^0$ and $P_\pm$ be defined like in (2.7.3) and (2.7.11), respectively, and give rise to the free and Furry representations $\hat{\Psi}^0$ in $\mathcal{F}_0$ and $\hat{\Psi}$ in $\mathcal{F}$, respectively. Both representations are unitarily equivalent and therefore realizable in the same Fock space $\mathcal{F}_0$ if and only if*[9]

$$P_+P_-^0 \in H.S. \quad \textit{and} \quad P_+^0P_- \in H.S. \tag{2.7.17}$$

[9] H.S. denotes the Hilbert-Schmidt class, i.e. operators with finite H.S. norm.

6A *Furthermore (Klaus-Scharf), then there exists a self-adjoint Hamiltonian* $\hat{H}$ *in* $\mathcal{F}_0$ *which generates the evolution*

$$\hat{\Psi}_t(f) = \hat{\Psi}(e^{iHt}f) = e^{i\hat{H}t}\hat{\Psi}(f)e^{-i\hat{H}t} \tag{2.7.18}$$

and its construction is given explicitly by implementing the Bogoliubov transformation generated by the change of projectors for the creation and annihilation operators.
6B *The evolution generator* $\hat{H}$ *exists in* $\mathcal{F}_0$ *(Bongaarts) if and only if*

$$P_+^0 e^{-iHt} P_-^0 \in H.S. \qquad \forall t, \tag{2.7.19}$$

but for this case no explicit construction of $\hat{H}$ *is given.*

The condition (2.7.17) implies (2.7.19), what is shown below. Whether (2.7.19) is more general or they are equivalent is not known, though there exist some arguments for their equivalence.

Lemma 2 *If* $P_+ - P_+^0 \in H.S.$ *and* H *self-adjoint on* $\mathcal{H}$ *then* $P_+^0 e^{-iHt} P_-^0 \in H.S.$ *for all* t.

Proof:
e^{-iHt} is unitary, so

$$(P_+ - P_+^0)e^{-iHt} = P_+ e^{-iHt} - P_+^0 e^{-iHt} \in \text{H.S.} \tag{2.7.20}$$

$$\Rightarrow P_+ e^{-iHt} P_-^0 - P_+^0 e^{-iHt} P_-^0 \in \text{H.S.} \tag{2.7.21}$$

P_+ commutes with e^{-iHt}, so

$$P_+ P_-^0 e^{-iHt} - P_+^0 e^{-iHt} P_-^0 \in \text{H.S.} \tag{2.7.22}$$

$P_+ P_-^0 \in$ H.S. (see theorem 2), hence $P_+ P_-^0 e^{-iHt} \in$ H.S.. Therefore

$$P_+^0 e^{-iHt} P_-^0 \in \text{H.S.} \ \square \tag{2.7.23}$$

A comment on the interaction picture is in place here. One may ask if $V = H - H_0$ can be implemented to generate a unitary evolution in $\mathcal{F}_0$ in an analogous way to (2.7.18), i.e. if there exists a self-adjoint $\hat{V}$ in $\mathcal{F}_0$ such that

$$\hat{\Psi}(e^{iVt}f) = e^{i\hat{V}t}\hat{\Psi}(f)e^{-i\hat{V}t}. \tag{2.7.24}$$

The answer is, in general, negative, what follows from a theorem by Boongarts [Bon70, Th. 5] stating that for any V being a $\mathcal{C}_0^\infty$ function there exists no $\hat{V}$ satisfying (2.7.24) (while $\hat{H}_0$ and $\hat{H}$ exist!).

Regular potentials

For the purpose of establishing a particle interpretation we are interested in the condition (2.7.17), guaranteeing equivalence of both representations. It is an implicit constraint on the external potential, which influences the properties of H. Potentials V for which $H = H_0 + V$ satisfy the condition (2.7.17) are called *regular*. Unfortunately, the question about the most general condition implying (2.7.17) is open. Only restricted sufficient conditions on V guaranteeing its regularity are known. We cite the most important of them.

Nenciu and Scharf [NS78] show that the necessary condition for regularity is

$$\int \frac{|\mathbf{p}|^2}{1+|\mathbf{p}|^{1+\varepsilon}} \, |\hat{V}(\mathbf{p})|^2 \, d^3p < \frac{C}{\varepsilon} \tag{2.7.25}$$

for any $\varepsilon > 0$ and C independent of ε. $\hat{V}(\mathbf{p})$ denotes Fourier transform of $V(\mathbf{x})$. It implies that static magnetic fields are never regular! Only electric potentials ($\mathbf{A} = 0$, $V \neq 0$) can be considered as candidates.

On the other hand,

$$\int \frac{|\mathbf{p}|^2}{1+|\mathbf{p}|^{1-\varepsilon}} \, |\hat{V}(\mathbf{p})|^2 \, d^3p < \infty \tag{2.7.26}$$

for some $\varepsilon > 0$ is a sufficient condition for the potential V being regular. A conjecture of Nenciu and Scharf is that a necessary and sufficient condition for a potential being regular is

$$\int \frac{|\mathbf{p}|^2}{1+|\mathbf{p}|} \, |\hat{V}(\mathbf{p})|^2 \, d^3p < \infty. \tag{2.7.27}$$

That was an open problem, but we give a counterexample in theorem 19 (section 6.2.1).

The square well potential

A square-well potential defined as

$$V(x) = \begin{cases} V_0 & \text{if} \quad |x| \leq a, \\ 0 & \text{if} \quad |x| > a, \end{cases} \tag{2.7.28}$$

whose Fourier transform is

$$\hat{V}(\mathbf{p}) = V_0 \left(\frac{4\pi a}{|\mathbf{p}|}\right)^{3/2} J_{3/2}(|\mathbf{p}|a) \sim \begin{cases} 1 & \text{as} \quad |\mathbf{p}| \approx 0 \\ |\mathbf{p}|^{-2} & \text{as} \quad |\mathbf{p}| \to \infty, \end{cases} \tag{2.7.29}$$

does not satisfy the conjectured condition (2.7.27) due to the behaviour of $\hat{V}(\mathbf{p})$ at infinity, which is related to the discontinuity in $V(\mathbf{x})$. It satisfies the necessary condition (2.7.25), but it does not satisfy the sufficient condition (2.7.26). Therefore regularity of the square well potential remains here open. We will come back to the problem in section 6.2.1.

If the square well is smoothed out at $|\mathbf{x}| = a$ then the Fourier transform falls off fast enough that the sufficient condition (2.7.26) holds. We show that it is enough to make

the potential only continuous by modifying it in the neighbourhood of $r = a$ in order to make it regular. Consider a slightly modified square well potential

$$V(r) = \begin{cases} -V_0, & r < a - \delta \\ -\frac{V_0}{2} + \frac{V_0}{2}\frac{(r-a)}{\delta}, & |r-a| \leq \delta \\ 0, & r > a + \delta \end{cases} \tag{2.7.30}$$

with some small $\delta > 0$. Now an essential integral

$$4\pi \int_0^\infty |V'(r)|^2 \; r^2 \; dr = \mathcal{O}(\delta^{-1}) \tag{2.7.31}$$

is finite for every $\delta > 0$. On the other hand we have

$$4\pi \int_0^\infty |V'(r)|^2 \; r^2 \; dr = \int_{\mathbb{R}^3} |\nabla V(\mathbf{x})|^2 \; d^3x = ||\nabla V||_2^2. \tag{2.7.32}$$

Using the property of Fourier transforms $||f||_2 = ||\hat{f}||_2$ [RS75, IX.4] we obtain

$$\begin{aligned} 4\pi \int_0^\infty |V'(r)|^2 \; r^2 \; dr = ||\mathbf{p}\hat{V}||_2^2 &= \int_{\mathbb{R}^3} |\mathbf{p}\hat{V}(\mathbf{p})|^2 \; d^3p \\ &= \int_{\mathbb{R}^3} |\mathbf{p}|^2 |\hat{V}(\mathbf{p})|^2 \; d^3p > \int_{\mathbb{R}^3} \frac{|\mathbf{p}|^2}{1+|\mathbf{p}|^{1-\epsilon}} |\hat{V}(\mathbf{p})|^2 \; d^3p \end{aligned} \tag{2.7.33}$$

for every $0 < \epsilon \leq 1$. Finally, we have shown

$$\int_{\mathbb{R}^3} \frac{|\mathbf{p}|^2}{1+|\mathbf{p}|^{1-\epsilon}} |\hat{V}(\mathbf{p})|^2 \; d^3p = \mathcal{O}(\delta^{-1}) < \infty \tag{2.7.34}$$

for every $\delta > 0$ and $0 < \epsilon \leq 1$ what is the sufficient condition (2.7.26) for regularity of V.

The Coulomb potential

Coulomb potential $V(\mathbf{x}) = A/|\mathbf{x}|$ has a Fourier transform $\hat{V}(\mathbf{p}) = -4\pi A/|\mathbf{p}|^2$ and analogously to the square well satisfies the necessary condition (2.7.25), but does not satisfy the sufficient condition (2.7.26) as well as the conjecture (2.7.27) because of a slow fall-off at infinity in $\hat{V}$. If the Coulomb potential is regularized at $\mathbf{x} = 0$, e.g. smoothed out and kept bounded, such that the integral (2.7.31) is finite, then in an analogous way it fulfills the sufficient condition (2.7.26) and is regular.

2.7.3 Time-dependent Hamiltonians

If the Hamiltonian depends on time then so does its spectrum. If the particle and antiparticle subspaces are to be defined by spectral projectors then they will also depend on time. It will generate a different Fock representation at every instant of time t. A pair of such two Fock representations is only then equivalent if the unitary evolution operator $U(t_2, t_1)$ is implementable in any of the Fock spaces. According to the literature [Bon70, FS79] it is rarely the case. The situation looks much better if the time-dependent Hamiltonian is

either asymptotically static (as $t \to \pm\infty$) or static in the initial (*in*) and final (*out*) period of the evolution (i.e. for $|t| > T$). Assume $\lim_{t\to\pm\infty} H(t) = H_0$, i.e. the external field is asymptotically switched off. Then, instead of the evolution operator $U(t_2, t_1)$, the wave operators $W_\pm(t)$ defined as a strong limit

$$W_\pm(t) \equiv \operatorname*{s-lim}_{t_0\to\pm\infty} U(t, t_0)\, U_0(t_0, t) \tag{2.7.35}$$

can be used and they have better properties regarding implementation. It follows from the fact that their existence, i.e. existence of the strong limit in (2.7.35), already imposes restrictions on the external potential in H. This will be discussed in section 3.5.

In the following we define a few most natural particle interpretations and study their equivalence (we use the nomenclature of [FS79]).

The *in*-representation

It bases on the projectors $P^0_\pm$ corresponding to the spectral subspaces of H_0. The field operator evolves according to the free evolution operator

$$\hat\Psi^{in}_t(f) = \hat\Psi^{in}_{t_0}(U^*_0(t, t_0)\, f) \tag{2.7.36}$$

and is decomposed at every time into the particle and antiparticle operators by

$$\hat\Psi^{in}_t(f) = \hat b^{in}_t(P^0_+\, f) + \hat d^{in\,*}_t(P^0_-\, f). \tag{2.7.37}$$

Then the particles in the *in*-regime are well defined, as was discussed in section 2.7.1. Next, we can establish a connection with the so-called interpolating field, which evolves according to the full evolution operator

$$\hat\Psi_t(f) = \hat\Psi_{t_0}(U^*(t, t_0)\, f). \tag{2.7.38}$$

Both can be identified in the far past, i.e. by the condition

$$\lim_{t\to-\infty} [\hat\Psi_t(f) - \hat\Psi^{in}_t(f)] = 0. \tag{2.7.39}$$

It has the following consequence for arbitrary time t

$$\begin{aligned} \hat\Psi_t(f) &= \lim_{t_0\to-\infty} \hat\Psi_{t_0}(U^*(t, t_0)\, f) = \lim_{t_0\to-\infty} \hat\Psi^{in}_{t_0}(U^*(t, t_0)\, f) \\ &= \lim_{t_0\to-\infty} \hat\Psi^{in}_t(U^*_0(t_0, t)\, U^*(t, t_0)\, f) = \hat\Psi^{in}_t(W^*_-(t)\, f). \end{aligned} \tag{2.7.40}$$

The interpolating *in*-representation

We have not specified completely the interpolated representation yet, because we have not defined its projectors. Define the particle and antiparticle subspaces as evolved from those

defined by the *in*-representation. Therefore we split both fields in the relation (2.7.40) using the corresponding projectors

$$\hat{b}_t(P_+(t)\ f) = \hat{b}^{in}_t(P^0_+\ W^*_-(t)\ f) \tag{2.7.41}$$
$$\hat{d}_t(P_-(t)\ f) = \hat{d}^{in}_t(P^0_-\ W^*_-(t)\ f). \tag{2.7.42}$$

These relations define the projectors $P_\pm(t)$ which are time-dependent. To find their values explicitly, we transform

$$\hat{\Psi}_t(P_\pm(t)\ f) = \hat{\Psi}^{in}_t(P^0_\pm\ W^*_-(t)\ f) = \hat{\Psi}_t(W_-(t)\ P^0_\pm\ W^*_-(t)\ f). \tag{2.7.43}$$

Since this relation holds for all $f \in \mathcal{H}$, it follows

$$P_\pm(t) = W_-(t)\ P^0_\pm\ W^*_-(t) \tag{2.7.44}$$

or

$$\begin{aligned} P_\pm(t) &= \underset{t_0\to-\infty}{\text{s-lim}}\ U(t,t_0)\ U_0(t_0,t)\ P^0_\pm\ U_0(t,t_0)\ U(t_0,t) \\ &= \underset{t_0\to-\infty}{\text{s-lim}}\ U(t,t_0)\ P^0_\pm\ U(t_0,t), \end{aligned} \tag{2.7.45}$$

because U_0 commutes with $P^0_\pm$. It means that to decide whether a state corresponding to a wave function f at time t is interpreted as a particle or an antiparticle, it is evolved to the far past, there projected on the subspace of free particles or antiparticles and finally evolved back to time t.

The *out*-representation

Analogously to *in*, we can define the *out*-representation by

$$\hat{\Psi}^{out}_t(f) = \hat{\Psi}^{out}_{t_0}(U^*_0(t,t_0)\ f) \tag{2.7.46}$$

and

$$\hat{\Psi}^{out}_t(f) = \hat{b}^{out}_t(P^0_+ f) + \hat{d}^{out\,*}_t(P^0_- f). \tag{2.7.47}$$

Then the connection with the interpolating field is defined by

$$\lim_{t\to\infty}[\hat{\Psi}_t(f) - \hat{\Psi}^{out}_t(f)] = 0 \tag{2.7.48}$$

and leads to

$$\hat{\Psi}_t(f) = \hat{\Psi}^{out}_t(W^*_+(t)\ f). \tag{2.7.49}$$

The interpolating *out*-representation

The interpolating *out*-representation is analogous to the interpolating *in* and is defined by the correspondence of the particle and antiparticle subspaces with those which evolved from those defined in the *out*-representation, i.e. by

$$\hat{b}_t(P_+(t)\ f) = \hat{b}_t^{out}(P_+^0\ W_+^*(t)\ f) \tag{2.7.50}$$
$$\hat{d}_t(P_-(t)\ f) = \hat{d}_t^{out}(P_-^0\ W_+^*(t)\ f). \tag{2.7.51}$$

The projectors $P_\pm(t)$ are again time-dependent and can be found by

$$\hat{\Psi}_t(P_\pm(t)\ f) = \hat{\Psi}_t^{out}(P_\pm^0\ W_+^*(t)\ f) = \hat{\Psi}_t(W_+(t)\ P_\pm^0\ W_+^*(t)\ f), \tag{2.7.52}$$

which holds for all $f \in \mathcal{H}$, therefore

$$P_\pm(t) = W_+(t)\ P_\pm^0\ W_+^*(t) = \underset{t_0\to\infty}{\text{s-lim}}\, U(t,t_0)\ P_\pm^0\ U(t_0,t). \tag{2.7.53}$$

The Furry (static) representation

This representation is based on a time-dependent projector which is defined at every time t separately by projection on the spectral subspaces of the instantaneous $H(t)$, as if the Hamiltonian and the external field were frozen at that time

$$\widetilde{P}_+(t) \equiv P_{[E_0,\infty)}(H(t)), \qquad \widetilde{P}_-^0(t) \equiv P_{(-\infty,E_0)}(H(t)). \tag{2.7.54}$$

Equivalence of the particle interpretations

The *in* and interpolating-*in* representations are unitarily equivalent, since the Bogoliubov transformation between them defined in (2.7.41), (2.7.42) is trivial and does not contain any off-diagonal terms mixing particles with antiparticles. Hence, they can be realized in the same Fock space $\mathcal{F}^{in}$. Analogously, the *out* and the interpolating-*out* representations are unitarily equivalent due to (2.7.50), (2.7.51) and can be both realized in $\mathcal{F}^{out}$. So there remain three classes of representations, *in*, *out* and Furry, which equivalence is not evident and requires more detailed analysis.

Furry representation is equivalent to the *in*-representation if the corresponding projectors satisfy

$$\widetilde{P}_+(t)\ P_-(t) \in \text{H.S.} \quad \text{and} \quad \widetilde{P}_-(t)\ P_+(t) \in \text{H.S.}, \tag{2.7.55}$$

what is equivalent to

$$\widetilde{P}_+(t)\ W_-(t)\ P_-^0 \in \text{H.S.} \quad \text{and} \quad \widetilde{P}_-(t)\ W_-(t)\ P_+^0 \in \text{H.S.}. \tag{2.7.56}$$

Fierz and Scharf [FS79] prove that it is the case if the time-dependent potential $V(t,\mathbf{x})$, understood as a 4x4 matrix acting on Dirac bispinors, satisfies the following criteria.

Theorem 7 *When*

(a) $\exists T_0$ *such that* $V(t,\mathbf{x}) = 0$ *for all* $t < T_0$,

(b) $V(t,\cdot)$ *is continuous and twice piecewise continuously differentiable with respect to* t,

(c) the Fourier transformed $\hat{V}^{(\alpha)}(t,\mathbf{k}) \in L^2(\mathbb{R}^3)^{16} \cap L^1(\mathbb{R}^3)^{16}$, $\alpha = 0,1,2$, $\forall T_0 \leq t \leq T$,

(d) $E = E_0$ *is not in the spectrum of* $H(T)$ *(if it is, it must be decided to which spectral subspace* $\widetilde{P}_-(T)$ *or* $\widetilde{P}_+(T)$ *the eigensubspace of* E_0 *belongs),*

(e) $H(T)$ *has an eigenfunction expansion (what implies additional restrictions on* V*, e.g.* $V(T,\mathbf{x}) \in L^1(\mathbb{R}^3)^{16}$ *is a sufficient condition),*

then the Furry and in-representations are unitarily equivalent at any time $t \in [T_0, T]$.

These are quite general conditions under which both representations are equivalent. They get destroyed e.g. when the potential varies in a discontinuous way. An example of a time-dependent square well potential is considered further, in section 2.8.2, where similar conditions on $V(t)$ are studied.

Analogously, the equivalence between the Furry and *out*-representation can be shown. If both pairs are equivalent, then, of course, the *in* and *out*-representations are equivalent.

Covariant particle interpretation

Fierz and Scharf [FS79] analyze the consequences of Lorentz transformations, which lead to the change of representations via unitary operators representing Lorentz transformations in $\mathcal{H}$. While the *in* and *out*-representations behave covariantly, the Furry representation does not. The transformed Furry representation is no more Furry representation in presence of time-dependent potentials. It means that the transformed vacuum becomes a many-particle state. While for static potentials one reference frame is distinguished and the Furry representation can be based on it, for time-dependent potentials no special reference frame and hence no special Furry representation can be chosen. Therefore, the only covariant particle interpretations in presence of time-dependent potentials are the (interpolating) *in* and *out*-representations, what confirms that the notion of particles has only asymptotic meaning.

2.8 Scattering in Fock space

Unitary equivalence of the *in*- and *out*-representations can be considered independently of their equivalence with the Furry representation, as we have proceeded in the previous section. The two can be formally identified by the interpolating field using (2.7.40), (2.7.49)

$$\hat{\Psi}_t(f) = \hat{\Psi}_t^{in}(W_-^*(t)\, f) \quad \text{and} \quad \hat{\Psi}_t(f) = \hat{\Psi}_t^{out}(W_+^*(t)\, f), \tag{2.8.1}$$

what gives

$$\hat{\Psi}_t^{out}(f) = \hat{\Psi}_t(W_+(t)\, f) = \hat{\Psi}_t^{in}(W_-^*(t)\, W_+(t)\, f) = \hat{\Psi}_t^{in}(S^*(t)\, f), \tag{2.8.2}$$

where we have introduced the classical (single-particle) scattering operator (3.5.18)

$$S(t) \equiv W_+^*(t)\, W_-(t) = \underset{\substack{t_1\to-\infty\\ t_2\to+\infty}}{\text{s-lim}}\, U_0(t,t_2)\, U(t_2,t_1)\, U_0(t_1,t). \tag{2.8.3}$$

Its existence, i.e. existence of the strong limits, follows from the existence of the wave operators $W_\pm(t)$ and presents restrictions on the time-dependent potential, what will be discussed later, in section 3.5. For the case of a static external field, and hence static H, it is easy to show that $S(t)$ is in fact independent of t

$$S(t) = U_0(t,0)\, S(0)\, U_0(0,t) = e^{-iH_0t} S(0) e^{iH_0t} = S(0), \tag{2.8.4}$$

because H_0, and hence $\exp(\pm iH_0t)$, commute with $S(0)$ (for proof see [Tha92, Th. 8.3] or [RS79, XI.3]). For time-dependent $H(t)$ we must keep the time-dependence of $S(t)$ explicitly in the notation or choose a distinguished time t_0 to which we refer. Usually it is $t = 0$.

Particles in the *in* and *out*-representations are defined in a time-independent way like in section 2.7.1

$$\begin{aligned}
\hat{b}_n^{in} &\equiv \hat{b}_n^{in}(t) = \hat{b}_t^{in}(P_+^0\, \varphi_n^{in}(t)) && (2.8.5)\\
\hat{d}_n^{in} &\equiv \hat{d}_n^{in}(t) = \hat{d}_t^{in}(P_-^0\, \varphi_n^{in}(t)) && (2.8.6)\\
\hat{b}_n^{out} &\equiv \hat{b}_n^{out}(t) = \hat{b}_t^{out}(P_+^0\, \varphi_n^{out}(t)) && (2.8.7)\\
\hat{d}_n^{out} &\equiv \hat{d}_n^{out}(t) = \hat{d}_t^{out}(P_-^0\, \varphi_n^{out}(t)) && (2.8.8)
\end{aligned}$$

and the corresponding wave functions satisfy

$$\begin{aligned}
\varphi_n^{in}(t) &= U_0(t,t_0)\, \varphi_n^{in}(t_0) \equiv U_0(t,0)\, \phi_n^{in} && (2.8.9)\\
\varphi_n^{out}(t) &= U_0(t,t_0)\, \varphi_n^{out}(t_0) \equiv U_0(t,0)\, \phi_n^{out}. && (2.8.10)
\end{aligned}$$

Then the Bogoliubov transformation between them induced by (2.8.2) can be found in the

following way

$$\begin{aligned}
\hat{b}_n^{out} &= \hat{b}_n^{out}(t) = \hat{b}_t^{out}(P_+^0\ \varphi_n^{out}(t)) \\
&= \hat{\Psi}_t^{out}(P_+^0\ \varphi_n^{out}(t)) = \hat{\Psi}_t^{in}(S^*(t)\ P_+^0\ \varphi_n^{out}(t)) \\
&= \hat{b}_t^{in}(P_+^0\ S^*(t)\ P_+^0\ \varphi_n^{out}(t)) + \hat{d}_t^{in^*}(P_-^0\ S^*(t)\ P_+^0\ \varphi_n^{out}(t)) \\
&= \hat{b}_t^{in}\left(\sum_k \left(\varphi_k^{in}(t), P_+^0\ S^*(t)\ P_+^0\ \varphi_n^{out}(t)\right)\ \varphi_k^{in}(t)\right) \\
&+ \hat{d}_t^{in^*}\left(\sum_k \left(\varphi_k^{in}(t), P_-^0\ S^*(t)\ P_+^0\ \varphi_n^{out}(t)\right)\ \varphi_k^{in}(t)\right) \\
&= \sum_k \left(P_+^0\ S^*(t)\ P_+^0\ \varphi_n^{out}(t), \varphi_k^{in}(t)\right) \cdot \hat{b}_t^{in}(P_+^0\ \varphi_k^{in}(t)) \\
&+ \sum_k \left(P_-^0\ S^*(t)\ P_+^0\ \varphi_n^{out}(t), \varphi_k^{in}(t)\right) \cdot \hat{d}_t^{in^*}(P_-^0\ \varphi_k^{in}(t)) \\
&= \sum_k \underbrace{\left(\varphi_n^{out}(t), P_+^0\ S(t)\ P_+^0\ \varphi_k^{in}(t)\right)}_{\equiv [S(t)_{++}]_{nk}} \cdot \hat{b}_k^{in} + \sum_k \underbrace{\left(\varphi_n^{out}(t), P_+^0\ S(t)\ P_-^0\ \varphi_k^{in}(t)\right)}_{\equiv [S(t)_{+-}]_{nk}} \cdot \hat{d}_k^{in^*}.
\end{aligned} \tag{2.8.11}$$

The matrix elements $[S(t)_{\pm\pm}]_{nk}$ can be simplified, e.g.

$$\begin{aligned}
[S(t)_{+-}]_{nk} &= \left(\varphi_n^{out}(t), P_+^0\ S(t)\ P_-^0\ \varphi_k^{in}(t)\right) \\
&= \lim_{\substack{t_1\to-\infty \\ t_2\to+\infty}} \left(U_0(t,0)\ \phi_n^{out}, P_+^0\ U_0(t,t_2)\ U(t_2,t_1)\ U_0(t_1,t)\ P_-^0\ U_0(t,0)\ \phi_k^{in}\right) \\
&= \lim_{\substack{t_1\to-\infty \\ t_2\to+\infty}} \left(\phi_n^{out}, P_+^0\ U_0(0,t_2)\ U(t_2,t_1)\ U_0(t_1,0)\ P_-^0\ \phi_k^{in}\right) \\
&= \left(\phi_n^{out}, P_+^0\ S(0)\ P_-^0\ \phi_k^{in}\right) = [S(0)_{+-}]_{nk} \equiv (S_{+-})_{nk}.
\end{aligned} \tag{2.8.12}$$

Then, the Bogoliubov transformation takes finally the form

$$\hat{b}_n^{out} = \sum_k (S_{++})_{nk}\ \hat{b}_k^{in} + \sum_k (S_{+-})_{nk}\ \hat{d}_k^{in^*} \tag{2.8.13}$$

$$\hat{d}_n^{out^*} = \sum_k (S_{-+})_{nk}\ \hat{b}_k^{in} + \sum_k (S_{--})_{nk}\ \hat{d}_k^{in^*}. \tag{2.8.14}$$

It is implementable, and thus the *in* and *out*-representations are unitarily equivalent, if and only if (cf. theorem 1)

$$S_{+-} \in \text{H.S.} \quad \text{and} \quad S_{-+} \in \text{H.S.}. \tag{2.8.15}$$

Then there exists a unitary operator $\hat{S}$ in $\mathcal{F}^{in}$ which implements S:

$$\hat{\Psi}^{in}(S^* f) = \hat{S}^* \hat{\Psi}^{in}(f) \hat{S}. \tag{2.8.16}$$

2.8.1 Particle production

For practical calculations of scattering processes it is important that the whole information about the scattering in Fock space is encoded in the one-particle scattering operator S, which alone defines the Bogoliubov transformation. To see it we calculate as an example the expectation value of the number of particles created from an initial vacuum state $\Omega \equiv \Omega^{in}$ in an implemented scattering process. Define "the number of particles in state ϕ_n^{out} operator" as

$$\begin{aligned}\hat{N}_n^{out} &\equiv \hat{b}_n^{out^*}\, \hat{b}_n^{out} + \hat{d}_n^{out^*}\, \hat{d}_n^{out} \\ &= \hat{b}_{t=0}^{out\ ^*}(P_+^0\ \phi_n)\, \hat{b}_{t=0}^{out}(P_+^0\ \phi_n) + \hat{d}_{t=0}^{out\ ^*}(P_-^0\ \phi_n)\, \hat{d}_{t=0}^{out}(P_-^0\ \phi_n)\end{aligned} \tag{2.8.17}$$

or split to particle and antiparticle number operators

$$\hat{N}_{(+)n}^{out} \equiv \hat{b}_n^{out^*}\, \hat{b}_n^{out} \quad \text{for} \quad \phi_n^{out} \in \mathcal{H}_+ \tag{2.8.18}$$

$$\hat{N}_{(-)n}^{out} \equiv \hat{d}_n^{out^*}\, \hat{d}_n^{out} \quad \text{for} \quad \phi_n^{out} \in \mathcal{H}_-. \tag{2.8.19}$$

Here we have assumed for simplicity of the notation that the bases $\{\phi_n^{in}\}$ and $\{\phi_n^{out}\}$ are identical, what can be relaxed at any time. Then its expectation value in the state evolved from vacuum Ω^{in} which is $\hat{S}\Omega^{in}$ in the Schrödinger picture can be calculated as follows

$$\begin{aligned}N_{(+)n}^{out} &\equiv \left(\hat{S}\ \Omega, \hat{N}_{(+)n}^{out}\ \hat{S}\ \Omega\right) = \left(\hat{S}\ \Omega, \hat{b}_n^{out^*}\ \hat{b}_n^{out}\ \hat{S}\ \Omega\right) \\ &= \left(\hat{S}\ \Omega, \hat{b}_0^{out^*}(P_+^0\ \phi_n)\ \hat{b}_0^{out}(P_+^0\ \phi_n)\ \hat{S}\ \Omega\right) \\ &= \left(\Omega, \hat{S}^*\ \hat{\Psi}_0^{out^*}(P_+^0\ \phi_n)\ \hat{S}\ \hat{S}^*\ \hat{\Psi}_0^{out}(P_+^0\ \phi_n)\ \hat{S}\ \Omega\right) \\ &= \left(\Omega, \hat{\Psi}_0^{out^*}(S^*\ P_+^0\ \phi_n)\ \hat{\Psi}_0^{out}(S^*\ P_+^0\ \phi_n)\ \Omega\right) \\ &= \Big(\Omega, \Big[\hat{b}_0^{out^*}(P_+^0\ S^*\ P_+^0\ \phi_n) + \hat{d}_0^{out}(P_-^0\ S^*\ P_+^0\ \phi_n)\Big] \\ &\qquad \Big[\hat{b}_0^{out}(P_+^0\ S^*\ P_+^0\ \phi_n) + \hat{d}_0^{out^*}(P_-^0\ S^*\ P_+^0\ \phi_n)\Big]\ \Omega\Big) \\ &= \left(\Omega, \hat{d}_0^{out}(P_-^0\ S^*\ P_+^0\ \phi_n)\ \hat{d}_0^{out^*}(P_-^0\ S^*\ P_+^0\ \phi_n)\Omega\right) \\ &= \left(\Omega, \hat{d}_0^{out}\left(\sum_k (\phi_k, P_-^0\ S^*\ P_+^0\ \phi_n)\ \phi_k\right)\ \hat{d}_0^{out^*}\left(\sum_l (\phi_l, P_-^0\ S^*\ P_+^0\ \phi_n)\ \phi_l\right)\Omega\right) \\ &= \sum_{k,l} (\phi_k, P_-^0\ S^*\ P_+^0\ \phi_n)\ (P_-^0\ S^*\ P_+^0\ \phi_n, \phi_l)\left(\Omega, \hat{d}_0^{out}\left(P_-^0\ \phi_k\right)\ \hat{d}_0^{out^*}\left(P_-^0\ \phi_l\right)\Omega\right) \\ &= \sum_{k,l} (P_-^0\ S^*\ P_+^0\ \phi_n, \phi_l)\ (\phi_k, P_-^0\ S^*\ P_+^0\ \phi_n)\ \delta_{kl} \\ &= (P_-^0\ S^*\ P_+^0\ \phi_n, P_-^0\ S^*\ P_+^0\ \phi_n) \\ &= ||P_-^0\ S^*\ P_+^0\ \phi_n||^2.\end{aligned} \tag{2.8.20}$$

It measures the norm of the vector $\phi_n \in \mathcal{H}_+$ scattered "back in time" to the far past and projected onto the antiparticle subspace $\mathcal{H}_-$. Analogously, we can find the expectation

value of the number of antiparticles in state ϕ_n created from vacuum in a scattering process

$$N^{out}_{(-)n} = ||P^0_+ \, S^* \, P^0_- \, \phi_n||^2, \tag{2.8.21}$$

which expresses the norm of a vector $\phi_n \in \mathcal{H}_-$ scattered "back in time" and projected on the particle subspace $\mathcal{H}_+$.

Interesting is to calculate the total number of particles and antiparticles created from vacuum in a scattering process given by S

$$N^{out}_{(+)} \equiv \sum_n N^{out}_{(+)n} = \sum_n ||P^0_- \, S^* \, P^0_+ \, \phi_n||^2 = ||(S^*)_{-+}||^2_{HS} = ||S_{+-}||^2_{HS} \tag{2.8.22}$$

$$N^{out}_{(-)} \equiv \sum_n N^{out}_{(-)n} = \sum_n ||P^0_+ \, S^* \, P^0_- \, \phi_n||^2 = ||(S^*)_{+-}||^2_{HS} = ||S_{-+}||^2_{HS}. \tag{2.8.23}$$

It turns out that these numbers are just the same as those appearing in the conditions (2.8.15) for implementability of S, which now can be rewritten as

$$N^{out}_{(+)} < \infty \quad \text{and} \quad N^{out}_{(-)} < \infty. \tag{2.8.24}$$

It means that a classical scattering process S in $\mathcal{H}$ is implementable by a unitary operator $\hat{S}$ in Fock space $\mathcal{F}$ if and only if the total number of particles and antiparticles created from vacuum are finite.

2.8.2 Implementability of S

The condition of implementability of S as a unitary operator in Fock space (2.8.15) is an implicit restriction on the time-dependent Hamiltonian $H(t)$ and consequently on the potential $V(t)$. We quote a theorem of Seipp [Sei82, Th. 7], [Tha92, Th. 8.25] giving sufficient conditions on $V(t)$

Theorem 8 *Consider the external field V as a 4x4 matrix acting on the Dirac bispinors. Let $V(t)$ be strongly continuous and two times piecewise strongly differentiable in t such that $d^2V(t)/dt^2$ is piecewise strongly continuous. Denote*

$$W^{(n)}(t) \equiv \frac{d^n V(t)}{dt^n}, \qquad n = 0, 1, 2. \tag{2.8.25}$$

If $\widetilde{W}^{(n)}(t,\cdot) \in L^1(\mathbb{R}^3)^{16} \cap L^2(\mathbb{R}^3)^{16}$ (i.e. each component of the Fourier transforms $\widetilde{W}^{(n)}(t,\mathbf{p})$ is integrable and square integrable with respect to $\mathbf{p}$) and

$$\int_{-\infty}^{+\infty} ||\widetilde{W}^{(n)}(t,\cdot)||_k \, dt < \infty \quad \textit{for} \quad n = 0, 1, 2, \quad k = 1, 2, \tag{2.8.26}$$

then S_{-+} and S_{+-} are Hilbert-Schmidt.

Example – Time-dependent square well potential

Consider an example of a time-dependent square well potential

$$V(t,\mathbf{x}) \equiv U(t)\cdot v(\mathbf{x}) \quad \text{with} \quad v(\mathbf{x}) \equiv \Theta(a-|\mathbf{x}|). \tag{2.8.27}$$

The conditions of the above theorem translate into

$$\int_{-\infty}^{+\infty} \left|\frac{d^n U(t)}{dt^n}\right| dt \;<\; \infty \quad \text{with} \quad n=0,1,2, \tag{2.8.28}$$

$$\int_{\mathbb{R}^3} |\widetilde{v}(\mathbf{p})|^k \, d^3p \;<\; \infty \quad \text{with} \quad k=1,2. \tag{2.8.29}$$

Both ($k=1,2$) conditions (2.8.29), which in short can be written as $\widetilde{v} \in L^1(\mathbb{R}^3)\cap L^2(\mathbb{R}^3)$, are satisfied by the Fourier transformed square well

$$\widetilde{v}(\mathbf{p}) = 4\pi\left[\frac{\sin(a|\mathbf{p}|)}{|\mathbf{p}|^3} - \frac{a\cos(a|\mathbf{p}|)}{|\mathbf{p}|^2}\right]. \tag{2.8.30}$$

Conditions (2.8.28) can be in short rewritten as[10] $U \in W^{2,1}(\mathbb{R})$ and imply among other things that

- $U(t),\ dU(t)/dt,\ d^2U(t)/dt^2 \to 0$ as $t \to \pm\infty$,
- $U(t)$ and $dU(t)/dt$ are piecewise continuous.

[10] $W^{p,k}$ denote Sobolev spaces

Chapter 3

Evolution and scattering in the classical Dirac equation

In order to implement evolution and scattering processes within the quantized Dirac field theory introduced in the previous chapter, evolution and scattering operators for the classical Dirac equation are needed. Physical intuition suggests that spontaneous particle creation happens when the ground state of the classical Hamiltonian reaches the negative continuum. In this chapter we will study the spectrum of the classical Hamiltonian and check if self-adjointness and unitary evolution are guaranteed also for overcritical potentials.

3.1 Self-adjointness of the Dirac-operator

The free Hamiltonian is defined as in (1.1.4) and the full Hamiltonian as in (1.1.3). The potential is defined in (1.1.5) and is treated as a multiplication 4x4 matrix operator with the components V_{kl}, $k, l = 1, ..., 4$. In this section either assume V as time-independent or consider every $V(t)$ separately treating t as a parameter.

The free Dirac Hamiltonian H_0 is essentially self-adjoint on the domain of smooth bispinorial functions on $\mathbb{R}^3$ with compact support [Tha92, Th. 1.1]

$$\mathcal{D}(H_0) = \mathcal{C}_0^\infty(\mathbb{R}^3)^4. \tag{3.1.1}$$

This domain is dense in the first Sobolev space

$$H^1(\mathbb{R}^3)^4 = \left\{ f \in L^2(\mathbb{R}^3)^4 \,\middle|\, \frac{\partial f}{\partial x^i} \in L^2(\mathbb{R}^3)^4 \right\}, \tag{3.1.2}$$

i.e. in the space of all square integrable bispinorial functions on $\mathbb{R}^3$ with square integrable distributional first derivatives. Hence, there exists a unique self-adjoint extension of H_0, call it $\widetilde{H_0}$, into the domain $H^1(\mathbb{R}^3)^4$. It is not essential to give the explicit form of $\widetilde{H_0}$. As it is unique, it is practically enough to think of its formal definition H_0, which describes

properly the action on the square integrable and differentiable functions, which we usually consider. From now on, for the sake of simplicity of the notation, we skip the tilde and write H_0 thinking of it as a self-adjoint operator on $H^1(\mathbb{R}^3)^4$.

The full Hamiltonian $H \equiv H_0 + V$ keeps some of the properties of H_0, because for small V it can be considered as a perturbation of H_0. Yet, we are interested not only in small V, i.e. weak potentials, but rather on the contrary, in strong potentials. Therefore, it is important to formulate criteria describing qualitative changes in the properties of H depending on the strength of V.

Regarding self-adjointness it is the question of a measure of V, which decides whether the perturbation is small or big. A general criterion is given by the fundamental Kato-Rellich theorem [RS75, Th. X.12]

Theorem 9 *Let H_0 be self-adjoint, V symmetric and V be H_0-bounded with relative bound $a < 1$, i.e. for some $a, b \in \mathbb{R}$ and $a < 1$*

$$||V\ f|| \leq a\ ||H_0\ f|| + b\ ||f|| \qquad \forall f \in \mathcal{H}. \tag{3.1.3}$$

Then $H = H_0 + V$ is self-adjoint on $\mathcal{D}(H_0)$.

It follows a theorem giving a more explicit condition on V [Tha92, Th. 4.2]

Theorem 10 *Let*

$$|V_{ik}(\mathbf{x})| \leq \frac{a}{2|\mathbf{x}|} + b \qquad \forall\, \mathbf{x} \in \mathbb{R}^3 \setminus \{0\}, \qquad i,k = 1, ..., 4, \tag{3.1.4}$$

for some $b > 0$ and $a < 1$. Then $H = H_0 + V$ is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{0\})^4$ and self-adjoint on $\mathcal{D}(H_0)$.

On the other hand, if no singularities are present, it holds [Tha92, Th. 4.3]

Theorem 11 *Let*

$$V_{ik} \in \mathcal{C}^\infty(\mathbb{R}^3), \qquad i,k = 1, ..., 4. \tag{3.1.5}$$

Then $H = H_0 + V$ is essentially self-adjoint on $\mathcal{C}^\infty(\mathbb{R}^3)^4$.

From the above two theorems it becomes clear that not the strength of the potential itself is essential for the self-adjointness of H, as in theorem 11 arbitrary smooth potentials are allowed, but it is the strength of the singularity in V. The condition in theorem 10 is optimal if all components V_{ik} are considered together (i.e. there exist potentials with $|V_{ik}(\mathbf{x})| \leq (1/2 + \epsilon)/|\mathbf{x}|$ with arbitrary small ϵ such that H is no longer self-adjoint), but it is not optimal if V is a pure electric potential, i.e. $V = eA_0\mathbf{1}$ and $A_i = 0$. Then there is a more general theorem [Sch72b]

Theorem 12 *Let V can be expressed as $V = V_1 + V_2$, where $V_1 \in \mathcal{C}^0(\mathbb{R}^3 \setminus \{0\})$ and $V_2 \in L^\infty(\mathbb{R}^3)$ (i.e. bounded) with*

$$|V_1(\mathbf{x})| \leq \frac{a}{|\mathbf{x}|}, \qquad \forall \mathbf{x} \in \mathbb{R}^3 \tag{3.1.6}$$

and $a \in (0, \sqrt{3}/2)$. *Then* $H = H_0 + V$ *is essentially self-adjoint on* $\mathcal{C}_0^\infty(\mathbb{R}^3 \setminus \{0\})^4$ *and self-adjoint on* $\mathcal{D}(H_0)$.

Condition on V_2 can be replaced by $V_2 \in L^p_{loc}(\mathbb{R}^3)$ with $p > 3$ [Wei03, Th. 20.4]. Even weaker conditions may be considered if the potential oscillates at infinity. For a more general theorem in such case see [Sch72b].

3.1.1 Coulomb potential from a point-like charge

Essential self-adjointness of $H_0 + V$ depends only on the local behaviour of V [Che77]. It turns out that the borderline case is represented by potentials having a Coulomb-like singularity[1] [Nar74]. Theorem 12 covers Coulomb potentials

$$V(\mathbf{x}) = -\frac{Z\alpha}{|\mathbf{x}|} \tag{3.1.7}$$

up to $Z\alpha < \sqrt{3}/2$, that is $Z \leq 118$. Higher values of Z lead to the following problem. Solving the radial Dirac equation, boundary conditions at $r = 0$ and at $r = \infty$ must be considered. Since $r = \infty$ is always a limit-point case of the differential equation, $r = 0$ is limit-point only for $0 \leq Z\alpha \leq \sqrt{3}/2$ but limit-circle for $Z\alpha > \sqrt{3}/2$, i.e. for $Z \geq 119$. In general a limit-circle case does not pick a unique boundary condition and this must be introduced additionally, leading thereby to a chosen self-adjoint extension. Nevertheless, for $\sqrt{3}/2 < Z\alpha < 1$ ($119 \leq Z \leq 137$) the limit-circle case is "weak" and one of the solutions diverges faster is than the other. Eliminating the faster divergent one gives rise to a kind of a distinguished boundary condition and a distinguished self-adjoint extension of H [Sch72a]. Alternatively, considering the limit $R \to 0$ in a cut-off procedure regularizing the Coulomb potential for $r < R$ one can also construct a self-adjoint extension of H [Wüs75]. Both imply finiteness of the potential energy in all states of $\mathcal{D}(H_0)$ and turn out to be equivalent. Another distinguished self-adjoint extension based on the finiteness of the kinetic energy has been constructed in [Nen76] and shown to be unique. In [KW79] it has been shown that all these procedures lead to the same self-adjoint extension.

For $Z > 137$ the above constructions do not work and other kinds of self-adjoint extensions must be considered. In principle, this procedure is arbitrary and there is a one-parameter family ($\theta \in [0, 2\pi)$) of possible self-adjoint extensions. Several examples can be found in the literature, where authors introduced a special distinguishing condition: orthogonality of eigenvectors [Cas50], special behaviour at the singularity [Nar74], continuity of the eigenvalues [BBZ81], limit procedure for a regularized singularity [Wüs75, Gär79] or other [Sch72a]. For a more detailed review cf. [Tha92, notes to sec. 4.3].

[1] We do not consider here more singular potentials at all, where the corresponding Hamiltonians are never self-adjoint, mainly due to lack of physical motivation. For more details, we refer to [Cas50].

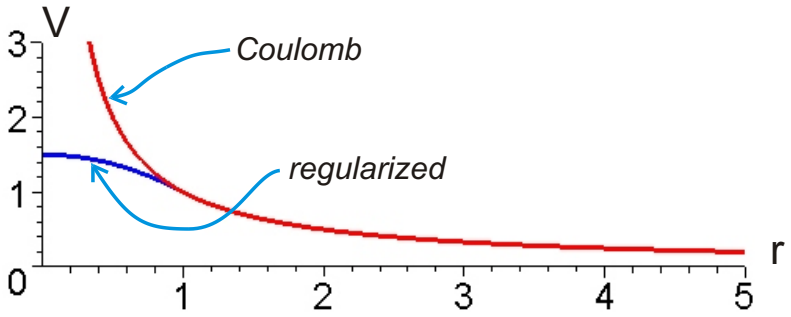


Figure 3.1: Point-like Coulomb vs. regularized potential of a homogeneously charged ball.

3.1.2 Potential of many Coulomb centers

The construction of the self-adjoint extension and its uniqueness for potentials consisting of a sum of Coulomb centers with $Z_i < 137$ has been proved by Nenciu in [Nen77] using a finite kinetic energy condition and by Klaus [Kla80a] using a (regularizing) cut-off procedure.

3.1.3 Potential of an extended charge

All problems with the need of self-adjoint extensions disappear when the Coulomb potential is smoothed out at $r = 0$. Theorem 11 covers that situation: the Hamiltonian is always self-adjoined (for any strength of the potential!). Physically, it corresponds to an extended charge what is always the case for charged nuclei. Replacing the point-like charge Z with a homogeneously charged ball of radius R gives a nonsingular potential

$$V_{(Z,R)}(r) = \begin{cases} \frac{Z\alpha}{r} & \text{for} \quad r > R, \\ \frac{Z\alpha}{2R}\left(3 - \frac{r^2}{R^2}\right) & \text{for} \quad r < R. \end{cases} \tag{3.1.8}$$

3.1.4 Particle with an anomalous magnetic moment

The anomalous magnetic moment is an effect of QED corrections to the Dirac equation. It can, however, be modelled in the classical Dirac equation as interaction between the anomalous magnetic moment μ_a and the electromagnetic field by introduction of a perturbation term in the Hamiltonian. In presence of the spherically symmetric electric potential the Hamiltonian (reduced to a single-spinor operator form "2x2") has the form

$$H = H_0 + V(r)\mathbf{1} - \mu_a \begin{pmatrix} 0 & V'(r) \\ V'(r) & 0 \end{pmatrix}. \tag{3.1.9}$$

In case of a Coulomb potential $V(r)$ the $V'(r)$ terms behave like r^{-2} and are highly singular. Nevertheless, they act in a regularizing way so that the total Hamiltonian H

stays self-adjoint for any Coulomb (as well as r^{-n}) potentials of arbitrary strength [Tha92, sec. 5.3.2]. This holds true also for many Coulomb centers [Beh85]. Since electron does have a small but nonzero anomalous magnetic moment it has to be considered seriously, because it changes qualitatively some mathematical properties of the Hamiltonian.

3.1.5 Self-adjointness of an overcritical potential

Finally, we can draw the conclusion that **self-adjointness of $H = H_0 + V$ is not endangered by strong potentials**. The only source of problems are potentials with strong point-like singularities, which physically are regularized by a finite size of the charge distribution (nuclei). Moreover, taking into account a small anomalous magnetic moment of the Dirac particle (electron) dismisses any problems with the self-adjointness.

3.2 Spectrum

The spectrum $\sigma(H)$ of the self-adjoint operator H can be split into the point spectrum $\sigma_p(H)$ containing all eigenvalues and the continuous spectrum $\sigma_{cont}(H)$ so that $\sigma(H) = \overline{\sigma_p(H)} \cup \sigma_{cont}(H) \subset \mathbb{R}$ (self-adjoint operators have an empty residual spectrum [RS72, Th. VI.8]). It is convenient to introduce also an alternative splitting, namely into the essential spectrum σ_{ess} containing the continuous spectrum σ_{cont}, all limit points of σ_p and eigenvalues of infinite multiplicity. Its complement is the discrete spectrum σ_{disc} so that $\sigma(H) = \sigma_{ess}(H) \cup \sigma_{disc}(H)$ (see [RS72, VII.2-3] or [Ric78, 8.1, 11.4-5] for definitions and discussion or [GP90, App. C] for a short review of the operator theory).

The essential spectrum of the free Dirac Hamiltonian H_0 is $\sigma_{ess}(H_0) = (-\infty, -1] \cup [1, \infty)$. It is very stable under perturbations of the operator, what means that the essential spectrum of the full Hamiltonian $\sigma_{ess}(H) \equiv \sigma_{ess}(H_0 + V) = \sigma_{ess}(H_0)$ for a wide class of potentials V. A sufficient condition is that $V(x) \to 0$ as $|x| \to 0$, but there exist also weaker conditions allowing even singularities in $V(x)$ at big distances which do not change the essential spectrum [Tha92, 4.3.4].

On the other hand, [Tho76, BG87] proved under fairly general conditions on $V(x)$ that there are no eigenvalues embedded in the continuous spectrum $\sigma_{cont}(H) = (-\infty, -1] \cup [1, \infty)$, what implies that the point spectrum $\sigma_{pp}(H) \subset (-1, 1)$ with possible concentration points at ± 1 (what is the case for Coulomb potentials).

Moreover, considering Hamiltonians $H_\lambda \equiv H_0 + \lambda V$ with $V(x) \leq 0$ ($V(x) \geq 0$ is analogous) Klaus [Kla80b] proved that there are infinitely many eigenvalues which enter the interval $(-1, 1)$ from above ($E = +1$), infinitely many which leave it at the bottom ($E = -1$) and all move monotonically from +1 to -1 as $\lambda \to \infty$. For spherically symmetric potentials $V(x)$ none of the eigenvalues can remain within $(-1, +1)$ as $\lambda \to \infty$.

3.2.1 Overcriticality

From the last three paragraphs it follows that the eigenvalues of $H_\lambda \equiv H_0 + V_\lambda \equiv H_0 + \lambda V$, which can be only in $(-1, +1)$, leave the interval as λ increases. They disappear from the spectrum, because they cannot be embedded in the continuous spectrum. A Hamiltonian H_λ and a potential V_λ for which at least one eigenvalue has disappeared, but was present for some $\lambda' < \lambda$, we call **overcritical**. The limiting case corresponding to the value $\lambda = \lambda_{cr}$ at which the eigenvalue tends to -1 when $\lambda \to \lambda_{cr}$ will be referred to as **critical**. So the potential V_λ becomes overcritical as the first, lowest lying eigenvalue disappears at -1 (for $\lambda = \lambda_{cr}$) and remains overcritical for all $\lambda > \lambda_{cr}$.

In fact, a disappeared eigenvalue leaves its mark in the analytic structure of the resolvent, giving rise to a resonance which we will discuss below. Moreover, it modifies the continuum wave functions, especially in the spectral neighbourhood of its disappearance point -1, so that despite of a lack of one eigenvector the set of all generalized eigenvectors of H remains complete and still can represent any vector in $\mathcal{H}$.

3.2.2 Spectral decomposition

Indeed, if the operator H is self-adjoint then there exists a projector valued spectral measure [Ric78, Ch. 9]

$$E_\lambda = P_{(-\infty,\lambda]}(H) \tag{3.2.1}$$

which provides a resolution of the identity

$$\mathbf{1} = \int_{-\infty}^{+\infty} dE_\lambda \tag{3.2.2}$$

and according to the spectral theorem [RS72, Th. VII.7-8]

$$H = \int_{-\infty}^{+\infty} \lambda \; dE_\lambda \qquad \text{as well as} \qquad f(H) = \int_{-\infty}^{+\infty} f(\lambda) \; dE_\lambda. \tag{3.2.3}$$

The measure E_λ can be uniquely decomposed into the following parts [Ric78, Ch. 9.9]

$$E_\lambda \text{ is discontinuous at } \lambda \quad \Leftrightarrow \quad \lambda \in \sigma_{pp}(H) \tag{3.2.4}$$

$$E_\lambda \text{ is strongly continuous but not in norm at } \lambda \quad \Leftrightarrow \quad \lambda \in \sigma_{cont}(H) \tag{3.2.5}$$

$$E_\lambda \text{ is continuous in norm at } \lambda \quad \Leftrightarrow \quad \lambda \in \mathbb{R} \setminus \sigma(H) \tag{3.2.6}$$

what gives $E = E_{pp} + E_{cont}$. Accordingly, there exists a unique decomposition of the Hilbert space $\mathcal{H} = \mathcal{H}_{pp} \bigoplus \mathcal{H}_{cont}$ [RS72, Th. VII.4] and a countable set of orthogonal projectors $Q_n : \mathcal{H} \to \mathcal{H}_{pp}$ on the eigenvalue subspaces such that $HQ_n = \lambda_n Q_n$. Then

$$\mathbf{1} = \sum_{\lambda_n \in \sigma_{pp}(H)} Q_n + \int_{\sigma_{cont}(H)} dE_\lambda \tag{3.2.7}$$

and

$$H = \sum_{\lambda_n \in \sigma_{pp}(H)} \lambda_n Q_n + \int_{\sigma_{cont}(H)} \lambda \; dE_\lambda. \tag{3.2.8}$$

Assuming that there exists a basis $|\phi_\lambda\rangle$, $\lambda \in \sigma(H)$ of generalized eigenfunctions of H such that

$$H|\phi_\lambda\rangle = \lambda|\phi_\lambda\rangle \tag{3.2.9}$$

(but not necessary $|\phi_\lambda\rangle \in \mathcal{H}$) one can express the measure [Ric78, 10.12]

$$E_\lambda|\chi\rangle = \int_{-\infty}^{\lambda} |\phi_\lambda\rangle\langle\phi_\lambda|\chi\rangle \; d\mu(\lambda) \quad \forall \chi \in \mathcal{H}, \tag{3.2.10}$$

where μ is some measure on $\mathbb{R}$. This justifies the Dirac notation, where the formal identity

$$dE_\lambda = |\phi_\lambda\rangle\langle\phi_\lambda| \; d\mu(\lambda) \tag{3.2.11}$$

leads to

$$\mathbf{1} = \int_{-\infty}^{+\infty} |\phi_\lambda\rangle\langle\phi_\lambda| \; d\mu(\lambda) \;\; = \sum_{\lambda_n \in \sigma_{pp}(H)} |\phi_{\lambda_n}\rangle\langle\phi_{\lambda_n}| \; \Delta\mu_n + \int_{\sigma_{cont}(H)} |\phi_\lambda\rangle\langle\phi_\lambda| \; d\mu(\lambda), \tag{3.2.12}$$

$$H = \int_{-\infty}^{+\infty} \lambda|\phi_\lambda\rangle\langle\phi_\lambda| \; d\mu(\lambda) = \sum_{\lambda_n \in \sigma_{pp}(H)} \lambda_n|\phi_{\lambda_n}\rangle\langle\phi_{\lambda_n}| \; \Delta\mu_n + \int_{\sigma_{cont}(H)} \lambda|\phi_\lambda\rangle\langle\phi_\lambda| \; d\mu(\lambda). \tag{3.2.13}$$

For $\lambda \in \sigma_{pp}$ the states $|\phi_\lambda\rangle \in \mathcal{H}_{pp}$ are eigenvectors of H, called *bound state wave functions*. For $\lambda \in \sigma_{cont}$ the states $|\phi_\lambda\rangle$ are so-called *continuum wave functions* and do not belong to $\mathcal{H}$, because $\langle\phi_\lambda|\phi_\lambda\rangle$ is not finite. First the *wave packets* belong to $\mathcal{H}$

$$\int_{\sigma_{cont}} a(\lambda) \; |\phi_\lambda\rangle \; d\mu(\lambda) \in \mathcal{H}_{cont} \qquad \Leftrightarrow \qquad \int_{\sigma_{cont}} |a(\lambda)|^2 \; d\mu(\lambda) < \infty. \tag{3.2.14}$$

Then

$$\int_{\sigma(H)} d\mu(\lambda) \; |\phi_\lambda\rangle\langle\phi_\lambda| = \sum_{\lambda_n \in \sigma_{pp}(H)} \mu(\lambda_n) \; |\phi_{\lambda_n}\rangle\langle\phi_{\lambda_n}| + \int_{\sigma_{cont}(H)} d\mu(\lambda) \; |\phi_\lambda\rangle\langle\phi_\lambda|. \tag{3.2.15}$$

The spectral measure μ is, in general, not unique up to multiplication by a function of λ, but this freedom is removed by imposing the *normalization conditions* for the wave functions

$$\mu(\lambda_n) \; |\phi_{\lambda_n}\rangle\langle\phi_{\lambda_n}|\phi_{\lambda_m}\rangle = \delta_{nm} \; |\phi_{\lambda_m}\rangle \qquad \text{for} \qquad \lambda_n, \lambda_m \in \sigma_{pp}, \tag{3.2.16}$$

$$\mu(\lambda) \; |\phi_\lambda\rangle\langle\phi_\lambda|\phi_{\lambda'}\rangle = \delta(\lambda - \lambda') \; |\phi_{\lambda'}\rangle \qquad \text{for} \qquad \lambda, \lambda' \in \sigma_{cont}. \tag{3.2.17}$$

The existence of generalized eigenvectors forming an orthonormal basis in $\mathcal{H}$ depends on further properties of H. For H_0 the basis is constructed via the spatial Fourier transform [Tha92, sec. 1.4.1]. For $H = H_0 + V$ completeness has been shown for $|V(x)| \leq \nu \, e^{-\alpha|x|}/|x|$ with $0 \leq \nu < 2/\pi$ [Nen75] and for $V(x) \in \mathcal{C}_0^\infty$ in [Pic05, Ch. 6] by construction of a generalized Fourier transform.

3.3 Resonances

3.3.1 Analytic structure of the resolvent and Green's function

The spectrum of H can also be analyzed from the point of view of analytic properties of the resolvent

$$R(\lambda) \equiv \frac{1}{H - \lambda \mathbf{1}}. \tag{3.3.1}$$

This operator is bounded for all λ in the resolvent set $\rho(H) \equiv \mathbb{C} \setminus \sigma(H)$ and unbounded for $\lambda \in \sigma(H)$. One can study analytic properties of the weighted resolvent

$$R_\psi(\lambda) \equiv (\psi, (H-\lambda)^{-1}\psi) = (\psi, R(\lambda)\psi) \quad \text{and} \quad R^0_\psi(\lambda) \equiv (\psi, (H_0-\lambda)^{-1}\psi) \tag{3.3.2}$$

for some $\psi \in A$, a dense set in $\mathcal{H}$, and construct their analytic (meromorphic) continuations from $\{\lambda \in \mathbb{C} \mid \mathrm{Im}\lambda > 0\}$ to $\{\lambda \in \mathbb{C} \mid \mathrm{Im}\lambda \leq 0\}$ [HS95, Th. 16.4].

For $\lambda \in \mathbb{C}$ in the vicinity of the essential spectrum $\sigma_{ess}(H)$ the value of $R_\psi(\lambda)$ grows like $|\mathrm{Im}\lambda|^{-1}$. At the points of the discrete spectrum $\lambda \in \sigma_{disc}(H)$ the weighted resolvent $R_\psi(\lambda)$ has poles for all $\psi \in A$ and

$$P_\lambda = \frac{1}{2\pi i} \oint_{|\mu-\lambda|=\epsilon} R(\mu)\, d\mu \tag{3.3.3}$$

for some small $\epsilon > 0$ gives a spectral projector projecting on the eigensubspace to the eigenvalue λ of H. If for all $\psi \in A$ the analytically continued $R_\psi(\lambda)$ has a pole at some $\lambda = \lambda_R$ ($\mathrm{Im}\lambda_R < 0$) while $R^0_\psi(\lambda_R)$ is analytic then λ_R is called *resonance* or a *resonance pole* [RS78, XII.6].

The existence of analytic continuations (by explicit construction), the association of the poles of these continuations with the eigenvalues of some non-self-adjoint operators obtained from H by complex dilations and the identification of these eigenvalues as resonances, are results of the Aguilar-Balslev-Combes-Simon theory [HS95, Ch. 16, 17]. One can show that the poles of the resolvent are identical with those of the scattering operator by using the relation [AJS77, Prop. 6.11]

$$S = \mathbf{1} + \operatorname*{s-lim}_{\eta\to 0^+} \operatorname*{s-lim}_{\delta\to 0^+} \int \left(R^0_{E-i\eta} - R^0_{E+i\eta}\right)\left(V - VR_{E+i\delta}V\right) d\mu(E). \tag{3.3.4}$$

Often it can be shown that these poles are identical with the poles of the meromorphic continuation of the Green's function or the S operator (for more details and further references we refer to [RS78, notes to Ch. XII] and [HS95, notes to Ch.16]). The Green's function is defined as the integral kernel of the resolvent

$$(R(\lambda)\ \psi)(x) \equiv \int G(\lambda, x, y)\ \psi(y)\ dy. \tag{3.3.5}$$

It shows some kind of a singular behaviour at $\lambda \in \sigma_{ess}(H)$. Analogously to the weighted resolvent, it can be continued analytically trough $\sigma_{ess}(H)$ from $\mathrm{Im}\lambda > 0$ to $\mathrm{Im}\lambda \leq 0$. When $\sigma_{ess}(H) \neq \mathbb{R}$ then $G(\lambda, \cdot, \cdot)$ becomes a multivalued function for $\mathrm{Im}\lambda < 0$ with a branch cut at $\sigma_{ess}(H)$. Moreover, it has poles at $\lambda \in \sigma_{disc}(H)$ as well as at resonances.

3.3.2 Perturbation of the eigenvalues

A very important question is how the bound states (discrete spectrum) and resonances behave and transform into each other under perturbations of the potential δV. This is essential in order to understand changes in the spectrum in time-dependent processes when V varies in time and $\delta V \sim dV/dt$. As we have already mentioned above, the essential spectrum σ_{ess} is highly stable under perturbations of the potential V. In contrast, the discrete spectrum σ_{disc} is rather sensitive: eigenvalues may move along the real axis or disappear turning into resonances. In other words, the real poles of $G(\lambda, \cdot, \cdot)$ may move along $\mathbb{R}$ or leave $\mathbb{R}$ and go to $\mathbb{C} : \mathrm{Im}\lambda < 0$. For a wide class of parameterized perturbations giving rise to the analytic family (in the sense of Kato) $H(\beta)$ the regular perturbation theory applies [RS78, Ch. XII.2]. Its main result is the convergent[2] Rayleigh-Schrödinger series for perturbed isolated eigenvalues. In case of an analytic family $H(\beta) = H(0) + \beta W$ the first terms of the series give

$$\lambda(\beta) = \lambda(0) + \beta\ (\phi(0), W\phi(0)) + \mathcal{O}(\beta^2), \tag{3.3.6}$$

where $\phi(0)$ is the unperturbed eigenvector to the eigenvalue $\lambda(0)$ of $H(0)$. However, for some perturbations the series diverges and is only asymptotic (roughly the problem is usually connected with a change of the domain of $H(\beta)$ as the perturbation is switched on), but an eigenvalue $\lambda(\beta) \in \mathbb{R}$ exists for all $H(\beta)$. We do not go into more detail referring the reader to [RS78, Ch. XII]. Yet for some "singular" perturbations the real isolated eigenvalue disappears completely from the spectrum as soon as the perturbation is switched on, while the spectrum becomes continuous around the point of the unperturbed eigenvalue $\lambda(0) \in \sigma_{ess}(\beta > 0)$ (e.g. as in the Stark effect). Another situation when a similar phenomenon occurs is an eigenvalue embedded in the continuous spectrum already for $\beta = 0$, i.e. $\lambda(0) \in \sigma_{ess}(0)$, which disappears as soon as the perturbation is switched on (e.g. helium atom). In both cases the eigenvalue becomes a complex resonance. There are two strategies which we want to mention how to keep track of its position.

Spectral concentration

The first one uses the notion of *spectral concentration* and says that in the "new" continuum $\sigma_{ess}(\beta > 0)$ a vector $\phi(\beta)$ can be found in the subspace

$$P_{(\lambda(0)+\alpha\beta-f(\beta),(\lambda(0)+\alpha\beta+f(\beta)}(H(\beta)), \qquad f(\beta) = o(\beta) \tag{3.3.7}$$

(α being the first Rayleigh-Schrödinger coefficient), i.e. localized spectrally around the point $\lambda(0) + \alpha\beta \in \sigma_{ess}(\beta)$, which goes strongly to the unperturbed eigenvector $\phi(0)$ as $\beta \to 0$ and

$$\lim_{\beta\to 0} ||(H(\beta) - \lambda(0) - \alpha\beta)\phi(\beta)||/\beta = 0. \tag{3.3.8}$$

[2]Nonzero radius of convergence in parameter β.

It means that for every $\beta > 0$ there exists $\phi(\beta)$, as approximate eigenvector of $H(\beta)$ to the eigenvalue $\lambda(0) + \alpha\beta$, which can be constructed as a wave packet localized spectrally in an interval centered at $\lambda(0) + \alpha\beta \in \sigma_{ess}(\beta)$ and having a width $f(\beta) \to 0$ as $\beta \to 0$. This can be used as a "practical" definition of the resonance state for some numerical calculations.

Complex pole

The second method is based on the fact that vanishing of an isolated or embedded eigenvalue from the spectrum and turning into a resonance corresponds to a move of the pole $\lambda(\beta)$ of the weighted resolvent $R_\psi(\lambda, \beta)$ or of the Green's function $G_\beta(\lambda, x, y)$ from the real axis to the complex plane. Using the dilation theory one can construct a family of non-self-adjoint operators which have a complex eigenvalue at the point of the resonance [RS78, Ch. XII.6]. Unfortunately, for this kind of eigenvalues one cannot directly apply the standard perturbation theory. However, one can obtain a Puiseux series containing non-integer powers of the parameter β for the resonance position $\lambda(\beta)$ [How74a], though p of its leading terms may consist of integer powers of β. If $f(\beta) = o(\beta^p)$ but $f(\beta)/\beta^{p+1} \to \infty$ it is called *spectral concentration to order p* [Nen81]. In the case of Auger ionization in the helium atom a spectral concentration to the first order [Sim73] occurs. The first Rayleigh-Schrödinger coefficient α_1 is real, so the second coefficient α_2 is the first that may have a non-vanishing imaginary part. It follows that, for small β, the imaginary part of the resonance pole behaves like

$$\Gamma \equiv 2 \text{ Im } \lambda(\beta) \approx 2 \ \beta^2 \text{ Im } \alpha_2. \tag{3.3.9}$$

This is the *Fermi golden rule*. Γ describes approximately the decay rate of the unperturbed eigenvector $\phi(0)$ under evolution generated by a time-independent Hamiltonian $H(\beta)$ as well as the spectral width of a wave packet approximating the resonance state. The connection is based on the observation that a first order pole in the scattering operator at a complex resonance position $\lambda(\beta) = E_{res} \equiv E_R + iE_I$ causes the following approximate structure of the scattering amplitude

$$a(E) = \frac{C}{E - (E_R + iE_I)} + f(E), \tag{3.3.10}$$

where $f(E)$ is analytic at $E = E_{res}$. If the pole is near the real axis, i.e. $E_I = \Gamma/2 \approx 0$, then

$$|a(E)|^2 \approx \frac{|C|^2}{(E - E_R)^2 + \frac{1}{4}\Gamma^2} \tag{3.3.11}$$

we obtain a Breit-Wigner resonance distribution. For more details on the Fermi golden rule stating positivity of Γ we refer to [RS78, XII.6], [How74a], [SW98] and [CS01].

Relative phase-shifts

There exists an alternative way of estimating the position of the resonances based on the analysis of the relative asymptotic phase-shifts of the continuum wave functions. It

has been used e.g. for identifying resonances in the Coulomb potential [RMG81] and is explained in [GMR85]. The main point is the observation that in presence of a resonance the continuum wave functions (i.e. the generalized eigenvectors corresponding to the continuous spectrum) become modified in such a way that they present a special structure of asymptotic phase-shift, namely $\exp(i(pr + \delta(E)))$ and $\delta(E)$ jumps by π (say from 0 to π) in the vicinity of the resonance position. More exactly, the point where $\delta(E) = \pi/2$ coincides with the real part E_R of the resonance position. The width Γ of the peak in $\sin^2(\delta(E))$ approximates the imaginary part E_I of the position of the resonance.

We conclude that **the resonances are continuations in β of eigenvalues $\lambda(\beta)$ of self-adjoint $H(\beta)$.**

3.3.3 Perturbation of eigenvalues at the edge of continuum $\varepsilon = -1$

A special case of perturbed eigenvalues turning into resonances are eigenvalues $\varepsilon(\lambda_0)$ of a self-adjoint $H(\lambda_0) = H_0 + \lambda_0 V$ embedded in the essential spectrum $\sigma_{ess} = (-\infty, -1] \cup [1, +\infty)$ at one of its end points[3]. We are interested in the case $\varepsilon(\lambda_0) = -1$ which we defined in the previous section (sec. 3.2.1) as *critical*. Moreover, we assume that the "coupling constant" λ_0 is positive and for $\lambda < \lambda_0$ there exists an isolated eigenvalue $\varepsilon(\lambda) > -1$. It can be guaranteed by assuming that the potential $V(x)$ is negative everywhere.

As $\lambda \to \lambda_0^-$ the eigenvalue $\varepsilon(\lambda) \to -1^+$, but we need to know some more details on the asymptotic behaviour and whether the eigenvalue exists for $\lambda = \lambda_0$. Klaus in [Kla85, Th. 1.1] shows that there are two cases:

1. $\varepsilon(\lambda) \cong -1 + c(\lambda_0 - \lambda) + \mathcal{O}(\lambda_0 - \lambda)^{3/2}$ with $c > 0$ and $\varepsilon(\lambda)$ has a convergent expansion in $(\lambda_0 - \lambda)^{1/2}$, but is non-analytic at $\lambda = \lambda_0$,

2. $\varepsilon(\lambda) \cong -1 + c(\lambda_0 - \lambda)^2$ with $c > 0$ and $\varepsilon(\lambda)$ is analytic at $\lambda = \lambda_0$.

So the two cases differ in the slope $d\varepsilon(\lambda)/d\lambda$ at which the critical value is reached:

$$\text{case 1)} \quad \lim_{\lambda \to \lambda_0} \frac{d\varepsilon(\lambda)}{d\lambda} = -c < 0, \qquad \text{case 2)} \quad \lim_{\lambda \to \lambda_0} \frac{d\varepsilon(\lambda)}{d\lambda} = 0. \tag{3.3.12}$$

Only in case 1 the critical Hamiltonian $H(\lambda_0)$ has an eigenvalue $\varepsilon(\lambda_0) = -1$, i.e. there exists an eigenvector with a finite norm. Analogous results hold at the other continuum edge $\varepsilon = +1$. Moreover, if the potential $V(x)$ is spherically symmetric and κ is the angular parameter then the above cases hold correspondingly

1. for all $|\kappa| > 1$ at $\varepsilon = \pm 1$, for $\kappa = -1$ at $\varepsilon = -1$, and for $\kappa = +1$ at $\varepsilon = +1$,

2. for $\kappa = -1$ at $\varepsilon = +1$ and for $\kappa = +1$ at $\varepsilon = -1$.

[3] Note a change of notation at that point: ε – eigenvalue or resonance (instead of previous λ), λ – parameter (instead of previous β). It is caused by our attempt to use the original notation of cited sources, mainly [RS78].

It means that the case 1. occurs always except when $\kappa = \pm 1$ at the edge $\varepsilon = \mp 1$. From [Kla85, Th. 4.3] we know that the lowest eigenvalue corresponds always to $|\kappa| = 1$, while the sign of κ may, in general, be arbitrary. However, in all known examples it is $\kappa = -1$ which gives the lowest eigenvalue and becomes critical at the smallest (positive) value of λ. Therefore, we will assume it in the following what allows us to concentrate on case 1. only. By this assumption Mur and Popov [MP76] calculated approximately the coefficient c.

It is an important fact that $\varepsilon(\lambda)$ is not analytic[4] at $\lambda = \lambda_0$. It allows for existence of a complex resonance described by continuation of $\varepsilon(\lambda)$ for $\lambda > \lambda_0$ while for $\lambda \leq \lambda_0$ we have a real eigenvalue. (Since this is not true in case 2. there is no complex resonance in that case!) Since the coefficient c by the linear term in the expansion of $\varepsilon(\lambda)$ with respect to $\lambda - \lambda_0$ is real, the first imaginary term is of order $\mathcal{O}(\lambda - \lambda_0)^{3/2}$ and it has , in general, a nonzero coefficient. Hence we obtain a universal scaling

$$\Gamma(\lambda)/2 \equiv \mathrm{Im}(\varepsilon(\lambda)) \sim \mathrm{Re}(\varepsilon(\lambda) + 1)^{3/2} \sim (\lambda - \lambda_0)^{3/2}, \tag{3.3.13}$$

which describes the estimated position of the resonance in the complex plane for $\lambda \gtrsim \lambda_0$ and proves the Fermi golden rule, which happens to scale in the same way as in the Schrödinger equation with a threshold eigenvalue [JN05]. The position of the resonance $\varepsilon(\lambda)$ can also be obtained as a solution of a transcendental equation [How74a, CS01]. In our example studied in chapter 5.3 this equation takes a relatively simple form, though still being transcendental and must be solved numerically.

We conclude that when the potential becomes overcritical the golden Fermi rule holds and the threshold eigenvalue (bound state energy) perturbs to a (complex) resonance whose real part ("resonance energy") lies within the negative continuum.

3.3.4 Meaning of resonances in evolution

Although it is difficult to show rigorously how the existence of resonances contributes to the evolution picture, a formal result sheds some light on it. The evolution group e^{-iHt} (for time-independent Hamiltonians H) can be represented via the Laplace transform as

$$(\psi, e^{-iHt}\psi) = \frac{-1}{2\pi i} \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-iEt}\, \mathrm{Im}(\psi, (H - E - i\epsilon)^{-1}\psi)\, dE. \tag{3.3.14}$$

If the resolvent $(H-E-i\epsilon)^{-1}$ can be continued across the real axis (or σ_{ess}) to $\mathrm{Im}E < 0$ and has poles there, deformation of the integration contour and the residual theorem will lead to a sum of contributions from separate poles. Their time-dependence will be $e^{-itE_R - tE_I}$ where E_R and E_I are the real and imaginary parts of E, thus giving an exponential decay of the amplitude.

[4] Probably a hidden assumption of analyticity led to an incorrect scaling in [GMR85].

3.4 Evolution

The Dirac equation with a time-independent self-adjoint Hamiltonian H

$$i\frac{\partial}{\partial t}\Psi(t) = H\Psi(t) \tag{3.4.1}$$

treated as a Cauchy problem with a given initial vector $\Psi(t_0) \in \mathcal{D}(H) \subset \mathcal{H}$ has, according to Stone's theorem [RS72, Th. VIII.7], a unique solution of the form

$$\Psi(t) = U(t)\Psi(t_0) = e^{-iH(t-t_0)}\Psi(t_0), \tag{3.4.2}$$

where $U(t)$ is a strongly continuous one-parameter unitary group, satisfying, amongst others, $U(t_0) = \mathbf{1}$ and $U(t+s) = U(t)U(s)$.

The case of a time-dependent Hamiltonian $H(t)$

$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \tag{3.4.3}$$

is much more complicated, since not every self-adjoint $H(t)$ generates evolution [DG97, B.3]. If it does, the evolution can be described by a two-parameter family of unitary operators $U(t_1, t_2)$ called a *unitary propagator* and satisfying

- $U(t_1, t_2)$ is unitary and strongly continuous in t_1, t_2,
- $U(t_2, t_1) = U^*(t_1, t_2)$ and $U(t, t) = 1$,
- $U(t_1, t_2)U(t_2, t_3) = U(t_1, t_3)$.

(These are the conditions assumed in section 2.6 by defining evolution in the Fock space.) It gives the solution of (3.4.3)

$$\Psi(t) = U(t, t_0)\Psi(t_0). \tag{3.4.4}$$

The sufficient conditions for existence of the unitary propagator are given in [Tha92, Th. 4.9] and [RS75, X.12]. In the case when $H(t) \equiv H_0 + V(t)$ it suffices that H_0 be self-adjoint and $V(t)$ bounded, self-adjoint and strongly continuous [Tha92, Th. 4.10] or $V(t) \in L^1_{loc}(\mathbb{R}, B(\mathcal{H}))$ (Bochner integrable) [DG97, B.3].

3.4.1 Adiabatic theorem(s)

In the case of adiabatic evolution one considers processes driven by a slowly changing Hamiltonian, usually written as $H_\epsilon(t) \equiv H(\epsilon t)$ with small ϵ. Mathematically, this type of evolution is equivalent to that satisfying the adiabatic equation

$$i\epsilon\frac{\partial}{\partial t}\Psi(t) = H\Psi(t), \tag{3.4.5}$$

which is obtained by the substitution $t \to t/\epsilon$. The spectrum and spectral subspaces of $H_\epsilon(t)$ change slowly in time. Since for static Hamiltonians $H_0(t) = H(0)$ the evolution is

confined to any spectral subspace of $H(0)$, e.g. an initial eigenvector evolves remaining an eigenvector forever, a similar behaviour is expected for the adiabatic evolution as $\epsilon \to 0$. Let $P_A(t)$ be a spectral projector of $H_\epsilon(t)$ on $A(t) \subset \sigma(H_\epsilon(t))$, where $A(t)$ changes continuously following the changing spectrum of $H_\epsilon(t)$. Let $U_\epsilon(t)$ be a unitary evolution operator solving (3.4.5). Choose an initial vector $\psi(0) \in P_A(0)\mathcal{H}$. Then it is expected that after the evolution, which is usually parameterized such that $t \in [0,1]$, the final vector $\psi(1) = U_\epsilon(1)\psi(0)$ is approximately in $P_A(1)$, i.e.

$$||U_\epsilon(1)P_A(0) - P_A(1)U_\epsilon(1)|| \equiv \delta(\epsilon) \to 0 \quad \text{as} \quad \epsilon \to 0. \tag{3.4.6}$$

There are several theorems covering different kinds of spectral projections $P_A(t)$ providing a bound on the function $\delta(\epsilon)$. In the simplest case of $H(t)$ having a purely discrete spectrum with $P_A(t)$ being a projector onto a chosen eigenvector to an eigenvalue being a piecewise differentiable function of time and without level crossings the adiabatic theorem says that $\delta(\epsilon) = \mathcal{O}(\epsilon)$ [GP91, Ch. 11.10].

A more general theorem of Nenciu [Nen80b] treats the situation of a finite number of disjoint components $\sigma_i(t)$ of the spectrum of $H_\epsilon(t)$ having a finite (spectral) distance between each other, but allowing e.g. separated continuous parts. The corresponding projectors $P_i(t)$ are assumed to be norm twice differentiable in time. Then the adiabatic limit holds, i.e. $\lim_{\epsilon\to 0} \delta(\epsilon) = 0$. In a more refined versions of the adiabatic theorem Nenciu gives better estimates for δ. In [Nen81] he proves the existence of projections $P_A^n(t)$ such that $\delta(\epsilon) = \mathcal{O}(\epsilon^n)$ for every $n \in \mathbb{N}$. In [Nen93] he constructs an asymptotic series in ϵ for the projector $P(t)$ such that $\delta(\epsilon) = \mathcal{O}\left(\exp\left(-\frac{k}{\epsilon^a}\right)\right)$ for some $k > 0$ and $a \geq 0$ which is related to the regularity of the resolvent of $H_\epsilon(t)$. For analytic potentials and evolution from $t = -\infty$ to $t = +\infty$ Joye and Pfister [JP91] show that $\delta(\epsilon) = \mathcal{O}\left(\epsilon^2 \exp\left(-\frac{a}{\epsilon}\right)\right)$.

Avron and Elgart in [AE99a] prove a theorem for finite rank projections $P_A(t)$ which allows for an embedded eigenvalue, an eigenvalue at the threshold of the continuum, or a finite number of eigenvalue crossings requiring only $P_A(t)$ to be continuous at the crossing points. Then the adiabatic limit holds: $\lim_{\epsilon\to 0} \delta(\epsilon) = 0$. The rate of convergence of $\delta(\epsilon)$ depends on the kind of level crossing and for the linear crossing it is $\delta(\epsilon) = \mathcal{O}(\sqrt{\epsilon})$ (Born-Fock theorem) [AE98]. Another theorem of Avron and Elgart [AE99b] assuming an eigenvalue at the threshold of the continuous spectrum gives a better estimate $\delta(\epsilon) = \mathcal{O}(\epsilon)$. For a review and references to further versions of adiabatic theorems we refer to [AE99a] and [Teu02].

3.5 Scattering

Scattering theory is a big field of research with extensive literature present. We cite here only those facts which will be important in our further considerations. For a more complete picture we refer the reader to [Tha92, Ch. 8] containing scattering theory for the Dirac equation, to [AJS77] containing a very good and richly commented introduction to the

scattering theory, to [RS79] containing the mathematical approach with many theorems and proofs, and to [Yaf04] for a brief review of main mathematical results.

3.5.1 Time-independent Hamiltonians

We first consider the simpler and most studied case in the scattering theory, namely that of a time-independent Hamiltonian $H = H_0 + V$, where H_0 is a free Dirac Hamiltonian and V is a static potential. Then there are two unitary propagators

$$U(t) = e^{-iHt} \quad \text{and} \quad U_0(t) = e^{-iH_0 t}, \tag{3.5.1}$$

which describe the full and free evolution, respectively.

The wave operators

The goal of the scattering theory is to relate a state $f \in \mathcal{H}$ at time $t = 0$ to a state $g_\pm \in \mathcal{H}$ which evolved from f to $t \to \pm\infty$ and evolves freely according to H_0, so that

$$\lim_{t\to\pm\infty} ||U(t)f - U_0(t)g_\pm|| = \lim_{t\to\pm\infty} ||f - U^*(t)\ U_0(t)g_\pm|| = 0. \tag{3.5.2}$$

Therefore it is useful to define operators

$$W_\pm = \operatorname*{s-lim}_{t\to\pm\infty} U^*(t)\ U_0(t) = \operatorname*{s-lim}_{t\to\pm\infty} e^{iHt}e^{-iH_0 t}, \tag{3.5.3}$$

called *Møller wave operators*[5]. There appear two natural questions: about the existence and range of these operators. Existence requires existence of the strong limit, i.e. when acting on every vector from $\mathcal{H}$. The range of $W_\pm$ can maximally be the part of $\mathcal{H}$ corresponding to the continuous spectrum of H_0, which we denote $\mathcal{H}_{cont} \equiv P_{cont}(H_0)\mathcal{H}$. If Range$W_\pm = \mathcal{H}_{cont}$ then the wave operators are called *asymptotically complete*. All depends on the properties of the pair (H, H_0), which in the given Dirac case reduce to the properties of V.

Roughly speaking, the existence of $W_\pm$ depends essentially on the behaviour of $V(x)$ at infinity, hardly at all on its local behaviour. Sufficient conditions for existence of $W_\pm$ are

- V is trace-class [Yaf04, Th. 1.4];
- $|V|(1 + |\cdot|)^{-1/2+\epsilon} \in L^2(\mathbb{R}^3)$ for some $\epsilon > 0$ (Kuroda's criterion) [Eck74a].

When $W_\pm$ exist they are partial isometries from $\mathcal{H}$ to Range$W_\pm \subset \mathcal{H}_{cont}$, i.e. $W_\pm^* W_\pm = \mathbf{1}$ on $\mathcal{H}$ and $W_\pm W_\pm^*$ are projectors on Range$W_\pm$ [Tha92, Th. 8.2]. Moreover, they satisfy the following intertwining relations

$$HW_\pm = W_\pm H_0, \qquad e^{-iHt}W_\pm = W_\pm e^{-iH_0 t}. \tag{3.5.4}$$

The sufficient conditions for the asymptotic completeness are:

[5] It is the so-called *time-dependent* version. For the *time-independent* definition by means of the resolvent and spectral integrals we refer to [AJS77, Ch. 6].

- $(H-z)^{-n}-(H_0-z)^{-n}$ is trace-class for some $n=1,2,...$ [Tha92, Th. 8.4], [Yaf04, Th. 1.5], [Wei03, Th. 22.19],
- $\int_0^\infty ||V(H_0-z)^{-1}\chi(|\mathbf{x}|>R)||\,dR<\infty$ (short-range) [Tha92, Th. 8.20],
- Define[6] $V_\alpha^2(x)\equiv\int_{B(x,1)}\frac{|V(y)|^2}{|x-y|^{1+\alpha}}\,dy$. The following holds [Eck74b]:

  0) $|V|(1+|\cdot|)^{-1/2+\epsilon}\in L^2(\mathbb{R}^3)$ for some $\epsilon>0$,

  a) $\exists\alpha\in(0,1]:\sup_{x\in\mathbb{R}^3}V_\alpha(x)<\infty$ (Stummel condition),

  b) $\int_{B(x,1)}|V(y)|^2\,dy\to 0$ as $|x|\to\infty$,

  c) $\int_{\mathbb{R}^3}\frac{|V(y)|}{|x-y|}\,dy\le M_1\ \forall x\in\mathbb{R}^3$ and tends to 0 as $|x|\to\infty$,

  d) $\int_{\mathbb{R}^3}\frac{|V(y)|}{|x-y|^2}\,dy\le M_2\ \forall x\in\mathbb{R}^3$ and tends to 0 as $|x|\to\infty$,

  where the condition b) can be replaced with

  b') $V_\alpha(x)\to 0$ as $|x|\to\infty$.

  The following three classes satisfy these general conditions:

  1) $\begin{cases}|V(x)|\le C|x|^{-2-\epsilon} & \text{for}\quad |x|>R,\\ V_\alpha(x)\le C_1 & \text{for}\quad |x|\le R+1,\end{cases}$ with $R>1, C, C_1, \epsilon>0, \alpha\in(0,1]$,

  2) $|V|\subset L^p(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$ with $p>3$,

  3) $\int_{\mathbb{R}^3}|V(y)|^q(1+|y|)^p\,dy<\infty$ with $q>3$ and $p>2q-3$,

- $V\in L^3_{loc}(\mathbb{R}^3)$ and $|V(x)|\le C|x|^{-2-\epsilon}$ for $|x|>R$ and $C,\epsilon>0$; in case of spherically symmetric potentials it is enough that $|V(r)|\le C|r|^{-1-\epsilon}$ [Pea77],
- Spherically symmetric potentials satisfying $\int_c^\infty r^\epsilon|V(r)|\,dr<\infty\ \forall c>0$ with some $\epsilon>0$ and one of the following conditions [Pea77]:

  a) $V(r)=g/r+W(r)$, where $0\le g\le j+1/2$ and $\int_0^\infty|W(r)|\,dr<\infty$ ($\int_0^\infty|W(r)\log(r)|\,dr<\infty$ for $|g|=j+1/2$) or

  b) $V(r)\equiv V_0(r)+W(r)$, where $|rV_0(r)|<g<\sqrt{2j}$ and $\int_0^\infty r^{\sqrt{(j+1/2)^2-g^2}-(j+1/2}|W(r)|\,dr<\infty$ or

  c) $V(r)\equiv V_0(r)+W(r)$, where $|rV_0(r)|>g>j+1/2$, $(rV_0(r))^{-1}$ has bounded variation and $\int_0^\infty r^{-\epsilon}|W(r)|\,dr<\infty$ for some $\epsilon>0$.

The Coulomb potential $V(\mathbf{x})=\gamma/|\mathbf{x}|$ is not of a short-range and does not satisfy any of the above conditions. The wave operators $W_\pm$ defined in (3.5.3) do not exist as strong limits, what has been first observed for the Schrödinger equation by Dollard [Dol64] and holds in the Dirac case as well [DV66]. The reason is that due to the long-range interaction the evolution at big distances never becomes truly free, what can be seen already on the

[6] $B(x,r)$ denotes a ball with center x and radius r.

classical level of a (relativistic) point particle. In oder to obtain strong limits of the kind (3.5.3) modifiers of the asymptotic free evolution must be introduced. For a potential having Coulomb asymptotics, i.e. $V(\mathbf{x}) = \gamma/|\mathbf{x}|$ for $|\mathbf{x}| \geq R > 0$ the wave operators

$$\tilde{W}_\pm \equiv \lim_{t\to\pm\infty} e^{iHt}\tilde{U}_0(t) \tag{3.5.5}$$

exist and are complete [Tha92, Th. 8.21], where the modified free evolution

$$\tilde{U}_0(t) \equiv \tilde{U}_0^+(t)P_{\mathbb{R}+}(H_0) + \tilde{U}_0^-(t)P_{\mathbb{R}-}(H_0) \tag{3.5.6}$$

$$\tilde{U}_0^\pm(t) = e^{\mp i\sqrt{\mathbf{p}^2+1}\ t} \exp\left[-i\int_0^t V\left(\frac{\pm\mathbf{p}s}{\sqrt{\mathbf{p}^2+1}}\right)\ ds\right]. \tag{3.5.7}$$

The integral appearing in $\tilde{U}_0^\pm(t)$ evaluates to a logarithmic term in $\sqrt{\mathbf{p}^2+1}$.

For general long-range potentials one must modify the free evolution in (3.5.3). Depending on the decay of the potential at infinity there exist several methods, the simplest being the Dollard modifiers (introduced above in the Coulomb case). For even slower decaying potentials one can replace e^{-H_0t} with $e^{-iS(t,\hat{\mathbf{p}})}$ with $S(t,\mathbf{p})$ being a solution of an appropriate Hamilton-Jacobi equation, obtaining a time-dependent modifier, or construct Isozaki-Kitada integral operators $J_\pm$ and define

$$\tilde{W}_\pm \equiv \operatorname*{s-lim}_{t\to\pm\infty} e^{iHt}J_\pm e^{-iH_0t}, \tag{3.5.8}$$

obtaining time-independent modifiers. We refer to [DG97, Ch. 4] for an extensive review of those methods[7]. For the Dirac equation with long-range potentials existence and completeness of modified wave operators of the Isozaki-Kitada type as pseudo-differential operators constructed in terms of approximate eigenfunctions of H has been proved in [GY01]. The potentials are only required to have any power-law decay at infinity and be $\mathcal{C}^\infty$ functions such that

$$|D^nV(\mathbf{x})| \leq C_n(1+|\mathbf{x}|^2)^{-|n|/2-\rho}, \qquad C_n,\rho > 0 \qquad \forall n \in \mathbb{N}^3 \tag{3.5.9}$$

and $D_k \equiv -i\partial/\partial x^k$.

The scattering operator

If $W_\pm$ are asymptotically complete then RangeW_+ = RangeW_- = $\mathcal{H}_{cont}$ and one can define the scattering operator

$$S = W_+^*W_- = \operatorname*{s-lim}_{\substack{t_1\to-\infty\\ t_2\to+\infty}} e^{+iH_0t_2}e^{-iH(t_2-t_1)}e^{-iH_0t_1}, \tag{3.5.10}$$

which is defined on the whole $\mathcal{H}$ and unitary. The intertwining relations take the form

$$H_0S = SH_0, \qquad e^{-iH_0t}S = Se^{-iH_0t} \tag{3.5.11}$$

and reflect the conservation of energy in the scattering processes.

[7] In [DG97] they are applied to the Schrödinger equation, but the ideas of the modifiers are quite general and can be extended to the Dirac equation.

3.5.2 Time-dependent Hamiltonians

Now, we consider Hamiltonians $H(t)$ which via the potential $V(t)$ depend on time. While the free evolution $U_0(t) = e^{-iH_0 t}$ is identical as in the static case, the full evolution is described via the unitary propagator $U(t_1, t_2)$ defined in (3.4.3)-(3.4.4).

The wave operators

We define the wave operators analogously to (3.5.3)

$$W_\pm = \underset{t\to\pm\infty}{\text{s-lim}}\, U(0,t)\; e^{-iH_0 t}. \tag{3.5.12}$$

Their existence and unitarity are proved for the Schrödinger equation in the case of asymptotic switching, i.e. $V(t,\mathbf{x}) \equiv e^{-\epsilon|t|}\tilde{V}(\mathbf{x})$ [Dol66], for potentials satisfying

$$||V(t,\cdot)||_p \in L^{r+\epsilon}(\mathbb{R}^3) \cap L^{r-\epsilon}(\mathbb{R}^3) \quad \text{or} \quad ||V(t,\cdot)||_\infty \in L^1(\mathbb{R}^3) \cap L^{1+\epsilon}(\mathbb{R}^3) \tag{3.5.13}$$

with $p > 3/2$, $r = 2p/(2p-3)$, $\epsilon > 0$ [How74b], and for potentials $V(t,\mathbf{x}) \equiv V_0(t,\mathbf{x}) + V_1(t,\mathbf{x})$ such that

$$\int_0^\infty ||V_0(t,\cdot)||_\infty \, dt < \infty, \quad \int_0^\infty ||\nabla_x V_1(t,\mathbf{x}\cdot)||_\infty \sqrt{1+t^2}\, dt < \infty \tag{3.5.14}$$

and $V_1(\cdot, x_0) \in L^1_{loc}(\mathbb{R}_+)$ for some $x_0 \in \mathbb{R}^3$ [DG97, Ch. 3]. In [Nen80a] Nenciu argues that the proof of Dollard [Dol66] can be automatically repeated for the Dirac equation with asymptotically switched potentials $V(t,\mathbf{x}) \equiv \varphi(t)\tilde{V}(\mathbf{x})$ satisfying

$$\tilde{V}_{ij}(\mathbf{x}) \in L^p(\mathbb{R}^3) \cap L^2(\mathbb{R}^3), \qquad p > 3 \tag{3.5.15}$$

and the switching factor $\varphi(s)$ satisfying for every $s \in \mathbb{R}$

$$0 \le \varphi(s) \le 1, \quad \lim_{s\to 0}\varphi(s) = 1, \quad \lim_{s\to\pm\infty}\varphi(s) = 0, \tag{3.5.16}$$

$\varphi(s)$ twice differentiable and

$$\sup_{s\in\mathbb{R}} |\varphi'(s)| < \infty, \quad \lim_{s\to\pm\infty}\varphi'(s) = 0, \quad \int_{-\infty}^{+\infty} \left(|\varphi'(s)|^2 + |\varphi''(s)|\right)\, ds < \infty. \tag{3.5.17}$$

The gaussian switching factor $\varphi(t) = \exp(-t^2)$ satisfies the above conditions, while the exponential switching factor $\varphi(t) = \exp(-|t|)$ does not, because it is not differentiable at $t = 0$.

The scattering operator

The unitary wave operators $W_\pm$ give rise to a unitary scattering operator

$$S = W_+^* W_- = \underset{\substack{t_1\to-\infty \\ t_2\to+\infty}}{\text{s-lim}}\, e^{+iH_0 t_2} U(t_2,t_1) e^{-iH_0 t_1}. \tag{3.5.18}$$

3.5.3 The adiabatic scattering

Consider evolution generated by a the time-dependent Hamiltonian

$$H_\epsilon(t) \equiv H_0 + \varphi(\epsilon t)\tilde{V}(\mathbf{x}) \tag{3.5.19}$$

with the switching factor $\varphi(t)$ defined as in the previous section by (3.5.16)-(3.5.17). It gives rise to wave operators $W_\epsilon^\pm$ which are unitary for every $\epsilon > 0$ (cf. previous section and [Nen80a]). Consequently, there exists a unitary scattering operator $S_\epsilon = (W_\epsilon^+)^* W_\epsilon^-$ for every $\epsilon > 0$. The adiabatic scattering theory addresses the question whether the adiabatic operators $W_\epsilon^\pm, S_\epsilon$ for small ϵ converge to those describing the static case $\epsilon = 0$, i.e. $W_0^\pm, S_0$, in the limit when $\epsilon \to 0$. Dollard in [Dol66] proves for $\varphi(\epsilon t) = \exp(-\epsilon|t|)$ that $W_\epsilon^\pm$ converge strongly to $W_0^\pm$ as $\epsilon \to 0$. This proof holds analogously for $\varphi(t) = \exp(-t^2)$ and can be generalized to arbitrary switching factors $\varphi(t)$ satisfying (3.5.16)-(3.5.17) [Nen80a]. It is worth noting that except regularity conditions on $\varphi(t)$ the integral condition in (3.5.17) requires sufficiently fast decay as $t \to \pm\infty$. If this is violated one can construct counterexamples to completeness of the wave operators [Yaf78], [DG97, Ch. 3.8]. So we take it for granted that the strong limit exists

$$\text{s-}\lim_{\epsilon\to 0} W_\epsilon^\pm = W_0^\pm \equiv W^\pm. \tag{3.5.20}$$

It follows a weak limit for the adjoined operators

$$\text{w-}\lim_{\epsilon\to 0} (W_\epsilon^\pm)^* = (W_0^\pm)^* = (W^\pm). \tag{3.5.21}$$

From both above limits it follows a weak limit for the scattering operators

$$\text{w-}\lim_{\epsilon\to 0} S_\epsilon = S_0 \equiv S. \tag{3.5.22}$$

Then, since all S_ϵ and S are unitary, one can show that the strong limit holds

$$\text{s-}\lim_{\epsilon\to 0} S_\epsilon = S_0 = S. \tag{3.5.23}$$

These types of convergence will be important in the proof of spontaneous particle creation defined via the adiabatic limit. Crucial will be the fact that despite the strong convergence there is, in general, no convergence in norm of S_ϵ to S_0.

Chapter 4

Overcritical fields and spontaneous particle creation

The goal of this chapter is to find physical processes which show the effect of vacuum decay and spontaneous particle creation exclusively due to an overcritical potential. In section 4.1 we analyze how the structure of the ground (vacuum) state changes in presence of an overcritical potential. In section 4.2 we consider several processes with static as well as suddenly switched on (and off) static overcritical potentials and conclude that they are unsatisfactory for observation of the spontaneous particle creation. The main obstacles are either no particle creation or an intensive additional pair creation due to the strongly time-dependent switching process. Next, in 4.3 we consider properties of general time-dependent scattering processes and show that they also fail to produce stable signatures of particle creation due to overcriticality. Further, in 4.4 we study and successfully define spontaneous particle creation in adiabatic processes, yet they lead to physically questionable pair production as the adiabatic limit is approached. Finally, in 4.5 we consider extension of these ideas to non-adiabatic processes involving overcritical potentials and argue that they are the best candidate for demonstrating the appearance of spontaneous particle creation in physical processes. In the next chapter we will study such processes numerically.

Concluding, we in principle agree with Fierz and Scharf [FS79] that spontaneous pair creation must be defined on the basis of a change in the structure of the (implemented) scattering operator $\hat{S}$ and not solely by diving of an eigenvalue of the static Hamiltonian, for the simple reason that only the former has the ability of describing particle creation processes. Yet we show that both phenomena coincide in the physically relevant situations.

4.1 Vacuum structure in presence of a static potential

As all needed mathematical tools have been prepared, we are ready to attack the key question if overcritical potentials lead to a spontaneous particle production. First, consider

static overcritical potentials. We follow the analysis of Klaus and Scharf in [KS77b].

Consider a one-parameter family of Hamiltonians

$$H_\lambda = H_0 + \lambda V \tag{4.1.1}$$

and assume V is smooth enough so that λV is regular for every $\lambda > 0$ (in the sense defined in section 2.7.2). As we have observed by the examples, the strength of the potential, and hence also its overcriticality, has nothing to do with regularity, as long as the potential stays smooth enough.

Consider projectors $P_\pm(\lambda)$ projecting on the positive and negative spectral subspaces of the corresponding Hamiltonian

$$P_\pm(\lambda) = \frac{1 + \mathrm{sgn}(H_\lambda)}{2}, \qquad P_\pm(\lambda)\mathcal{H} = \mathcal{H}_\pm(\lambda), \tag{4.1.2}$$

which are distinguished by the property that the corresponding vacuum states $\Omega_\lambda \in \mathcal{F}_\lambda$ are ground states of the respective implemented Hamiltonians $\hat{H}_\lambda$. For every projector $P_\pm(\lambda)$ we get a different representation in Fock space $\mathcal{F}_\lambda$, but since any two Hamiltonians differ by a regular potential $H_\lambda - H_{\lambda'} = (\lambda - \lambda')V$, all representations $\mathcal{F}_\lambda$ are unitarily equivalent. So we can consider all operators acting in one Fock space, say in $\mathcal{F}_0$, which we call the free Fock space. This special projector we denote $P^0_\pm \equiv P_\pm(0)$ and the subspaces $\mathcal{H}^0_\pm \equiv \mathcal{H}_\pm(0)$.

For every λ choose an orthonormal basis $\{\phi^\pm_n(\lambda)\}$ in $\mathcal{H}_\pm(\lambda)$. Define the particles as states created from the vacuum by the creation operators

$$\hat{b}^*_n(\lambda) = \hat{b}^*(P_+(\lambda)\phi^+_n(\lambda)) \quad \text{and} \quad \hat{d}^*_n(\lambda) = \hat{d}^*(P_-(\lambda)\phi^-_n(\lambda)) \tag{4.1.3}$$

and denote for simplicity the free particles and antiparticles by

$$\hat{b}^*_n \equiv \hat{b}^*_n(0) \quad \text{and} \quad \hat{d}^*_n \equiv \hat{d}^*_n(0). \tag{4.1.4}$$

4.1.1 The charged vacuum

Let us now study the structure of the vacuum as the parameter λ grows from zero. It can be shown that for potentials V_λ, which are H_0–bounded (see theorem 9),

$$||P_\pm(\lambda) - P^0_\pm|| < 1 \tag{4.1.5}$$

for small λ. Therefore, no vector $f \in \mathcal{H}$ exists, which belongs to $\mathcal{R}_+(\lambda) \equiv \mathcal{H}^0_+ \cap \mathcal{H}_-(\lambda)$ or $\mathcal{R}_-(\lambda) \equiv \mathcal{H}^0_- \cap \mathcal{H}_+(\lambda)$ (cf. theorem 3), hence $n_\pm \equiv \dim \mathcal{R}_\pm(\lambda) = 0$.

We can calculate the charge of the vacuum Ω_λ, which is a vector in $\mathcal{F}_0$, with respect to the charge operator $\hat{Q}_0$ corresponding to free particles

$$(\Omega_\lambda, \hat{Q}_0\, \Omega_\lambda) = \left(\hat{U}(\lambda)\, \Omega_0, \hat{Q}_0\, \hat{U}(\lambda)\, \Omega_0\right), \tag{4.1.6}$$

where the unitary operator $\hat{U}(\lambda) : \mathcal{F}_0 \to \mathcal{F}_0$ implements the Bogoliubov transformation between the fields corresponding to $P^0_\pm$ and $P_\pm(\lambda)$. Making use of theorem 3 we find

$$\hat{U}(\lambda)\,\Omega_0 = C_0(\lambda)\,\exp\left(\sum_{k,l=1}^{\infty} A(\lambda)_{kl}\hat{b}^*_k\hat{d}^*_l\right)\Omega_0 \tag{4.1.7}$$

with $\hat{U}_0(\lambda) = 1$ and $C_0(\lambda)$ guaranteeing proper normalization. Then

$$\begin{aligned} Q_{vac} &= (\Omega_\lambda, \hat{Q}_0\,\Omega_\lambda) \\ &= \left(C_0(\lambda)\,\exp\left[\sum_{k,l=1}^{\infty} A(\lambda)_{kl}\hat{b}^*_k\hat{d}^*_l\right]\Omega_0, \hat{Q}_0\,C_0(\lambda)\,\exp\left[\sum_{k,l=1}^{\infty} A(\lambda)_{kl}\hat{b}^*_k\hat{d}^*_l\right]\Omega_0\right) \\ &= 0, \end{aligned} \tag{4.1.8}$$

because, as can be observed easily, all particles and antiparticles are created by $\hat{U}(\lambda)$ from Ω_0 in pairs, so that the vector Ω_λ decomposed in $\mathcal{F}_0$ has non-vanishing coefficients only in subspaces $\mathcal{F}^{(n,m)}$, where $n = m$. Therefore, it is neutral.

The situation changes, if we consider bigger λ and hence stronger potentials λV, exactly at the value of λ, call it λ_1, where the wave function $\varphi_1(\lambda)$ of the lowest lying bound state of H_λ moves from $\mathcal{H}_+(\lambda)$ to $\mathcal{H}_-(\lambda)$ and its energy crosses the borderline between the two spectral subspaces, which we have chosen in (4.1.2) at $E = 0$ *(weak overcriticality)*. Let P_1 be a projection on the state $\varphi_1(\lambda)$. Then, when λ crosses the value λ_1 the projectors change discontinuously

$$P_+(\lambda_1^+) = P_+(\lambda_1^-) - P_1 \tag{4.1.9}$$

$$P_-(\lambda_1^+) = P_-(\lambda_1^-) + P_1, \tag{4.1.10}$$

where we have introduced a shorthand notation $\lambda_1^\pm$ for the limits $\lim_{\epsilon\to 0} ...(\lambda_1 \pm \epsilon)$, which should be taken of the whole expression containing $\lambda_1^\pm$. At the same time, the subspace $\mathcal{R}_+(\lambda_1^+)$ becomes nontrivial (see [KS77b, Appendix] for proof) and its dimension changes to $n_+ = \dim(P_1\mathcal{H}) = 1$ (assuming the state $\varphi_1(\lambda_1)$ is not energetically degenerate), while $n_- = 0$ remains unchanged. As a consequence, the vacuum transformation (4.1.7) changes qualitatively, because $\hat{U}_0(\lambda)$ becomes nontrivial ($\neq 1$). Since $n_+ = 1$ the sum in the exponent starts from $k = 2$. Because $n_- + n_+$ changes parity (from even to odd), it implies further changes in $\hat{U}(\lambda)$, namely operators B, C and D in theorem 3 change sign. This has the consequence that commutation of all creation operators except $\hat{b}^*_1$ with the exponential terms leads to an additional "-", which cancels with the one appearing in commutation with the new $\hat{U}_0(\lambda_1^+)$. But the last change has no consequences, when $\hat{U}(\lambda_1^+)$ acts on the vacuum vector Ω_0

$$\Omega_{\lambda_1^+} = \hat{U}(\lambda_1^+)\,\Omega_0 = C_0(\lambda_1^+)\,\hat{U}_0(\lambda_1^+)\,\exp\left(\sum_{\substack{k=2\\l=1}}^{\infty} A(\lambda_1^+)_{kl}\hat{b}^*_k\hat{d}^*_l\right)\Omega_0 \tag{4.1.11}$$

with

$$\hat{U}_0(\lambda_1^+) = \hat{b}_1^* + \hat{b}_1, \tag{4.1.12}$$

what reduces to $\hat{U}_0(\lambda_1^+) = \hat{b}_1^*$ when acting on the vacuum Ω_0 (operator $\hat{U}_0(\lambda_1^+)$ commutes with the exponent). The new, (weakly) overcritical vacuum is then positively charged

$$\begin{aligned} Q_{vac} &= (\Omega_{\lambda_1^+}, \hat{Q}_0\, \Omega_{\lambda_1^+}) \\ &= \left(C_0(\lambda_1^+)\, \hat{b}_1^* \exp\left[\sum_{\substack{k=2 \\ l=1}}^{\infty} A(\lambda_1^+)_{kl} \hat{b}_k^* \hat{d}_l^* \right] \Omega_0, \hat{Q}_0\, C_0(\lambda_1^+)\, \hat{b}_1^* \exp\left[\sum_{\substack{k=2 \\ l=1}}^{\infty} A(\lambda_1^+)_{kl} \hat{b}_k^* \hat{d}_l^* \right] \Omega_0 \right) \\ &= 1. \end{aligned} \tag{4.1.13}$$

On the other hand, the subcritical neutral vacuum $\Omega_{\lambda_1^-}$ does not go over into the overcritical charged vacuum $\Omega_{\lambda_1^+}$, even when the operator A could be made arbitrary small (e.g. in adiabatic evolution). It can be shown [KS77b, sec. 3] that

$$\begin{aligned} \Omega_{\lambda_1^-} = \; & C_0(\lambda_1^-)\, C_0^{-1}(\lambda_1^+) \left(1 + \sum_{l=1}^{\infty} A(\lambda_1^-) \hat{b}_1^* \hat{d}_l^* \right) \\ & \exp\left(\sum_{\substack{k=2 \\ l=1}}^{\infty} \left[A(\lambda_1^-)_{kl} - A(\lambda_1^+)_{kl} \right] \hat{b}_k^* \hat{d}_l^* \right) \hat{d}_1^*(\lambda_1^+)\, \Omega_{\lambda_1^+}, \end{aligned} \tag{4.1.14}$$

therefore, apart from particle-antiparticle pairs, one additional antiparticle is created. This antiparticle is defined with respect to the projector $P_-(\lambda_1^+)$ corresponding to $H_{\lambda_1^+}$. A similar relation holds between the overcritical and free vacua

$$\Omega_0 = C_0^{-1}(\lambda_1^+) \exp\left(- \sum_{\substack{k=2 \\ l=1}}^{\infty} A(\lambda_1^+)_{kl} \hat{b}_k^* \hat{d}_l^* \right) \hat{d}_1^*(\lambda_1^+)\, \Omega_{\lambda_1^+}, \tag{4.1.15}$$

where again, beside particle-antiparticle pairs, one antiparticle is created. Therefore, the charge (of the free vacuum)

$$q(\lambda) \equiv (\Omega_0, \hat{Q}_\lambda\, \Omega_0) \tag{4.1.16}$$

with respect to H_λ (i.e. in presence of the potential λV) changes from $q(0) = q(\lambda_1^-) = 0$ to

$$q(\lambda_1^+) = (\Omega_0, \hat{Q}_{\lambda_1^+}\, \Omega_0) = -1, \tag{4.1.17}$$

i.e. it has jump at $\lambda = \lambda_1$. This means that one antiparticle is created. It remains to clarify, to which wave function $\psi \in \mathcal{H}$ the antiparticle creation operator $\hat{d}_1^*(\lambda_1^+)$ corresponds. It must belong to $\mathcal{H}_+^0 \cap \mathcal{H}_-(\lambda_1^+)$, so it must satisfy

$$P_+^0 \psi = \psi \quad \text{and} \quad P_-(\lambda_1^+)\psi = \psi. \tag{4.1.18}$$

Therefore it cannot be equal to the diving bound state φ_1, because the latter can be decomposed

$$\varphi_1 = P_-^0\varphi_1 + P_+^0\varphi_1 \tag{4.1.19}$$

and, in general, both its components are non-zero, so it would violate the first condition in (4.1.18). Assuming ψ has the form $\psi = \varphi_1 + \chi$, where χ is orthogonal to φ_1

$$P_1\chi = 0, \tag{4.1.20}$$

it follows from the second condition in (4.1.18)

$$P_-(\lambda_1^+)(\varphi_1 + \chi) = \varphi_1 + P_-(\lambda_1^+)\chi \stackrel{!}{=} \psi = \varphi_1 + \chi, \tag{4.1.21}$$

and hence

$$P_-(\lambda_1^+)\chi = \chi. \tag{4.1.22}$$

From (4.1.20) and (4.1.22) we see that

$$\chi = [P_-(\lambda_1^+) - P_1]\chi = P_-(\lambda_1^-)\chi, \tag{4.1.23}$$

that is, it lies in the negative spectral subspace of $H_{\lambda_1^+}$ orthogonal to the dived bound state, which is nothing else than the negative continuum. Summarizing, the created antiparticle $\hat{d}_1^*(\lambda_1^+)$ corresponds to a wave function, which consists partially of the wave function of the dived bound state and partially lies in the negative continuum of $H_{\lambda_1^+}$.

Now, we show that for $\lambda > \lambda_1$ when no more vectors change the subspace between λ_1^+ and λ, there always exists a vector $\psi \in \mathcal{R}_+(\lambda) = \mathcal{H}_+^0 \cap \mathcal{H}_-(\lambda)$.

Lemma 3 *When for some* $\lambda > \lambda_1$

$$||P_\pm(\lambda_1^-) - P_\pm^0|| < 1 \quad \textit{and} \quad ||P_\pm(\lambda) - P_\pm(\lambda_1^+)|| < 1 \tag{4.1.24}$$

and at $\lambda = \lambda_1$ *relations (4.1.9)-(4.1.10) hold then there exists a vector* $\psi \in \mathcal{R}_+(\lambda) = \mathcal{H}_+^0 \cap \mathcal{H}_-(\lambda)$.

Proof: From $||P_\pm(\lambda_1^-) - P_\pm^0|| < 1$ follows that there is no vector in $P_\pm(\lambda_1^-)\mathcal{H} \cap P_\mp^0\mathcal{H}$, hence $\ker(P_\pm(\lambda_1^-)P_\pm^0) = \emptyset$ and $\operatorname{ind}(P_+(\lambda_1^-)P_+^0) = 0$. Analogously, $\operatorname{ind}(P_+(\lambda)P_+(\lambda_1^+)) = 0$. On the other hand, we have $\operatorname{ind}(P_+(\lambda_1^+)P_+(\lambda_1^-)) = 1$. Then, according to corollary 2

$$\begin{aligned}
\operatorname{ind}(P_+(\lambda)P_+^0) &= -\operatorname{Tr}(P_+(\lambda) - P_+^0) \\
&= -\operatorname{Tr}(P_+(\lambda) - P_+(\lambda_1^+)) - \operatorname{Tr}(P_+(\lambda_1^+) - P_+(\lambda_1^-)) - \operatorname{Tr}(P_+(\lambda_1^-) - P_+^0) \\
&= \operatorname{ind}(P_+(\lambda)P_+(\lambda_1^+)) + \operatorname{ind}(P_+(\lambda_1^+)P_+(\lambda_1^-)) + \operatorname{ind}(P_+(\lambda_1^-)P_+^0) \\
&= 0 + 1 + 0 = 1.
\end{aligned} \tag{4.1.25}$$

So, $\dim\ker(P_+(\lambda)P_+(\lambda_1^+)) \geq 1$ and hence there exists $\psi \in \mathcal{R}_+(\lambda) = \mathcal{H}_+^0 \cap \mathcal{H}_-(\lambda)$. □

We conclude that going over from a free or subcritical Hamiltonian H_λ with $\lambda < \lambda_1$ to an overcritical one with $\lambda > \lambda_1$ one new (i.e. defined with respect to the overcritical projection $P_-(\lambda_1^+)$) antiparticle appears

$$\boxed{q(\lambda) = (\Omega_0, \hat{Q}_\lambda\, \Omega_0) = -1, \qquad \lambda > \lambda_1}\,, \tag{4.1.26}$$

while the corresponding (new) vacuum state becomes positively charged

$$\boxed{Q_{vac} = (\Omega_\lambda, \hat{Q}_0\, \Omega_\lambda) = 1, \qquad \lambda > \lambda_1}\,. \tag{4.1.27}$$

There remains a question regarding the physical conditions under which the above calculated results can be measured. Specifying, first, what are the real particles which will be seen in the measurement, and second, what will be the time evolution of such a process where the Hamiltonian varies between two values? To answer the first question precisely, one should deeply analyze the measurement process: write the function or interaction of a detector installed in the experiment in terms of the field operators, find the eigenstates of the interaction Hamiltonian and argue (as is usually done in the studies of decoherence and entanglement processes) that these states will be observed in the experiment. We adopt a simplified point of view and assume that those particles are real and show up in the measurement which correspond to the (generalized) eigenstates of a current full Hamiltonian. The answer to the second question is essential for the problem of overcritical particle creation. From the "static" point of view, which concerns only properties of different Hamiltonians, but ignores the time evolution leading from one to the other, it seems that already the *weak overcriticality* with at least one bound state $E_0 < 0$ should lead to spontaneous antiparticle creation (what is claimed in [KS77b]). But, as will be shown in the remaining sections of this chapter, this phenomenon is physically irrelevant and only the *strong overcriticality*, with at least one bound state dived into the negative continuum, leads to physically relevant particle creation.

4.1.2 Vacuum polarization

By means of the vacuum polarization and the total charge of the vacuum Q_{vac} introduced in section 2.5.2 we can confirm the results (4.1.26)-(4.1.27) from the previous section 4.1.1 in another way. From (2.5.14) and (2.5.18) we know that

$$Q^\lambda_{vac} = \int d^3x\; \rho^\lambda(\mathbf{x}) = \mathrm{Tr}\left[P_+(\lambda) - P^0_+\right], \tag{4.1.28}$$

where $P_\pm(\lambda), P^0_\pm$ are projections on the spectral subspaces of the corresponding Hamiltonians H_λ, H_0 and are defined by

$$P_-(\lambda) \equiv P_{(-\infty,E_0]}(H_\lambda), \qquad P_+(\lambda) \equiv P_{(E_0,+\infty)}(H_\lambda), \qquad P^0_\pm \equiv P_\pm(0). \tag{4.1.29}$$

The operator $P_+(\lambda) - P^0_+$ was studied in [KS77b] and it was shown that every time an eigenvalue crosses the value E_0 as λ grows the charge of the vacuum Q_{vac} changes by one.

The same has been proved rigorously in [Hai04], including a renormalization method, because $P_+(\lambda) - P_+^0$ is, in general, not a trace-class operator. (We know that it is Hilbert-Schmidt for all regular potentials, i.e. for those which guarantee unitary equivalence of the representations based on $P_\pm(\lambda)$ and $P_\pm^0$, cf. theorem 2). Both results can be stated as

$$\begin{aligned} Q_{vac}^\lambda = N(\lambda) \equiv & (\text{number of eigenvalues of } H_{\lambda'} \text{ which crossed } E_0 \text{ from above}) \\ & -(\text{number of eigenvalues of } H_{\lambda'} \text{ which crossed } E_0 \text{ from below}) \\ & \text{as } \lambda' \text{ increased from 0 to } \lambda. \end{aligned} \tag{4.1.30}$$

The only difference between the authors concerns the choice of the critical value E_0, by crossing of which a particle state becomes an antiparticle state and vice versa. As we have already remarked at the end of the previous section 4.1.1, there is no way to answer the question of the "correct" choice of E_0 on that level, as long as all representations based on various $P_\pm(\lambda)$ defined like in (4.1.29) are unitarily equivalent. The answer whether there exist physical processes leading to the observation of the spontaneous particle creation must necessarily treat the change of projectors as a time-dependent process (although discontinuous) and are studied in the next sections of this chapter. At the end of the section 4.4.2 we arrive at the result that (in the case of negative potentials) the choice $E_0 = -1$ (strong overcriticality) is the one which is physically relevant for observation of the charged vacuum with spontaneously created particles scattered to infinity. For all choices of E_0 in the interval $(-1, +1)$ (weak overcriticality) there appears a formally charged vacuum, but it is accompanied by a bound antiparticle, ensuring overall neutrality. It should be possible to observe this phenomenon by calculating the total charge of the vacuum and the particles

$$Q_{tot} \equiv Q_{vac}^\lambda + q(\lambda) = (\Omega_\lambda, \hat{Q}_0\, \Omega_\lambda) + (\Omega_0, \hat{Q}_\lambda\, \Omega_0) = 0 \tag{4.1.31}$$

restricted to some finite region, say a ball with radius R, and taking the limit $t \to \infty$. The result in the (weakly or strongly) overcritical case should have the form

$$Q_{tot}(R,t) \equiv Q_{vac}^\lambda(R) + q(\lambda, R, t) = 1 - ||\psi(t)||_R^2, \tag{4.1.32}$$

where $||\psi(t)||_R^2$ is the norm of the spontaneously created antiparticle state restricted to the ball of radius R. In the limit $t \to \infty$ we expect a different behaviour for the bound state in the weakly overcritical case ($E_0 \in (-1, +1)$) and in the strongly overcritical case ($E_0 = -1$)

$$\lim_{t\to\infty} ||\psi(t)||_R^2 = \begin{cases} 1 - \mathcal{O}(R^{-\alpha}), \quad \alpha > 0, & \text{for weak overcriticality,} \\ 0 \quad \forall R > 0, & \text{for strong overcriticality,} \end{cases} \tag{4.1.33}$$

therefore leading to the total charge in every finite region after a long time

$$Q_{tot}(R) \equiv \lim_{t\to\infty} Q_{tot}(R,t) = \begin{cases} \mathcal{O}(R^{-\alpha}), \quad \alpha > 0, & \text{for weak overcriticality,} \\ 1 \quad \forall R > 0, & \text{for strong overcriticality.} \end{cases} \tag{4.1.34}$$

4.2 Quasi-static potentials

4.2.1 Evolution in a constant potential

Consider a static $H(t) = H_\lambda$ for all t. Then the evolution in $\mathcal{H}$ is described by $U_\lambda(t_2, t_1) = \exp(iH_\lambda(t_2 - t_1))$. Creation of particles from vacuum can be measured with

$$U_{\pm\mp} = P_\pm(\lambda)\, U_\lambda(-T, T)\, P_\mp(\lambda), \tag{4.2.1}$$

which in this case is zero, because $P_\pm(\lambda)$ commute with the Hamiltonian H_λ and its exponent

$$P_\pm(\lambda)\, U_\lambda(-T, T)\, P_\mp(\lambda) = U_\lambda(-T, T)\, P_\pm(\lambda)\, P_\mp(\lambda) = 0. \tag{4.2.2}$$

Hence, using (2.6.36) and (2.6.14) we obtain

$$\Delta N = ||U_{-+}||^2_{HS} + ||U_{+-}||^2_{HS} = 0, \qquad \Delta Q = ||U_{+-}||^2_{HS} - ||U_{-+}||^2_{HS} = 0, \tag{4.2.3}$$

what shows that no particle production is possible in such processes, independently on the fact if H_λ is overcritical or not.

4.2.2 Scattering in a constant potential

Scattering in a "constant potential" is defined by (3.5.10)

$$S_\lambda = \operatorname*{s-lim}_{\substack{t_1\to-\infty \\ t_2\to+\infty}} e^{iH_0 t_2} e^{-iH_\lambda(t_2-t_1)} e^{-iH_0 t_1} \tag{4.2.4}$$

and corresponds in fact to a scattering on a potential switched on and off at infinity ($t \to \pm\infty$) with keeping asymptotic definition of free particles with respect to H_0 (see next section 4.2.3). Assume that S_λ given above exists (see section 3.5.1 for conditions). Then $P^0_\pm\, S_\lambda\, P^0_\mp$ exist as well. It turns out that S_λ commutes with H_0 ([Tha92, Th. 8.3] or [RS79, XI.3]) and hence with $P^0_\pm$. Therefore,

$$(S_\lambda)_{\pm\mp} \equiv P^0_\pm\, S_\lambda\, P^0_\mp = 0, \tag{4.2.5}$$

what guarantees that $(S_\lambda)_{\pm\mp}$ are Hilbert-Schmidt and the operator S_λ is implementable by a unitary $\hat{S}_\lambda$ in $\mathcal{F}_0$. Unfortunately it implies also

$$\Delta N = ||S_{-+}||^2_{HS} + ||S_{+-}||^2_{HS} = 0, \qquad \Delta Q = ||S_{+-}||^2_{HS} - ||S_{-+}||^2_{HS} = 0, \tag{4.2.6}$$

i.e. no particle creation at all.

No particle creation in static external fields

In more detail, the corresponding Bogoliubov transformation between the *in* and *out* particles does not mix the particle and antiparticle creation or annihilation operators, i.e.

$$\hat{b}'(P^0_+ f) = \hat{b}(P^0_+ S^*_\lambda P^0_+ f) + \hat{d}^*(P^0_- S^*_\lambda P^0_+ f) = \hat{b}(S^*_\lambda P^0_+ P^0_+ f) + \hat{d}^*(S^*_\lambda \underbrace{P^0_- P^0_+}_{=0} S^*_\lambda f) = \hat{b}(S^*_\lambda P^0_+ f) \tag{4.2.7}$$

$$\hat{d}^{*\prime}(P^0_- f) = \hat{b}(P^0_+ S^*_\lambda P^0_- f) + \hat{d}^*(P^0_- S^*_\lambda P^0_- f) = \hat{b}(S^*_\lambda \underbrace{P^0_+ P^0_-}_{=0} f) + \hat{d}^*(S^*_\lambda P^0_- P^0_- S^*_\lambda f). = \hat{d}^*(S^*_\lambda P^0_- f) \tag{4.2.8}$$

Therefore, as the theorem of Bongaarts states ([Bon70] or [Tha92, Th. 10.10]), no particles are created in such a scattering process

$$\begin{aligned}(\Omega_0, \hat{N}'\Omega_0) &= \left(\Omega_0, \sum_n \left[\hat{b}^{*\prime}(P^0_+ f_n)\hat{b}'(P^0_+ f_n) + \hat{d}^{*\prime}(P^0_- f_n)\hat{d}'(P^0_- f_n)\right]\Omega_0\right) \\ &= \left(\Omega_0, \sum_n \left[\hat{b}^*(P^0_+ S^*_\lambda f_n)\hat{b}(P^0_+ S^*_\lambda f_n) + \hat{d}^*(P^0_- S^*_\lambda f_n)\hat{d}(P^0_- S^*_\lambda f_n)\right]\Omega_0\right) \\ &= 0.\end{aligned} \tag{4.2.9}$$

The above theorem is quite strong – it of course requires implementability of S_λ, but this is guaranteed once the classical scattering operator S_λ exists. It is a bit surprising, because there are some known examples of the static fields, which are expected to produce particles, although there do not exist rigourous proofs. We consider the most known two: the Klein's paradox and the Schwinger effect.

Klein's paradox

For simplicity, consider a one- instead of 3-dimensional physical space, what does not change the nature of the problem, and a potential

$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ U & \text{for} \quad x > a \\ \text{monotonically growing} & \text{for} \quad 0 \le x \le a, \end{cases} \tag{4.2.10}$$

with $U > 0$. As one can find already on the classical level, there exists a current D, if $U > 2$ ($U > 2mc^2$ in physical units), that is when there exists an energetic gap such that solutions with energies in the gap behave as electrons for $x \to -\infty$ and as positrons as $x \to +\infty$. In the linear case $V(x) = vx$ for $0 \le x \le a$ the current is $D \sim \exp(-C/v)$ with some $C > 0$ [Sau31, Szc32]. In a smooth case, $V(x) \sim \tanh(vx)$, it has a form, which becomes universal for big momenta and behaves again like $D \sim \exp(-C/v) \sim \exp\left(-C/\left.\frac{dV}{dx}\right|_{x=0}\right)$ [Sau32]. This is the reason for expecting, at least intuitively, a flow of particles created in presence of the strong static potential. Yet this problem cannot be solved within the one-particle classical Dirac theory. In order to construct a many-particle

picture of a scattering process in Fock space, the classical scattering operator S must be implemented. Unfortunately, it does not exist in the form (4.2.4) (i.e. the corresponding strong limits do not exist). Bongaarts and Ruijsenaars have studied this problem rigorously [BR76] and have introduced modified wave operators $W_{\pm}$, which allowed to define some modified scattering operator $\widetilde{S}$. Unfortunately, they prove, for $U > 2$ this operator is not implementable by any unitary operator $\hat{S}$ in $\mathcal{F}_0$, therefore, **the scattering process in a potential causing the "Klein paradox" cannot be described in the Fock space of free fields**.

Independently of the fact, whether such a potential is physical or not, the reason for the unsuccessful trial to describe the scattering can be the failure of QED in external fields to handle processes with too high rate of created particles. If particles (or particle-antiparticle pairs) were continuously produced, their number after an infinitely long time, which is needed in the scattering, would be infinite and the Hilbert-Schmidt norms of $S_{\pm\mp}$ would necessarily have to be infinite, causing the scattering operator to be non-implementable in Fock space. Physically, the many created charged particles would modify the external electromagnetic field and surely avoid further creation. Since QED in external fields does not include this backreaction effect, it is not surprising that it leads to mathematical problems and fails to describe the physical situation. At the moment, it seems that the only way to solve this problem rigorously is to adopt QED corrections describing properly the backreaction of the created charges on the electromagnetic field, as it is the case in full QED. This is unfortunately too complicated to be solved in even such a simple static problem.

The Schwinger effect

An analogous problem occurs in the well-known Schwinger effect [Sch51], where the one-dimensional potential has the form

$$V(x) = Ax. \tag{4.2.11}$$

The line of arguments followed in the previous paragraph can be repeated.

4.2.3 Sudden switch on and off of the potential

Consider now processes with a sudden switch on and off of the potential: $H_0 \to H_\lambda \to H_0$, which differ from the scattering in the previous section only by the fact that switching happens at finite times, say $-T, +T$

$$H_\lambda(t) = \begin{cases} H_0 & \text{for} \quad t < -T, \\ H_\lambda & \text{for} \quad -T < t < T, \\ H_0 & \text{for} \quad t > T. \end{cases} \tag{4.2.12}$$

The evolution is solved by means of two unitary propagators

$$U_\lambda(t_2,t_1) = \exp(iH_\lambda(t_2-t_1)), \qquad \text{for} \qquad |t_1|,|t_2| < T \tag{4.2.13}$$

$$U_0(t_2,t_1) = \exp(iH_0(t_2-t_1)), \qquad \text{for} \qquad t_1,t_2 < T \quad \text{or} \quad t_1,t_2 > T. \tag{4.2.14}$$

A full propagator in the interesting case $t_1 < -T$, $t_2 > T$ takes the form

$$U_{\lambda,T}(t_2,t_1) = U_0(t_2,T)\, U_\lambda(T,-T)\, U_0(-T,t_1). \tag{4.2.15}$$

Such processes always create particles and antiparticles, because, in general,

$$[U_{\lambda,T}(t_2,t_1)]_{\pm\mp} = P^0_\pm\, U_{\lambda,T}(t_2,t_1)\, P^0_\mp = U_0(t_2,T)\, P^0_\pm\, U_\lambda(T,-T)\, P^0_\mp\, U_0(-T,t_1) \neq 0 \tag{4.2.16}$$

and

$$\Delta N = |||[U_{\lambda,T}(t_2,t_1)]_{-+}||^2_{HS} + |||[U_{\lambda,T}(t_2,t_1)]_{+-}||^2_{HS} > 0. \tag{4.2.17}$$

Moreover, the particles are always created in pairs, what will be discussed in more generality in section 4.3, so that $|||[U_{\lambda,T}(t_2,t_1)]_{+-}||_{HS} = |||[U_{\lambda,T}(t_2,t_1)]_{-+}||_{HS}$ and hence

$$\Delta Q = |||[U_{\lambda,T}(t_2,t_1)]_{+-}||^2_{HS} - |||[U_{\lambda,T}(t_2,t_1)]_{-+}||^2_{HS} = 0. \tag{4.2.18}$$

In fact, processes relevant for particle production happen only in the period $t \in [-T,T]$, what can be easily seen by calculating the expressions appearing in (4.2.17)

$$\begin{aligned} |||[U_{\lambda,T}(t_2,t_1)]_{\pm\mp}||_{HS} &= ||P^0_\pm\, U_{\lambda,T}(t_2,t_1)\, P^0_\mp||_{HS} \\ &= ||P^0_\pm\, U_0(t_2,T)\, U_\lambda(T,-T)\, U_0(-T,t_1)\, P^0_\mp||_{HS} \\ &= ||U_0(t_2,T)\, P^0_\pm\, U_\lambda(T,-T)\, P^0_\mp\, U_0(-T,t_1)||_{HS} \\ &= ||P^0_\pm\, U_\lambda(T,-T)\, P^0_\mp||_{HS} \end{aligned} \tag{4.2.19}$$

and observing that they do not depend on t_1, t_2 (as long as $t_1 < -T$, $t_2 > T$).

It can be shown that the limits $t_1 \to -\infty$ and $t_2 \to \infty$ of $U_{\lambda,T}(t_2,t_1)$ do not exist, because of complex phases of the type $\exp(\pm iEt_k)$, attached to the vectors, which do not converge (actually, the strong limit does not exist, the weak limit is zero). To be able to consider processes extending to infinitely long times one has to go over from the evolution to the scattering operator

$$\begin{aligned} S_{\lambda,T} &\equiv \underset{\substack{t_1\to-\infty \\ t_2\to+\infty}}{\text{s-lim}}\, U_0(0,t_2)\, U_{\lambda,T}(t_2,t_1)\, U_0(t_1,0) \\ &= \underset{\substack{t_1\to-\infty \\ t_2\to+\infty}}{\text{s-lim}}\, U_0(0,t_2)\, U_0(t_2,T)\, U_\lambda(T,-T)\, U_0(-T,t_1)\, U_0(t_1,0) \\ &= U_0(0,T)\, U_\lambda(T,-T)\, U_0(-T,0). \end{aligned} \tag{4.2.20}$$

Again, particle creation during the whole scattering is identical to that one of the evolution

in $t \in [-T, T]$

$$\begin{aligned} |||[S_{\lambda,T}]_{\pm\mp}||_{HS} &= ||P^0_{\pm}\ S_{\lambda,T}\ P^0_{\mp}||_{HS} \\ &= ||P^0_{\pm}\ U_0(0,T)\ U_\lambda(T,-T)\ U_0(-T,0)\ P^0_{\mp}||_{HS} \\ &= ||U_0(0,T)\ P^0_{\pm}\ U_\lambda(T,-T)\ P^0_{\mp}\ U_0(-T,0)||_{HS} \\ &= ||P^0_{\pm}\ U_\lambda(T,-T)\ P^0_{\mp}||_{HS}, \end{aligned} \tag{4.2.21}$$

and hence

$$|||[S_{\lambda,T}]_{\pm\mp}||_{HS} = |||[U_{\lambda,T}(t_2,t_1)]_{\pm\mp}||_{HS}, \tag{4.2.22}$$

what implies

$$\Delta Q_{\lambda,T} = |||[S_{\lambda,T}]_{+-}||^2_{HS} - |||[S_{\lambda,T}]_{-+}||^2_{HS} = 0. \tag{4.2.23}$$

$$\Delta N_{\lambda,T} = |||[S_{\lambda,T}]_{-+}||^2_{HS} + |||[S_{\lambda,T}]_{+-}||^2_{HS} > 0. \tag{4.2.24}$$

From (4.2.20) and (4.2.4) it is straightforward to observe that

$$S_\lambda = \underset{T\to\infty}{\text{s-lim}}\, S_{\lambda,T} \equiv S_{\lambda,\infty}, \tag{4.2.25}$$

i.e. the so-called "scattering on a constant potential" is just scattering on a potential switched on and off at infinity ($t \to \pm\infty$).

The particle and charge production for $S_{\lambda,\infty}$ was trivial

$$\Delta N_{\lambda,\infty} = 0, \qquad \Delta Q_{\lambda,\infty} = 0. \tag{4.2.26}$$

The limit $T \to \infty$ in (4.2.23) is straightforward and gives immediately (4.2.26). To show that $\Delta N_{\lambda,T} \to \Delta N_{\lambda,\infty} = 0$ as $T \to \infty$ in (4.2.24) we need some calculation.

Theorem 13

$$\lim_{T\to\infty} \Delta N_{\lambda,T} = \lim_{T\to\infty} |||[S_{\lambda,T}]_{-+}||^2_{HS} + |||[S_{\lambda,T}]_{+-}||^2_{HS} = 0. \tag{4.2.27}$$

Proof:
By virtue of (4.2.22) it is enough to show that

$$\lim_{T\to\infty} |||[U_{\lambda,T}(t_2,t_1)]_{\pm\mp}||^2_{HS} = 0. \tag{4.2.28}$$

Using a basis $\{f_E\}$ of generalized eigenfunctions of H_λ and writing $T = t_2 - t_1$ we have (all integrals below are calculated over the spectrum of H_λ with a corresponding spectral

measure $d\mu(E)$ what we omit for simplicity)

$$
\begin{aligned}
&||[U_{\lambda,T}(t_2,t_1)]_{-+}||^2_{HS} = ||P^0_- U_{\lambda,T}(t_2,t_1)P^0_+||^2_{HS} \\
&= \int dE\ dE'\ |(f_{E'}, P^0_- U_{\lambda,T}(t_2,t_1)P^0_+ f_E)|^2 \\
&= \int dE\ dE'\ \left| \int dE''\ (f_{E'}, P^0_- U_{\lambda,T}(t_2,t_1) f_{E''})(f_{E''}, P^0_+ f_E) \right|^2 \\
&= \int dE\ dE'\ \left| \int dE''\ \left(f_{E'}, P^0_- e^{-iE''T} f_{E''}\right)(f_{E''}, P^0_+ f_E) \right|^2 \\
&= \int dE\ dE'\ \int dE'''\ \overline{e^{-iE'''T}(f_{E'}, P^0_- f_{E'''})(f_{E'''}, P^0_+ f_E)} \\
&\qquad\qquad \cdot \int dE''\ e^{-iE''T}(f_{E'}, P^0_- f_{E''})(f_{E''}, P^0_+ f_E) \\
&= \int dE\ dE'\ dE''\ dE'''\ e^{-i(E''-E''')T}(P^0_- f_{E'''}, f_{E'})(P^0_+ f_E, f_{E'''})(f_{E'}, P^0_- f_{E''})(f_{E''}, P^0_+ f_E) \\
&= \int dE\ dE'\ dE''\ dE'''\ e^{-i(E''-E''')T}(P^0_+ f_{E''}, f_E)(f_E, P^0_+ f_{E'''})(P^0_- f_{E'''}, f_{E'})(f_{E'}, P^0_- f_{E''}) \\
&= \int dE''\ dE'''\ e^{-i(E''-E''')T}(P^0_+ f_{E''}, P^0_+ f_{E'''})(P^0_- f_{E'''}, P^0_- f_{E''}) \\
&= \int dE\ dE'\ e^{-i(E-E')T}(P^0_+ f_E, f_{E'})(f_{E'}, P^0_- f_E) \\
&\equiv \int dE\ dE'\ e^{-i(E-E')T} F(E,E') \equiv \widetilde{F}(T,-T) \equiv G(T),
\end{aligned}
\tag{4.2.29}
$$

what shows that the estimated function $G(T)$ can be written as a (generalized) Fourier transform $\widetilde{F}(T,-T)$ of some function $F(E,E')$. We prove that $G(T) \to 0$ as $T \to \infty$ by showing that $\widetilde{F} \in \mathcal{C}_\infty(\mathbb{R}^2)$, i.e. a smooth function vanishing at infinity. It is the case when $F \in L^1(\mathbb{R}^2)$ [RS75, Th. IX.7]. So we must only show that the following integral is finite

$$
\begin{aligned}
\int dE\ dE'\ |f(E,E')| &= \int dE\ dE'\ |(P^0_+ f_E, f_{E'})(f_{E'}, P^0_- f_E)| \\
&= \int_{f_E \in \mathcal{H}_-} dE \int_{f_{E'} \in \mathcal{H}_-} dE'\ |(P^0_+ P_- f_E, P_- f_{E'})(P_- f_{E'}, P^0_- P_- f_E)| \\
&+ \int_{f_E \in \mathcal{H}_-} dE \int_{f_{E'} \in \mathcal{H}_+} dE'\ |(P^0_+ P_- f_E, P_+ f_{E'})(P_+ f_{E'}, P^0_- P_- f_E)| \\
&+ \int_{f_E \in \mathcal{H}_+} dE \int_{f_{E'} \in \mathcal{H}_-} dE'\ |(P^0_+ P_+ f_E, P_- f_{E'})(P_- f_{E'}, P^0_- P_+ f_E)| \\
&+ \int_{f_E \in \mathcal{H}_+} dE \int_{f_{E'} \in \mathcal{H}_+} dE'\ |(P^0_+ P_+ f_E, P_+ f_{E'})(P_+ f_{E'}, P^0_- P_+ f_E)|.
\end{aligned}
\tag{4.2.30}
$$

We use the following estimates for the first

$$\begin{aligned}
&|(P_+^0 P_- f_E, P_- f_{E'})(P_- f_{E'}, \underbrace{P_-^0}_{1-P_+^0} P_- f_E)| \\
&= |(P_+^0 P_- f_E, P_- f_{E'})(P_- f_{E'}, P_- f_E) - (P_+^0 P_- f_E, P_- f_{E'})(P_- f_{E'}, P_+^0 P_- f_E)| \\
&\leq |(P_+^0 P_- f_E, P_- f_{E'})|\delta(E-E') + |(P_- f_{E'}, P_+^0 P_- f_E)|^2
\end{aligned} \tag{4.2.31}$$

and for the second term

$$\begin{aligned}
&|(P_+^0 P_- f_E, P_+ f_{E'})(P_+ f_{E'}, \underbrace{P_-^0}_{1-P_+^0} P_- f_E)| \\
&= |(P_+^0 P_- f_E, P_+ f_{E'}) \underbrace{(P_+ f_{E'}, P_- f_E)}_{0} - (P_+^0 P_- f_E, P_+ f_{E'})(P_+ f_{E'}, P_+^0 P_- f_E)| \\
&= |(P_+ f_{E'}, P_+^0 P_- f_E)|^2.
\end{aligned} \tag{4.2.32}$$

The third and fourth terms are transformed analogously using the substitution $P_+^0 = 1 - P_-^0$ instead. We obtain

$$\begin{aligned}
&\int dE\ dE'\ |f(E,E')| \\
&\quad \leq \int_{f_E \in \mathcal{H}_-} dE \int_{f_{E'} \in \mathcal{H}_-} dE' \ \left[|(P_+^0 P_- f_E, P_- f_{E'})|\delta(E-E') + |(P_- f_{E'}, P_+^0 P_- f_E)|^2\right] \\
&\quad + \int_{f_E \in \mathcal{H}_-} dE \int_{f_{E'} \in \mathcal{H}_+} dE' \ |(P_+ f_{E'}, P_+^0 P_- f_E)|^2 \\
&\quad + \int_{f_E \in \mathcal{H}_+} dE \int_{f_{E'} \in \mathcal{H}_-} dE' \ |(P_- f_{E'}, P_-^0 P_+ f_E)|^2 \\
&\quad + \int_{f_E \in \mathcal{H}_+} dE \int_{f_{E'} \in \mathcal{H}_+} dE' \ \left[|(P_-^0 P_+ f_E, P_+ f_{E'})|\delta(E-E') + |(P_+ f_{E'}, P_-^0 P_+ f_E)|^2\right] \\
&\leq \int_{f_E \in \mathcal{H}_-} dE\ |(P_+^0 P_- f_E, P_+^0 P_- f_E)| + \int_{f_E \in \mathcal{H}_-} dE \int_{f_{E'} \in \mathcal{H}_-} dE' \ |(f_{E'}, P_- P_+^0 P_- f_E)|^2 \\
&+ \int_{f_E \in \mathcal{H}_-} dE \int_{f_{E'} \in \mathcal{H}_+} dE' \ |(f_{E'}, P_+^0 P_- f_E)|^2 \\
&+ \int_{f_E \in \mathcal{H}_+} dE \int_{f_{E'} \in \mathcal{H}_-} dE' \ |(f_{E'}, P_-^0 P_+ f_E)|^2 \\
&+ \int_{f_E \in \mathcal{H}_+} dE\ |(P_-^0 P_+ f_E, P_-^0 P_+ f_E)| + \int_{f_E \in \mathcal{H}_+} dE \int_{f_{E'} \in \mathcal{H}_+} dE' \ |(f_{E'}, P_+ P_-^0 P_+ f_E)|^2 \\
&= ||P_+^0 P_-||_{HS}^2 + ||P_+^0 P_-||_{HS}^2 + ||P_+^0 P_-||_{HS}^2 \\
&+ ||P_-^0 P_+||_{HS}^2 + ||P_-^0 P_+||_{HS}^2 + ||P_-^0 P_+||_{HS}^2 < \infty,
\end{aligned} \tag{4.2.33}$$

because for regular potentials $P_\pm^0 P_\mp$ are Hilbert-Schmidt. □

For answering the question of implementability of $U_{\lambda,T}(t_2, t1)$ or $S_{\lambda,T}$ (equivalent because of (4.2.22)) one cannot use the theorem 8, because necessary conditions are violated

by the discontinuous time variation of the potential's strength (see example below theorem 8 for more details). However, using parts of the proof of the above theorem we can prove the following

Theorem 14 *The above defined unitary operator $S_{\lambda,T}$ is implementable, i.e. $[S_{\lambda,T}]_{\pm\mp}$ are Hilbert-Schmidt.*

Proof:
Using (4.2.22) it is enough to show that $[U_{\lambda,T}(t_2,t_1)]_{\pm\mp}$ are Hilbert-Schmidt (and hence $U_{\lambda,T}(t_2,t_1)$ is implementable. In the proof of theorem 13 we have shown (4.2.29)

$$||[U_{\lambda,T}(t_2,t_1)]_{-+}||^2_{HS} = \int dE\ dE'\ e^{-i(E-E')T} F(E,E'). \tag{4.2.34}$$

So in order to prove finiteness of $||[U_{\lambda,T}(t_2,t_1)]_{-+}||_{HS}$ it is enough to show that

$$\left| \int dE\ dE'\ e^{-i(E-E')T} F(E,E') \right| \leq \int dE\ dE'\ |F(E,E')| = ||F||_1 \tag{4.2.35}$$

is finite. This has been already shown in (4.2.30)-(4.2.33). □

We will come back to this question later studying the example of a spherical potential well in section 6.3.

Spectrum of created particles

At this place we want to introduce the notion of a *spectrum of created (anti-)particles*. It is a distribution, in the scale of energy, of the (anti-)particle creation probability (2.8.20)-(2.8.21)

$$N^+_E = ||P^0_-\ S^*_{\lambda,T}\ P^0_+\ \phi^+_E||^2, \qquad N^-_E = ||P^0_+\ S^*_{\lambda,T}\ P^0_-\ \phi^-_E||^2, \tag{4.2.36}$$

for $\phi^\pm_E \in \mathcal{H}^0_\pm$, where $\{\phi_E\}$ is a basis of (generalized) eigenvectors of H_0. These distributions can be rewritten as

$$\begin{aligned} N^+_E &= \int_\sigma |(\phi_{E'}, P^0_-\ S^*_{\lambda,T}\ P^0_+\ \phi_E)|^2\ d\mu_0(E') = \int_{\sigma_-} |(\phi_{E'}, S^*_{\lambda,T}\ \phi_E)|^2\ dE' \\ &= \int_{\sigma_-} |S^{EE'}_{\lambda,T}|^2 dE' \qquad \text{for } E \in \sigma_+, \\ N^-_E &= \int_{\sigma_+} |S^{EE'}_{\lambda,T}|^2 dE' \qquad \text{for } E \in \sigma_-, \end{aligned} \tag{4.2.37}$$

where $\sigma = \sigma(H_0) = (-\infty,-1] \cup [1,\infty)$, $\sigma_\pm = \sigma(P^0_\pm H_0)$, $d\mu_0(E) = dE$ and $S^{EE'}_{\lambda,T}$ are matrix elements of $S_{\lambda,T}$. For the considered switch on and off processes they can be exactly calculated if we introduce $\{\chi_E\}$ as a basis of (generalized) eigenvectors of H_λ. Then they read

$$S^{EE'}_{\lambda,T} = \int_{\sigma_\lambda} (\phi_E, \chi_{E''}) e^{i(E+E'-2E'')T} (\chi_{E''}, \phi_{E'})\ d\mu_\lambda(E''), \tag{4.2.38}$$

where $\sigma_\lambda = \sigma(H_\lambda) = (-\infty, -1] \cup [1, \infty) \cup \{E_n, n = 1, 2, ...$ (for bound states)$\}$ and $d\mu_\lambda(E)$ is a corresponding spectral measure. Then

$$N_E^- = \int_{\sigma_+} dE' \int_{\sigma_\lambda} d\mu_\lambda(E_1'') \int_{\sigma_\lambda} d\mu_\lambda(E_2'')\, e^{-i(E_1''-E_2'')T} \cdot (\phi_E, \chi_{E_2''})(\chi_{E_2''}, \phi_{E'})(\phi_{E'}, \chi_{E_1''})(\chi_{E_1''}, \phi_E) \quad (4.2.39)$$

We see that if $T = 0$ (what corresponds to a static Hamiltonian H_0 with no jumps) then the complex phase vanishes and the two integrals over $d\mu_\lambda(E_i'')$, $i = 1, 2$ reduce to identity due to completeness of the basis χ_E. Finally, the remaining scalar products $(\phi_E, \phi_{E'})$ give zero, because $\phi_E \in H_-^0$ and $\phi_{E'} \in H_+^0$ are orthogonal. The limit $T \to \infty$ must also give zero, but that is due to cancellation of the fast-varying phases and is not so obvious to see.

4.2.4 Sudden switch on of the potential

The situation which we have analyzed in section 4.1.1 comparing two Hamiltonians H_0 and H_λ with corresponding particle definitions and vacua can be interpreted in terms of a process which proceeds in time. To obtain as a result the set of particles created from vacuum Ω_0, which is described by (4.1.11), we must start the time process from the free Hamiltonian H_0 and initial vacuum state Ω_0, and finish with the (weakly) overcritical Hamiltonian $H_{\lambda_1^+}$. Since the Bogoliubov transformation between the free particles and antiparticles $\hat{b}_k^*, \hat{d}_k^*$ and those at $\lambda = \lambda_1^+$ is nothing else than projections following from the change of projectors $P_\pm^0$ to $P_\pm(\lambda_1^+)$, the corresponding time-dependent process must be a sudden change of the Hamiltonian from H_0 to $H_{\lambda_1^+}$, which otherwise remains constant, i.e.

$$H(t) = \begin{cases} H_0 & \text{for} \quad t < 0 \\ H_{\lambda_1^+} & \text{for} \quad t > 0 \end{cases} \quad (4.2.40)$$

with the whole time-process lasting from some $-T < 0$ to some $T > 0$. As discussed in section 4.1.1, such a process creates particle-antiparticle pairs and one special antiparticle, with respect to the final static Hamiltonian $H_{\lambda_1^+}$. The unitary evolution operator in $\mathcal{H}$ has the form

$$U_T \equiv U(T, -T) = U_{\lambda_1^+}(T, 0)\, U_0(0, -T) \equiv \exp(-iH_{\lambda_1^+}T) \exp(-iH_0T), \qquad T > 0. \quad (4.2.41)$$

The charge creation can be calculated directly

$$\begin{aligned}\Delta Q[U] &= |||[U_T]_{+-}||^2_{HS} - |||[U_T]_{-+}||^2_{HS} \\ &= ||P_+(\lambda_1^+)\, U_T\, P^0_-||^2_{HS} - ||P_-(\lambda_1^+)\, U_T\, P^0_+||^2_{HS} = \\ &= ||P_+(\lambda_1^+)\, e^{-iH_{\lambda_1^+}T} e^{-iH_0T}\, P^0_-||^2_{HS} - ||P_-(\lambda_1^+)\, e^{-iH_{\lambda_1^+}T} e^{-iH_0T}\, P^0_+||^2_{HS} \\ &= ||e^{-iH_{\lambda_1^+}T}\, P_+(\lambda_1^+)\, P^0_-\, e^{-iH_0T}||^2_{HS} - ||e^{-iH_{\lambda_1^+}T}\, P_-(\lambda_1^+)\, P^0_+\, e^{-iH_0T}||^2_{HS} \\ &= ||P_+(\lambda_1^+)\, P^0_-||^2_{HS} - ||P_-(\lambda_1^+)\, P^0_+||^2_{HS} \\ &= -1,\end{aligned} \tag{4.2.42}$$

what agrees with (2.6.13).

If we define the scattering operator by

$$S \equiv \underset{\substack{T_1\to-\infty\\ T_2\to+\infty}}{\text{s-lim}}\, U_{\lambda_1^+}(0,T_2)\, U(T_2,T_1)\, U_0(T_1,0) \tag{4.2.43}$$

then it reduces to

$$S = \underset{\substack{T_1\to-\infty\\ T_2\to+\infty}}{\text{s-lim}}\, U_{\lambda_1^+}(0,T_2)\, U_{\lambda_1^+}(T_2,0)\, U_0(0,T_1)\, U_0(T_1,0) = \mathbf{1}. \tag{4.2.44}$$

It holds only under the assumption that the potential is switched on once and remains so forever. Although it looks trivial, it has nontrivial matrix elements if one calculates them with respect to different bases. S maps formally $\mathcal{H} = \mathcal{H}^0_+ \oplus \mathcal{H}^0_-$ on $\mathcal{H} = \mathcal{H}^{\lambda_1^+}_+ \oplus \mathcal{H}^{\lambda_1^+}_-$, where $\mathcal{H}^0_\pm \equiv P^0_\pm \mathcal{H}$ and $\mathcal{H}^{\lambda_1^+}_\pm \equiv P_\pm(\lambda_1^+)\mathcal{H}$. With orthonormal bases $\{\phi^\pm_n\} \in \mathcal{H}^0_\pm$ and $\{\chi^\pm_n\} \in \mathcal{H}^{\lambda_1^+}_\pm$ we find

$$[S_{\pm\pm'}]_{mn} \equiv (\chi^\pm_m, S\phi^{\pm'}_n) = (\chi^\pm_m, \phi^{\pm'}_n), \tag{4.2.45}$$

what reflects the fact that the whole process reduces to a single projection operation. The charge creation is then very simple to calculate

$$\begin{aligned}\Delta Q[S] &= ||S_{+-}||^2_{HS} - ||S_{-+}||^2_{HS} \\ &= ||P_+(\lambda_1^+)\, P^0_-||^2_{HS} - ||P_-(\lambda_1^+)\, P^0_+||^2_{HS} \\ &= -1.\end{aligned} \tag{4.2.46}$$

Here, the same comment must be made as at the end of section 4.1.1, that the final state ψ, in which the antiparticle is created, is not identical with the weakly overcritical bound state ϕ_1 ($-1 < E_1 < 0$), but it partially belongs to the negative continuum. Physically, it is expected that in such strongly time dependent evolution processes with a sudden jump of the potential the energy $E_p > 0$ of the created positron may be higher than for the corresponding positron ground state, i.e. $E_p > |E_1|$. Hence, there may appear a non-vanishing probability that the antiparticle will get scattered ($E_p > 1$). Moreover, additional pair creation (due to the big time variation of the potential) is expected, too.

Both, the evolution U_T and scattering S are implementable when

$$|||[U_T]_{\pm\mp}||_{HS} = ||S_{\pm\mp}||_{HS} = ||P_\pm(\lambda_1^+)\, P^0_\mp||_{HS}, \tag{4.2.47}$$

i.e. when the switched potential is regular (in the sense of theorem 6).

4.3 Scattering on general time-dependent potentials

4.3.1 Switch on and off of the potential

In this section we consider general scattering processes defined by evolution $U(t_2, t_1)$ in a general time-dependent potential $V(t)$. The Hamiltonian $H(t) \equiv H_0 + V(t)$ is therefore time-dependent, but since we assume $V(t) \to 0$ as $t \to \pm\infty$ the initial and final Hamiltonians, which will define particle states, are equal: $H(-\infty) = H(+\infty) = H_0$. We assume $S_{\pm\mp}$ are Hilbert-Schmidt, hence S is implementable and gives unitary $\hat{U}$ according to theorem 3 (with $V = 1$). Further, we assume $\dim\ker S_{++} > 0$ so that the $\hat{U}_0$ part of the operator $\hat{U}$ is non-trivial and creates particles from vacuum due to overcriticality of the potential. It turns out that in these processes particles are created only in pairs with antiparticles, so that the total charge does not change. It follows from the commutation $\hat{Q}\hat{U} = \hat{U}\hat{Q}$, which is proved in a subcritical case in [Sch95]. In general case we follow the proof of Seipp [Sei82].

Consider a family of scattering processes $S(\lambda)$ generated by $H_\lambda(t) = H_0 + \lambda V(t)$. $S(\lambda)$ can be constructed by a (norm convergent) Dyson series

$$S(\lambda) = \sum_{n=0}^{\infty} (-i\lambda)^n S_n \tag{4.3.1}$$

$$S_n \equiv \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \ldots \int_{-\infty}^{t_{n-1}} dt_n \widetilde{V}(t_1) \ldots \widetilde{V}(t_n), \tag{4.3.2}$$

with

$$\widetilde{V}(t) \equiv e^{itH_0} V(t) e^{-itH_0}. \tag{4.3.3}$$

It can be shown that such $S(\lambda)$ is analytic in λ. Therefore, it is also continuous in λ. Further, $S(\lambda)_{++}, S(\lambda)^*_{++}, S(\lambda)_{--}$ and $S(\lambda)^*_{--}$ are analytic and continuous in λ, too.

Theorem 15

$$\mathrm{ind}\,(S(\lambda)_{++}) = 0 \quad \textit{and} \quad \mathrm{ind}\,(S(\lambda)_{--}) = 0. \tag{4.3.4}$$

Proof:
The index is constant on a continuous family of (Fredholm) operators. Since $S(0) = \mathbf{1}$ it holds

$$\mathrm{ind}\,(S(0)_{++}) = \dim\ker S(0)_{++} - \dim\ker S(0)^*_{++} = 0, \tag{4.3.5}$$

$$\mathrm{ind}\,(S(0)_{--}) = \dim\ker S(0)_{--} - \dim\ker S(0)^*_{--} = 0. \tag{4.3.6}$$

Then, by continuity in λ, we get (4.3.4). □

From the above theorem together with theorem 5 follows immediately that

$$\Delta Q[S(\lambda)] = -\mathrm{ind}\,(S(\lambda)_{++}) = \mathrm{ind}\,(S(\lambda)_{--}) = 0, \tag{4.3.7}$$

i.e. that the scattering processes $S(\lambda)$ do not change the total charge and particles may be created only in pairs with antiparticles.

In other words, from the above theorem follows

$$\begin{aligned} \dim\ker S(\lambda)_{++} &= \dim\ker S(\lambda)^*_{++} = \dim\ker S(\lambda)_{--} && (4.3.8)\\ n_+ &= n_-, && (4.3.9) \end{aligned}$$

i.e. the number of special particles and antiparticles states are equal, what can also be stated as (cf. (2.3.69)-(2.3.70))

$$\exists f \in \mathcal{H}_+ :\ (S_{-+})^* S_{-+} f = f \qquad \Leftrightarrow \qquad \exists g \in \mathcal{H}_- :\ (S_{+-})^* S_{+-} g = g. \tag{4.3.10}$$

Consider now $S \equiv S(1)$ and assume it is strong ($\dim\ker S_{++} + \dim\ker S_{--} > 0$). In order to find the particle production from vacuum in the scattering process S we need to calculate $\hat{U}\Omega$. To construct the implementer $\hat{U}$ we need to apply theorem 3 for $U = S$ and $V = 1$. With $n_* \equiv n_+ = n_-$ we find

$$\begin{aligned} \hat{U}\,\Omega &= C_0\ \hat{d}^*_{n_*} \dots \hat{d}^*_1 \hat{b}^*_{n_*} \dots \hat{b}^*_1\ \exp\left(\sum_{k,l} D_{kl} \hat{b}^*{}_k \hat{d}^*{}_l\right)\Omega \\ &= C_0\ \hat{d}^*_{n_*} \dots \hat{d}^*_1 \hat{b}^*_{n_*} \dots \hat{b}^*_1\ \prod_{k,l}\left(1 + D_{kl} \hat{b}^*{}_k \hat{d}^*{}_l\right)\Omega. \end{aligned} \tag{4.3.11}$$

Physically, two interesting questions arise. First, if the n_* special pairs created by $\hat{d}^*_{n_*} \dots \hat{d}^*_1\ \hat{b}^*_{n_*} \dots \hat{b}^*_1$ have any special properties in contrast to (in general, infinite number of) pairs created by $\prod_{k,l}\left(1 + D_{kl}\hat{b}^*{}_k \hat{d}^*{}_l\right)$ to make them physically distinguishable in detection experiments? Second, if (the number and corresponding wave functions of) the special pairs are stable under small perturbations of the potential?

To the first question one can say, that the probability of creation of the special (anti-)particles is 1, while for all other it is less than 1 (but may be arbitrarily near 1). Although in a single detection there is (mathematically) no reason to expect different properties of the particles of both kinds.

The answer to the second question makes the special particles observationally even more marginal, namely it turns out that the number n_* of the special pairs is very unstable under perturbations of the potential and is almost always equal to zero. To show that consider again a class of scattering processes $S(\lambda)$ which are generated by time-dependent potentials of a different strength ($\sim \lambda$). The set of values of λ for which there are special particle states turns out to be only discrete, what is stated in the following

Theorem 16 *The set of values of λ for which $n_* = \dim\ker S(\lambda)_{++} > 0$ is discrete.*

Proof: $\dim\ker S(\lambda)_{++} > 0$ implies that there exists $f \in \mathcal{H}_+$ such that $(S(\lambda)_{-+})^* S(\lambda)_{-+} f = f$, i.e. $(S(\lambda)_{-+})^* S(\lambda)_{-+} = P_+ S^*(\lambda) P_- S(\lambda) P_+$ has an eigenvalue 1, but this is possible either for a discrete set of values of λ or for all λ, what follows from the analytic Fredholm

theorem [RS72, Th.VI.14]. The latter is never the case, because for $\lambda = 0$ the operator is $P_+S^*(0)P_-S(0)P_+ = P_+P_-P_+ = 0$. □

Moreover, it is only possible when [Sei82, Th.3]

$$\int_{-\infty}^{+\infty} ||\lambda V(t)||\, dt \geq \ln(2), \tag{4.3.12}$$

i.e. for

$$|\lambda| \geq \frac{\ln(2)}{\int_{-\infty}^{+\infty} ||V(t)||\, dt}. \tag{4.3.13}$$

From the above theorem follows that **even if for some λ there are special particle states, they get destroyed when one perturbs the potential $\lambda V(t)$ by infinitesimally changing λ. Creation of special (anti-)particles seems to be independent from whether the potential becomes overcritical during the evolution.**

4.3.2 Switch on of the potential

The situation changes completely, compared to the previous section, if the potential only switches on, but does not switch off during the evolution

$$\lim_{t\to-\infty} V(t) = 0, \qquad \lim_{t\to+\infty} V(t) \equiv V_\infty \neq 0 \tag{4.3.14}$$

and therefore the Hamiltonian defined as $H_\lambda(t) = H_0 + \lambda V(t)$ reaches two different limits as $t \to \pm\infty$

$$H_0 = H_\lambda(-\infty) \neq H_\lambda(+\infty) = H_0 + \lambda V_\infty \equiv H_\lambda^\infty. \tag{4.3.15}$$

The initial projectors

$$P_\pm \equiv P_\pm(H_0) = \frac{1 \pm \mathrm{sgn}(H_0)}{2} \tag{4.3.16}$$

remain unchanged, but differ from the final ones

$$P'_\pm(\lambda) \equiv P_\pm(H_\lambda^\infty) = \frac{1 \pm \mathrm{sgn}(H_\lambda^\infty)}{2}. \tag{4.3.17}$$

Now, the scattering operator is defined as

$$S(\lambda) = \underset{\substack{t_1\to-\infty \\ t_2\to+\infty}}{\text{s-lim}} e^{iH_\lambda^\infty t_2} U_\lambda(t_2, t_1) e^{-iH_0 t_1}. \tag{4.3.18}$$

The partial operators are defined as

$$S(\lambda)_{\pm'\pm} \equiv P'_{\pm'}(\lambda)\; S(\lambda)\; P_\pm \tag{4.3.19}$$

and are no more analytic nor even continuous in λ, because the projectors $P'_\pm(\lambda)$ are discontinuous at the critical values of λ, what has been discussed in section 4.1.1. Therefore it is no longer possible to show $\mathrm{ind}\,(S(\lambda)_{++}) = 0$ (cf. theorem 15), and hence the scattering process $S(\lambda)$ may change the total charge (which is calculated with respect to two different

vacua). It is the situation when the final vacuum becomes a charged state relative to the initial one, discussed in section 4.1.

Unfortunately, the special states in these processes, in general, bear the same property as those in the previous section – they are highly unstable under small perturbations of the potential. In the following we argue in analogy to theorem 16, but first we have to construct the series representation for $S(\lambda)$ being analytic in λ. The Dyson series constructed in (4.3.1)-(4.3.2) cannot be used now, because the integrals in (4.3.2) diverge as $t \to \infty$. This follows from the fact that $V(t) \to V_\infty \neq 0$ and hence $V(t)$ is not integrable (i.e. $\int_{-\infty}^{+\infty} V(t)dt$ diverges). Therefore we need to modify this construction. The (Dyson) series expansion for the evolution operator is

$$U_\lambda(t,s) \equiv e^{-itH_0}\widetilde{U_\lambda^-}(t,s)e^{isH_0} \tag{4.3.20}$$

$$\widetilde{U_\lambda^-}(t,s) = \sum_{n=0}^{\infty}(-i\lambda)^n \int_s^t dt_1 \int_s^{t_1} dt_2 \ldots \int_s^{t_{n-1}} dt_n \widetilde{V}(t_1)\ldots\widetilde{V}(t_n), \tag{4.3.21}$$

with

$$\widetilde{V}(t) \equiv e^{itH_0}V(t)e^{-itH_0} \quad \text{and} \quad H_\lambda(t) = H_0 + \lambda V(t). \tag{4.3.22}$$

It can be used to define the "past" wave operator

$$W(\lambda)_- \equiv \underset{s\to-\infty}{\text{s-lim}}\, U_\lambda(0,s)e^{-isH_0} = \underset{s\to-\infty}{\text{s-lim}}\, \widetilde{U_\lambda^-}(0,s), \tag{4.3.23}$$

which is analytic in λ. For the "future" wave operator we need a different expansion, with H_0 replaced by H_λ^∞ and $V(t)$ by $V'(t) \equiv V(t) - V_\infty$, to guarantee convergence of the integrals at $t \to \infty$

$$U_\lambda(t,s) \equiv e^{-itH_\lambda^\infty}\widetilde{U_\lambda^+}(t,s)e^{isH_\lambda^\infty} \tag{4.3.24}$$

$$\widetilde{U_\lambda^+}(t,s) = \sum_{n=0}^{\infty}(-i\lambda)^n \int_s^t dt_1 \int_s^{t_1} dt_2 \ldots \int_s^{t_{n-1}} dt_n \widetilde{V_\infty}(t_1)\ldots\widetilde{V_\infty}(t_n), \tag{4.3.25}$$

with

$$\widetilde{V_\infty}(t) \equiv e^{itH_\lambda^\infty}V'(t)e^{-itH_\lambda^\infty} \quad \text{and} \quad H\lambda(t) = H_\lambda^\infty + \lambda V'(t). \tag{4.3.26}$$

By this definition $V'(t) \to 0$ as $t \to \infty$. Now, the "future" wave operator reads

$$W(\lambda)_+ \equiv \underset{s\to+\infty}{\text{s-lim}}\, U_\lambda(0,s)e^{-isH_\lambda^\infty} = \underset{s\to+\infty}{\text{s-lim}}\, \widetilde{U_\lambda^+}(0,s), \tag{4.3.27}$$

which is analytic in λ, too. Finally, we obtain the scattering operator

$$S(\lambda) = (W(\lambda)_+)^* W(\lambda)_- = \underset{\substack{s\to-\infty\\ t\to+\infty}}{\text{s-lim}}\, (\widetilde{U_\lambda^+}(0,t))^* \widetilde{U_\lambda^-}(0,s) \tag{4.3.28}$$

and it is analytic in λ. This fact will be used in the following.

As a next step we need to study if the scattering process $S(\lambda)$ implemented in Fock space by $\hat{S}_\lambda$ creates single particles, especially if it happens due to the overcriticality of the final potential V_∞. The analysis of the structure of the implementer $\hat{S}_\lambda$ is more complicated than in the previous section, because we pose a different question here:

Does $\hat{S}_\lambda$, acting on the initial vacuum Ω defined by H_0, produce special (anti-)particles with respect to the final vacuum Ω'_λ defined by H^∞_λ? That is

$$\hat{S}_\lambda \Omega = C_0 \, \hat{d}'^*_m \dots \hat{d}'^*_1 \hat{b}'^*_n \dots \hat{b}'^*_1 \, \Omega'_\lambda \, ? \tag{4.3.29}$$

(where, for simplicity, we have skipped the factor $\prod_{k,l} \left(1 + D_{kl} \hat{b}'^*_k \hat{d}'^*_l\right)$ producing pairs with probability less than 1).

The nontrivial point is that the special (anti-)particle states $\hat{b}'^*_n, \hat{d}'^*_m$ are defined with respect to the final vacuum Ω'_λ (in short "final" particles) and are different from the "initial" particles $\hat{b}^*_n, \hat{d}^*_m$ defined with respect to Ω. Theorem 3 does not provide a method for the construction of the operator $\hat{S}_\lambda$ in such a form. Therefore we consider a following modified process: we attach to the scattering process $S(\lambda) : \mathcal{H}^0_+ \oplus \mathcal{H}^0_- \to \mathcal{H}^\lambda_+ \oplus \mathcal{H}^\lambda_-$ (with bases $\{\phi^\pm_n\} \in \mathcal{H}^0_\pm$ and $\{\chi^\pm_n\} \in \mathcal{H}^\lambda_\pm$) another process mapping back on the initial Hilbert subspaces, namely $V(\lambda) : \mathcal{H}^\lambda_\pm \to \mathcal{H}^0_\pm$ and defined by $V(\lambda)\chi^\pm_n = \phi^\pm_n$ (dependence of V on λ originates from the definition of the basis vectors $\chi^\pm_n \in \mathcal{H}^\lambda_\pm$). So we obtain $U(\lambda) = V(\lambda)S(\lambda)$ whose implementer $\hat{U}_\lambda$ can be constructed via theorem 3. Also the implementer $\hat{V}_\lambda$ can be constructed by the same theorem. Since $\hat{U}_\lambda = \hat{V}_\lambda \hat{S}_\lambda$ we can find $\hat{S}_\lambda = \hat{V}^*_\lambda \hat{U}_\lambda$. Since the action of $\hat{V}^*_\lambda$ on the operators and on the vacuum has a compact form

$$\hat{V}^*_\lambda \hat{b}^*_n \hat{V}_\lambda = \hat{b}'^*_n, \qquad \hat{V}^*_\lambda \hat{d}^*_n \hat{V}_\lambda = \hat{d}'^*_n, \qquad \hat{V}^*_\lambda \Omega = \Omega'_\lambda, \tag{4.3.30}$$

we observe that acting with $\hat{V}_\lambda$ on both sides of (4.3.29) we get

$$\hat{U}_\lambda \Omega = \hat{V}_\lambda \hat{S}_\lambda \Omega = \hat{V}_\lambda \left(C_0 \, \hat{d}'^*_m \dots \hat{d}'^*_1 \hat{b}'^*_n \dots \hat{b}'^*_1 \, \Omega'_\lambda \right) = C_0 \, \hat{d}^*_m \dots \hat{d}^*_1 \hat{b}^*_n \dots \hat{b}^*_1 \, \Omega, \tag{4.3.31}$$

i.e. $\hat{U}_\lambda$ produces m special ("initial") antiparticles and n special ("initial") particles from vacuum. In the following we consider the case $m = 1$ and $n = 0$. The reasoning for any m and n is analogous, but just this case is especially interesting in connection with overcritical potentials .

Since the antiparticle creating process $U(\lambda)$ consists of two steps, $S(\lambda)$ and $V(\lambda)$, there appears a natural question if the antiparticle is created completely in one of the two steps or somehow partially in both, so that it fully appears only after both steps. It turns out that the latter is impossible and

Theorem 17 *A single special antiparticle created by $U = VS$ must be created either by S or by V. It follows from*

$$\operatorname{ind}(P'_+ U P_+) = \operatorname{ind}(P'_+ S P_+) + \operatorname{ind}(P'_+ V P_+). \tag{4.3.32}$$

Proof: Using the theorem 2 we find

$$\begin{aligned} -\mathrm{ind}\,(P'_+UP_+) &= \mathrm{Tr}(U^*P'_+U - P_+) = \mathrm{Tr}(S^*V^*P'_+VS - P_+) \\ &= \mathrm{Tr}(S^*V^*P'_+VS - S^*P_+S) + \mathrm{Tr}(S^*P_+S - P_+) \\ &= \mathrm{Tr}(S^*(V^*P'_+V - P_+)S) + \mathrm{Tr}(S^*P_+S - P_+) \\ &= \mathrm{Tr}(V^*P'_+V - P_+) + \mathrm{Tr}(S^*P_+S - P_+) \\ &= -\mathrm{ind}\,(P'_+VP_+) - \mathrm{ind}\,(P_+SP_+). \end{aligned} \tag{4.3.33}$$

Since U creates a single special antiparticle we have $\mathrm{ind}\,(P'_+UP_+) = 1$, but in

$$\mathrm{ind}\,(P'_+UP_+) = \mathrm{ind}\,(P'_+VP_+) + \mathrm{ind}\,(P_+SP_+) \tag{4.3.34}$$

every index is an integer number. Thus, at least one of the indices on the right-hand side must be greater or equal 1, what means that either V or S creates (at least) one special antiparticle. □

Next, by an analytic argument we will show that the special (anti-)particles created by $\hat{S}_\lambda$ w.r.t. the initial vacuum Ω are unstable under small variations of λ, while those created by $\hat{V}_\lambda$ are stable if the final potential is overcritical. In other words, the stable creation of special (anti-)particles, if it should take place, is not due to the scattering process itself, but to the (overcritical) structure of the final vacuum Ω'_λ.

For $S(\lambda)$ we repeat the reasoning behind theorem 16. The fact that $\hat{S}_\lambda$ creates special antiparticles is equivalent to that $(S(\lambda)_{-+})^*S(\lambda)_{-+}$ has eigenvalue 1 (cf. (2.3.69)). This operator

$$(S(\lambda)_{-+})^*S(\lambda)_{-+} = P_+S^*(\lambda)P_-S(\lambda)P_+ \tag{4.3.35}$$

is analytic in λ, because $S(\lambda)$ is analytic, what has been shown above. Therefore by the analytic Fredholm theorem it can have eigenvalue 1 either for all λ or only for isolated values of λ. The first case does not hold, because for $\lambda = 0$ the operator is $P_+S^*(0)P_-S(0)P_+ = P_+P_-P_+ = 0$. The same can be shown for the creation of special particles (i.e. for $S(\lambda)_{+-}$ instead of $S(\lambda)_{-+}$). So we have shown that the creation of special "initial" particles and antiparticles by $\hat{S}_\lambda$ in highly unstable under small perturbations of λ.

The situation with $V(\lambda)$ is different. Since $P_\pm V(\lambda) = V(\lambda)P'_\pm(\lambda)$, the operator

$$(V(\lambda)_{-+})^*V(\lambda)_{-+} = P_+V^*(\lambda)P_-V(\lambda)P_+ = P_+V^*(\lambda)V(\lambda)P'_-(\lambda)P_+ = P_+P'_-(\lambda)P_+ \tag{4.3.36}$$

has eigenvalue 1 if and only if there exists a vector $\psi_\lambda \in \mathcal{H}^0_+ \cap \mathcal{H}^\lambda_-$ for which $P'_-(\lambda)P_+\psi_\lambda = \psi_\lambda$. As has been discussed in section 4.1.1, this is the case for overcritical potentials, i.e. when $\lambda > \lambda_1$, where λ_1 is defined by the condition that the energy of the lowest bound state (the smallest eigenvalue of H_λ) crosses zero. At $\lambda = \lambda_1$ the projectors $P'_\pm(\lambda)$, otherwise analytic in λ, change discontinuously. Therefore there is not much use of the analytic Fredholm theorem. It is clear that for $\lambda < \lambda_1$ the above operator has no eigenvalue 1 and

for all $\lambda > \lambda_1$ it has. Exactly the same holds for the creation of special antiparticles by $\hat{V}_\lambda$

$$\hat{V}_\lambda\Omega = \begin{cases} \Omega, & \lambda < \lambda_1, \\ \hat{d}^*(\psi'_\lambda)\Omega, & \lambda > \lambda_1, \end{cases} \tag{4.3.37}$$

with $\psi'_\lambda \equiv V(\lambda)\psi_\lambda \in \mathcal{H}^0_-$. In other words, it is due to change of structure of the final vacuum Ω'_λ with respect to Ω

$$\Omega = \begin{cases} V^*_\lambda\Omega = \Omega'_\lambda, & \lambda < \lambda_1, \\ V^*_\lambda\hat{d}^*(\psi'_\lambda)\Omega = \hat{d}'^*(\psi_\lambda)\Omega'_\lambda, & \lambda > \lambda_1. \end{cases} \tag{4.3.38}$$

Now, we can combine the two results for $\hat{S}_\lambda$ and $\hat{V}_\lambda$. It turns out that the stable creation of special antiparticles from vacuum can happen only when the creation is due to $\hat{V}_\lambda$, what is the case for overcritical final potentials ($\lambda > \lambda_1$). But we cannot forget that then $\hat{S}_\lambda$ must fulfill further conditions in order to allow $\hat{U}_\lambda = \hat{V}_\lambda\hat{S}_\lambda$ for special antiparticle creation. Let us now consider what the conditions must be (assuming $\lambda > \lambda_1$ in the following). Antiparticle creation

$$\hat{U}_\lambda\Omega = \hat{d}^*(\psi'_\lambda)\Omega \tag{4.3.39}$$

is equivalent to

$$\begin{aligned} \hat{S}_\lambda\Omega = \hat{V}^*_\lambda\hat{U}_\lambda\Omega = \hat{V}^*\left(\hat{d}^*(\psi'_\lambda)\Omega\right) = \hat{d}'^*(\psi_\lambda)\Omega'_\lambda \\ \text{(or, alternatively:)} \quad = \hat{V}^*_\lambda\hat{U}_\lambda\hat{V}_\lambda\hat{V}^*_\lambda\Omega = (\hat{V}^*_\lambda\hat{U}_\lambda\hat{V}_\lambda)\Omega'_\lambda = \hat{d}'^*(\psi_\lambda)\Omega'_\lambda \end{aligned} \tag{4.3.40}$$

but from (4.3.38) follows that $\hat{d}'^*(\psi_\lambda)\Omega'_\lambda = \Omega$, what gives

$$\hat{S}_\lambda\Omega = \Omega \tag{4.3.41}$$

(where we consequently ignore creation of pairs with probability less than 1 by factors of the form $\prod_{k,l}\left(1 + A_{kl}\hat{b}^*_k\hat{d}^*_l\right)$).

At this point we see for the first time the *spontaneous* character of the special (anti-)particle creation in these processes, namely $\hat{S}_\lambda$ produces no special (anti-)particles with respect to Ω, but produces some with respect to Ω'_λ

$$\hat{S}_\lambda\Omega = \begin{cases} \Omega & \text{(no (anti-)particles)}, \\ \hat{d}'^*(\psi_\lambda)\Omega'_\lambda & \text{(one special antiparticle)}. \end{cases} \tag{4.3.42}$$

In fact, creation of the antiparticle is due to the difference between the initial and final ground states $\Omega = \hat{d}'^*(\psi_\lambda)\Omega'_\lambda \neq \Omega'_\lambda$, what is physically described as a *decay of the vacuum state* Ω, which is a ground state with respect to the initial Hamiltonian, but ceases to be a ground state with respect to the final Hamiltonian, to the charged Ω'_λ. Therefore, the creation of such special (anti-)particles is called *spontaneous* particle creation.

While the total charge in terms of the initial particle definition cannot change even in the evolution to the final overcritical potential

$$\begin{aligned} q(t) &\equiv (\hat{U}_\lambda\,\Omega, \hat{Q}\,\hat{U}_\lambda\,\Omega) = (\Omega, \hat{U}_\lambda^*\,\hat{Q}\,\hat{U}_\lambda\,\Omega) \\ &= ||(U_\lambda)_{+-}||^2_{HS} - ||(U_\lambda)_{-+}||^2_{HS} = -\mathrm{ind}\,((U_\lambda)_{++}) = 0 \end{aligned} \tag{4.3.43}$$

according to theorem 15, it changes in terms of the final particles, defined with respect to the final vacuum,

$$\begin{aligned} q'(t) &\equiv (\hat{U}_\lambda\,\Omega, \hat{Q}'\,\hat{U}_\lambda\,\Omega) = (\Omega, \hat{U}_\lambda^*\,\hat{V}_\lambda^*\,\hat{Q}\,\hat{V}_\lambda\,\hat{U}_\lambda\,\Omega) \\ &= ||(V_\lambda U_\lambda)_{+-}||^2_{HS} - ||(V_\lambda U_\lambda)_{-+}||^2_{HS} = \\ &= ||P_+ V_\lambda U_\lambda P_-||^2_{HS} - ||P_- V_\lambda U_\lambda P_+||^2_{HS} = \\ &= ||V_\lambda P'_+ U_\lambda P_-||^2_{HS} - ||V_\lambda P'_- U_\lambda P_+||^2_{HS} = \\ &= ||P'_+ U_\lambda P_-||^2_{HS} - ||P'_- U_\lambda P_+||^2_{HS} = -\mathrm{ind}\,(P'_+ U_\lambda P_+) = -1 \end{aligned} \tag{4.3.44}$$

in our case, what confirms that one antiparticle is created with respect to Ω'_λ. Therefore it cannot be claimed, on the basis of (4.3.43), that no spontaneous particle creation may occur (as was done in [CO82]), because one has always to consider particles defined with respect to the final Hamiltonian, i.e. with respect to the final vacuum state, as is done in (4.3.44).

To have a successful antiparticle creation according to the above scheme, it must hold

$$V(\lambda)_{-+}\psi_\lambda = \psi'_\lambda \quad \text{with} \quad ||\psi'_\lambda|| = ||\psi_\lambda|| = 1, \tag{4.3.45}$$

or

$$\psi_\lambda = (V(\lambda)_{-+})^*\psi'_\lambda \tag{4.3.46}$$

and

$$||U(\lambda)_{-+})^*\psi'_\lambda|| = ||P_+ U(\lambda)^* P_-\psi'_\lambda|| = 1. \tag{4.3.47}$$

Since

$$(U(\lambda)_{-+})^*\psi'_\lambda = P_+ S(\lambda)^* V^*(\lambda) P_-\psi'_\lambda = P_+ S^*(\lambda) P_+\psi_\lambda, \tag{4.3.48}$$

we get the expected condition on $S(\lambda)$

$$||P_+ S^*(\lambda) P_+\psi_\lambda|| = 1. \tag{4.3.49}$$

It can be reformulated as a condition that

$$P_{\psi_\lambda} S(\lambda) P_+ S^*(\lambda) P_{\psi_\lambda} \tag{4.3.50}$$

(P_{ψ_λ} means projection on state ψ_λ) has an eigenvalue 1 (with the obvious eigenvector ψ_λ). Because this operator is analytic in λ (P_{ψ_λ} is analytic, because ψ_λ is), we again by use of the analytic Fredholm theorem conclude that it is the case either for all λ or only for isolated values of λ. In the latter case the whole special antiparticle creation by $\hat{U}_\lambda$ (and

thus the special "final" antiparticle creation with respect to Ω'_λ by $\hat{S}_\lambda$) will be unstable under small variations of λ. The first case is not so simple to eliminate, but it seems highly improbable that any, not specially prepared (as e.g. in adiabatic scattering), will have this property. Unfortunately, we were unable to eliminate this possibility in general by a rigorous proof. Nonetheless, using the above argumentation, **we conclude that the special "final" (anti-)particle creation (with respect to Ω'_λ) in the scattering process where the potential is only switched on is, in general (except specially prepared processes), unstable under small variations of λ. On the other hand, if it should be possible then only for potentials, whose final value is overcritical.**

4.4 Scattering in the adiabatic limit

Our goal is to find scattering processes which lead to (stable) production of special particles and/or antiparticles exclusively due to the overcriticality of the potential, i.e. to *spontaneous* particle creation. From the previous section we know that in the processes with switch on and off of the potential (standard scattering) the special particles and antiparticles must be created in equal numbers, i.e. in pairs. However, in these processes also many other *(dynamical)* pairs are created, due to the time-dependence of the potential. Although these two kinds of pairs can be distinguished mathematically (probability of special pairs is exactly 1, while of all other pairs is less than 1), they cannot be distinguished in the detection experiments, because all other parameters can be identical. In case of a non-standard scattering with only switch on of the potential the special (anti-)particles do not have to be created in pairs, so e.g. one antiparticle can be created with respect to the new final vacuum (which itself gets charged w.r.t. the initial one). It would be a clear experimental signature of spontaneous particle creation, if an odd number of created (anti-)particles could be observed or the total charge would change. Unfortunately, in both types of the scattering processes the creation of special (anti-)particles is unstable under small variations of the potential's strength, what means that an arbitrarily small change in the strength of the potential during the evolution destroys the effect of creation of special (anti-)particles. It seems to make the effect physically irrelevant, what has been postulated in [SS82].

Before we will try to overcome these problems, we should ask the question, which properties, from the physical point of view, are relevant for observing the signatures of spontaneous (anti-)particle creation. In a stronger sense, it should be a stable (under small perturbations of the potential) creation of only special pairs, in the switch-on-off case, and only special antiparticles (with the change of the total charge) in the switch-on case. In a weaker sense, we can try to relax the stability condition and check what happens near the point, where spontaneous creation of special (anti-)particles happens. This will be discussed in the last section of this chapter. Now, consider the possibilities of the spontaneous particle creation in the stronger sense.

The most obvious way to eliminate the dynamical pairs is to consider time-independent potentials. Unfortunately, as we have seen in section 4.2.2, static potentials do not create any particles, neither dynamical nor special. Therefore, the next serious candidate is the adiabatic scattering process, because it is free from the above problems and has a chance of special (anti-)particle creation. A family of scattering operators $S_\epsilon(\lambda)$ parameterized by ϵ, the time-scale, is defined in a standard way by the evolution generated by the Hamiltonian $H_{\lambda,\epsilon}(t) \equiv H_0 + \lambda V_\epsilon(t)$ with $V_\epsilon(t) \equiv V(\epsilon t)$. The adiabatic scattering is defined by the limit

$$S(\lambda) \equiv \lim_{\epsilon \to 0} S_\epsilon(\lambda), \tag{4.4.1}$$

what is, in general, different from $S_0(\lambda)$, i.e. scattering in the static potential $V_0(t) = V(0)$. Such $S(\lambda)$ is , in general, no longer analytic in λ (a limit of analytic functions does not have to be analytic). Therefore arguments based on analyticity (through the analytic Fredholm theorem) leading to instability of creation of the special (anti-)particles cannot be used. Moreover, creation of dynamical pairs is suppressed and tends in the adiabatic limit to zero, in contrast to the special (anti-)particles, which should survive the limit. In the following we consider the adiabatic limit in the switch-on-off as well as in the switch-on scattering.

4.4.1 Adiabatic switch on and off of the potential

Intuitive picture in the adiabatic limit

Let us recall the pictures from the introduction (chapter 1). We plot the spectrum of $H(t)$ (i.e. energy eigenvalues and both continua) against time t. From the adiabatic theorem (cf. section 3.4.1) we know that "jumps" between the bound states (arrow from filled to empty circle) are suppressed in the adiabatic limit and that the wave function of the Dirac equation $\Psi(t)$ follows a continuously varying eigenvector $\psi_n(t)$ (bound state). This theorem holds as long as eigenvalues $E_n(t)$ stay isolated and do not touch the continuum, what is the case for overcritical potentials.

In the situation of figure 4.1 the lowest lying eigenvalue $E_0(t)$ vanishes in continuum, i.e. $E_0(t) \to -1$ as $t \to -T^-$, and then reappears, i.e. $E_0(t) \to -1$ as $t \to T^+$, with some $T > 0$. Assume the system $\Psi(t) = \psi_0(t)$ at some early $t < -T$. The adiabatic theorem states that $\Psi(t) = \psi_0(t)$ for all $t < -T$. Then, in the overcritical phase $t \in (-T, T)$, the wave function $\Psi(t)$ is represented by a wave packet in the negative continuum. Such wave packets are known to "decay", because the amplitudes of their constituents (the generalized eigenfunctions in continuum) dephase and produce functions, which are orthogonal to the initial ones. Finally, it is a crucial question, if the wave function follows the eigenvalue $E_0(t)$ diving out of the continuum at $t > T$, i.e. if $\Psi(t) = E_0(t)$ for all $t > T$. It is expected that it will not be the case and $\Psi(t)$ will be kept in the negative continuum forever, yet there is no adiabatic theorem describing such situation in general, only on base of the spectral properties of $H(t)$.

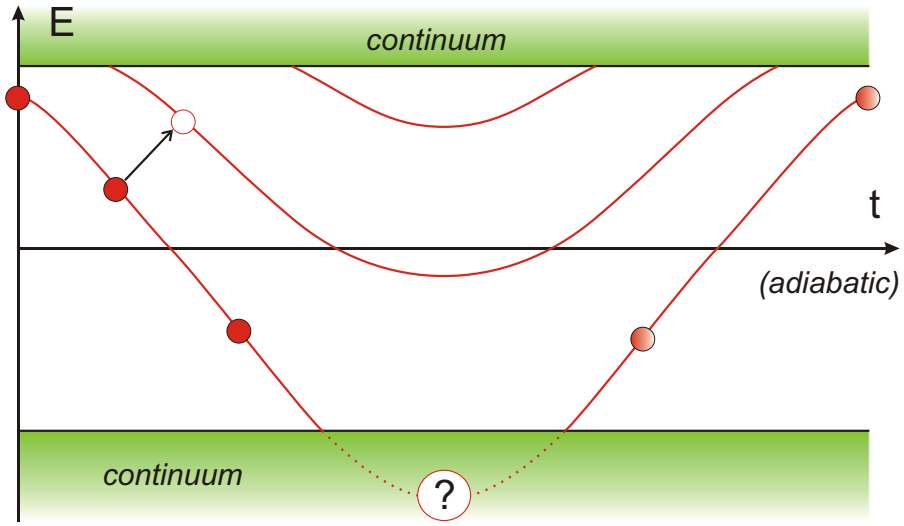


Figure 4.1: Time-dependence of the spectrum of the Hamiltonian $H(t)$.

Extending to infinite times $t \to \pm\infty$, assume that $V(t) \to 0$ as $t \to \pm\infty$ and that the bound state $E_0(t)$ vanishes asymptotically in the positive continuum. Then, if the expected scenario is true, the scattering operator S maps an initial state from the positive continuum $\phi \equiv W_-^*(t)\Psi(t) = \lim_{t\to-\infty} e^{itH_0}\Psi(t) \in \mathcal{H}_+^0$ onto a final state in the negative continuum $\chi \equiv W_+^*(t)\Psi(t) = \lim_{t\to+\infty} e^{itH_0}\Psi(t) \in \mathcal{H}_-^0$, i.e. $S_{-+}\phi = \chi$, what implies a spontaneous creation of an antiparticle in state χ. (Additionally, a particle will be created, cf. section 4.3 and theorem 15, or see below, so that finally a spontaneously created pair appears.)

To provide a picture in terms of particle creation processes, we have to modify the previous picture slightly, adopting consequences of the quantization of the Dirac field, namely that both continua are empty and that crossing the energy-line $E = 0$ (denoted on figure 4.2 by a dashed line above the time-axis) states change the subspace between $\mathcal{H}_+^0$ and $\mathcal{H}_-^0$. In a sense, the latter implies inversion of the occupation of such a state, because at time $t = t_0$ the state $\Omega_{t_0^-}$ in Fock space goes over to $d_1'^* \, \Omega_{t_0^+}$, where Ω_t is a vacuum with respect to the Hamiltonian $H(t)$, that is a no-particle state becomes a one-antiparticles state and vice versa. The notion of particles refers always to the instantaneous vacuum Ω_t defined with respect to the current Hamiltonian $H(t)$.

Figure 4.2 schematically shows the process of spontaneous pair creation in the adiabatic limit due to the potential which becomes overcritical for some period of time. The initial state is a vacuum (the bound state is not occupied). As the energy of the bound state crosses zero (potential becomes weakly overcritical) there appears an antiparticle (the bound state becomes occupied). As the eigenvalue vanishes in the negative continuum (potential becomes strongly overcritical) the antiparticle state corresponds to a wave packet, which decays in time. In the adiabatic limit it is expected that the phase lasts

long enough (actually infinitely long) for the wave packet to decay completely. Later, as the bound state dives out, it is not occupied, since the whole wave function is trapped in the lower continuum. It still corresponds to a antiparticle in a scattering state. Finally, as the bound state crosses the level $E = 0$ again, it becomes occupied and the final state is a particle in a bound state and an antiparticle in the scattering state.

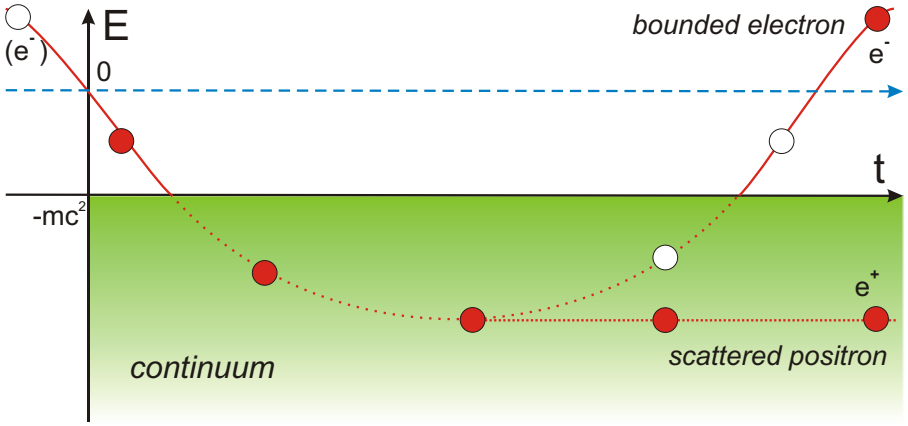
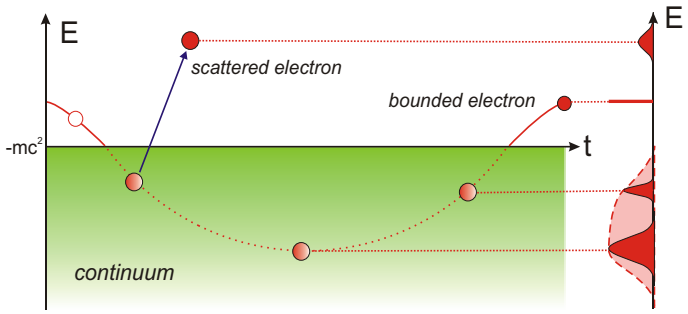


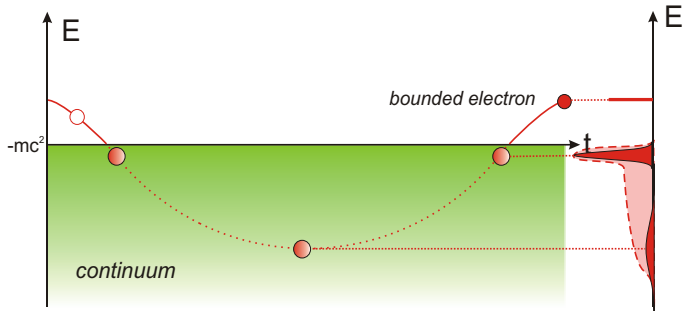
Figure 4.2: A scheme of the spontaneous pair creation in the adiabatic limit.

This is the spontaneous creation of a pair due to an overcritical potential in the adiabatic limit. The physical interpretation within the Fock space representation follows from the simple fact from the classical Dirac theory, namely that the (classical) scattering operator S maps some initial state from the positive continuum ($\phi \in \mathcal{H}^0_+$) onto a final state in the negative continuum ($\chi \in \mathcal{H}^0_-$).

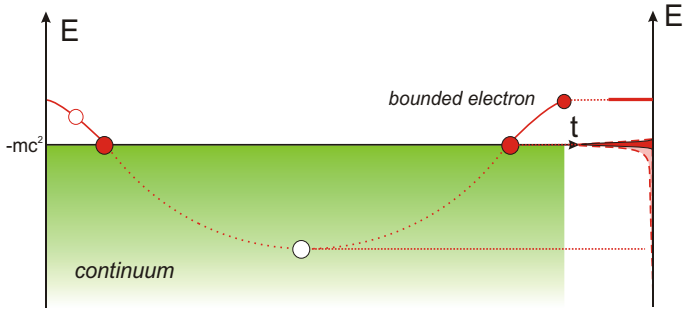
However, there appears a problem, which seems specific to the adiabatic limit. It can be explained by the following non-rigorous reasoning. Assume, the wave packet approximately follows (i.e. is localized around) the position of the resonance in the continuum during the overcritical phase. It should be expected that it decays along the whole way and at each stage contributes to the final wave function which will stay trapped in the continuum. This simplification is not very far from reality, because the decay is based on dephasing of the amplitudes in a wave packet, so in other words such a wave packet decoheres and therefore adds to contributions from other wave packets in a decoherent way.



As the adiabatic limit is approached the variation of the potential becomes slower and the overcritical phase lasts longer. Hence, the wave packet has at each stage (i.e. each value of the potential) more and more time to decay. It should be expected that more and more of the wave function will decay already at the early overcritical stage, thus producing a final wave function localized near the edge of the lower continuum.



Consequently, in the adiabatic limit, the final wave function should be peaked at the edge of the negative continuum.



Physically it would imply that the spontaneously created antiparticles have energy $E \to 1^+$ (i.e. $E \to mc^2$ in physical units) and hence momentum (almost) zero.

But then, there appears a doubt, if the wave function really gets trapped in the continuum and does not follow the emerging bound state. The reason for this is the following. It is known, that wave packets arising from diving of a bound state into the continuum approximate the shape of the resonance wave function (which is a remnant of the bound state). Their position is localized (in the energies) around the real part of the resonance's complex energy E_R and their width Γ is proportional to its imaginary part E_I. If in the adiabatic limit the decay occurs near the edge of the continuum then $E_R \approx -1$. It is known that $E_I \to 0$ as $E_R \to -1$, what implies that the width of the wave packet $\Gamma \to 0$. Then the wave packet needs more time to decay, since the decay time scales as $T_{decay} \sim 1/\Gamma$. The proof of spontaneous particle creation in the adiabatic limit must solve this puzzle.

Definition of spontaneous particle creation by the adiabatic limit

Consider a family of time-dependent potentials parameterized by ϵ

$$V_\epsilon(t) = V(\epsilon t). \tag{4.4.2}$$

Usually one defines the adiabatic switching by introducing an explicit exponential switching factor

$$V_\epsilon(t, \mathbf{x}) \equiv e^{-\epsilon^2 t^2}\ \tilde{V}(\mathbf{x}). \tag{4.4.3}$$

We will not restrict our considerations to this special form, assuming only that the potential $V(t, \mathbf{x})$ tends to zero sufficiently fast as $t \to \pm\infty$ so that the wave operators $W^{\pm}_{\lambda,\epsilon}(\lambda)$ are complete and the scattering operator $S_{\lambda,\epsilon}$ exists and is unitary (cf. section 3.5). Without restriction of generality we will assume that $V(t)$ is strongest at $t = 0$, what means that the lowest eigenvalue $E^\lambda_0(t)$ of $H_\lambda(t)$, if exists, satisfies

$$\min_t E^\lambda_0(t) = E^\lambda_0(0). \tag{4.4.4}$$

Obviously, the family of scattering operators $S_{\lambda,\epsilon}$ in $\mathcal{H}$ gives rise to a family of implementers $\hat{S}_{\lambda,\epsilon}$ in Fock space $\mathcal{F}$. We hope to overcome the obstacles from the previous section regarding spontaneous pair creation as we expect $S_{\lambda,\epsilon}$ having a non-trivial limit

$$\lim_{\epsilon\to 0} S_{\lambda,\epsilon} \neq S_{\lambda,0} \tag{4.4.5}$$

and thus

$$1 = \lim_{\epsilon\to 0} ||P_\pm S_{\lambda,\epsilon} P_\mp|| \neq ||P_\pm S_{\lambda,0} P_\mp|| = 0. \tag{4.4.6}$$

Consequently we expect the same for the implementers

$$\lim_{\epsilon\to 0} \hat{S}_{\lambda,\epsilon} \neq \hat{S}_{\lambda,0} \tag{4.4.7}$$

and thus

$$0 = \lim_{\epsilon\to 0} (\Omega, \hat{S}_{\lambda,\epsilon}\Omega) \neq (\Omega, \hat{S}_{\lambda,0}\Omega) = 1. \tag{4.4.8}$$

The natural way to define spontaneous particle creation rigorously is the survival of particle creation in the adiabatic limit, since creation of the dynamical pairs tends to zero, what follows from the adiabatic theorem. Following Nenciu [Nen80a], we define a measure

$$r_\lambda = 1 - \lim_{\epsilon\to 0} \left| \left(\Omega, \hat{S}_{\lambda,\epsilon}\Omega\right) \right|^2 \tag{4.4.9}$$

giving the probability of creation of any particles in the adiabatic limit. It can be shown that the condition $r_\lambda = 0$ is equivalent to $N_\lambda = 0$, where N_λ is the total number of particles created from vacuum. Nenciu conjectures that there exists a critical value $\lambda = \lambda_{cr}$ such that

$$\lim_{\epsilon\to 0} r_\lambda = \begin{cases} 0 & \text{for} \quad 0 < \lambda < \lambda_{cr}, \\ 1 & \text{for} \quad \lambda > \lambda_{cr}. \end{cases} \tag{4.4.10}$$

It is expected that the first case occurs if the potential is strongly subcritical during the whole evolution, i.e. $E_0^\lambda(t)$ exists for all t and $E_0^\lambda(t) > -1$, and the second case if $V(t)$ is strongly overcritical for some $t \in (-T, T)$ with $T > 0$, i.e. $E_0^\lambda(t)$ disappears in the lower continuum for $t \in (-T, T)$. It means that λ_{cr} should be equal to $\widetilde{\lambda}_1$, i.e. when $E_0^\lambda(0) \to -1$ as $\lambda \to \widetilde{\lambda}_1$ (cf. (4.4.4)).

From this conjecture it follows that r_λ has a jump at $\lambda = \lambda_{cr}$. The subcritical part agrees with the adiabatic theorem, from which follows that particle creation tends to zero as $\epsilon \to 0$. On the contrary, the overcritical part seems to contradict it, but this is just the situation when assumptions for the adiabatic theorem are not fulfilled, namely the eigenvalue $E_0^\lambda(t)$ dives into the continuum $(-\infty, -1]$ and so does not stay isolated for all t.

There was an attempt by Nenciu in 1987 to prove this conjecture [Nen87], but he was not able to control the evolution at the point t_0 of diving of the eigenvalue, i.e. when $E_0^\lambda(t) \to -1$ as $t \to t_0$. Instead, he introduced a small jump $\sim \delta$ in the strength of the potential at $t = t_0$ and kept the potential in the overcritical phase time-independent. It allowed him to overcome the difficulty at the edge of the continuum, but destroyed the adiabatic character of the process and introduced again dynamical pair production, however he showed that the production rate of the dynamical pairs tends to zero as $\delta \to 0$. Yet, since the potential was kept only slightly overcritical and time-independent, the result is far from being satisfactory for explaining the general situation of diving of an eigenvalue. Later Prodan in 2000 [Pro99] tried again by splitting the adiabatic limit into two independent limits ($\epsilon_1, \epsilon_2 \to 0$), one in the past and one in the future (for corresponding wave operators), but was able to prove the conjecture only by taking a special order of the two limits. He showed that for every $\epsilon_1, \epsilon_2 > 0$ there exists a vector $\phi_{\epsilon_1} \in \mathcal{H}_+^0$ such that

$$\lim_{\epsilon_1 \to 0} \lim_{\epsilon_2 \to 0} ||P_-(W_{\lambda,\epsilon_2}^+)^* W_{\lambda,\epsilon_1}^- P_+ \phi_{\epsilon_1}|| = 1, \tag{4.4.11}$$

what suggests that ϕ_{ϵ_1} is transported adiabatically from $\mathcal{H}_+^0$ in the past to $\mathcal{H}_-^0$ in the future by $(W_{\lambda,\epsilon_2}^+)^* W_{\lambda,\epsilon_1}^-$, which in the adiabatic limit $\epsilon_1, \epsilon_2 \to 0$ gives $(W_\lambda^+)^* W_\lambda^- = S_\lambda$, only when the limit $\epsilon_2 \to 0$ in the future wave operator W_{λ,ϵ_2}^+ is taken before the limit $\epsilon_1 \to 0$ in the past wave operator W_{λ,ϵ_1}^-. At this point he asked the question how far this proof is from the required situation $\epsilon_1 = \epsilon_2$. We showed [Pro04] that this technique is useless. How misleading such a procedure is can be seen by calculating, using the same technique, that

$$\lim_{\epsilon_1 \to 0} \lim_{\epsilon_2 \to 0} ||P_-(W_{\lambda,\epsilon_2}^-)^* W_{\lambda,\epsilon_1}^- P_+ \phi_{\epsilon_1}|| = 1, \tag{4.4.12}$$

what means that ϕ_{ϵ_1} is transported adiabatically from $\mathcal{H}_+^0$ in the past to $\mathcal{H}_-^0$ in the past(!) by $(W_{\lambda,\epsilon_2}^-)^* W_{\lambda,\epsilon_1}^-$, what is absurd. Such a limit has nothing to do with the true definition of the adiabatic limit where $\epsilon_1 = \epsilon_2$. Setting $\epsilon_1 = \epsilon_2 \equiv \epsilon$ in the above equation we obtain

$$\lim_{\epsilon \to 0} ||P_-(W_{\lambda,\epsilon}^-)^* W_{\lambda,\epsilon}^- P_+ \phi_{\epsilon_1}|| = \lim_{\epsilon \to 0} ||P_- P_+ \phi_\epsilon|| = 0, \tag{4.4.13}$$

what is physically reasonable.

Proof ideas and problems

In this paragraph we give a sketch of the proof and point at the essential problems. It is a fundamental result of the scattering theory in QED of external fields, that

$$(\Omega, \hat{S}\,\Omega) = \begin{cases} 0 & \text{if} \quad S_{+-}(S_{+-})^* \quad \text{has an eigenvalue 1,} \\ \det\left[1 + (S_{++})^{-1} S_{+-} (S_{+-})^* (S_{++})^{*-1}\right]^{-1/2} & \text{otherwise.} \end{cases} \tag{4.4.14}$$

Since the Fredholm determinant in the second case is rather difficult to treat, it is convenient to replace it with some estimations. It can be shown [Nen87]

$$||A||_{H.S.} \to 0 \quad \Rightarrow \quad (\Omega, \hat{S}\,\Omega) \to 1 \qquad \text{(no particle production)} \tag{4.4.15}$$

$$||A|| \to 1 \quad \Rightarrow \quad (\Omega, \hat{S}\,\Omega) \to 0 \qquad \text{(“complete” particle production)} \tag{4.4.16}$$

Making use of the above facts, to prove the conjecture in the adiabatic limit it remains to show:

- In the subcritical case: $||P_\pm\, S_{\lambda,\epsilon}\, P_\mp||_{H.S.} \overset{\epsilon\to 0}{\longrightarrow} 0$. Then $(\Omega, \hat{S}_{\lambda,\epsilon}\,\Omega) \overset{\epsilon\to 0}{\longrightarrow} 1$.
- In the overcritical case: $||P_\pm\, S_{\lambda,\epsilon}\, P_\mp|| \overset{\epsilon\to 0}{\longrightarrow} 1$. Then $(\Omega, \hat{S}_{\lambda,\epsilon}\,\Omega) \overset{\epsilon\to 0}{\longrightarrow} 0$.

The proof in the subcritical case is simple. There, by the adiabatic theorem, the adiabatic limit reduces to the static case.

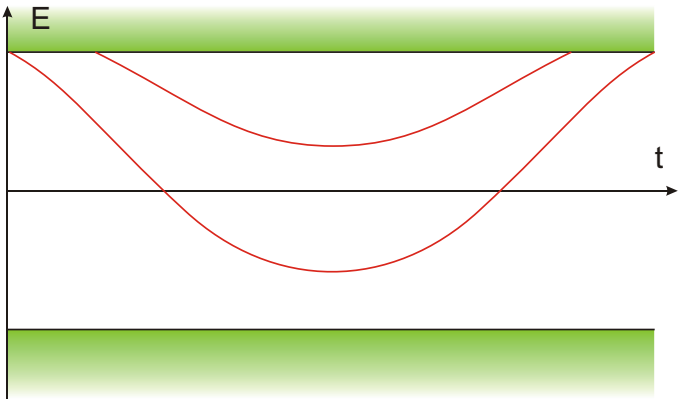


Figure 4.3: Strongly subcritical evolution.

If “negative” and “positive” parts of the spectrum stay separated, then

$$\lim_{\epsilon\to 0} ||P_\pm\, S_{\lambda,\epsilon}\, P_\mp||_{H.S.} \;=\; ||P_\pm\, S_{\lambda,0}\, P_\mp||_{H.S.} \;=\; 0 \tag{4.4.17}$$

The overcritical case is much more difficult. Until very recently (2005) there was no proof of the fact

$$||P_\pm\, S_{\lambda,\epsilon}\, P_\mp|| \overset{\epsilon\to 0}{\longrightarrow} 1. \tag{4.4.18}$$

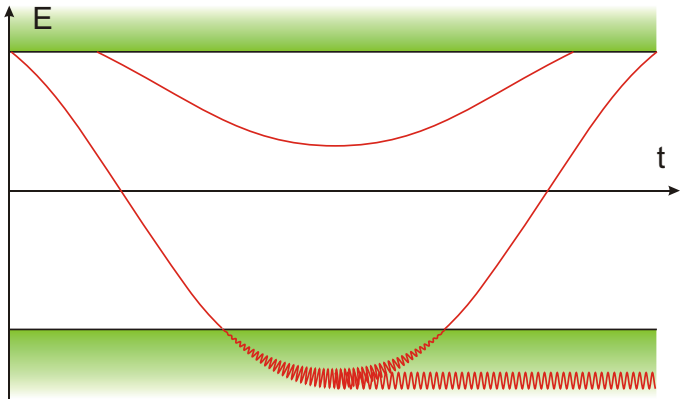


Figure 4.4: Strongly overcritical evolution.

Problems in the theory

First, we want to address problems which make the proof difficult. It is obvious that only the lowest lying eigenvalue (lowest line on fig. 4.4) contributes to the result. Therefore consider a simplified situation where only one eigenvalue was present, which for $t \to \pm\infty$ vanishes in the positive continuum $[1, \infty)$ (what is a consequence of asymptotic vanishing of the potential) and in some period $t \in [-T, T]$ vanishes in the lower continuum $(-\infty, -1]$. (One could also consider situations where the potential tends asymptotically to some limiting value, such that the limiting Hamiltonian has bound states (dotted line on the figure below). Though, this would not eliminate the following difficulties, because scattering in presence of bound states has its own problems.)

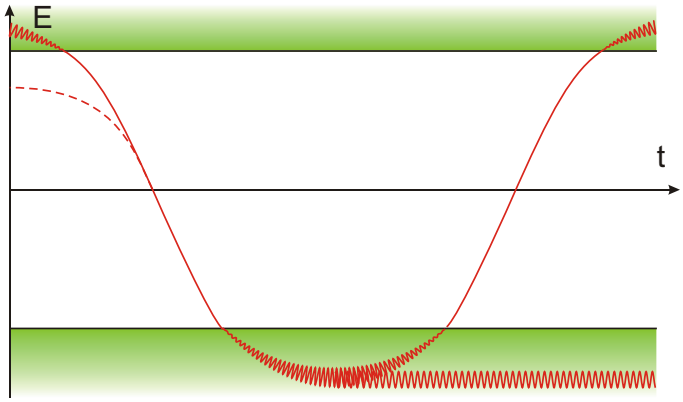


Figure 4.5: Strongly overcritical evolution (only the lowest eigenvalue shown).

In order to prove $||P_- \; S_{\lambda,\epsilon} \; P_+|| \overset{\epsilon\to 0}{\longrightarrow} 1$ one must find a vector $\phi \in \mathcal{H}^0_+$ which will be fully transported to $\chi \in \mathcal{H}^0_-$ by $S_{\lambda,\epsilon}$ for every small $\epsilon > 0$ and $\lambda > \lambda_{cr}$. This is not a simple task, because it turns out that $S_{\lambda,\epsilon}$ tends weakly to the static $S_{\lambda,0}$, what implies that all scalar products of interest are in the adiabatic limit zero

$$S_{\lambda,\epsilon} \overset{\text{weakly}}{\longrightarrow} S_{\lambda,0} \quad \Rightarrow \quad \forall_{\chi,\phi\in\mathcal{H}} \; \langle \chi | P_- \; S_{\lambda,\epsilon} \; P_+ \; \phi \rangle \overset{\epsilon\to 0}{\longrightarrow} \langle \chi | P_- \; S_{\lambda,0} \; P_+ \phi \rangle = 0. \qquad (4.4.19)$$

Even worse, $S_{\lambda,\epsilon}$ tends also strongly to the static $S_{\lambda,0}$, what implies that no initial vector $\phi \in \mathcal{H}^0_+$ can be transported to the lower continuum in the adiabatic limit

$$S_{\lambda,\epsilon} \overset{\text{strongly}}{\longrightarrow} S_{\lambda,0} \quad \Rightarrow \quad \forall_{\phi\in\mathcal{H}} \, ||P_- \, S_{\lambda,\epsilon} \, P_+ \, \phi|| \overset{\epsilon\to 0}{\longrightarrow} 0. \tag{4.4.20}$$

This is not valid if the initial state can be a bound state ϕ_0, but independently of this the problem remains in the opposite direction

$$S^*_{\lambda,\epsilon} \overset{\text{strongly}}{\longrightarrow} S^*_{\lambda,0} \quad \Rightarrow \quad \forall_{\chi\in\mathcal{H}} \, ||P_+ \, S^*_{\lambda,\epsilon} \, P_- \, \chi|| \overset{\epsilon\to 0}{\longrightarrow} 0 \quad \Rightarrow \quad N_\chi \overset{\epsilon\to 0}{\longrightarrow} 0 \tag{4.4.21}$$

where it has the consequence that the number of particles created in a given final state $\chi \in \mathcal{H}^0_-$ is zero in the adiabatic limit. Yet there is no convergence of $S_{\lambda,\epsilon}$ to the static $S_{\lambda,0}$ in norm, what finally allows the total number of particles created from vacuum to be non-zero

$$S_{\lambda,\epsilon} \overset{\text{norm}}{\nrightarrow} S_{\lambda,0} \quad \Rightarrow \quad ||P_- \, S_{\lambda,\epsilon} \, P_+|| \overset{\epsilon\to 0}{\nrightarrow} 0 \quad \Rightarrow \quad N^\epsilon_\pm \overset{\epsilon\to 0}{\nrightarrow} 0, \quad (\Omega, \hat{S}_{\lambda,\epsilon} \, \Omega) \overset{\epsilon\to 0}{\nrightarrow} 1 \tag{4.4.22}$$

Observe that the total number of created positrons $N^\epsilon_- = ||S_{\lambda,\epsilon}||^2_{HS} = \sum_n ||P_- S_{\lambda,\epsilon} P_+ f_n||^2$ tends, according to (4.4.20), term-wise to zero, but does not converge as a sum as $\epsilon \to 0$. This shows how subtle the effect of spontaneous particle creation in the adiabatic limit is. From the above it follows that the limit $||P_- \, S_{\lambda,\epsilon} \, P_+|| \overset{\epsilon\to 0}{\longrightarrow} 1$ cannot be shown by construction of initial and final vectors $\phi \in \mathcal{H}^0_+$, $\chi \in \mathcal{H}^0_-$ such that $S_{\lambda,\epsilon}\phi = \chi$. Rather one has to accept that the initial and final vectors are "somewhere in the continuum" and depend on ϵ. Then one must show that

$$\forall \, \epsilon > 0 \quad \exists \, \phi_\epsilon \in \mathcal{H}^0_+, \; \chi_\epsilon \in \mathcal{H}^0_- : \quad S_{\lambda,\epsilon} \, \phi_\epsilon = \chi_\epsilon. \tag{4.4.23}$$

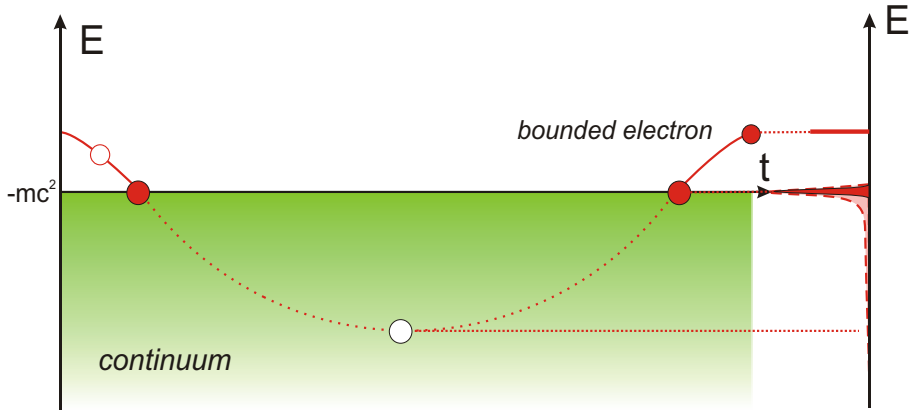
The proof

Only very recently, in 2005, Pickl [Pic05] was able to proof the conjecture in full generality what regards the strength of the potential and its time-dependence. Yet, could consider only compactly supported potentials (excluding e.g. the (regularized-)Coulomb potential). Assuming that the eigenvalue dives to the continuum with a finite slope, i.e. $dE_0(t)/dt \to \gamma < 0$ as $E_0(t) \to -1^+$ (cf. section 3.3.3 and equation (3.3.12)), he showed that the decay of the wave function $\Psi(t)$ (in the sense $||\Psi(t)||_\infty = O(1)$) occurs after $t \sim \epsilon^{-2/3}$, what is less than the duration of the overcritical phase $T \sim \epsilon^{-1}$. Hence the wave packet decays completely and in the adiabatic limit

$$\lim_{\epsilon\to 0} (\psi_0(t), \Psi(t)) = 0 \qquad \forall \, t > T/\epsilon, \tag{4.4.24}$$

i.e. the wave function $\Psi(t)$ does not dive out with the reappearing bound state $\psi_0(t)$ (at $\epsilon t > T$), but remains trapped in the negative continuum. The proof is relatively complicated technically (about 80 pages of text) and we will not cite it here. As we mentioned at the beginning of this section, it solves the problem of a slow decay of narrow

peaks at the edge of continuum ($T_{decay} \sim 1/\Gamma$ and $\Gamma \to 0$ as $E_R \to -1^-$). It also confirms our expectation that **in the adiabatic limit the wave function finally trapped in the negative continuum will be localized at its edge, implying that the spectrum of the spontaneously created antiparticles will have energies peaked at $E \approx 1^+$ (i.e. $E \approx mc^2$ in physical units) and hence momenta (almost) equal to zero**.



The scenario

Concluding, we present the scenario of particle creation in subsequent phases of the evolution. Adiabatic processes have the advantage of possessing a well defined and physically meaningful vacuum vector at every time, namely Ω_t defined by the current projector $P_\pm(t)$ with respect to the spectrum of the instantaneous Hamiltonian $H(t)$. These vacua are related to the initial one $\Omega \equiv \Omega_{-\infty}$ by

$$\Omega_t = \hat{W}_-^*(t)\,\Omega, \tag{4.4.25}$$

where $\hat{W}_-(t)$ is an implementer of the past wave operator $W_-(t) \equiv \lim_{s\to-\infty} U(t,s)e^{i(t-s)H_0}$ and $U(t,s)$ is the adiabatic evolution operator (their special implementation properties will be discussed in the next section 4.4.2). Accordingly, particles $\hat{b}_t(P_+(t)\,\varphi)$ and antiparticles $\hat{d}_t(P_-(t)\,\varphi)$ are defined with respect to the instantaneous vacuum Ω_t. Then, we distinguish the following stages, characterized by the behaviour of the state vector $\Phi(t) = \hat{W}_-(t)\,\Omega$ and the lowest eigenvalue $E_0(t)$:

- initial: $\Phi(-\infty) = \Omega$,
- weakly subcritical ($E_0(t) > 0$): $\Phi(t) = \Omega_t$,
- weakly overcritical ($-1 < E_0(t) < 0$): $\Phi(t) = \hat{d}'^*(P_-(t)\,\psi_0(t))\,\Omega_t$ – one antiparticle in a bound state $\psi_0(t)$ w.r.t. the charged vacuum Ω_t,
- strongly overcritical ($E_0(t)$ dived into the negative continuum): $\Phi(t) = \hat{d}'^*(P_-(t)\,\Psi(t))\,\Omega_t$, (where $\Psi(t) \in \mathcal{H}_-(t)$) – one antiparticle in a scattering state $\Psi(t)$ w.r.t. the charged vacuum Ω_t,

- weakly overcritical ($-1 < E_0(t) < 0$): $\Phi(t) = \hat{d}'^*(P_-(t)\ \Psi(t))\ \Omega_t$ – one antiparticle in a scattering state $\Psi(t)$ w.r.t. the charged vacuum Ω_t,
- weakly subcritical ($E_0(t) > 0$): $\Phi(t) = \hat{b}'^*(P_+(t)\ \psi_0(t))\ \hat{d}'^*(P_-(t)\ \Psi(t))\ \Omega_t$ – one antiparticle in a scattering state $\Psi(t)$ and one particle in a bound state $\psi_0(t)$ w.r.t. the neutral vacuum Ω_t,
- **final:** $\boxed{\Phi(\infty) = \hat{b}'^*(P_+\ \psi_0(\infty))\ \hat{d}'^*(P_-\ \chi)\ \Omega}$ **– one antiparticle in a scattering state χ and one particle in a bound or scattering state $\psi_0(\infty)$ w.r.t. the neutral vacuum Ω_t.**

Problems in the numerics

The above discussed subtlety of the effect of spontaneous particle creation in the adiabatic limit causes huge problems in the numerical simulation of the evolution or scattering. First note, that the limit in norm of a sequence of operators (here: the adiabatic limit $\epsilon \to 0$) can differ from the strong limit only on the infinite dimensional Hilbert space $\dim \mathcal{H} = \infty$. Theoretically this condition is satisfied in the Dirac theory, but in numerical calculations one always has $\dim \mathcal{H}_{num} < \infty$, because there is no way to simulate a true continuum, which must be replaced with a finite (e.g. cut-off in energies) discretized one. It implies that **using any asymptotically static basis in the discretized continuum, independent of ϵ, there is no possibility of observing the spontaneous particle creation by performing a (numerical) adiabatic limit**.

The reason can be understood in terms of decay of a wave packet in continuum. The wave packet in the negative continuum representing ϕ_ϵ evolved to times $t \approx 0$ decays in the adiabatic limit, because as ϵ tends to zero the duration of the overcritical phase increases, so the wave packet is evolved for longer and longer times. But wave packets in continuum decay and after a long time never come back to the initial shape, what is the necessary condition to build a localized wave function corresponding to the bound state eventually diving out of the continuum. The "decayed" wave packet remains forever in the negative continuum and builds asymptotically χ_ϵ. On the contrary, in a numerical finite dimensional discretized continuum no wave packet decay occurs – it returns periodically near its initial shape. Therefore standard numerical procedures cannot show the effect of spontaneous particle creation in the adiabatic limit.

However, there is a possibility of making better numerics, modifying the way of approaching the adiabatic limit. Assume that the discretized continuum states correspond to generalized eigenvectors to discrete values of energy. Let the energy levels be equidistant with gaps ΔE. Observe, that although no true decay of wave packets is possible, the evolution in the discrete system is a good approximation to the continuous one for times $t \lesssim 1/\Delta E$ (it is a characteristic time-scale of the discrete evolution, after which the artificial oscillations begin). Hence, it cannot be a good approximation in the adiabatic limit, where the numerical time of evolution T must grow as $1/\epsilon$, when $\epsilon \to 0$.

But one can modify this procedure by making the discretization gap ΔE dependent on ϵ, namely $\Delta E(\epsilon) \sim \epsilon \sim 1/T$. Then one can reach a good approximation for times $t \lesssim 1/\Delta E(\epsilon) \sim 1/\epsilon \sim T$. Unfortunately, numerical expense of such a scheme is huge and grows like $\sim 1/\epsilon^4$. This scaling makes reaching of the adiabatic limit in a numerical simulation practically impossible.

4.4.2 Adiabatic switch on of the potential

Actually, the adiabatic switch on process is a part of the adiabatic switch on and off process, which he have discussed in the previous section 4.4.1. Here, we want to discuss the (above postponed) procedure and physical consequences of implementation of the evolution operator $U(t_2, t_1)$ and of the wave operator $W_-(t)$ in the general situation of an adiabatically switched on potential.

Assume that at the initial time t_1 the Hamiltonian is $H(t_1) = H_0 + V(t_1) \equiv H_1$, the corresponding spectral projectors are $P_\pm$ and the vacuum is denoted by Ω. At the final time t_2 the Hamiltonian is $H(t_2) = H_0 + V(t_2) \equiv H_2$, the projectors are $P'_\pm$ and the vacuum Ω'. The evolution $U(t_2, t_1)$ is adiabatic, what means

$$U(t_2, t_1) P_{\varrho(t_1)}(H_1) = P_{\varrho(t_2)}(H_2) U(t_2, t_1), \tag{4.4.26}$$

where $P_{\varrho(t)}(H(t))$ describes a spectral projection on part $\varrho(t)$ of the spectrum of $H(t)$, which varies continuously and stays isolated from the rest of the spectrum during the evolution. Assume, at $t = t_1$ there are bound states ψ_n ($n = 0, 1, 2, ..., N$, where N finite or infinite) with energies $0 < E_n < 1$ and they moves continuously without crossing to ψ'_n with E'_n at $t = t_2$. Let $0 < E'_n < 1$ for $n = 1, 2, ...$ and consider different values of E'_0. From the adiabaticity of the evolution follows for the bound states

$$U(t_2, t_1) P_{\psi_n} = P_{\psi'_n} U(t_2, t_1) \quad \text{for} \quad n = 0, 1, 2, ... \tag{4.4.27}$$

where $P_{\psi_n} = P_{E_n}(H_1)$ is a projection on state ψ_n. It means that $U(t_2, t_1)$ maps the bound states onto each other

$$U(t_2, t_1) \psi_n = \psi'_n \quad \text{for} \quad n = 0, 1, 2, ... \tag{4.4.28}$$

Since the continuous spectra of H_1 and H_2 are equal, it holds

$$U(t_2, t_1) P_{\sigma_\pm} = P'_{\sigma_\pm} U(t_2, t_1), \tag{4.4.29}$$

where we have simplified the notation introducing $P_{\sigma_\pm} \equiv P_{\sigma_\pm}(H_1)$ and $P'_{\sigma_\pm} \equiv P_{\sigma_\pm}(H_2)$ with $\sigma_+ \equiv [1, \infty)$ and $\sigma_- \equiv (-\infty, -1]$). In order to construct the implementer $\hat{U}$ of $U(t_2, t_1)$ by theorem 3 we need the partial evolution operators

$$U_{\pm' \pm} \equiv P'_{\pm'} U(t_2, t_1) P_\pm, \tag{4.4.30}$$

which in case of the adiabatic evolution can be calculated explicitly. We only need to consider three physically different cases:

A) weakly subcritical: $0 < E_0' < 1$,

B) weakly overcritical: $-1 < E_0' < 0$,

C) strongly overcritical: E_0' dissolved in the negative continuum.

Then, using (4.4.27) and (4.4.29) and writing U for $U(t_2, t_1)$, we obtain

A) weakly subcritical: $0 < E_0' < 1$,

$$\begin{aligned}
U_{--} &= P'_{\sigma_-} U P_{\sigma_-} = U(P_{\sigma_-})^2 = U P_{\sigma_-} = U P_- \\
U_{++} &= \left(P'_{\sigma_+} + \sum_{n=0}^{N} P_{\psi'_n}\right) U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = P'_{\sigma_+} U P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi'_n} U P_{\psi_n} \\
&= U\left((P_{\sigma_+})^2 + \sum_{n=0}^{N} (P_{\psi_n})^2\right) = U P_+ \\
U_{+-} &= \left(P'_{\sigma_+} + \sum_{n=0}^{N} P_{\psi'_n}\right) U P_{\sigma_-} = U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) P_{\sigma_-} = 0 \\
U_{-+} &= P'_{\sigma_-} U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = U P_{\sigma_-} \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = 0
\end{aligned} \tag{4.4.31}$$

hence $\dim\ker U_{--} = \dim\ker U_{++} = 0$ and no special states exist.

B) weakly overcritical: $-1 < E_0' < 0$,

$$\begin{aligned}
U_{--} &= \left(P'_{\sigma_-} + P_{\psi'_0}\right) U P_{\sigma_-} = U\left(P_{\sigma_-} + P_{\psi_0}\right)(P_{\sigma_-}) = U P_- \\
U_{++} &= \left(P'_{\sigma_+} + \sum_{n=1}^{N} P_{\psi'_n}\right) U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = P'_{\sigma_+} U P_{\sigma_+} + \sum_{n=1}^{N} P_{\psi'_n} U P_{\psi_n} \\
&= U\left((P_{\sigma_+})^2 + \sum_{n=1}^{N} (P_{\psi_n})^2\right) = U(P_+ - P_{\psi_0}) \\
U_{+-} &= \left(P'_{\sigma_+} + \sum_{n=1}^{N} P_{\psi'_n}\right) U P_{\sigma_-} = U \left(P_{\sigma_+} + \sum_{n=1}^{N} P_{\psi_n}\right) P_{\sigma_-} = 0 \\
U_{-+} &= (P'_{\sigma_-} + P_{\psi'_0}) U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = U(P_{\sigma_-} + P_{\psi_0}) \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = U P_{\psi_0}
\end{aligned} \tag{4.4.32}$$

hence $\dim\ker U_{--} = 0$, $\dim\ker U_{++} = 1$ and one special state exists: $U_{-+}\psi_0 = \psi'_0$.

C) strongly overcritical: E_0' dissolved in the negative continuum, namely $U(t_2, t_1)\psi_0 =$

$\widetilde{\psi'_0} \in P'_{\sigma_-}\mathcal{H}$,

$$
\begin{aligned}
U_{--} &= P'_{\sigma_-} U P_{\sigma_-} = U\left(P_{\sigma_-} + P_{\psi_0}\right)(P_{\sigma_-}) = UP_- \\
U_{++} &= \left(P'_{\sigma_+} + \sum_{n=1}^{N} P_{\psi'_n}\right) U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = P'_{\sigma_+} U P_{\sigma_+} + \sum_{n=1}^{N} P_{\psi'_n} U P_{\psi_n} \\
&= U\left((P_{\sigma_+})^2 + \sum_{n=1}^{N} (P_{\psi_n})^2\right) = U(P_+ - P_{\psi_0}) \\
U_{+-} &= \left(P'_{\sigma_+} + \sum_{n=1}^{N} P_{\psi'_n}\right) U P_{\sigma_-} = U\left(P_{\sigma_+} + \sum_{n=1}^{N} P_{\psi_n}\right) P_{\sigma_-} = 0 \\
U_{-+} &= P'_{\sigma_-} U \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = U(P_{\sigma_-} + P_{\psi_0}) \left(P_{\sigma_+} + \sum_{n=0}^{N} P_{\psi_n}\right) = UP_{\psi_0}
\end{aligned}
\tag{4.4.33}
$$

hence $\dim\ker U_{--} = 0$, $\dim\ker U_{++} = 1$ and one special state exists: $U_{-+}\psi_0 = \widetilde{\psi'_0}$.

Summarizing, in all cases the auxiliary operators of theorem 3 describing the dynamical pair creation and annihilation are trivial $A = D = 0$, what is a special property of the adiabatic evolution. The operators B and C, describing separate evolution of particles and antiparticles, respectively, are non-zero, but they do not play any role if $\hat{U}$ acts on the vacuum. The special part of $\hat{U}$, namely $\hat{U}_0$, describing creation of a special (anti-)particle is trivial $\hat{U}_0 = \mathbf{1}$ in case A and non-trivial $\hat{U}_0 = \hat{d}^*(V\psi'_0)$ in cases B and C, where we need to introduce the operator V describing the change of the projectors from $P_\pm$ to $P'_\pm$ and guaranteeing the expression of the final state in terms of the final vacuum by $\hat{V}^*\Omega = \Omega'$ (cf. section 4.3.2 for more details). Therefore, the state evolved from vacuum in the adiabatic evolution from t_1 to t_2 is

$$
\boxed{
\Phi = \hat{V}^*\,\hat{U}\,\Omega = \begin{cases} \hat{V}^*\,\Omega = \Omega' & \text{in case A,} \\ \hat{V}^*\left(\hat{d}^*(V\psi'_0)\,\Omega\right) = & \begin{cases} \hat{d}'^*(\widetilde{\psi'_0})\,\Omega' & \text{in case B,} \\ \hat{d}'^*(\psi'_0)\,\Omega' & \text{in case C.} \end{cases} \end{cases}
}
\tag{4.4.34}
$$

We conclude that **in the weakly subcritical case (A) nothing interesting happens and vacuum remains vacuum, hence we call this vacuum stable**. In cases B and C an antiparticle is created with respect to the final vacuum, while the vacuum state Ω' itself becomes positively charged relative to Ω, so that the total charge with respect to Ω is conserved in the evolution. It seems that the vacuum in these both cases becomes unstable during the evolution and decays to a different one by producing an antiparticle. Yet it is not obvious that it has physically the same meaning in both cases. **In the strong overcriticality case (C) the created antiparticle is in a scattering state $\widetilde{\psi'_0}$ and when evolved further, after long enough time, will depart to spatial infinity, where it can be detected in experiment. In contrast,**

in the weak overcriticality case (B) the antiparticle occupies a bound state ψ'_0 and together with the positively charged vacuum Ω' forms a stable composite, which probably cannot be detected by any charge-based measurement. Such interpretation is in agreement with the fact that two unitarily equivalent representations of CAR describe the same physical situation and cannot be distinguished. **The weakly overcritical (B) and weakly subcritical (A) situations are unitarily equivalent** (cf. section 2.4.5), so the structure of the final state is a matter of choice of the final projector. If we chose instead of $P'_\pm = (1 \pm \mathrm{sgn}(H_1))/2$, what gives

$$P'_+ = P_{[0,\infty)}(H_1) \quad \text{and} \quad P'_- = P_{(-\infty,0)}(H_1), \tag{4.4.35}$$

a different pair (used by Greiner *et al.* [GMR85, RMG74, RMG81])

$$P''_+ = P_{(-1,\infty)}(H_1) \quad \text{and} \quad P''_- = P_{(-\infty,-1]}(H_1), \tag{4.4.36}$$

we would have a vacuum as a final state, as in case A. Since by theorem 2 the projectors give rise to equivalent representations of CAR, all physical consequences must be the same.

4.5 Spontaneous particle creation in a weaker sense

The "weaker sense" means that we relax the stability condition for creation of (anti-)particles in a special state and check what happens near such a point.

Until now we have only considered the creation of (anti-)particles in special states, what was possible in overcritical as well as subcritical potentials. Yet, this phenomenon, in general, turned out to be unstable under small perturbations of the potential. The only situation, when stability was guaranteed, i.e. a pair particle-antiparticle was always created, was the adiabatic limit of a scattering process in presence of an overcritical potential. But, due to the slowness of the switching on to overcriticality, the whole wave function (in the Dirac equation) decays already at the edge of the continuum giving rise to production of antiparticles with vanishing momentum. The result, although mathematically correct, is not fully satisfactory from the physical point of view for two reasons. First, adiabatic processes are not realizable in experiment and the adiabatic limit itself does not provide enough information about general slow processes. Although, in the proof of Pickl [Pic05] one can find estimates on the decay of the wave function for small adiabatic parameters ϵ and use them to estimate the energy distribution of the created antiparticles, which will obviously be localized at the edge of the negative continuum, one cannot extrapolate them to bigger values of ϵ corresponding to quicker processes. Second, the adiabatic result depends on the position and properties of the resonance appearing in the negative continuum due to overcriticality only at the edge of the continuum – later, it is completely independent of how the resonance behaves. It is in deep disagreement with a more intuitive result for quick processes, where the resonance becomes a remnant of the dissolved bound state, "carries" in form of a wave packet its (nearly whole) amplitude and decays accordingly

to its spectral width, finally contributing to the creation of antiparticles with the same spectral distribution. Of course, we do not indent and cannot discredit a proved result in the adiabatic limit. We only point out that it is of limited use in understanding of pair creation in general time-dependent overcritical potentials with physical parameters.

Pair creation in special states is described schematically by

$$\hat{S}\,\Omega = C_0\,\hat{b}^*(\chi^+)\,\hat{d}^*(\chi^-)\,\Omega, \tag{4.5.1}$$

(where we neglect possible other pairs in non-special states), and is due to the fact that $\chi^\pm \in \mathcal{H}^0_\pm$ are eigenvectors of $S_{\pm\mp}(S_{\pm\mp})^*$ to the eigenvalue 1. It means that S maps a vector (one for each sign) from $\mathcal{H}^0_\pm$ to $\mathcal{H}^0_\mp$, so there exist $\phi^\pm \in \mathcal{H}^0_\pm$ such that $S_{\pm\mp}\phi^\mp = \chi^\pm$. In section 4.3 we have shown that such a phenomenon is unstable with respect to small changes in the potential's strength λ. Perturbing the potential slightly results in destroying the existence of eigenvalues 1 of $S_{\pm\mp}(S_{\pm\mp})^*$ and making them smaller than 1. By continuity in λ, the vectors $\chi^\pm$ and ϕ^+ will change only slightly, but it cannot be avoided that each of them will get an admixture belonging in to the other spectral subspace $\mathcal{H}^0_\pm$. Now, there will exist a pair of vectors $\phi'^\pm \in \mathcal{H}^0_\pm$ such that

$$S'\phi'^\pm = \chi'^\pm = (P_+ + P_-)\chi'^\pm \equiv \chi'^\pm_+ + \chi'^\pm_- \equiv \alpha^\pm\chi''^\pm_+ + \beta^\pm\chi''^\pm_- \tag{4.5.2}$$

with $||\chi''^\pm_+|| = ||\chi''^\pm_+|| = 1$ and $|\alpha^\pm|, |\beta^\pm| < 1$, $|\alpha^\pm|^2 + |\beta^\pm|^2 = 1$. By continuity in λ the norms of the "admixtures" $||\chi'^+_-|| = |\beta^-|$ and $||\chi'^-_+|| = |\alpha^+|$ should be small, i.e. $\alpha^+, \beta^- \approx 0$. Implementation of S' gives essentially a "regular" pair creation (i.e. no special states)

$$\hat{S}'\,\Omega = C'_0\ :\exp\left(D\,\hat{b}^*(\chi''^+_+)\,\hat{d}^*(\chi''^+_-)\right):\Omega = C'_0\,\left(1 + D\,\hat{b}^*(\chi''^+_+)\,\hat{d}^*(\chi''^+_-)\right)\Omega, \tag{4.5.3}$$

where (cf. theorem 3)

$$D = (\chi''^+_-, S'_{-+}(S'_{++})^{-1}\chi''^+_+) = \left(\chi''^+_-, S'_{-+}\frac{1}{\alpha^+}\phi'^+\right) = \left(\chi''^+_-, \frac{\beta^+}{\alpha^+}\chi''^+_-\right) = \frac{\beta^+}{\alpha^+} \tag{4.5.4}$$

is very big, because $\alpha^+ \approx 0$. (The limit $\alpha^+ \to 0$ is non-trivial, what is manifested by change in the structure of $\hat{S}$, as shown in [Sei82].) The normalization constant C'_0 satisfies

$$1 = ||\hat{S}'\,\Omega||^2 = |C'_0|^2(1 + |D|^2), \tag{4.5.5}$$

what gives

$$|C'_0| = \frac{1}{\sqrt{1+|D|^2}} = \frac{1}{\sqrt{1+\frac{|\beta^+|^2}{|\alpha^+|^2}}} = \frac{|\alpha^+|}{\sqrt{|\alpha^+|^2+|\beta^+|}} = |\alpha^+|. \tag{4.5.6}$$

Therefore, we can rewrite (4.5.3) as

$$\hat{S}'\,\Omega = e^{i\vartheta}\left(\alpha^+ + \beta^+\,\hat{b}^*(\chi''^+_+)\,\hat{d}^*(\chi''^+_-)\right)\Omega, \tag{4.5.7}$$

what explicitly shows that in the neighbourhood of the case when special pairs (4.5.1) are created with probability 1, the probability of a pair creation is still big ($|\beta^+|^2 \approx 1$).

On the one hand, this result can be applied for any potentials (sub- or overcritical) in any processes (quick or slow), where it implies that the special pair creation (4.5.1) is reached smoothly as a limit of a non-special pair creation (4.5.3) by small variation of the potential [Sei82] (confirmed also numerically in case of heavy ion collisions [RMMG81]). Therefore, no abrupt change in the rate of the pair creation occurs and no essential difference between sub- and overcritical potentials is observed, what has been used as a main argument against the existence (or significance) of the spontaneous pair creation [SS82]. This reasoning is not acceptable, mainly due to a very restrictive definition of the spontaneous particle creation *(stronger sense)* and too wide class of possible scattering processes considered.

On the other hand, the neighbourhood of the special case discussed above can be interpreted as a neighbourhood of an adiabatic process, i.e. a general slow scattering process (but different from the adiabatic limit), which according to the above result should produce a pair with a big probability due to the overcriticality of the potential. At the same time, no (or almost no) pair will be created in a slow subcritical process. **Therefore a jump in the rate of the pair creation occurs at the edge between sub- and overcritical processes. This we call *spontaneous particle creation in a weaker sense*. The *stronger sense* is defined by the condition of special states, or in other words, by probability 1 for pair creation and is realized only in the adiabatic limit.**

One can ask, how far one can depart from the adiabatic limit, i.e. how quick a scattering process can be, to give still a significant probability for pair creation due to overcriticality. The first answer could be that as the process becomes quick one looses control over the jumps between all possible states during the evolution of the Dirac wave function, so the probabilities of finding $S\phi^+$ in the positive and negative continua become of the same order, i.e. $\alpha^+ \approx \beta^+$. But this does not differ from quick subcritical processes, what suggests that slowness (or adiabaticity) is the necessary condition to have an essential overcritical pair creation. Yet, in practice the situation is more advantageous due to a resonance which appears for the overcritical potentials and modifies the negative continuum wave functions in such a way that they contain most of the wave function evolved from an initial bound state, even in a very quick diving process. To see the effect if suffices to consider a sudden jump process, being the worst possible case as a limit of extremely quick processes, in which a bound state disappears immediately for the switched on overcritical potential. The amount of the initial bound state ψ_0 in the overcritical negative continuum (projection: P'_-) is usually big, i.e. $||P'_-\psi_0|| \approx 1$ (cf. section 6.2.2). It bears some similarity to subcritical situations, where the potential changes quickly. In the limit of a sudden jump the amplitude to find the wave function of an initial bound state in the final bound state

is (ψ_0', ψ_0), which can be estimated by the perturbation theory

$$(\psi_0', \psi_0) = 1 + \mathcal{O}(\Delta V). \tag{4.5.8}$$

There is one essential difference between slow evolution of bound states and of resonances (by which we will here mean wave packets corresponding to a dived bound state in the continuum). For bound states the slower the process is the more stable the state becomes, in the sense that by the adiabatic theorem the amplitude of a wave function evolved from an initial bound state $\psi_0(0)$ in a final bound state $\psi_0(T)$ behaves like

$$||U(T,0)\ \psi_0(0) - \psi_0(T)|| = \mathcal{O}\left(\frac{1}{T}\right), \tag{4.5.9}$$

what implies

$$A_0(T) \equiv (\psi_0(T), U(T,0)\ \psi_0(0)) = 1 + \mathcal{O}\left(T^{-2}\right) \overset{T\to\infty}{\longrightarrow} 1. \tag{4.5.10}$$

For resonances the effect of slow evolution is the opposite, because a wave packet ψ_R, in contrast to a bound state, decays (hence we call it unstable)

$$A_R(T) \equiv (\psi_R(T), U(T,0)\ \psi_R(0)) \overset{T\to\infty}{\longrightarrow} 0. \tag{4.5.11}$$

It is relatively simple to show it for evolution in presence of a constant potential where $U(T,0) = \exp(-iTH)$ and $\psi_R(T) = \psi_R(0)$. Decomposing the wave packet in continuum (ϕ_E are continuum wave functions)

$$\psi_R(t) = \int_\sigma a(E)\phi_E\ dE, \tag{4.5.12}$$

where $\sigma \subset \sigma_{cont}(H)$, and $\int_\sigma |a(E)|^2\ dE = 1$, we find

$$\begin{aligned} A_R(T) = (\psi_R(0), U(T,0)\ \psi_R(0)) &= \int_\sigma\int_\sigma \overline{a(E')}a(E)\left(\phi_{E'}, e^{-iTH}\phi_E\right)\ dE'\ dE \\ &= \int_\sigma\int_\sigma \overline{a(E')}a(E)e^{-iTE}\underbrace{(\phi_{E'}, \phi_E)}_{\delta(E'-E)}\ dE'\ dE \\ &= \int_\sigma |a(E)|^2 e^{-iTE}\ dE = \mathcal{O}\left(T^{-1}\right) \overset{T\to\infty}{\longrightarrow} 0. \end{aligned} \tag{4.5.13}$$

In fact, the estimation by $\mathcal{O}(T^{-1})$ is the weakest one, assuming only that $a(E)$ is square integrable. However, since the resonance is spectrally localized and usually smoothly distributed one gets stronger estimates, e.g. for a Breit-Wigner type distribution

$$a(E) = \frac{a_0}{\Gamma^2 + (E - E_0)^2} \qquad \to \qquad A_R(T) \sim e^{-\Gamma T} \tag{4.5.14}$$

and for Gaussian packets even faster.

These estimations hold only for constant (in that case overcritical) potentials with a static resonance. Yet, we are interested in situations where the resonance moves in the

continuum due to the varying overcritical potential. Although, no (analogous to bound states) adiabatic theorem for resonances is known, we will try to describe non-rigorously what happens to the amplitude $A_R(t)$ of a moving resonance during a slow evolution. Therefore, we will follow the ideas of a constructive proof of the adiabatic theorem given in [GP91]. Let the time interval $t \in [0, T]$ be parameterized by $t \equiv T\tau$ with $\tau \in [0, 1]$ and consider now τ as evolution parameter and T as a constant. Decompose the evolution operator into three parts

$$U_T(\tau) \equiv V(\tau)S_T(\tau)W_T(\tau) \tag{4.5.15}$$

which satisfy the following evolution equations

$$i\frac{dV(\tau)}{d\tau} = K(\tau)V(\tau), \quad V(0) = \mathbf{1}, \quad K(\tau) \equiv i\int_{\sigma(\tau)} \frac{dP_E(\tau)}{d\tau} P_E(\tau)d\mu(E), \tag{4.5.16}$$

where $P_E(\tau)$ are projectors on the basis states $\phi_E(\tau)$, which are chosen to be eigenvectors (bound states) or generalized eigenvectors (continuum) of the Hamiltonian $H(\tau)$, $\sigma(\tau) = \sigma(H(\tau))$ is the spectrum of $H(\tau)$ and $d\mu(E)$ is the corresponding spectral measure.

$$i\frac{dS_T(\tau)}{d\tau} = T\widetilde{H}(\tau)S_T(\tau), \quad S_T(0) = \mathbf{1}, \quad \widetilde{H}(\tau) \equiv V^*(\tau)HV(\tau) \tag{4.5.17}$$

and

$$i\frac{dW_T(\tau)}{d\tau} = -\widetilde{K}_T(\tau)W_T(\tau), \quad W_T(0) = \mathbf{1}, \quad \widetilde{K}_T(\tau) \equiv S_T^*(\tau)V^*(\tau)K(\tau)V(\tau)S_T(\tau). \tag{4.5.18}$$

The three operators $V(\tau), S_T(\tau), W_T(\tau)$ play the following roles. $V(\tau)$ rotates (in the Hilbert space) the eigenvectors of the initial Hamiltonian $H(0)$ to the corresponding eigenvectors of $H(\tau)$, for bound states according to continuity of the eigenvalues $E_n(\tau)$ and in continuum to the same value of E. It means that

$$P_{E_n}(\tau)V(\tau) = V(\tau)P_{E_n}(0) \quad \text{for} \quad |E_n| < 1, \tag{4.5.19}$$

$$P_E(\tau)V(\tau) = V(\tau)P_E(0) \quad \text{for} \quad |E| \geq 1. \tag{4.5.20}$$

$S_T(\tau)$ evolves the states $\phi_E(0)$ according to $\widetilde{H}(\tau)$, of which they are eigenvectors, hence it simply equips them with a phase $\exp(-iT\theta_E(\tau))$, where $\theta_E(\tau) \equiv \int_0^\tau E(\tau')d\tau'$

$$S_T(\tau) = \int_{\sigma(\tau)} e^{-iT\theta_E(\tau)} P_E(\tau)d\mu(E). \tag{4.5.21}$$

Finally, $W_T(\tau)$ describes time-changes exclusively due to the variation of the basis vectors $\phi_E(\tau)$. Summarizing, the action of the evolution operator $U_T(\tau)$ splits into three actions:

- jumps between basis states due to their time-change ($W_T(\tau)$),
- quasi-free evolution due to the action of the Hamiltonian ($S_T(\tau)$)
- and rotation to follow the changing basis vectors ($V(\tau)$).

The idea of the proof of a standard adiabatic theorem is to show (by cancellation of phases of all jump-between-states amplitudes) that $W_T(\tau) = \mathbf{1} + \mathcal{O}(1/T)$. Then $U_T(\tau) \cong V(\tau)S_T(\tau)$ as $T \to \infty$ and, acting on the eigenvectors,

$$U_T(\tau)P_{E_n}(0) \cong V(\tau)S_T(\tau)P_{E_n}(0) = e^{iT\theta_{E_n}(\tau)}V(\tau)P_{E_n}(0) = e^{iT\theta_{E_n}(\tau)}P_{E_n}(\tau). \quad (4.5.22)$$

Then the amplitude of the evolved bound state (4.5.10) can be estimated to

$$\begin{aligned} A_0(T) &= (\psi_0(T), U_T(1)\psi_0(0)) = \left(\psi_0(T), V(1)S_T(1)\left(\mathbf{1} + \mathcal{O}\left(\frac{1}{T}\right)\right)\psi_0(0)\right) \\ &= \left(1 + \mathcal{O}\left(\frac{1}{T}\right)\right)(V^*(1)\psi_0(T), S_T(1)\psi_0(0)) \\ &= \left(1 + \mathcal{O}\left(\frac{1}{T}\right)\right)(\psi_0(0), e^{-iT\theta_0(1)}\psi_0(0)) \\ &= \left(1 + \mathcal{O}\left(\frac{1}{T}\right)\right)e^{-iT\theta_0(1)}. \end{aligned} \quad (4.5.23)$$

In the case of a resonance we must use a projector on the wave packet $\psi_R(\tau)$ instead of a bound state, which has different properties especially with respect to $S_T(\tau)$, because it is not an eigenvector of $H(\tau)$ and therefore the action of $S_T(\tau)$ does not reduce to a simple multiplication by a phase factor. Although, using the above construction we can analogously calculate the amplitude (4.5.11) of the evolved time-dependent resonance. Taking $\tau = 1$ we find

$$\begin{aligned} A_R(T) &= (\psi_R(T), U(T,0)\,\psi_R(0)) \\ &= (\psi_R(T), U_T(1)\psi_R(0)) = (\psi_R(T), V(1)S_T(1)W_T(1)\psi_R(0)) \\ &= (S_T^*(1)V^*(1)\psi_R(T), W_T(1)\psi_R(0)) = (S_T^*(1)\psi_R(0), W_T(1)\psi_R(0)) \end{aligned} \quad (4.5.24)$$

The left-hand side of the scalar product can be expanded in the basis $\phi_E(0)$ using (4.5.12)

$$\begin{aligned} S_T^*(1)\psi_R(0) &= \int_{\sigma(\tau)} e^{iT\theta_E(1)}P_E(0)d\mu(E)\int_{\sigma(\tau)} a_{E'}(0)\phi_{E'}(0)d\mu(E') \\ &= \int_{\sigma(\tau)} e^{iT\theta_E(1)}a_E(0)\phi_E(0)d\mu(E). \end{aligned} \quad (4.5.25)$$

About the right-hand side we know that it decays like $W_T(\tau) = \mathbf{1} + \mathcal{O}(1/T)$ for big T. Thus

$$\begin{aligned} A_R(T) &= \left(\int_{\sigma(\tau)} e^{iT\theta_E(1)}a_E(0)\phi_E(0)d\mu(E), \left(\mathbf{1} + \mathcal{O}\left(\frac{1}{T}\right)\right)\psi_R(0)\right) \\ &= \left(1 + \mathcal{O}\left(\frac{1}{T}\right)\right)\cdot\left(\int_{\sigma(\tau)} e^{iT\theta_E(1)}a_E(0)\phi_E(0)d\mu(E), \int_{\sigma(\tau)} a_{E'}(0)\phi_{E'}(0)d\mu(E')\right) \\ &= \left(1 + \mathcal{O}\left(\frac{1}{T}\right)\right)\cdot \underbrace{\int_{\sigma(\tau)} e^{iT\theta_E(1)}|a_E(0)|^2\phi_E(0)d\mu(E)}_{\mathcal{O}(T^{-1}) \text{ or } \mathcal{O}(e^{-\Gamma T})}. \end{aligned} \quad (4.5.26)$$

About the last integral we know that it generally behaves like $\mathcal{O}(T^{-1})$, but for a Breit-Wigner distribution of $a_E(0)$, which is a typical shape of a resonance, it decays exponentially (cf. (4.5.14)). Finally we obtain

$$A_R(T) = \left(\mathbf{1} + \mathcal{O}\left(\frac{1}{T}\right)\right) \cdot \mathcal{O}(e^{-\Gamma T}). \tag{4.5.27}$$

Now we see clearly the difference between the adiabatic evolution of bound states (4.5.23) and resonances (4.5.27). Although the first factor (due to W_T) guarantees that there are almost no jumps due to the time-variation of the basis during the evolution, the second terms (due to S_T) differ essentially. Since a bound state is an eigenvector, whose adiabatic evolution becomes trivial and reduces to multiplication by a phase factor, the resonance is represented by a wave packet and decays usually exponentially in long and slow evolution.

We can conclude that evolving a wave function, starting from a bound state which dissolves in the negative continuum when the potential becomes overcritical, transforms it to a wave packet representing a resonance. This resonance moves deeper and deeper into the continuum as the strength of the potential increases further, yet the wave packet does not necessarily follow it. As we see from (4.5.27), there are essentially two factors preventing an optimal result to reach $A_R(T) \approx 1$, what requires both factors being big (≈ 1). In slow processes (tending to adiabaticity in a limit) the first factor tends to 1, but the second factor becomes very small due to the decay of the wave packet. In contrast, in quick processes (tending to a sudden jump in a limit) the second factor tends to 1 (because $S_T(1) \to \mathbf{1}$ as $T \to 0$), but the first one becomes less than one. Actually, the latter case seems more optimistic, because $W_T(\tau) \to V^*(\tau)$ as $T \to 0$. Therefore

$$\begin{aligned} A_R(T) &= (\psi_R(T), V(1)S_T(1)W_T(1)\psi_R(0)) \to (\psi_R(T), V(1)\mathbf{1}V^*(1)\psi_R(0)) \\ &= (\psi_R(T), \psi_R(0)) \end{aligned} \tag{4.5.28}$$

as $T \to 0$, what is not only non-zero, but can even be relatively big, when the difference between the initial and final Hamiltonians ΔV is not too big. In such case the perturbation theory gives the estimation

$$(\psi_R(T), \psi_R(0)) = 1 + \mathcal{O}(\Delta V). \tag{4.5.29}$$

We conclude with a somewhat surprising result that **the probability to observe the wave function in a final resonance state (localized apart from the edge of the continuum), which evolved from an initial bound state and eventually dived into the continuum, is bigger for quick processes than for slow ones. In the latter case the probability tends to zero due to the decay of the wave packet during its whole evolution along the moving resonance, mainly near the edge of the continuum, where the resonance appears. In case of quick processes it is unknown which rate of time-variation gives the optimal result, i.e. the maximal probability.**

The last question is difficult to answer in the above framework. The optimal result, when the product of both factors in (4.5.27) becomes maximal, can be an interplay between both, i.e. an optimal combination of the decay and the loss due to basis-rotation. However, we expect, that the optimal result is reached in the sudden-jump limit, but we were unable to proof it rigorously.

The question of optimal excitation of a final resonance state will be studied in the numerical part (part II) of this work. It has a big significance for the (spontaneous) pair creation in presence of overcritical potentials, because the amplitude of the resonance is the upper bound for the amplitude of pair creation. More precisely, the amplitude of pair creation with an antiparticle in the resonance state is just the part of the resonance, which has decayed during the overcritical period and this is bounded by the excitation amplitude of the resonance. To learn about the behaviour of this amplitude from the numerics we will consider potentials which vary from an initial subcritical value to an overcritical one at different rates, then stay overcritical to allow the wave packet decay (and contribute to an antiparticle production), and finally return to the initial subcritical value, producing an accompanying particle (in a bound state, when done adiabatically).

Part II

Examples and numerical study

Chapter 5

Dirac equation with a spherically symmetric square well potential

In this chapter we construct solutions to the Dirac equation in presence of a spherically symmetric potential well, which will be used in the next chapter, where we are going to study particle production in time-dependent overcritical potentials. The two-parameter class of the potential wells is sufficient to cover all cases of interest. The spatial profile of the potential is chosen to be a spherically symmetric square potential well, for which it is relatively simple to find all normalized wave functions – solutions of the stationary Dirac equation, to be used as a basis in the Hilbert space. We first give an introduction to the Dirac equation in presence of spherically symmetric potentials and construct the partial wave decomposition based on algebraic properties of the Dirac operator. Then we solve the Dirac equation for a two-parameter class of spherically symmetric potential wells, giving an orthogonal and normalized complete set of wave functions. Further, we analyze the structure and behaviour of bound states and by analytic continuation find resonances in the overcritical potentials.

5.1 Dirac equation in spherical symmetry

We consider the Dirac equation for a particle in the electromagnetic field

$$\left[\gamma^\mu \left(i\hbar\partial_\mu - \frac{e}{c}A_\mu(x)\right) - mc\right]\Psi(x) = 0 \tag{5.1.1}$$

where Ψ is a bispinor (Ψ_α, $\alpha = 1, .., 4$) and x stands for 4-coordinates in Minkowski space. It can be rewritten in the form

$$i\hbar\frac{\partial\Psi}{\partial t}(x) = \left[c\alpha^i\hat{p}_i + mc^2\beta + eA_0(x) + e\alpha^i A_i(x)\right]\Psi(x) \equiv \hat{H}\Psi(x), \tag{5.1.2}$$

where

- the total Hamiltonian: $\hat{H} = \hat{H}_0 + W$,

- the free Hamiltonian: $\hat{H}_0 = c\alpha^i \hat{p}_i + mc^2\beta$,
- the momentum operator: $\hat{p}_i = -i\hbar\partial_i$,
- the Dirac matrices: $\alpha^i = \gamma^0\gamma^i$, $\beta = \gamma^0$,
- and the potential: $W(x) = eA_0(x) + e\alpha^i A_i(x)$.

Let the potential be purely electric ($A_i(x) = 0$) and spherically symmetric: $W(x) = eA_0(x) \equiv V(r)$. The spherical symmetry allows for the decomposition of the Hilbert space (of Ψ at a given time)

$$\mathcal{H} = L^2(\mathbb{R}^3)^4 \simeq L^2(\mathbb{R}^1_+) \otimes L^2(S^2)^4. \tag{5.1.3}$$

There exist two operators which commute with the spherically symmetric Hamiltonian: the total orbital momentum operator $\vec{J} = \vec{L} + \vec{S}$ and the spin-orbit operator $K = \beta(2\vec{S}\cdot\vec{L} + 1)$ (with $\vec{L} = \mathbf{x} \wedge \vec{p}$ and $\vec{S} = \frac{1}{4i}(\vec{\alpha} \wedge \vec{\alpha})$). They are related by $K = \beta(\vec{J}^2 - \vec{L}^2 + \frac{1}{4})$.

We choose a complete set of orthonormal eigenvectors

$$\vec{J}^2\Phi_{m_j} = j(j+1)\Phi_{m_j}, \qquad j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, ... \tag{5.1.4}$$

$$J_3\Phi_{m_j} = m_j\Phi_{m_j}, \qquad m_j = -j, -j+1, ..., j \tag{5.1.5}$$

Every subspace (j, m_j) is 4-times degenerate ($\mathbb{C}^\infty(S^2)^4$ is 4-dimensional). Because K commutes with $\vec{J}$, we choose

$$K\Phi_{m_j,\kappa_j} = -\kappa_j\Phi_{m_j,\kappa_j}, \qquad \kappa_j = \pm(j + \frac{1}{2}). \tag{5.1.6}$$

The set (j, m_j, κ_j) is still 2-times degenerate. We write the vectors in the form

$$\Phi_{m_j,\kappa_j} = c^+\Phi^+_{m_j,\kappa_j} + c^-\Phi^-_{m_j,\kappa_j}, \tag{5.1.7}$$

where

$$\Phi^+_{m_j,\mp(j+\frac{1}{2})} = \begin{pmatrix} i\chi^{m_j}_{j\mp\frac{1}{2}} \\ 0 \end{pmatrix}, \quad \Phi^-_{m_j,\mp(j+\frac{1}{2})} = \begin{pmatrix} 0 \\ \chi^{m_j}_{j\pm\frac{1}{2}} 0 \end{pmatrix}, \tag{5.1.8}$$

and

$$\chi^{m_j}_{j-\frac{1}{2}} = \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j+m_j}\, Y^{m_j-\frac{1}{2}}_{j-\frac{1}{2}} \\ \sqrt{j-m_j}\, Y^{m_j+\frac{1}{2}}_{j-\frac{1}{2}} \end{pmatrix}, \tag{5.1.9}$$

$$\chi^{m_j}_{j+\frac{1}{2}} = \frac{1}{\sqrt{2j+2}} \begin{pmatrix} \sqrt{j+1-m_j}\, Y^{m_j-\frac{1}{2}}_{j+\frac{1}{2}} \\ -\sqrt{j+1+m_j}\, Y^{m_j+\frac{1}{2}}_{j+\frac{1}{2}} \end{pmatrix}. \tag{5.1.10}$$

Y_l^m $(l = 0, 1, 2, ...;\ m = -l, -l+1, ..., l)$ are spherical harmonics defined by means of the associated Legendre polynomials P_l^m

$$Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}P_l^m(cos\theta), \quad m>0 \tag{5.1.11}$$

$$P_l^m(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{m+l}}{dx^{m+l}}(x^2-1)^l \tag{5.1.12}$$

$$Y_l^{-m}(\theta,\phi) = (-1)^m\overline{Y_l^m(\theta,\phi)} \tag{5.1.13}$$

Then the "angular" part of the Hilbert space splits into a direct sum of the subspaces spanned by the eigenvectors to the eigenvalues (j, m_j, κ_j)

$$[L^2(S^2)] = \bigoplus_{j=\frac{1}{2},\frac{3}{2},...}^{\infty}\ \bigoplus_{m_j=-j}^{j}\ \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} \mathcal{K}_{m_j,\kappa_j}, \tag{5.1.14}$$

where

$$\mathcal{K}_{m_j,\kappa_j} = \left\{c^+\Phi^+_{m_j,\kappa_j} + c^-\Phi^-_{m_j,\kappa_j} | c^\pm \in \mathbb{C}\right\}. \tag{5.1.15}$$

The free Hamiltonian takes the form

$$H_0 = -i\hbar c(\vec{\alpha}\vec{e_r})\left(\partial_r + \frac{1}{r} - \frac{1}{r}\beta K\right) + \beta mc^2. \tag{5.1.16}$$

With respect to the basis $\left\{\Phi^+_{m_j,\kappa_j}, \Phi^-_{m_j,\kappa_j}\right\}$ in $\mathcal{K}$ the expressions β and $-i\vec{\alpha}\vec{e_r}$ read

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad -i\vec{\alpha}\vec{e_r} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{5.1.17}$$

and finally the total Hamiltonian

$$h_{m_j,\kappa_j} = \begin{pmatrix} mc^2 & \hbar c(-\partial_r + \frac{\kappa_j}{r}) \\ \hbar c(\partial_r + \frac{\kappa_j}{r}) & -mc^2 \end{pmatrix} + \begin{pmatrix} V(r) & 0 \\ 0 & V(r) \end{pmatrix}, \tag{5.1.18}$$

$$H = \bigoplus_{j=\frac{1}{2},\frac{3}{2},...}^{\infty}\ \bigoplus_{m_j=-j}^{j}\ \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} h_{m_j,\kappa_j}. \tag{5.1.19}$$

So every function in the Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^3)^4 \simeq L^2(\mathbb{R}^1_+) \otimes \left[\bigoplus_{j=\frac{1}{2},\frac{3}{2},...}^{\infty}\ \bigoplus_{m_j=-j}^{j}\ \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} \mathcal{K}_{m_j,\kappa_j}\right] \tag{5.1.20}$$

may be written in the form

$$\boxed{\Psi(r,\theta,\phi) = \sum_{j,m_j,\kappa_j}\left[\frac{1}{r}f^+_{m_j,\kappa_j}(r)\Phi^+_{m_j,\kappa_j}(\theta,\phi) + \frac{1}{r}f^-_{m_j,\kappa_j}(r)\Phi^-_{m_j,\kappa_j}(\theta,\phi)\right].} \tag{5.1.21}$$

If we consider Ψ to be time-dependent, then the functions $f^\pm$ will also depend on time. Because all $\Phi^\pm_{m_j,\kappa_j}$ are orthogonal, the Dirac equation (5.1.2) reduces to

$$\boxed{\begin{aligned} i\hbar\frac{\partial f^+_{m_j,\kappa_j}}{\partial t} &= mc^2 f^+_{m_j,\kappa_j} - \hbar c\frac{\partial f^-_{m_j,\kappa_j}}{\partial r} + \frac{\hbar c\kappa_j}{r} f^-_{m_j,\kappa_j} + V(r) f^+_{m_j,\kappa_j} \quad (5.1.22)\\ i\hbar\frac{\partial f^-_{m_j,\kappa_j}}{\partial t} &= -mc^2 f^-_{m_j,\kappa_j} + \hbar c\frac{\partial f^+_{m_j,\kappa_j}}{\partial r} + \frac{\hbar c\kappa_j}{r} f^+_{m_j,\kappa_j} + V(r) f^-_{m_j,\kappa_j}. \quad (5.1.23)\end{aligned}}$$

If we look for stationary solutions, we separate the time-dependence

$$\begin{aligned} f^+_{m_j,\kappa_j}(t,r) &= e^{-iEt/\hbar} f_{m_j,\kappa_j}(r) \quad (5.1.24)\\ f^-_{m_j,\kappa_j}(t,r) &= e^{-iEt/\hbar} g_{m_j,\kappa_j}(r). \quad (5.1.25)\end{aligned}$$

Then the system reduces to two coupled ODE's

$$\boxed{\begin{aligned} \hbar c\frac{\partial g(r)}{\partial r} - \frac{\hbar c\kappa_j}{r} g(r) + \left(E - mc^2 - V(r)\right) f(r) &= 0 \quad (5.1.26)\\ \hbar c\frac{\partial f(r)}{\partial r} + \frac{\hbar c\kappa_j}{r} f(r) - \left(E + mc^2 - V(r)\right) g(r) &= 0 \quad (5.1.27)\end{aligned}}$$

and we skipped the indices (m_j, κ_j). Introducing the dimensionless variables

$$\varepsilon = \frac{E}{mc^2}, \quad \upsilon(R) = \frac{V(r)}{mc^2}, \quad R = \frac{mc}{\hbar} r \tag{5.1.28}$$

we obtain a form more suitable for numerical integration

$$\boxed{\begin{aligned} \frac{\partial g(R)}{\partial R} - \frac{\kappa}{R} g(R) + (\varepsilon - 1 - \upsilon(R))\, f(R) &= 0 \quad (5.1.29)\\ \frac{\partial f(R)}{\partial R} + \frac{\kappa}{R} f(R) - (\varepsilon + 1 - \upsilon(R))\, g(R) &= 0 \quad (5.1.30)\end{aligned}}$$

This system can be separated for arbitrary potentials as follows. We can calculate $f(R)$ from (5.1.26) and insert into (5.1.27) and analogous for $g(R)$, obtaining

$$g''(R) - \frac{\kappa(\kappa-1)}{R^2} g(R) + \left[(\varepsilon - \upsilon(R))^2 - 1\right] g(R) - \left(g'(R) - \frac{\kappa}{R} g(R)\right) \frac{\upsilon'(R)}{\varepsilon - \upsilon(R) - 1} = 0 \tag{5.1.31}$$

$$f''(R) - \frac{\kappa(\kappa+1)}{R^2} f(R) + \left[(\varepsilon - \upsilon(R))^2 - 1\right] f(R) + \left(f'(R) + \frac{\kappa}{R} f(R)\right) \frac{\upsilon'(R)}{\varepsilon - \upsilon(R) + 1} = 0 \tag{5.1.32}$$

It may be rewritten in the Sturm-Liouville form

$$\begin{aligned} \left(\frac{g(R)'}{\varepsilon - \upsilon(R) - 1}\right)' + \frac{-\frac{\kappa(\kappa-1)}{R^2} + \left[(\varepsilon - \upsilon(I))^2 - 1\right] - \frac{\kappa}{R}\frac{\upsilon'(R)}{\varepsilon - \upsilon(R) - 1}}{\varepsilon - \upsilon(R) - 1} g(R) &= 0 \quad (5.1.33)\\ \left(\frac{f(R)'}{\varepsilon - \upsilon(R) + 1}\right)' + \frac{-\frac{\kappa(\kappa+1)}{R^2} + \left[(\varepsilon - \upsilon(R))^2 - 1\right] + \frac{\kappa}{R}\frac{\upsilon'(R)}{\varepsilon - \upsilon(R) + 1}}{\varepsilon - \upsilon(R) + 1} f(R) &= 0 \quad (5.1.34)\end{aligned}$$

Redefining

$$\tilde{g}(R) \equiv \frac{g(R)}{\sqrt{\varepsilon - \upsilon - 1}}, \qquad \tilde{f}(R) \equiv \frac{g(f)}{\sqrt{\varepsilon - \upsilon + 1}} \tag{5.1.35}$$

we finally get

$$\tilde{g}(R)'' + \left[-\frac{\kappa(\kappa-1)}{R^2} + \left[(\varepsilon - \upsilon(R))^2 - 1\right] - \frac{\kappa}{R}\frac{\upsilon'(R)}{\varepsilon - \upsilon(R) - 1} \right. \\ \left. -\frac{3}{4}\frac{(\upsilon'(R))^2}{(\varepsilon - \upsilon(R) - 1)^2} - \frac{1}{2}\frac{\upsilon''(R)}{\varepsilon - \upsilon(R) - 1} \right] \tilde{g}(R) = 0 \quad (5.1.36)$$

$$\tilde{f}(R)'' + \left[-\frac{\kappa(\kappa+1)}{R^2} + \left[(\varepsilon - \upsilon(R))^2 - 1\right] + \frac{\kappa}{R}\frac{\upsilon'(R)}{\varepsilon - \upsilon(R) + 1} \right. \\ \left. -\frac{3}{4}\frac{(\upsilon'(R))^2}{(\varepsilon - \upsilon(R) + 1)^2} - \frac{1}{2}\frac{\upsilon''(R)}{\varepsilon - \upsilon(R) + 1} \right] \tilde{f}(R) = 0 \quad (5.1.37)$$

Although the separation is always successful, the resulting equations represent a rather unusual eigenvalue problem which is difficult to solve. However, it may prove advantageous if the potential's derivatives take a simple form.

The decoupled equations may be useful in determining the asymptotic behaviour of solutions, e.g. the Coulomb potential $\upsilon(R) = Z/R$ leads for $R \to \infty$ to

$$\tilde{g}(R)'' + \left[-1 + \left(\varepsilon - \frac{Z}{R} \right)^2 - \frac{\kappa(\kappa-1)}{R^2} + O(R^{-3}) \right] \tilde{g}(R) = 0 \quad (5.1.38)$$

$$\tilde{f}(R)'' + \left[-1 + \left(\varepsilon - \frac{Z}{R} \right)^2 - \frac{\kappa(\kappa+1)}{R^2} + O(R^{-3}) \right] \tilde{f}(R) = 0 \quad (5.1.39)$$

and for $R \approx 0$

$$\tilde{g}(R)'' + \left[\frac{\frac{1}{4} - \kappa^2 + Z^2}{R^2} + O(R^{-1}) \right] \tilde{g}(R) = 0 \quad (5.1.40)$$

$$\tilde{f}(R)'' + \left[\frac{\frac{1}{4} - \kappa^2 + Z^2}{R^2} + O(R^{-1}) \right] \tilde{f}(R) = 0. \quad (5.1.41)$$

5.2 Square well potential

Consider a square potential well

$$\boxed{V(r) = -V_0 \Theta(a-r) = \begin{cases} -V_0, & r < a \\ 0, & r > a \end{cases}.} \quad (5.2.1)$$

Decomposing the wave function

$$\boxed{\Psi(t,r,\theta,\phi) = \frac{1}{r} e^{-iEt/\hbar} \sum_{j,m_j,\kappa_j} \left[f_{E,m_j,\kappa_j}(r) \Phi^{+}_{m_j,\kappa_j}(\theta,\phi) + g_{E,m_j,\kappa_j}(r) \Phi^{-}_{m_j,\kappa_j}(\theta,\phi) \right]} \quad (5.2.2)$$

and introducing dimensionless variables

$$\varepsilon = \frac{E}{mc^2}, \quad \upsilon(R) = \frac{V(r)}{mc^2}, \quad U = \frac{V_0}{mc^2}, \quad R = \frac{mc}{\hbar} r, \quad A = \frac{mc}{\hbar} a \quad (5.2.3)$$

the Dirac equation (5.1.2) for fixed quantum numbers (m_j, κ_j) reads

$$\boxed{\begin{aligned}\frac{\partial g(R)}{\partial R}-\frac{\kappa}{R}g(R)+(\varepsilon-1-\upsilon(R))\,f(R) &= 0 \quad (5.2.4)\\ \frac{\partial f(R)}{\partial R}+\frac{\kappa}{R}f(R)-(\varepsilon+1-\upsilon(R))\,g(R) &= 0 \quad (5.2.5)\end{aligned}}$$

Differentiating by R and eliminating first derivatives we obtain

$$\begin{aligned}g''(R)-\frac{\kappa(\kappa-1)}{R^2}g(R)+\left[(\varepsilon-\upsilon(R))^2-1\right]g(R)-\upsilon'(R)f(R) &= 0 \quad (5.2.6)\\ f''(R)-\frac{\kappa(\kappa+1)}{R^2}f(R)+\left[(\varepsilon-\upsilon(R))^2-1\right]f(R)+\upsilon'(R)g(R) &= 0, \quad (5.2.7)\end{aligned}$$

where prime denotes derivative with respect to R.

For the given potential (5.2.1) the last term with $\upsilon'(R)$ is always zero, except at the point $R=A$ which needs to be considered separately. Around that point we can integrate both equations from $A-\epsilon$ to $A+\epsilon$ and take the limit $\epsilon\to 0$. The result is that the first derivatives of g and f have a discontinuity there

$$\begin{aligned}\Delta g'(A) &= g'(A^+)-g'(A^-)=Uf(A) \quad (5.2.8)\\ \Delta f'(A) &= f'(A^+)-f'(A^-)=-Ug(A). \quad (5.2.9)\end{aligned}$$

Introducing new functions

$$g(R)=\sqrt{R}G(R), \qquad f(R)=\sqrt{R}F(R) \quad (5.2.10)$$

the first-order equations take the form

$$\begin{aligned}G'(R)-\frac{\kappa-\frac{1}{2}}{R}G(R)+[\varepsilon-1-\upsilon(R)]\,F(R) &= 0 \quad (5.2.11)\\ F'(R)+\frac{\kappa+\frac{1}{2}}{R}F(R)-[\varepsilon+1-\upsilon(R)]\,G(R) &= 0 \quad (5.2.12)\end{aligned}$$

and the second-order (decoupled) equations

- for $R<A$

$$\boxed{\begin{aligned}G''(R)+\frac{1}{R}G'(R)+\left[(\varepsilon+U)^2-1-\frac{(\kappa-\frac{1}{2})^2}{R^2}\right]G(R) &= 0 \quad (5.2.13)\\ F''(R)+\frac{1}{R}F'(R)+\left[(\varepsilon+U)^2-1-\frac{(\kappa+\frac{1}{2})^2}{R^2}\right]F(R) &= 0 \quad (5.2.14)\end{aligned}}$$

- for $R>A$

$$\boxed{\begin{aligned}G''(R)+\frac{1}{R}G'(R)+\left[\varepsilon^2-1-\frac{(\kappa-\frac{1}{2})^2}{R^2}\right]G(R) &= 0 \quad (5.2.15)\\ F''(R)+\frac{1}{R}F'(R)+\left[\varepsilon^2-1-\frac{(\kappa+\frac{1}{2})^2}{R^2}\right]F(R) &= 0. \quad (5.2.16)\end{aligned}}$$

These are Bessel equations. The most general solutions read

- for $R < A$

$$G(R) = A_1 J_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) + B_1 N_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \quad (5.2.17)$$

$$F(R) = C_1 J_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) + D_1 N_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \quad (5.2.18)$$

- for $R > A$ and $|\varepsilon| > 1$

$$G(R) = A_2 J_{|\kappa-\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) + B_2 N_{|\kappa-\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) \quad (5.2.19)$$

$$F(R) = C_2 J_{|\kappa+\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) + D_2 N_{|\kappa+\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) \quad (5.2.20)$$

- for $R > A$ and $|\varepsilon| < 1$

$$G(R) = A_3 I_{|\kappa-\frac{1}{2}|}(\sqrt{1-\varepsilon^2}R) + B_3 K_{|\kappa-\frac{1}{2}|}(\sqrt{1-\varepsilon^2}R) \quad (5.2.21)$$

$$F(R) = C_3 I_{|\kappa+\frac{1}{2}|}(\sqrt{1-\varepsilon^2}R) + D_3 K_{|\kappa+\frac{1}{2}|}(\sqrt{1-\varepsilon^2}R) \quad (5.2.22)$$

Where J, N are Bessel functions and I, K are modified Bessel functions.

Inserting the solutions (5.2.17-5.2.22) into the first-order coupled equations (5.2.11-5.2.12) connects the amplitudes of G and F

$$C_1 = \text{sign}\,(\kappa)\,\frac{\sqrt{(\varepsilon+U)^2-1}}{\varepsilon+U-1}A_1 \quad (5.2.23)$$

$$D_1 = \text{sign}\,(\kappa)\,\frac{\sqrt{(\varepsilon+U)^2-1}}{\varepsilon+U-1}B_1 \quad (5.2.24)$$

$$C_2 = \text{sign}\,(\kappa)\,\frac{\sqrt{\varepsilon^2-1}}{\varepsilon-1}A_2 \quad (5.2.25)$$

$$D_2 = \text{sign}\,(\kappa)\,\frac{\sqrt{\varepsilon^2-1}}{\varepsilon-1}B_2 \quad (5.2.26)$$

$$C_3 = \frac{\sqrt{1-\varepsilon^2}}{1-\varepsilon}A_3 \quad (5.2.27)$$

$$D_3 = -\frac{\sqrt{1-\varepsilon^2}}{1-\varepsilon}B_3. \quad (5.2.28)$$

To simplify the following expressions introduce abbreviations

$$\omega_1 = \sqrt{(\varepsilon+U)^2-1}, \quad \omega_2 = \sqrt{\varepsilon^2-1}, \quad \omega_3 = \sqrt{1-\varepsilon^2}. \quad (5.2.29)$$

Condition at $R = 0$

The square-integrability condition

$$\int \overline{\Psi(\mathbf{x})}\Psi(\mathbf{x})d^3x \sim \int_0^\infty \left(|f(r)|^2 + |g(r)|^2\right) dr \sim \int_0^\infty R\left(|F(R)|^2 + |G(R)|^2\right) dR < \infty \quad (5.2.30)$$

requires the asymptotic behaviour $F(R) \sim R^p$, $G(R) \sim R^q$ with $p, q > -1$.

The functions $N_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R)$ and $N_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R)$ can never simultaneously fulfill this requirement. It follows $B_1 = D_1 = 0$, hence

- for $R < A$

$$G(R) = A_1 J_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \tag{5.2.31}$$

$$F(R) = C_1 J_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \tag{5.2.32}$$

At $R = 0$ both solutions vanish $G(0) = F(0) = 0$.

5.2.1 Wave functions

Continuum

Wave functions with $|\varepsilon| > 1$ describe scattering states. Their energies belong to the continuous spectrum $(-\infty, -1) \cup (1, \infty)$. There is no additional boundary condition at infinity since all solutions $G(R), F(R)$ oscillate with a constant amplitude as $R \to \infty$.

The matching condition at $R = A$

$$F(R^-) = F(R^+), \qquad G(R^-) = G(R^+) \tag{5.2.33}$$

gives the values of A_2, B_2

$$A_2 \equiv A_1\widetilde{A_2} = -A_1 \text{sign}\,(\kappa)\,\frac{\pi}{2}A\omega_2 \cdot \left[J_{|\kappa-\frac{1}{2}|}(\omega_1 A)N_{|\kappa+\frac{1}{2}|}(\omega_2 A) - \frac{\varepsilon-1}{\varepsilon+U-1}\frac{\omega_1}{\omega_2}J_{|\kappa+\frac{1}{2}|}(\omega_1 A)N_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right] \tag{5.2.34}$$

$$B_2 \equiv A_1\widetilde{B_2} = A_1 \text{sign}\,(\kappa)\,\frac{\pi}{2}A\omega_2 \cdot \left[J_{|\kappa-\frac{1}{2}|}(\omega_1 A)J_{|\kappa+\frac{1}{2}|}(\omega_2 A) - \frac{\varepsilon-1}{\varepsilon+U-1}\frac{\omega_1}{\omega_2}J_{|\kappa+\frac{1}{2}|}(\omega_1 A)J_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right]. \tag{5.2.35}$$

Finally the form of the continuum wave functions is:

- for $R < A$

$$G(R) = A_1 J_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \tag{5.2.36}$$

$$F(R) = C_1 J_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \tag{5.2.37}$$

- for $R > A$

$$G(R) = A_2 J_{|\kappa-\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) + B_2 N_{|\kappa-\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) \tag{5.2.38}$$

$$F(R) = C_2 J_{|\kappa+\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) + D_2 N_{|\kappa+\frac{1}{2}|}(\sqrt{\varepsilon^2-1}R) \tag{5.2.39}$$

with

$$C_1 = \text{sign}\,(\kappa)\,\frac{\sqrt{(\varepsilon+U)^2-1}}{\varepsilon+U-1}A_1 \tag{5.2.40}$$

$$C_2 = \text{sign}\,(\kappa)\,\frac{\sqrt{\varepsilon^2-1}}{\varepsilon-1}A_2 \tag{5.2.41}$$

$$D_2 = \text{sign}\,(\kappa)\,\frac{\sqrt{\varepsilon^2-1}}{\varepsilon-1}B_2 \tag{5.2.42}$$

The last undefined constant A_1 will be determined by normalization.

Bound states

Square-integrable solutions with $|\varepsilon| \leq 1$ describe bound states. First, we show that they exist only for $\varepsilon > 1-U$. Consider the system of equations (5.4.3)-(5.4.4) and the boundary conditions $G(0) = F(0) = 0$ and $G(R), F(R) \to 0$ as $R \to \infty$. Assume $\varepsilon < 1 - U$. Asymptotic analysis at $R \cong 0$ shows that both functions must have the same sign, so assume they are positive. Since $\kappa(\kappa \pm 1) \leq 0$ and $(\varepsilon - v(R))^2 - 1 < 0$, both second derivatives $g''(R), f''(R) \geq 0$ for all $R \geq 0$ except $R = A$. It means that both first derivatives $g'(R), f'(R)$, which were positive in the vicinity of $R = 0$, grow until the point $R = A$. At this point both derivatives have a jump according to (5.2.8)-(5.2.9). $\Delta g'(R)$ is positive, $\Delta f'(R)$ is negative, so $g'(R)$ increases. For $R > A$, $g'(R)$ grows further and it never becomes negative, hence it will never fulfill the asymptotic boundary condition at infinity, namely $g(R) \to 0$. The argument for $\varepsilon = 1 - U$ is similar. Here the asymptotic analysis at $R = 0$ gives that $g(R) \equiv 0$ and it will stay zero for all $R < A$, because it solves the equation (5.4.3) there. Therefore we argue analogously, but for $f(R)$ instead of $g(R)$. The second derivative $f''(R) \geq 0$ for all $R \neq A$, so the first derivative $f'(R)$ grows for $R < A$, at $R = A$ it has no jump, because $g(A) = 0$, and further $f'(R)$ grows for $R > A$. It will never become negative, so it cannot fulfill the asymptotic boundary condition at infinity: $f(R) \to 0$.

We have shown that bound states may exist only for $\varepsilon > 1 - U$. Then $\omega_1 = \sqrt{(\varepsilon + U)^2 - 1}$ and $\omega_3 = \sqrt{1 - \varepsilon^2}$ are real. The functions $I_{|\kappa + \frac{1}{2}|}(\omega_3 R)$ and $I_{|\kappa - \frac{1}{2}|}(\omega_3 R)$ never fulfill the asymptotic condition at infinity ($G(R), F(R) \to 0$), so $A_3 = C_3 = 0$. Hence, the final form of the bound state wave functions is:

- for $R < A$

$$G(R) = A_1 J_{|\kappa - \frac{1}{2}|}(\sqrt{(\varepsilon + U)^2 - 1} R) \tag{5.2.43}$$

$$F(R) = C_1 J_{|\kappa + \frac{1}{2}|}(\sqrt{(\varepsilon + U)^2 - 1} R) \tag{5.2.44}$$

- for $R > A$

$$G(R) = B_3 K_{|\kappa - \frac{1}{2}|}(\sqrt{1 - \varepsilon^2} R) \tag{5.2.45}$$

$$F(R) = D_3 K_{|\kappa + \frac{1}{2}|}(\sqrt{1 - \varepsilon^2} R) \tag{5.2.46}$$

with

$$C_1 = \operatorname{sign}(\kappa) \frac{\sqrt{(\varepsilon + U)^2 - 1}}{\varepsilon + U - 1} A_1 \tag{5.2.47}$$

$$D_3 = -\frac{\sqrt{1 - \varepsilon^2}}{1 - \varepsilon} B_3. \tag{5.2.48}$$

Matching at $R = A$ gives the value of B_3

$$B_3 = A_1 \frac{J_{|\kappa - \frac{1}{2}|}(\omega_1 A)}{K_{|\kappa - \frac{1}{2}|}(\omega_3 A)} \tag{5.2.49}$$

and the implicit condition on the energy ε (quantization condition)

$$J_{|\kappa-\frac{1}{2}|}(\omega_1 A)K_{|\kappa+\frac{1}{2}|}(\omega_3 A) + \text{sign}\,(\kappa)\,\frac{1-\varepsilon}{\varepsilon+U-1}\frac{\omega_1}{\omega_3}J_{|\kappa+\frac{1}{2}|}(\omega_1 A)K_{|\kappa-\frac{1}{2}|}(\omega_3 A) = 0, \quad (5.2.50)$$

which needs to be solved in order to obtain the energy levels of the system.

The last undefined constant A_1 will be determined by normalization up to a complex phase, which will be chosen as to make A_1 real. This, together with the fact that ω_1 and ω_3 are real, guarantees that the functions $G(R)$ and $F(R)$ are real.

5.2.2 Normalization

To fix the last free coefficient A_1, the overall amplitude of the wave function, we need to impose a normalization condition. In order to do that we first introduce a restricted scalar product $\langle\psi|\psi'\rangle_{m_j,\kappa_j}$ in $\mathcal{K}_{m_j,\kappa_j}$. The full scalar product of the wave functions from $\mathcal{H}$

$$\Psi(r,\theta,\phi) = \sum_{j,m_j,\kappa_j}\left[\frac{1}{r}f_{m_j,\kappa_j}(r)\Phi^{+}_{m_j,\kappa_j}(\theta,\phi) + \frac{1}{r}g_{m_j,\kappa_j}(r)\Phi^{-}_{m_j,\kappa_j}(\theta,\phi)\right] \quad (5.2.51)$$

has the form

$$\begin{aligned}
\langle\langle\Psi|\Psi'\rangle\rangle &= \int_{\mathbb{R}^3} d^3x\overline{\Psi(\mathbf{x})}\Psi'(\mathbf{x}) \\
&= \int_0^\infty r^2 dr\int_{S^2} d\Omega\frac{1}{r}\sum_{j,m_j,\kappa_j}\left[\overline{f_{m_j,\kappa_j}(r)}\,\overline{\Phi^{+}_{m_j,\kappa_j}(\theta,\phi)} + \overline{g_{m_j,\kappa_j}(r)}\,\overline{\Phi^{-}_{m_j,\kappa_j}(\theta,\phi)}\right] \\
&\qquad\qquad \cdot\frac{1}{r}\sum_{j',m'_j,\kappa'_j}\left[f'_{m'_j,\kappa'_j}(r)\Phi^{+}_{m'_j,\kappa'_j}(\theta,\phi) + g'_{m'_j,\kappa'_j}(r)\Phi^{-}_{m'_j,\kappa'_j}(\theta,\phi)\right] \\
&= \sum_{j,m_j,\kappa_j}\int_0^\infty dr\left[\overline{f_{m_j,\kappa_j}(r)}f'_{m_j,\kappa_j}(r) + \overline{g_{m_j,\kappa_j}(r)}g'_{m_j,\kappa_j}(r)\right] \\
&= \frac{\hbar}{mc}\sum_{j,m_j,\kappa_j}\int_0^\infty RdR\left[\overline{F_{m_j,\kappa_j}(R)}F'_{m_j,\kappa_j}(R) + \overline{G_{m_j,\kappa_j}(R)}G'_{m_j,\kappa_j}(R)\right] \\
&\equiv \frac{\hbar}{mc}\sum_{j,m_j,\kappa_j}\langle\psi_{m_j,\kappa_j}|\psi'_{m_j,\kappa_j}\rangle
\end{aligned} \quad (5.2.52)$$

where

$$\psi_{m_j,\kappa_j}(r) = \begin{pmatrix} F_{m_j,\kappa_j}(R) \\ G_{m_j,\kappa_j}(R)\end{pmatrix} \quad (5.2.53)$$

and the restricted scalar product

$$\langle\psi|\psi'\rangle = \int_0^\infty \begin{pmatrix} F(R) \\ G(R)\end{pmatrix}^{\dagger}\begin{pmatrix} F'(R) \\ G'(R)\end{pmatrix} R\,dR = \int_0^\infty\left[\overline{F(R)}F'(R) + \overline{G(R)}G'(R)\right]R\,dR. \quad (5.2.54)$$

A_1 will be determined by the normalization up to a complex phase, which may be chosen arbitrarily, but independent on the energy ε.

Continuum

Since the continuum wave functions are not integrable, we normalize the scalar product of a pair of eigenvectors to energies $\varepsilon, \varepsilon'$ to a delta function

$$\langle \psi_\varepsilon | \psi_{\varepsilon'} \rangle = \delta(\varepsilon - \varepsilon'). \tag{5.2.55}$$

A rather lengthy calculation leads to the condition

$$A_1 = \sqrt{\frac{|\varepsilon - 1|}{2\left(|\widetilde{A_2}|^2 + |\widetilde{B_2}|^2\right)}}. \tag{5.2.56}$$

The complex phase has been chosen as to make A_1 always real.

Bound states

Bound states are integrable and we normalize them to unity

$$||\psi_\varepsilon||^2 \equiv \langle \psi_\varepsilon | \psi_\varepsilon \rangle = 1. \tag{5.2.57}$$

Again, a rather lengthy calculation gives

$$\begin{aligned} A_1 = \frac{\sqrt{2}}{A} \cdot \\ \Bigg\{ J_{|\kappa-\frac{1}{2}|}(\omega_1 A)^2 \left[-\frac{J_{|\kappa-\frac{1}{2}|-1}(\omega_1 A) J_{|\kappa-\frac{1}{2}|+1}(\omega_1 A)}{J_{|\kappa-\frac{1}{2}|}(\omega_1 A)^2} + \frac{K_{|\kappa-\frac{1}{2}|-1}(\omega_3 A) K_{|\kappa-\frac{1}{2}|+1}(\omega_3 A)}{K_{|\kappa-\frac{1}{2}|}(\omega_3 A)^2} \right] \\ + \frac{(\varepsilon+U)^2 - 1}{(\varepsilon+U-1)^2} J_{|\kappa+\frac{1}{2}|}(\omega_1 A)^2 \cdot \\ \left[-\frac{J_{|\kappa+\frac{1}{2}|-1}(\omega_1 A) J_{|\kappa+\frac{1}{2}|+1}(\omega_1 A)}{J_{|\kappa+\frac{1}{2}|}(\omega_1 A)^2} + \frac{K_{|\kappa+\frac{1}{2}|-1}(\omega_3 A) K_{|\kappa+\frac{1}{2}|+1}(\omega_3 A)}{K_{|\kappa+\frac{1}{2}|}(\omega_3 A)^2} \right] \Bigg\}^{-1/2} . \end{aligned} \tag{5.2.58}$$

Here, too, the complex phase has been chosen as to make A_1 always real (with $\omega_1, \omega_3 \in \mathbb{R}$).

5.2.3 Singular values of parameters ε, U

There are two (or counted with both sign combinations, four) special values of the parameters ε, U, where the Dirac equations become singular, namely: $(\varepsilon + U)^2 = 1$ and $\varepsilon^2 = 1$. They require separate analysis.

Special case: $(\varepsilon + U)^2 = 1$

This case is singular, because the equations (5.2.13)-(5.2.14) change their character at that point. They become scale invariant (change $R \to \lambda R$ is a symmetry) and their solutions (5.2.31)-(5.2.32) cannot be Bessel functions any more, but must rather have a form of a

power of R. The origin of the problem is that the values of ε satisfying $(\varepsilon+U)^2=1$ lie at the edge of a "local continuum" inside the potential well, which is simply shifted by U from the usual values ± 1. At the same time solutions outside the well, (5.2.38)-(5.2.39) and (5.2.45)-(5.2.46), behave regularly at these special values of ε.

There are two ways to deal with the problem: one can either solve the equations anew or calculate a limit in the general solutions as $(\varepsilon+U)^2\to 1$. We choose the second one, because we are interested if the limiting procedure produces a correct result (i.e. if the limit is regular), what is of some importance in numerical calculations.

Unfortunately, simply setting $(\varepsilon+U)^2=1$ does not produce reasonable wave functions, namely

$$G(R)=A_1 J_{|\kappa-\frac{1}{2}|}(0)=A_1\cdot 0, \qquad F(R)=C_1 J_{|\kappa+\frac{1}{2}|}(0)=C_1\cdot 0. \tag{5.2.59}$$

Though, it is not a real problem, because at the same time $A_1, C_1\to\infty$. In fact, it is a consequence of the choice of normalization, which, taken properly into account, restores reasonable wave functions. We will write asymptotic formulas for $G(R), F(R)$ and A_1, C_1 at $\omega_1=\sqrt{(\varepsilon+U)^2-1}\cong 0$, using (5.5.21), and observe that singular terms cancel, leading to well-behaved wave functions.

$$G(R) \;\cong\; A_1\frac{\omega_1^{\left|\kappa-\frac{1}{2}\right|}\,R^{|\kappa-\frac{1}{2}|}}{2^{|\kappa-\frac{1}{2}|}\,\Gamma(\left|\kappa-\frac{1}{2}\right|+1)} \tag{5.2.60}$$

$$F(R) \;\cong\; A_1\frac{\operatorname{sign}(\kappa)}{\varepsilon+U-1}\,\frac{\omega_1^{\left|\kappa+\frac{1}{2}\right|+1}\,R^{|\kappa+\frac{1}{2}|}}{2^{|\kappa+\frac{1}{2}|}\,\Gamma(\left|\kappa+\frac{1}{2}\right|+1)} \tag{5.2.61}$$

To find the asymptotic behaviour of A_1 we need to consider separately the cases $\varepsilon+U\cong\pm 1$ and $\operatorname{sign}(\kappa)=\pm 1$. While in $\varepsilon+U\cong -1$ the energy belongs certainly to the lower continuum ($\varepsilon<-1$), in $\varepsilon+U\cong 1$ it depends on the strength of the potential. But we know from a general analysis that there is no bound state with energy $\varepsilon=1-U$, therefore we analyze only the continuum case for $U>2$.

- $\varepsilon+U\cong -1$ (ε in lower continuum) and $\kappa>0$:

$$A_1\cong\frac{\sqrt{\frac{2}{|\varepsilon+1|}}\frac{1}{\pi A}\frac{2^{\kappa-\frac{1}{2}}\,\Gamma(\kappa+\frac{1}{2})}{\omega_1^{\kappa-\frac{1}{2}}\,A^{\kappa-\frac{1}{2}}}}{\sqrt{\left|N_{|\kappa+\frac{1}{2}|}(\omega_2 A)\right|^2+\left|J_{|\kappa+\frac{1}{2}|}(\omega_2 A)\right|^2}}\equiv\frac{2^{\kappa-\frac{1}{2}}\,\Gamma(\kappa+\frac{1}{2})}{\omega_1^{\kappa-\frac{1}{2}}}\cdot\widetilde{A_1}^{-+} \tag{5.2.62}$$

where $\widetilde{A_1}^{-+}$ is finite. Inserting this into (5.2.60) and (5.2.61) gives

$$G(R)\cong\widetilde{A_1}^{-+}\cdot R^{\kappa-\frac{1}{2}}, \qquad F(R)\cong 0. \tag{5.2.63}$$

Of course, this is the form of the solution only for $R<A$. For $R>A$ the usual formulas (5.2.38)-(5.2.39) for the wave functions may be used, although the normalization constants

A_2, B_2 need to be evaluated by a limit procedure, too, since they contain a product of A_1 and $J_{|\kappa\pm\frac{1}{2}|}(\omega_1 A)$

$$A_2 \cong -\widetilde{A_1}^{-+} \cdot \frac{\pi}{2}\omega_2 A A^{\kappa-\frac{1}{2}} N_{|\kappa+\frac{1}{2}|}(\omega_2 A) \tag{5.2.64}$$

$$B_2 \cong \widetilde{A_1}^{-+} \cdot \frac{\pi}{2}\omega_2 A A^{\kappa-\frac{1}{2}} J_{|\kappa+\frac{1}{2}|}(\omega_2 A). \tag{5.2.65}$$

- $\varepsilon + U \cong -1$ (ε in lower continuum) and $\kappa < 0$:

$$A_1 \cong \frac{\sqrt{\frac{2}{|\varepsilon+1|}}\frac{1}{\pi A}\frac{2^{-\kappa+\frac{1}{2}}\,\Gamma(-\kappa+\frac{3}{2})}{\omega_1^{-\kappa+\frac{1}{2}}\,A^{-\kappa+\frac{1}{2}}}}{\sqrt{\left|N_{|\kappa+\frac{1}{2}|}(\omega_2 A) + \frac{\varepsilon-1}{\omega_2}\frac{-\kappa+\frac{1}{2}}{A}N_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right|^2 + \left|J_{|\kappa+\frac{1}{2}|}(\omega_2 A) + \frac{\varepsilon-1}{\omega_2}\frac{-\kappa+\frac{1}{2}}{A}J_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right|^2}}$$

$$\equiv \frac{2^{-\kappa+\frac{1}{2}}\,\Gamma(-\kappa+\frac{3}{2})}{\omega_1^{-\kappa+\frac{1}{2}}} \cdot \widetilde{A_1}^{--} \tag{5.2.66}$$

where $\widetilde{A_1}^{--}$ is finite. Inserting this into (5.2.60) and (5.2.61) gives

$$G(R) \cong \widetilde{A_1}^{--} \cdot R^{-\kappa+\frac{1}{2}}, \qquad F(R) \cong \widetilde{A_1}^{--} \cdot \left(-\kappa+\frac{1}{2}\right) R^{-\kappa-\frac{1}{2}}. \tag{5.2.67}$$

Analogously to the previous case we find

$$A_2 \cong \widetilde{A_1}^{--} \cdot \frac{\pi}{2}\omega_2 A\left[A^{-\kappa+\frac{1}{2}} N_{|\kappa+\frac{1}{2}|}(\omega_2 A) + \frac{\varepsilon-1}{\omega_2}\left(-\kappa+\frac{1}{2}\right) A^{-\kappa-\frac{1}{2}} N_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right] \tag{5.2.68}$$

$$B_2 \cong -\widetilde{A_1}^{--} \cdot \frac{\pi}{2}\omega_2 A\left[A^{-\kappa+\frac{1}{2}} J_{|\kappa+\frac{1}{2}|}(\omega_2 A) + \frac{\varepsilon-1}{\omega_2}\left(-\kappa+\frac{1}{2}\right) A^{-\kappa-\frac{1}{2}} J_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right]. \tag{5.2.69}$$

- $\varepsilon + U \cong 1$ (ε in lower continuum, $U > 2$) and $\kappa < 0$:

Introduce an auxiliary variable $y \equiv \varepsilon + U - 1 \cong 0$. Then $\omega_1 \cong \sqrt{2y}$.

$$A_1 \cong \frac{\sqrt{2}^{\,-\kappa-\frac{3}{2}}\,\Gamma(-\kappa+\frac{1}{2})}{\sqrt{y}^{\,-\kappa-\frac{3}{2}}} \frac{\sqrt{\frac{2}{\varepsilon^2-1}}\frac{\omega_2}{\pi A^{-\kappa-\frac{3}{2}}}}{\sqrt{\left|N_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right|^2 + \left|J_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right|^2}}$$

$$\equiv \frac{\sqrt{2}^{\,-\kappa-\frac{3}{2}}\,\Gamma(-\kappa+\frac{1}{2})}{\sqrt{y}^{\,-\kappa-\frac{3}{2}}} \cdot \widetilde{A_1}^{+-} \tag{5.2.70}$$

where $\widetilde{A_1}^{+-}$ is finite. Inserting this into (5.2.60) and (5.2.61) gives

$$G(R) \cong 0, \qquad F(R) \cong -\widetilde{A_1}^{+-} \cdot R^{-\kappa-\frac{1}{2}}. \tag{5.2.71}$$

$$A_2 \cong -\widetilde{A_1}^{+-} \cdot \frac{\pi}{2}(\varepsilon-1) A^{-\kappa+\frac{1}{2}} N_{|\kappa-\frac{1}{2}|}(\omega_2 A) \tag{5.2.72}$$

$$B_2 \cong \widetilde{A_1}^{+-} \cdot \frac{\pi}{2}(\varepsilon-1) A^{-\kappa+\frac{1}{2}} J_{|\kappa-\frac{1}{2}|}(\omega_2 A). \tag{5.2.73}$$

- $\varepsilon + U \cong -1$ (ε in lower continuum, $U > 2$) and $\kappa > 0$:

$$A_1 \cong \frac{\sqrt{2}^{\kappa-\frac{1}{2}}\,\Gamma(\kappa+\frac{1}{2})}{\sqrt{y}^{\kappa-\frac{1}{2}}}\cdot \frac{\sqrt{\frac{2}{|\varepsilon+1|}}\frac{1}{\pi A^{\kappa+\frac{1}{2}}}}{\sqrt{\left|N_{|\kappa+\frac{1}{2}|}(\omega_2 A) - \frac{\varepsilon-1}{\omega_2}\frac{A}{\kappa+\frac{1}{2}}N_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right|^2 + \left|J_{|\kappa+\frac{1}{2}|}(\omega_2 A) - \frac{\varepsilon-1}{\omega_2}\frac{A}{\kappa+\frac{1}{2}}J_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right|^2}}$$
$$\equiv \frac{\sqrt{2}^{\kappa-\frac{1}{2}}\,\Gamma(\kappa+\frac{1}{2})}{\sqrt{y}^{\kappa-\frac{1}{2}}}\cdot \widetilde{A_1}^{++} \qquad (5.2.74)$$

where $\widetilde{A_1}^{++}$ is finite. Inserting this into (5.2.60) and (5.2.61) gives

$$G(R) \cong \widetilde{A_1}^{++}\cdot R^{\kappa-\frac{1}{2}}, \qquad F(R) \cong \widetilde{A_1}^{++}\cdot\frac{1}{\kappa+\frac{1}{2}}\,R^{\kappa+\frac{1}{2}}. \qquad (5.2.75)$$

$$A_2 \;\cong\; -\widetilde{A_1}^{++}\cdot\frac{\pi}{2}\omega_2 A^{\kappa+\frac{1}{2}}\left[N_{|\kappa+\frac{1}{2}|}(\omega_2 A) - \frac{\varepsilon-1}{\omega_2}\frac{A}{\kappa+\frac{1}{2}}N_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right] \qquad (5.2.76)$$

$$B_2 \;\cong\; \widetilde{A_1}^{++}\cdot\frac{\pi}{2}\omega_2 A^{\kappa+\frac{1}{2}}\left[J_{|\kappa+\frac{1}{2}|}(\omega_2 A) - \frac{\varepsilon-1}{\omega_2}\frac{A}{\kappa+\frac{1}{2}}J_{|\kappa-\frac{1}{2}|}(\omega_2 A)\right]. \qquad (5.2.77)$$

Special case: $\varepsilon^2 = 1$

In this case energy lies on the edge of the continuous spectrum. From the general theory it is not known whether the boundary point belongs to the spectrum or not. This value must be studied separately. By inserting the value $\varepsilon^2 = 1$ into (5.2.15)-(5.2.16) we find that the only acceptable solutions are

$$G(R) \sim R^{-|\kappa-\frac{1}{2}|}, \qquad F(R) =\sim R^{-|\kappa+\frac{1}{2}|} \qquad \text{for} \quad R > A. \qquad (5.2.78)$$

The exact formulas with the proper normalization can be obtained by taking the limit $\varepsilon \to \pm 1$ in the bound-state wave functions. Consider first the solutions (5.2.43)-(5.2.44) for $R < A$. The functions $J_{|\kappa\pm\frac{1}{2}|}(\omega_1 R)$ behave regularly, but some terms in the definition of the normalization constant A_1 become singular

$$K_{|\kappa\pm\frac{1}{2}|}(\omega_3 A) \to \infty \quad \text{as} \quad \omega_3 \to 0. \qquad (5.2.79)$$

Therefore we must make use of the asymptotic formula (5.5.24) to find the (finite) limit

$$A_1 \cong \frac{\sqrt{2}}{A}\left\{-J_{|\kappa-\frac{1}{2}|-1}(\omega_1 A)J_{|\kappa-\frac{1}{2}|+1}(\omega_1 A) + J_{|\kappa-\frac{1}{2}|}(\omega_1 A)^2\frac{\left|\kappa-\frac{1}{2}\right|}{\left|\kappa-\frac{1}{2}\right|-1}\right.$$
$$\left.+\frac{(\varepsilon+U)^2-1}{(\varepsilon+U-1)^2}\left[-J_{|\kappa+\frac{1}{2}|-1}(\omega_1 A)J_{|\kappa+\frac{1}{2}|+1}(\omega_1 A) + J_{|\kappa+\frac{1}{2}|}(\omega_1 A)^2\frac{\left|\kappa+\frac{1}{2}\right|}{\left|\kappa+\frac{1}{2}\right|-1}\right]\right\}^{-1/2}. \qquad (5.2.80)$$

The wave functions for $R > A$ become asymptotically

$$G(R) \cong A_1 \cdot J_{|\kappa-\frac{1}{2}|}(\omega_1 A)\left(\frac{R}{A}\right)^{-|\kappa-\frac{1}{2}|}, F(R) \cong A_1 \cdot \text{sign}\,(\kappa)\,\frac{\omega_1}{\varepsilon+U-1} J_{|\kappa+\frac{1}{2}|}(\omega_1 A)\left(\frac{R}{A}\right)^{-|\kappa+\frac{1}{2}|} \tag{5.2.81}$$

as $\varepsilon \to \pm 1$. In the calculation we have used the relation between different Bessel functions which is satisfied for every bound state, namely the "energy quantization" condition (5.2.50). From it follows

$$\frac{J_{|\kappa-\frac{1}{2}|}(\omega_1 A)}{J_{|\kappa+\frac{1}{2}|}(\omega_1 A)} \cong -\text{sign}\,(\kappa)\left(\frac{A}{2}\right)^{\text{sign}(\kappa)} \sqrt{\frac{\varepsilon+U+1}{\varepsilon+U-1}}\,\frac{\Gamma(\left|\kappa-\frac{1}{2}\right|)}{\Gamma(\left|\kappa+\frac{1}{2}\right|)} \cdot \begin{cases} 1/(1+\varepsilon), & \text{for} \quad \kappa < 0, \\ 1-\varepsilon, & \text{for} \quad \kappa > 0, \end{cases} \tag{5.2.82}$$

what gives in particular:

$$J_{|\kappa+\frac{1}{2}|}(\omega_1 A) = 0 \quad \text{for} \quad \kappa < 0, \varepsilon = -1 \quad \text{and} \quad J_{|\kappa-\frac{1}{2}|}(\omega_1 A) = 0 \quad \text{for} \quad \kappa > 0, \varepsilon = 1. \tag{5.2.83}$$

In other cases both $J_{|\kappa\pm\frac{1}{2}|}(\omega_1 A)$ are finite ($\neq 0$). The above has the consequence that $F(R > A) \equiv 0$ for $\kappa < 0, \varepsilon = -1$ and $G(R > A) \equiv 0$ for $\kappa > 0, \varepsilon = 1$.

5.2.4 Bound states – analysis

In this section we will study the structure of bound states of the square well potential, i.e. solutions for ε of the energy quantization equation (5.2.50)

$$J_{|\kappa-\frac{1}{2}|}(\omega_1 A) K_{|\kappa+\frac{1}{2}|}(\omega_3 A) + \text{sign}\,(\kappa)\,\frac{1-\varepsilon}{\varepsilon+U-1}\frac{\omega_1}{\omega_3} J_{|\kappa+\frac{1}{2}|}(\omega_1 A) K_{|\kappa-\frac{1}{2}|}(\omega_3 A) = 0, \tag{5.2.84}$$

as functions of the parameters U, A and κ. From the operator theory we know that bound-state energies belong to the point spectrum and are countable, hence we can use the notation ε_n, where n counts the bound states. We need a unique numeration procedure for every U, A and κ, which will be convenient for further analysis. We will use the natural one, basing on counting the bound states from the lowest lying with $n = 0$ upwards with increasing n, but with one modification, namely if a bound-state appears or disappears at the bottom of the spectrum as U or A vary, no renumbering will occur. This choice of numbering is consistent, if the dependence of ε_n on U, A is continuous and the are no level crossings, what is true within every partial wave subspace, i.e. for fixed value of κ [Tha92, sec. 4.7.3]. Then, for every U, A we will have $E_p, E_{p+1}, ..., E_q$ present in the spectrum, with $0 \leq p \leq q$, but not necessarily $p = 0$. Dependence on κ cannot be continuous since κ takes only integer values. Moreover, level crossing of eigenvalues corresponding to different values of κ is possible. Therefore, the numbering procedures for different κ are independent.

Continuity of $\varepsilon_n(U, A)$ can be shown as a consequence of differentiability, which is a stronger condition. To show that the derivative with respect to U or A is regular and finite it is sufficient to differentiate the formula (5.2.84) with respect to the parameter U

or A and calculate $\partial\varepsilon_n(U,A)/\partial U$ or $\partial\varepsilon_n(U,A)/\partial A$, respectively, what is a trivial algebraic operation. It is not difficult to show that both formulas are regular and finite for $|\varepsilon_n| < 1$ and $\varepsilon_n > 1 - U$. The cases $\varepsilon_n \to \pm 1$ must be treated by a limiting procedure and lead to finite results, too. Therefore $\varepsilon_n(U,A)$ are continuous and differentiable functions of U and A.

In what follows we will concentrate mainly on the dependence of $\varepsilon_n(U,A)$ on U. Therefore we will only write $\varepsilon_n(U)$, assuming that A is constant. First, from general quantum mechanics, for bound states described by $H\psi_n = E_n\psi_n$ we know that variation of the eigenvalue due to variation of the Hamiltonian is equal to $\delta E_n = \langle\psi_n|\delta H\psi_n\rangle$. In our case it leads to

$$\begin{aligned}\delta\varepsilon_n = \langle\psi_n|\delta\upsilon\ \psi_n\rangle &= -\delta U\cdot\int_0^\infty \left[\overline{F(R)}\ \Theta(A-R)\ F(R) + \overline{G(R)}\ \Theta(A-R)\ G(R)\right] R\,dR \\ &= -\delta U\cdot\int_0^A \left[|F(R)|^2 + |G(R)|^2\right] R\,dR\end{aligned} \tag{5.2.85}$$

and hence

$$\varepsilon_n'(U) \equiv \frac{\delta\varepsilon_n(U)}{\delta U} = -\int_0^A \left[|F(R)|^2 + |G(R)|^2\right] R\,dR < 0 \tag{5.2.86}$$

because the integrand is strictly positive. It proves that the bound-state energies $\varepsilon_n(U)$ are differentiable and that they are decreasing functions of the potential's strength U.

Now we want to answer the question whether the bound-state energies move downwards with increasing U starting from $\varepsilon = 1$ and reaching $\varepsilon = -1$ or reach asymptotically some other value within the interval $(-1,1)$. Before we carry on with the analysis, let's first restrict the considerations to the case $\kappa = -1$. It will turn out that among all angular momentum sectors just this one gives the lowest lying bound states (the strongest binding) and therefore contains the absolute ground state. Roughly, the reason is that for $\kappa = -1$ the effective repulsive centrifugal potential is the weakest. Therefore, this sector is of biggest interest for us. The mathematical task simplifies for a given value of κ, especially for $\kappa = -1$ for which the Bessel functions have the simplest trigonometric form, but we will see later that the general character of solutions remains essentially the same for other values of κ.

Case $\kappa = -1$

For $\kappa = -1$ the Bessel functions can be expressed as

$$J_{|\kappa+\frac{1}{2}|}(z) = J_{\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}}\sin(z), \qquad J_{|\kappa-\frac{1}{2}|}(z) = J_{\frac{3}{2}}(z) = \sqrt{\frac{2}{\pi z}}\left(\frac{\sin(z)}{z} - \cos(z)\right) \tag{5.2.87}$$

$$K_{|\kappa+\frac{1}{2}|}(z) = K_{\frac{1}{2}}(z) = \sqrt{\frac{\pi}{2z}}e^{-z}, \qquad K_{|\kappa-\frac{1}{2}|}(z) = K_{\frac{3}{2}}(z) = \sqrt{\frac{\pi}{2z}}\left(\frac{1}{z}+1\right)e^{-z} \tag{5.2.88}$$

and (5.2.84) reduces to

$$1 - \frac{A\sqrt{(\varepsilon_n + U)^2 - 1}}{\tan\left(A\sqrt{(\varepsilon_n + U)^2 - 1}\right)} = \frac{\varepsilon_n + U + 1}{\varepsilon_n + 1}\left(1 + A\sqrt{1 - \varepsilon_n^2}\right). \tag{5.2.89}$$

First, observe that for weak potentials there are no bound states:

- $a \approx 0$
  Making use of $\tan(x) \approx x$ for $x \approx 0$ we find from (5.2.89)
  $$0 \approx \frac{1 + \varepsilon_n + U}{1 + \varepsilon_n}, \tag{5.2.90}$$
  which has no solutions for $|\varepsilon_n| \leq 1$.

- $U \approx 0$
  From the general discussion about bound-states in 5.2.1 we know that $\varepsilon_n > 1 - U$, thus $\varepsilon_n \to 1$ as $U \to 0$. Therefore $\sqrt{(\varepsilon_n + U)^2 - 1} \approx 0$ and $\sqrt{1 - \varepsilon_n^2} \approx 0$. Using again $\tan(x) \approx x$ for $x \approx 0$ we obtain from (5.2.89)
  $$0 \approx 1, \tag{5.2.91}$$
  what means that there are no solutions.

To find for which parameters U, A first solutions appear, it is enough to consider the limit $\varepsilon_n \to 1^-$ in (5.2.89). The condition takes an implicit form

$$\tan\left(A\sqrt{U(U+2)}\right) = -2A\sqrt{\frac{U+2}{U}} \tag{5.2.92}$$

and cannot be solved analytically. Nevertheless, the existence of a sequence of solutions can be proved as follows. The r.h.s. is always negative. $A\sqrt{U(U+2)}$ increases monotonically and unboundedly in both variables A and $U > 0$. Thus the function $\tan(A\sqrt{U(U+2)})$ grows monotonically and is negative on every interval

$$A\sqrt{U(U+2)} \in \left((k - \frac{1}{2})\pi, k\pi\right), \qquad k \in \mathbb{Z} \tag{5.2.93}$$

and takes values in the whole $\mathbb{R}^-$. On the other hand, $-2A\sqrt{(U+2)/U}$, considered as a function of A starts at 0 for $A = 0$ and decreases monotonically towards $-\infty$ as A grows. Therefore the above equation has exactly one solution in every interval

$$A_k^+ \in \left(\frac{(k - \frac{1}{2})\pi}{\sqrt{U(U+2)}}, \frac{k\pi}{\sqrt{U(U+2)}}\right) \quad \text{for} \quad k > 0. \tag{5.2.94}$$

Considered as a function of U, the r.h.s. $-2A\sqrt{(U+2)/U}$ starts at $-\infty$ for $U \to 0^+$ and increases monotonically to $-2A$ as $U \to \infty$. Therefore there is at least one solution in every interval

$$U_k^+ \in \left(-1 + \sqrt{1 + \frac{(k - \frac{1}{2})^2\pi^2}{A^2}}, -1 + \sqrt{1 + \frac{k^2\pi^2}{A^2}}\right) \quad \text{for} \quad k > 0. \tag{5.2.95}$$

To prove that there is exactly one solution in every interval it is sufficient to observe that the l.h.s. function $\mathcal{L}(U)$ crosses the r.h.s. function $\mathcal{R}(U)$ always from below, i.e. $\mathcal{L}'(U) > \mathcal{R}'(U)$ at the points $\mathcal{L}(U) = \mathcal{R}(U)$. This can be easily shown by little algebra and use of the inequality $A\sqrt{U(U+2)} > \pi/2$, which follows from the relation (5.2.93) for the lowest possible value $k = 1$.

Finally, we have shown that there is an infinite, increasing sequence of parameters U or A, respectively, for which new bound states at $\varepsilon_n(U, A) = 1$ appear.

Now we can show that there are also infinite sequences of parameters U and A for which the bound-states disappear at $\varepsilon_n(U, A) = -1$. Analogously, consider the limit $\varepsilon_n \to -1^+$ in (5.2.89). It turns out that the r.h.s. becomes (+)infinite. On the l.h.s. it must correspond to zeros of $\tan(A\sqrt{(-1+U)^2-1})$, what gives a discrete set of solutions

$$A\sqrt{(-1+U)^2-1} = k\pi, \qquad k \in \mathbb{Z}. \tag{5.2.96}$$

It can be solved either for a sequence of values A

$$A_k^- = \frac{k\pi}{\sqrt{U(U-2)}}, \qquad k = 1, 2, 3, ... \tag{5.2.97}$$

or a sequence of values U

$$U_k^- = 1 + \sqrt{1 + \frac{k^2\pi^2}{A^2}}, \qquad k = 0, 1, 2, ... \tag{5.2.98}$$

These are so-called critical values for the strength of the potential, when a bound-state reaches the edge of the negative continuous spectrum $\varepsilon_n = -1$, although the value U_0 must be excluded from the set, because, as will become clear later, no bound state reaches the value -1 already for $U = 2$.

Observe that at the critical values of $U_k^{\pm}$ there exists always a bound-state with the exact energy $\varepsilon_n = \pm 1$, because the corresponding wave functions are square integrable, what has been generally shown by Klaus in [Kla85].

Next, let's differentiate the formula (5.2.89) with respect to the parameter U and A and calculate $\partial\varepsilon_n(U, A)/\partial U$ and $\partial\varepsilon_n(U, A)/\partial A$, respectively. The trigonometric functions in the result may be eliminated by use of (5.2.89).

• with respect to U:

$$\frac{\partial\varepsilon_n(U,A)}{\partial U} = \frac{(A\omega_3+1)^2\frac{(\varepsilon_n+U+1)^2}{(\varepsilon_n+1)^2} - (A\omega_3+1)\left[\frac{\varepsilon_n+U+1}{\varepsilon_n+1} + \frac{\omega_1^2}{(\varepsilon_n+1)(\varepsilon_n+U)}\right] + A^2\omega_1^2}{(A\omega_3+1)^2\frac{(\varepsilon_n+U+1)^2}{(\varepsilon_n+1)^2} - (A\omega_3+1)\left[\frac{\varepsilon_n+U+1}{\varepsilon_n+1} - \frac{U\omega_1^2}{(\varepsilon_n+1)^2(\varepsilon_n+U)}\right] + A^2\omega_1^2 + \frac{A\varepsilon_n\omega_1^2(\varepsilon_n+U+1)}{\omega_3(\varepsilon_n+1)(\varepsilon_n+U)}} \tag{5.2.99}$$

This formula looks complicated, but it can be easily shown that it is regular and finite for all $|\varepsilon_n| \leq 1$ and $\varepsilon_n > 1 - U$. Therefore $\varepsilon_n(U)$ is differentiable and thus also continuous.

Two special cases are important: the slope of the function when a new bound-state appears at $\varepsilon_n = 1$

$$\lim_{\varepsilon_n \to 1^-} \frac{d\varepsilon_n}{dU} = 0^-, \tag{5.2.100}$$

what implies that every new bound-state departs from the positive continuum smoothly, and the slope of the function as bound-state disappears at $\varepsilon_n = -1$

$$\lim_{\varepsilon_n \to -1^+} \frac{d\varepsilon_n}{dU} = -\frac{U-1}{2U-3} < 0, \tag{5.2.101}$$

because $U \geq 2$ in order to make $\varepsilon_n \to -1^+$ possible. It means that every bound-state energy reaching the top of the negative continuum crosses the line $\varepsilon_n = -1$ (from above) with a finite slope, what has been generally proved by Klaus in [Kla85]. These two results will be important for the analysis of adiabatic scattering processes.

• with respect to A:

$$\frac{\partial \varepsilon_n(A)}{\partial A} = \frac{(A\omega_3+1)^2 \frac{(\varepsilon_n+U+1)^2}{(\varepsilon_n+1)^2} - (2A\omega_3+1)\frac{\varepsilon_n+U+1}{\varepsilon_n+1} + A^2\omega_1^2}{\frac{A(\varepsilon_n+U)}{\omega_1^2}\left[(A\omega_3+1)^2 \frac{(\varepsilon_n+U+1)^2}{(\varepsilon_n+1)^2} - (A\omega_3+1)\frac{\varepsilon_n+U+1}{\varepsilon_n+1} + A^2\omega_1^2\right] + \frac{A^2\varepsilon_n(\varepsilon_n+U+1)}{\omega_3(\varepsilon_n+1)}} \tag{5.2.102}$$

This derivative is also regular and finite for $|\varepsilon_n| < 1$ and $\varepsilon_n > 1 - U$, hence $\varepsilon_n(U, A)$ are continuous and differentiable functions of U and A.

Treating ε_n as functions of U we have already found points where new bound-states appear $\varepsilon_n(U) = 1$ and where strongly bound states disappear $\varepsilon_n(U) = -1$, and we also know that the functions $\varepsilon_n(U)$ are continuous. To assign the first to the second we will show that the functions $\varepsilon_n(U)$ may take values only in some skewed bands on the plane (U, ε_n). Let's analyze single terms in the formula (5.2.89). Obviously

$$A\sqrt{(\varepsilon_n+U)^2-1} > 0, \quad 1 + A\sqrt{1-\varepsilon_n^2} > 1 \quad \text{and} \quad \frac{\varepsilon_n+U+1}{\varepsilon_n+1} > 1. \tag{5.2.103}$$

It follows that

$$\tan\left(A\sqrt{(\varepsilon_n+U)^2-1}\right) < 0. \tag{5.2.104}$$

It defines allowed intervals for the variable $A\omega_1$

$$A\sqrt{(\varepsilon_n+U)^2-1} \in \left((n+\frac{1}{2})\pi, (n+1)\pi\right), \qquad n \in \mathbb{Z}_0^+, \tag{5.2.105}$$

what can be solved for ε_n

$$\varepsilon_n \in \left(\sqrt{1+\frac{(n+\frac{1}{2})^2\pi^2}{A^2}} - U, \sqrt{1+\frac{(n+1)^2\pi^2}{A^2}} - U\right). \tag{5.2.106}$$

This relation defines skew bands, where solutions ε_n can be found. These bands coincide with the intervals U_k^+ at the value $\varepsilon_n = 1$, where new bound-states appear. Since we know that in every such interval there appears exactly one new bound-state, the bands

are disjoint and the functions $\varepsilon_n(U)$ are continuous, the conclusion is that in every band defined above there is exactly one curve $\varepsilon_n(U)$ starting at $\varepsilon_n(U_{n+1}^+)) = 1$ and finishing at $\varepsilon_n(U_{n+1}^-) = -1$ (figure 5.1). It guarantees a unique numbering of bound-states. It becomes here also transparent that the possible critical potential $U_0^- = 2$ must be excluded, because it does not lie within any band.

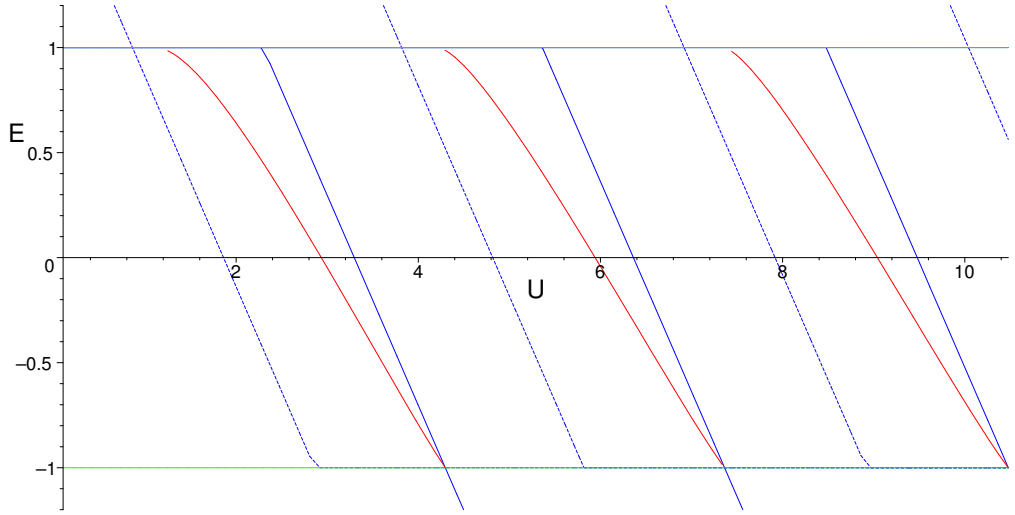


Figure 5.1: Bound states ε_n for different values of the potential's strength U (solid lines) and bounding regions according to (5.2.106) (dashed straight lines).

We want to add one more relation, which will be important in a numerical search for solutions of (5.2.89), namely the condition saying which bound-states (numbers) can be present for a given potential's strength. Taking into account that $-1 \leq \varepsilon_n \leq 1$ the last relation can be resolved for n

$$\frac{A}{\pi}\sqrt{(U-1)^2-1} - 1 \leq n \leq \frac{A}{\pi}\sqrt{(U+1)^2-1} - \frac{1}{2}. \tag{5.2.107}$$

Case $\kappa = 1$

For $\kappa = 1$ the quantization condition (5.2.84) takes a similar simple form

$$1 - \frac{A\sqrt{(\varepsilon_n+U)^2-1}}{\tan\left(A\sqrt{(\varepsilon_n+U)^2-1}\right)} = -\frac{\varepsilon_n+U-1}{1-\varepsilon_n}\left(1+A\sqrt{1-\varepsilon_n^2}\right). \tag{5.2.108}$$

The analysis of bound states can be performed in a fully analogous way, but there is no point to not present it here.

Other values of κ

The analysis of the full condition (5.2.84) for any κ cannot be done so easily, because the Bessel functions have more complicated properties than the trigonometric functions

appearing in cases $\kappa = \pm 1$. Though, some analogous results can be proved analytically, the rest must be verified numerically.

Equation (5.2.84) can be split into terms of a known sign

$$-\operatorname{sign}(\kappa)\ \underbrace{\frac{\sqrt{(\varepsilon+U)^2-1}}{\varepsilon+U-1}}_{+}\ \frac{J_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}A)}{J_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}A)} = \underbrace{\frac{\sqrt{1-\varepsilon^2}}{1-\varepsilon}}_{+}\ \underbrace{\frac{K_{|\kappa+\frac{1}{2}|}(\sqrt{1-\varepsilon^2}A)}{K_{|\kappa-\frac{1}{2}|}(\sqrt{1-\varepsilon^2}A)}}_{+}. \tag{5.2.109}$$

Then, the signs of the remaining terms must fulfill

$$\operatorname{sign}(\kappa)\cdot\operatorname{sign}\left(J_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}A)\right)\cdot\operatorname{sign}\left(J_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}A)\right) = -1 \tag{5.2.110}$$

in order to guarantee existence of a solution. For given κ and A the l.h.s of the above condition is a function of $\varepsilon+U$ and $\sqrt{(\varepsilon+U)^2-1}$ is a monotonic function of $\varepsilon+U$. The Bessel functions oscillate around zero, i.e. they change sign perpetually. Moreover, since the indices of both Bessel functions in this equation differ by 1, their zeros lie alternately on the real axis. It follows that there exist infinite number of intervals (a_n^-, b_n^-) of $\varepsilon+U$ such that both Bessel functions have the same sign with $A\sqrt{(a_n^+)^2-1}$ and $A\sqrt{(b_n^+)^2-1}$ being zeros of the corresponding Bessel functions. The complementary set on $\mathbb{R}^+$ is an infinite sum of intervals $(a_n^+, b_n^+) = (b_n^-, a_{n+1}^-)$ of $\varepsilon+U$ such that the Bessel functions have opposite signs. The first set presents a solution for the case $\operatorname{sign}(\kappa) < 0$ and the second for $\operatorname{sign}(\kappa) > 0$. Finally, we obtain intervals, for a given U, where possible values of bound state energies ε_n can be found, namely

$$\varepsilon_n \in \left(a_n^{\pm} - U, b_n^{\pm} - U\right), \tag{5.2.111}$$

where the sign is to be chosen equal to $\operatorname{sign}(\kappa)$. These are obviously skew bands in function of U, as it was the case for $\kappa = -1$.

5.2.5 Critical point

It is important to know for which values of U the critical points $\varepsilon_n = -1^+$ appear, especially what is their order with respect to the value of κ. Equation (5.2.109) is convenient for such analysis, because the l.h.s. is finite and r.h.s. is singular – both K-Bessel functions tend to zero as $\varepsilon \to -1^+$

$$\begin{aligned}\sqrt{\frac{U}{U-2}}\ \frac{J_{|\kappa+\frac{1}{2}|}(\sqrt{(U-1)^2-1}A)}{J_{|\kappa-\frac{1}{2}|}(\sqrt{(U-1)^2-1}A)} &= -\operatorname{sign}(\kappa)\lim_{\varepsilon\to-1^+}\frac{\sqrt{1-\varepsilon^2}}{1-\varepsilon}\ \frac{K_{|\kappa+\frac{1}{2}|}(\sqrt{1-\varepsilon^2}A)}{K_{|\kappa-\frac{1}{2}|}(\sqrt{1-\varepsilon^2}A)} \\ &= \frac{-\operatorname{sign}(\kappa)}{2A}\lim_{x\to0} x\cdot\frac{K_{|\kappa+\frac{1}{2}|}(x)}{K_{|\kappa-\frac{1}{2}|}(x)} = \begin{cases}0, & \kappa<0\\ -\frac{\kappa-\frac{1}{2}}{A}, & \kappa>0.\end{cases}\end{aligned} \tag{5.2.112}$$

The first case, $\kappa < 0$ has a straightforward solution

$$J_{|\kappa+\frac{1}{2}|}(\sqrt{(U-1)^2-1}A) = 0, \tag{5.2.113}$$

and gives an infinite sequence of critical values U_n (whose values must be calculated numerically). The other case, $\kappa > 0$, is more complicated, but with a little analysis it can also be shown that its solutions form an infinite sequence U_n.

In fact, we are mostly interested in the first critical value, i.e. the smallest critical value of U, say U_1, when the lowest bound state ε_1 reaches the negative continuum. This holds not only for all critical values U_n within a given value of κ, but also among all values of κ. Hence we ask the question, what is the order of values U_1 for different κ. Consider first $\kappa < 0$. The condition for criticality reduces to an equation for zeros of the Bessel function

$$J_{-\kappa-\frac{1}{2}}(x) = 0 \tag{5.2.114}$$

with $x \equiv \sqrt{(U-1)^2 - 1}A$ being a monotonically growing function of U and $-\kappa - \frac{1}{2} > 0$. From the theory of Bessel functions [Wat22] we know that the first positive zeros of $J_\nu(x)$ move monotonically left, towards $x = 0$ as the index ν grows. Moreover, the second zeros to any value of ν are always to the right of all first zeros to any value ν'. Therefore, calling x_n^κ the n-th (positive) zero of the above equation, we have

$$x_1^{-1} < x_1^{-2} < x_1^{-3} < ... < x_2^{-1} < x_2^{-2} < x_2^{-3} < ... \tag{5.2.115}$$

and because x is a monotonically growing function of U, we get the first critical values

$$U_1^{-1} < U_1^{-2} < U_1^{-3} < ... < U_2^{-1} < U_2^{-2} < U_2^{-3} < ... \tag{5.2.116}$$

It means that among all negative values of κ overcriticality happens first for $\kappa = -1$, then for $\kappa = -2$, etc. More involved analysis shows that solutions for $\kappa > 0$ are placed alternately to those for $-\kappa$, hence we finally obtain

$$U_1^{-1} < U_1^1 < U_1^{-2} < U_1^2 < U_1^{-3} < U_1^3 < ... < U_2^{-1} < U_2^1 < U_2^{-2} < U_2^2 < U_2^{-3} < U_2^3 < ... \tag{5.2.117}$$

i.e. overcriticality occurs always first for $\kappa = -1$, then for $\kappa = 1$, then $\kappa = -2$, then $\kappa = 2$, etc. It allows us to concentrate in the following mainly on the overcriticality in the sector $\kappa = 1$, as it happens for the weakest potentials.

5.3 Overcriticality and resonances

Since overcriticality happens always first (i.e. for the smallest value of U) for $\kappa = -1$, we will restrict our considerations in this section only to that sector. To give numerically some values, we choose the radius of the potential well $A = 1$ in the dimensionless variables, what corresponds to $a = \hbar/(mc) = \lambda_C$ being the Compton wavelength of the electron. On the one hand, this is the natural length scale in this problem, on the other, the structure of bound states is relatively simple – for every value of U only one bound state is present and new bound states appear at $\varepsilon = 1$ roughly as overcritical disappear at $\varepsilon = -1$ with

increasing U. The critical value for the strength of the potential is (5.2.98)

$$U_1^- = 1 + \sqrt{1 + \frac{\pi^2}{A^2}} \approx 4.297 \text{ (for } A = 1), \tag{5.3.1}$$

The slope at which the bound state $\varepsilon_1(U)$ reaches the edge of the continuum $\varepsilon = -1$ is (5.2.101)

$$\lim_{\varepsilon_1 \to -1^+} \frac{d\varepsilon_1(U)}{dU} = -\left.\frac{U-1}{2U-3}\right|_{U=U_1^-} \approx -0.589 < 0 \qquad \forall_{A>0}. \tag{5.3.2}$$

For overcritical potentials, i.e. for $U > U_1^-$, the bound state turns into a resonance, whose position we have defined in section 3.3 as a complex pole of the resolvent continued to the second Riemann sheet. In practice, it corresponds to a solution of the bound state (energy quantization) formula (5.2.89)

$$1 - \frac{A\sqrt{(\varepsilon+U)^2-1}}{\tan\left(A\sqrt{(\varepsilon+U)^2-1}\right)} = \frac{\varepsilon+U+1}{\varepsilon+1}\left(1 + A\sqrt{1-\varepsilon^2}\right), \tag{5.3.3}$$

continued analytically beyond the complex cut along $(-\infty, -1)$ in the variable ε. Here, the square roots $\sqrt{1-\varepsilon^2}$ and $\sqrt{(\varepsilon+U)^2-1}$ must be properly continued, what means that a special branch must be chosen. A typical $\sqrt{\cdot}$ function has a cut along the negative real axis $\mathbb{R}^-$. It leads to cuts along $(-\infty, -1)$ and $(1, \infty)$ in $\sqrt{1-\varepsilon^2}$ and $(-1-U, 1-U)$ and $-U + i\mathbb{R}$ in $\sqrt{(\varepsilon+U)^2-1}$. Since for overcritical potentials we have $U > 2$, there is an interval $(1-U, -1)$ through which we will go from the lower $\mathrm{Im}(\varepsilon) < 0$ to the upper $\mathrm{Im}(\varepsilon) > 0$ half plane choosing a universal branching. Since $\sqrt{(\varepsilon+U)^2-1}$ is analytic and single-valued there, only $\sqrt{1-\varepsilon^2}$ must be treated in a special way, namely by choosing the branch cut in the $\sqrt{\cdot}$ along the positive imaginary half-axis $i\mathbb{R}^+$, we make $\sqrt{(\varepsilon+U)^2-1}$ analytic when crossing the segment $(1-U, -1)$ (see figure 5.2). We expect complex resonances to be placed in the area $\varepsilon_R \equiv \mathrm{Re}(\varepsilon) \in (1-U, -1)$, $\varepsilon_I \equiv \mathrm{Im}(\varepsilon) > 0$. This picture is similar to that obtained in [HR85].

For $A = 1$ we have found the complex resonance energy as a continuation of the value of the bound state energy (for $U \in (4.00, 4.28)$), moving with increasing $U \in (4.29, 5.00)$ from the vicinity of the point $\varepsilon = -1$ (at $U = U_1^- \approx 4.29$) further to the left (ε_R decreases, as the bound state energy) and leaving the real axis, with increasing ε_I (figure 5.3).

Far from the point $\varepsilon = -1$ the resonance lies on a straight line $\varepsilon_I \approx -0.325\ (\varepsilon_R + 1) - 0.019$. In the vicinity of the critical point (figure 5.4), we find $\varepsilon_I \approx -0.58\ (-\varepsilon_R - 1)^{3/2}$, what confirms the theoretical prediction (3.3.13) $\varepsilon_I \sim (-\varepsilon_R - 1)^{3/2}$ and agrees with the scaling obtained explicitly for the square well potential in [AB65] as well as generally in [Kla85]. It disagrees with the result of Greiner *et al.* [GMR85], who by the method of perturbation theory at the boundary between the sub- and overcritical potential obtained scaling $\varepsilon_I \sim (-\varepsilon_R - 1)^2$. The reason may be that their method implicitly assumes analyticity of $\varepsilon(\lambda)$ what is not true at the threshold.

Alternatively, we can plot the real and imaginary values of the resonance position, ε_R and ε_I, against the strength of the potential U. In figures 5.5-5.6 we can observe the

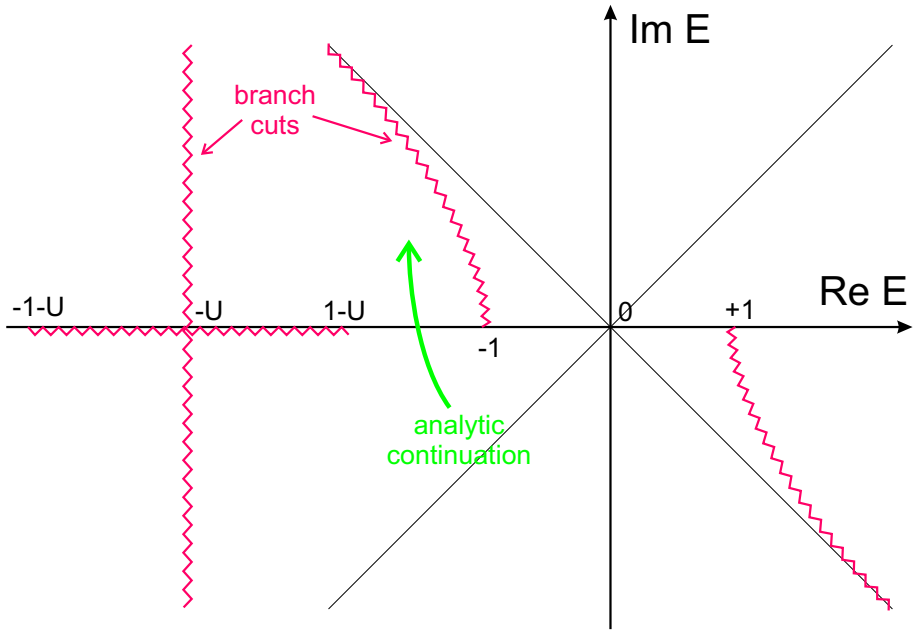


Figure 5.2: Chosen analytic continuation of $\sqrt{1-\varepsilon^2}$ and $\sqrt{(\varepsilon+U)^2-1}$.

bound state behaviour for $U \lesssim 4.29$ ($\varepsilon_I = 0$, ε_R decreasing) and the resonance behaviour ($\varepsilon_I \neq 0$) for $U \gtrsim 4.29$. For overcritical U the resonance $\varepsilon_R(U)$ continues decreasing at the same rate as the bound state did, almost linearly $\varepsilon_R(U) \approx -\left.\frac{U-1}{2U-3}\right|_{U=U_1^-} \cdot (U-U_1^-) - 1 \approx -0.589\ (U-U_1^-) - 1$, while the behaviour of $\varepsilon_I(U)$ is nonanalytic at the critical point, $\varepsilon_I(U) = 0$ for $U < U_1^-$ and $\varepsilon_I(U) \approx 0.26\ (U-U_1^-)^{3/2}$.

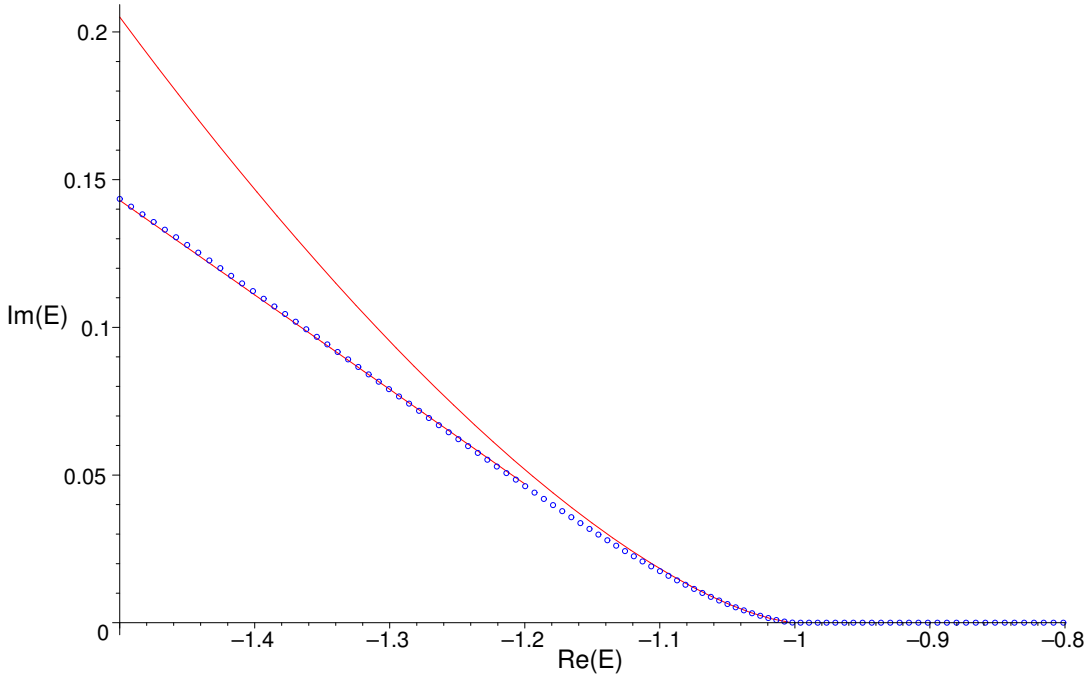


Figure 5.3: Position of the complex resonance (dots) for $U \in (4, 5)$ with linear and power-law fits (solid lines).

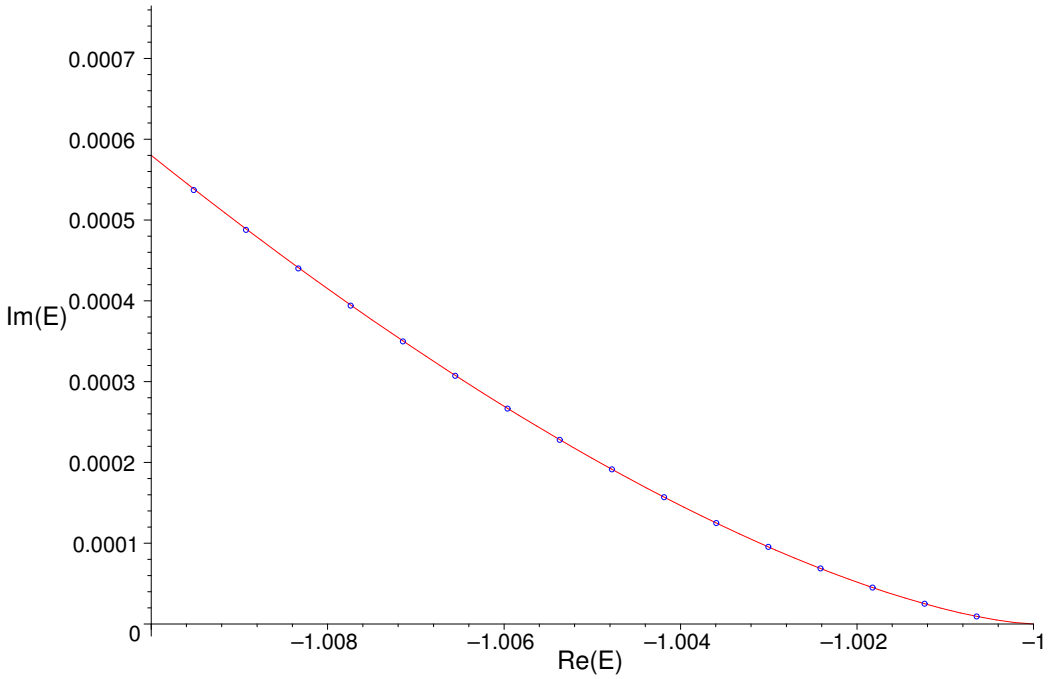


Figure 5.4: Position of the complex resonance (dots) in the vicinity of the critical point and a power-law fit $\varepsilon_I \sim (-\varepsilon_R - 1)^{3/2}$ (solid line).

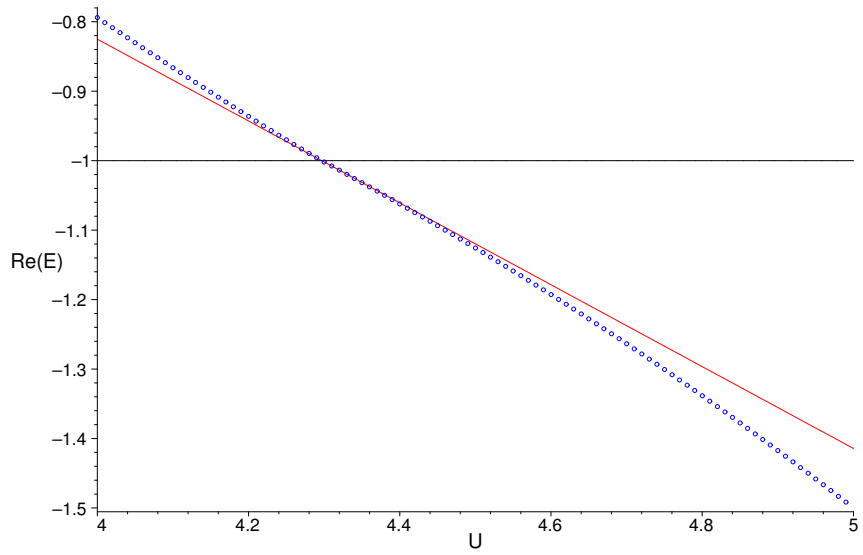


Figure 5.5: Real part of the position of the complex resonance (dots) and a linear fit (solid line).

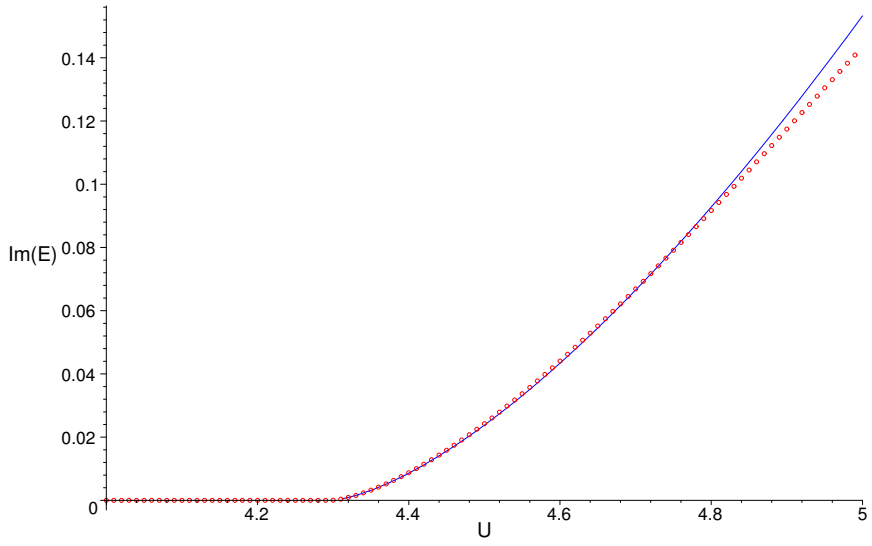


Figure 5.6: Imaginary part of the position of the complex resonance (dots) and a power-law fit $\varepsilon_I \sim (U - U_1^-)^{3/2}$ (solid line).

5.4 Regularity of the square well potential

At the end of this chapter we want to study the regularity (in the sense defined in section 2.7.2 and theorem 6) of the square well potential

$$V(r) = -V_0\ \Theta(a-r) = \begin{cases} -V_0, & r < a \\ 0, & r > a \end{cases} . \tag{5.4.1}$$

Since $V(r)$ is discontinuous its Fourier transform $\hat{V}(\mathbf{p})$ falls off like $1/|\mathbf{p}|^2$ for big $|\mathbf{p}|$ (2.7.29) and hence satisfies the necessary condition (2.7.25), but does not satisfy the sufficient condition (2.7.26) for being regular, so we must leave the problem open. On the other hand, we have shown in section 2.7.2 that smoothing out the discontinuity at $r = a$ by making the potential only continuous (2.7.30)

$$V(r) = \begin{cases} -V_0, & r < a-\delta \\ -\frac{V_0}{2} + \frac{V_0}{2}\frac{(r-a)}{\delta}, & |r-a| \le \delta \\ 0, & r > a+\delta \end{cases} \tag{5.4.2}$$

with some small $\delta > 0$, is enough to make the Fourier transform $\hat{V}(\mathbf{p})$ fall off faster and satisfy the sufficient condition for regularity (2.7.26).

It remains to check which influence the δ-regularization has on all the solutions of the Dirac equation presented in this chapter. To this end we consider the system of equations (5.2.6)

$$g''(R) - \frac{\kappa(\kappa-1)}{R^2}g(R) + \left[(\varepsilon - \upsilon(R))^2 - 1\right] g(R) - \upsilon'(R)f(R) = 0 \tag{5.4.3}$$

$$f''(R) - \frac{\kappa(\kappa+1)}{R^2}f(R) + \left[(\varepsilon - \upsilon(R))^2 - 1\right] f(R) + \upsilon'(R)g(R) = 0 \tag{5.4.4}$$

(written with dimensionless variables therefore R instead of r, etc.) The system can be solved first in the interval $R \in [0, A)$ starting from the boundary condition at $R = 0$ and then by matching at $R = A$ with the solutions for $R > A$. The first derivatives of g and f are discontinuous at $R = A$ (5.2.8) and their jumps $\Delta g, \Delta f$ determine the coefficients of the solutions for $R > A$. In the case of δ-regularized potential it can be easily shown that these jumps are modified so that

$$\Delta g_\delta - \Delta g = \mathcal{O}(\delta), \qquad \Delta f_\delta - \Delta f = \mathcal{O}(\delta). \tag{5.4.5}$$

In the same way behave all other parameters of the solutions which can depend on δ. It proves that the δ-regularization procedure is a regular perturbation and all solutions tend to those of the pure square well as $\delta \to 0$.

5.5 Appendix: Bessel functions

5.5.1 Bessel equation

The Bessel differential equation has the form

$$y''(z) + \frac{1}{z}y'(z) + \left(\alpha^2 - \frac{\nu^2}{z^2}\right) y(z) = 0. \tag{5.5.1}$$

A linearly independent pair of solutions are the Bessel function of the first kind (regular in $z = 0$) and of the second kind: $J_\nu(\alpha z), N_\nu(\alpha z)$ or the two Hankel functions $H_\nu^{(-)}(\alpha z), H_\nu^{(+)}(\alpha z)$.

The modified Bessel equation is obtained by the change $\alpha \to i\alpha$

$$y''(z) + \frac{1}{z}y'(z) - \left(\alpha^2 + \frac{\nu^2}{z^2}\right) y(z) = 0. \tag{5.5.2}$$

Its linearly independent solutions are $I_\nu(\alpha z)$ (regular at $z = 0$) and $K_\nu(\alpha z)$.

5.5.2 Connections between the Bessel functions

J and N

There is a connection between J and N

$$N_\nu(z) = \frac{\cos(\pi\nu)J_\nu(z) - J_{-\nu}(z)}{\sin(\pi\nu)}. \tag{5.5.3}$$

For the half-integer indices it reduces to

$$N_{|\kappa\pm\frac{1}{2}|}(z) = \text{sign}\,(\kappa)\,(-1)^\kappa J_{-|\kappa\pm\frac{1}{2}|}(z). \tag{5.5.4}$$

J, N and $\mathbf{H}^{(-)}$, $\mathbf{H}^{(+)}$

$$J_\nu(z) = \frac{H_\nu^{(+)}(z) + H_\nu^{(-)}(z)}{2}, \qquad N_\nu(z) = \frac{H_\nu^{(+)}(z) - H_\nu^{(-)}(z)}{2i}, \tag{5.5.5}$$

$$H_\nu^{(+)}(z) = J_\nu(z) + iN_\nu(z), \qquad H_\nu^{(-)}(z) = J_\nu(z) - iN_\nu(z). \tag{5.5.6}$$

J, N and I, K

$$I_\nu(z_\pm) = e^{\mp\nu\frac{i\pi}{2}} J_\nu(\pm iz_\pm), \qquad K_\nu(z_\pm) = \pm\frac{i\pi}{2} e^{\pm\nu\frac{i\pi}{2}} H_\nu^{(\pm)}(\pm iz_\pm) \tag{5.5.7}$$

$$J_\nu(iz_\pm) = e^{\pm\nu\frac{i\pi}{2}} I_\nu(\pm z_\pm), \qquad N_\nu(iz_\pm) = -\frac{2}{\pi} e^{\mp\nu\frac{i\pi}{2}} K_\nu(\pm z_\pm) \mp ie^{\pm\nu\frac{i\pi}{2}} I_\nu(\pm z_\pm) \tag{5.5.8}$$

for $\arg(z_+) \in (-\pi, \frac{\pi}{2})$ and $\arg(z_-) \in (-\frac{\pi}{2}, \pi)$.

Negative index

$$J_{-\nu}(z) = \cos(\pi\nu)J_\nu(z) - \sin(\pi\nu)N_\nu(z), \qquad N_{-\nu}(z) = \sin(\pi\nu)J_\nu(z) + \cos(\pi\nu)N_\nu(z), \tag{5.5.9}$$

$$I_{-\nu}(z) = e^{2\pi i\nu} I_\nu(z) + \frac{2}{\pi}\sin(\pi\nu)K_\nu(z), \qquad K_{-\nu}(z) = K_\nu(z) \tag{5.5.10}$$

Recurrence relations

$$J'_\nu(z) = \pm\frac{\nu}{z}J_\nu(z) \mp J_{\nu\pm1}(z), \qquad N'_\nu(z) = \pm\frac{\nu}{z}N_\nu(z) \mp N_{\nu\pm1}(z), \tag{5.5.11}$$

$$I'_\nu(z) = \pm\frac{\nu}{z}I_\nu(z) + I_{\nu\pm1}(z), \qquad K'_\nu(z) = \pm\frac{\nu}{z}K_\nu(z) - K_{\nu\pm1}(z). \tag{5.5.12}$$

They are equivalent to

$$\left[z^{\pm\nu}J_\nu(z)\right]' = \pm z^{\pm\nu}J_{\nu\mp1}(z), \qquad \left[z^{\pm\nu}N_\nu(z)\right]' = \pm z^{\pm\nu}N_{\nu\mp1}(z), \tag{5.5.13}$$

$$\left[z^{\pm\nu}I_\nu(z)\right]' = z^{\pm\nu}I_{\nu\mp1}(z), \qquad \left[z^{\pm\nu}K_\nu(z)\right]' = -z^{\pm\nu}K_{\nu\mp1}(z). \tag{5.5.14}$$

For half-integer indices

$$J'_{|\kappa-\frac{1}{2}|}(z) = \text{sign}\,(\kappa)\,\frac{|\kappa-\frac{1}{2}|}{z}J_{|\kappa-\frac{1}{2}|}(z) - \text{sign}\,(\kappa)\,J_{|\kappa+\frac{1}{2}|}(z) \tag{5.5.15}$$

$$J'_{|\kappa+\frac{1}{2}|}(z) = -\text{sign}\,(\kappa)\,\frac{|\kappa+\frac{1}{2}|}{z}J_{|\kappa+\frac{1}{2}|}(z) + \text{sign}\,(\kappa)\,J_{|\kappa-\frac{1}{2}|}(z) \tag{5.5.16}$$

(what holds for N in the same form).

Wronskians

Define the Wronskian of two functions by $W[f,g] \equiv fg' - f'g$.

$$W[J_\nu, N_\nu] = \frac{2}{\pi z}, \qquad W[I_\nu, K_\nu] = -\frac{1}{z}. \tag{5.5.17}$$

It follows a relation for half-integer indices

$$J_{|\kappa-\frac{1}{2}|}(z)N_{|\kappa+\frac{1}{2}|}(z) - J_{|\kappa+\frac{1}{2}|}(z)N_{|\kappa-\frac{1}{2}|}(z) = \text{sign}\,(\kappa)\,\frac{2}{\pi z}. \tag{5.5.18}$$

5.5.3 Integrals of Bessel functions

$$\int rJ_\nu(\alpha r)^2 dr =$$

$$\frac{r^2}{2}\left[J_\nu(\alpha r)^2 - J_{\nu+1}(\alpha r)J_{\nu-1}(\alpha r)\right] = \frac{r^2}{2}J'_\nu(\alpha r)^2 + \frac{1}{2}\left(r^2 - \frac{\nu^2}{\alpha^2}\right)J_\nu(\alpha r)^2 \tag{5.5.19}$$

$$\int rK_\nu(\alpha r)^2 dr =$$

$$\frac{r^2}{2}\left[K_\nu(\alpha r)^2 - K_{\nu+1}(\alpha r)K_{\nu-1}(\alpha r)\right] = -\frac{r^2}{2}K'_\nu(\alpha r)^2 + \frac{1}{2}\left(r^2 + \frac{\nu^2}{\alpha^2}\right)K_\nu(\alpha r)^2 \tag{5.5.20}$$

5.5.4 Asymptotic behaviour

For $z \approx 0$

$$J_\nu(z) \cong \frac{(z/2)^\nu}{\Gamma(\nu+1)}, \qquad N_\nu(z) \cong -\frac{1}{\pi}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu}, \qquad \text{for} \quad \text{Re}(\nu) > 0 \tag{5.5.21}$$

$$K_\nu(z) \cong \frac{1}{2}\Gamma(\nu)\left(\frac{z}{2}\right)^{-\nu}, \qquad \text{for} \quad \text{Re}(\nu) > 0 \tag{5.5.22}$$

For $z \to \infty$

$$J_\nu(z) \cong \frac{2}{\pi z}\cos\left(z - \frac{1}{2}\pi\nu - \frac{1}{4}\pi\right), \quad N_\nu(z) \cong \frac{2}{\pi z}\sin\left(z - \frac{1}{2}\pi\nu - \frac{1}{4}\pi\right) \quad \text{for } |\arg z| < \pi \tag{5.5.23}$$

$$K_\nu(z) \cong \frac{\pi}{2z}e^{-z}, \qquad I_\nu(z) \cong \frac{1}{2\pi z}e^{z} \qquad \text{for } |\arg z| < \pi/2 \tag{5.5.24}$$

For $\nu \to \infty$

$$J_\nu(z) \cong \frac{1}{\sqrt{2\pi\nu}}\left(\frac{ez}{2\nu}\right)^{\nu}, \qquad N_\nu(z) \cong -\sqrt{\frac{2}{\pi\nu}}\left(\frac{ez}{2\nu}\right)^{-\nu} \tag{5.5.25}$$

Chapter 6

Particle production in a time-dependent overcritical potential

In this chapter we want to study these details of the spontaneous particle creation, discussed in part I, which could not be decided analytically on a general level. Here, we construct a series of examples of time-dependent processes (sudden, quick, slow switch on and off of a sub- and overcritical potentials) by using always the same spatial potential and considering only various time-dependent amplitudes, what is sufficient to cover all cases of interest. The spatial profile of the potential is chosen to be the spherically symmetric square potential well, discussed in the previous chapter. We derive a system of differential equations to be implemented numerically for calculation of the scattering operator, discuss various sources of errors introduced by the numerical discretization and try to find estimations for them.

First, we consider sudden switch on and next switch on and off of an overcritical potential and calculate the spectrum of produced particles and antiparticles. We observe that for sufficiently long overcritical periods a peak forms in the antiparticle spectrum and we compare it with the shape of the resonance in the overcritical potential. Later, we consider continuous switch on and off processes, explaining how difficult the treatment of extremely narrow resonance peaks at the edge of the negative continuum is. We consider subcritical potentials in order to show an adiabatic limit in which no particles are created. Then we compare processes, where the overcritical potentials are switched on at different speed and are possibly frozen in the overcritical phase.

We prove, in agreement with the conclusions of section 4.5, that the wave packet in the negative continuum representing a dived bound state partially follows the moving resonance and partially decays at every stage of evolution. This continuous decay is more intensive in slow processes, while in quick processes the wave packet more precisely follows the resonance. In the adiabatic limit, the whole decay occurs already at the

edge of continuum, resulting in production of antiparticles with vanishing momentum. In contrast, in quick switch on processes with delay in the overcritical phase, the spectrum of the created antiparticles agrees best with the shape of the resonance.

6.1 Numerical evolution in a basis

The evolution equation for the wave function reads

$$H(t)\Psi(t,\mathbf{x}) = i\hbar\frac{\partial\Psi(t,\mathbf{x})}{\partial t}. \tag{6.1.1}$$

The Hamiltonian $H(t)$ is time-dependent and has the form $H(t) = H_0 + V(t)$. At every instant of time (t plays the role of a parameter) we can choose an infinite countable set of orthonormal vectors $\{\psi_k(t,\mathbf{x})\}$ in $\mathcal{H}$ forming a basis, because $\mathcal{H}$ is separable. With respect to that basis, or rather the one-parameter (t) family of bases, we can decompose the wave function (at every time) as

$$\Psi(t,\mathbf{x}) = \sum_k a_k(t)\ \psi_k(t,\mathbf{x}). \tag{6.1.2}$$

Although separability of $\mathcal{H}$ is generally a useful property, it does not help much in constructing a good basis for numerical calculations. The main reason is that it is very difficult to find an explicit representation of them, having necessary convergence and completeness properties. Even if it were possible, they would be numerically rather impractical, because it is not to expect that there would be a simple relation to e.g. eigenvectors of the Hamiltonian, which are of interest in calculations.

Instead of solving the evolution equation numerically using a basis, one could try to integrate it numerically in space discretizing $\mathbb{R}^3$. The drawback of this method is that one has to use a large number of points in $\mathbb{R}^3$ in order to encode the information on oscillating continuum wave functions. In a sense, the set of functions on the discretized $\mathbb{R}^3$ forms also a (incomplete) basis in $\mathcal{H}$ (e.g. in [BGGS03] over $5\cdot 10^6$ points in $\mathbb{R}^3$ had to be used).

Adiabatic basis

Therefore, we rather start with the spectral representation introduced in section 3.2.2 of the Hamiltonian $H(t)$ using its generalized eigenvectors $\psi_E(t,\mathbf{x})$ calculated at every instant of time t, building the so-called *adiabatic basis*

$$\begin{aligned}\Psi(t,\mathbf{x}) &= \int_{\sigma(t)} a_E(t)\ \psi_E(t,\mathbf{x})\ d\mu(E)\\ &= \int_{\sigma_{cont}(t)} a_E(t)\ \psi_E(t,\mathbf{x})\ d\mu(E) + \sum_{E_n\in\sigma_{disc}(t)} a_{E_n}(t)\ \psi_{E_n}(t,\mathbf{x}),\end{aligned} \tag{6.1.3}$$

where $\sigma(t) \equiv \sigma(H(t))$ is the spectrum of $H(t)$, which contains continuous part $\sigma_{cont}(t)$ and may contain discrete set of bound states $\sigma_{disc}(t)$, and $d\mu$ is the corresponding spectral

measure. Inserting this into the above evolution equation we obtain a system of evolution equations for the coefficients

$$\begin{aligned}\dot{a}_E(t) &= \frac{1}{i\hbar}\int_{\sigma(t)} \left\langle \psi_E \left| \left(H(t) - i\hbar\frac{\partial}{\partial t}\right) \psi_{E'} \right\rangle \right. a_{E'}(t)\, d\mu(E') \\ &= -\frac{i}{\hbar}\int_{\sigma(t)} \langle \psi_E | H(t) \psi_{E'}\rangle \, a_{E'}(t)\, d\mu(E') - \int_{\sigma(t)} \langle \psi_E | \dot{\psi}_{E'}\rangle \, a_{E'}(t)\, d\mu(E'),\end{aligned} \tag{6.1.4}$$

assumed that the basis vectors $\psi_E(t,\mathbf{x})$ are differentiable with respect to time. If $E \in \sigma_{disc}(t)$ this equation has the same form after the replacement $E \to \varepsilon_n$. In the literature, the amplitudes $a_E(t)$ are often referred to as excitations of *channels* and the above system of equations (for all $E \in \sigma(t)$) is called *coupled channel equations*.

If we choose the basis $\psi_E(t,\mathbf{x})$ to be generalized eigenvectors of $H(t)$ then the first term on the r.h.s. simplifies

$$\begin{aligned}\dot{a}_E(t) &= -\frac{i}{\hbar}\int_{\sigma(t)} E' \underbrace{\langle \psi_E | \psi_{E'}\rangle}_{\delta(E-E')} \, a_{E'}(t)\, d\mu(E') - \int_{\sigma(t)} \langle \psi_E | \dot{\psi}_{E'}\rangle \, a_{E'}(t)\, d\mu(E') \\ &= -\frac{i}{\hbar} E\, a_E(t) - \int_{\sigma(t)} \langle \psi_E | \dot{\psi}_{E'}\rangle \, a_{E'}(t)\, d\mu(E').\end{aligned} \tag{6.1.5}$$

With the redefinitions

$$a_E(t) \equiv b_E(t)\, e^{-i\chi_E(t)}, \qquad \chi_E(t) \equiv \frac{1}{\hbar}\, E\, (t - t_0), \qquad \text{for } E \in \sigma_{cont}, \tag{6.1.6}$$

$$a_{E_n}(t) \equiv b_{E_n}(t)\, e^{-i\chi_{E_n}(t)}, \qquad \chi_{E_n}(t) \equiv \frac{1}{\hbar}\int_{t_0}^{t} E_n(t')\, dt', \qquad \text{for } E \in \sigma_{disc}. \tag{6.1.7}$$

we can remove the first term and get

$$\dot{b}_E(t) = -\int_{\sigma(t)} e^{-i(\chi_E(t) - \chi_{E'}(t))} \langle \psi_E | \dot{\psi}_{E'}\rangle \, b_{E'}(t)\, d\mu(E'). \tag{6.1.8}$$

Static basis

Analogously, one can consider the *static basis* of generalized eigenvectors of the free Hamiltonian H_0, which gives the decomposition

$$\Psi(t,\mathbf{x}) = \int_{\sigma^0} a_E(t)\, \psi_E(t,\mathbf{x})\, d\mu^0(E) = \int_{\sigma_{cont}{}^0} a_E(t)\, \psi_E(t,\mathbf{x})\, d\mu(E), \tag{6.1.9}$$

where $\sigma^0 \equiv \sigma(H_0) = \sigma_{cont}{}^0 \equiv \sigma_{cont}(H_0)$ is the spectrum of H_0 which is purely continuous and $d\mu$ is the corresponding spectral measure. The coupled channel equations are different from in the adiabatic basis and take the form

$$\begin{aligned}\dot{a}_E(t) &= -\frac{i}{\hbar}\int_{\sigma_{cont}{}^0(t)} \langle \psi_E | (H_0 + V(t)) \psi_{E'}\rangle \, a_{E'}(t)\, d\mu(E') \\ &= -\frac{i}{\hbar} E\, a_E(t) - \frac{i}{\hbar}\int_{\sigma_{cont}{}^0(t)} \langle \psi_E | V(t) \psi_{E'}\rangle \, a_{E'}(t)\, d\mu(E').\end{aligned} \tag{6.1.10}$$

Introducing

$$a_E(t) \equiv c_E(t)\, e^{-iE(t-t_0)} \tag{6.1.11}$$

we remove the first term and get

$$\dot{c}_E(t) = -\frac{i}{\hbar}\int_{\sigma_{cont}{}^0(t)} e^{-i(E-E')t}\langle\psi_E|V(t)\psi_{E'}\rangle\; c_{E'}(t)\; d\mu(E'). \tag{6.1.12}$$

6.1.1 Construction of the (classical) scattering operator S

In the following we choose the adiabatic basis. Equations (6.1.4) and (6.1.8) can be used to solve the Dirac equation for a wave function. To calculate the evolution or the scattering operator numerically, we have to find its all matrix elements

$$U_{E'E} = \langle\psi_{E'}|U\;\psi_E\rangle, \qquad S_{E'E} = \langle\psi_{E'}|S\;\psi_E\rangle. \tag{6.1.13}$$

To reach this goal, the coupled channel equations can be used in the following way. Assume, we want to calculate matrix elements of the evolution operator $U \equiv U(t_1, t_0)$, so we have

$$\Psi(t_1) = U\;\Psi(t_0), \qquad U_{EE} \equiv \langle\psi_E(t_1)|U\;\psi_{E'}(t_0)\rangle \tag{6.1.14}$$

together with the representations

$$\Psi(t_0) \;\equiv\; \int_{\sigma(t_0)} a_E(t_0)\;\psi_E(t_0)\; d\mu(E), \tag{6.1.15}$$

$$\Psi(t_1) \;\equiv\; \int_{\sigma(t_1)} a_E(t_1)\;\psi_E(t_1)\; d\mu(E). \tag{6.1.16}$$

Inserting them into the above, we easily find

$$\begin{aligned} a_E(t_1) &= \left\langle \psi_E(t_1) \,\middle|\, U\int_{\sigma(t_0)} a_{E'}(t_0)\;\psi_{E'}(t_0)\; d\mu(E') \right\rangle \\ &= \int_{\sigma(t_0)} \langle\psi_E(t_1)\,|\,U\;\psi_{E'}(t_0)\rangle\;\; a_{E'}(t_0)\; d\mu(E') \\ &= \int_{\sigma(t_0)} U_{EE'}\; a_{E'}(t_0)\; d\mu(E'). \end{aligned} \tag{6.1.17}$$

Hence, the channel amplitudes $a_E(t_0)$ and $a_E(t_1)$ are uniquely connected by $U_{EE'}$. Unfortunately, we need rather an opposite kind of relation, giving from the numerically calculated $a_E(t_0)$, $a_E(t_1)$ the needed evolution operator. Therefore, we can consider special initial values of the amplitudes of the form

$$a_E(t_0) = \tilde{\delta}(E-E') \equiv \begin{cases} \delta(E-E'), & \text{for } E' \in \sigma_{cont}, \\ \delta_{EE'} \equiv \begin{cases} 1, & \text{if } E = E', \\ 0, & \text{if } E \neq E', \end{cases} & \text{for } E' \in \sigma_{disc} \end{cases} \tag{6.1.18}$$

for a given value E'. Then

$$a_E(t_1) = U_{EE'}, \tag{6.1.19}$$

what means that the numerical calculated $a_E(t_1)$ give "one row" of the matrix elements $U_{EE'}$ for a given E'. To obtain all matrix elements, one has to repeat this procedure for all $E' \in \sigma(t_1)$. Yet, it is numerically more favourable to perform the calculations for all values of E' simultaneously. We can namely introduce extended amplitudes $a_{E'E}(t)$ such that they initially assume special values

$$a_{E'E}(t_0) = \tilde{\delta}(E' - E), \tag{6.1.20}$$

or equivalently define a one-parameter family of wave functions

$$\Psi_{E'}(t) \equiv \int_{\sigma(t)} a_{E'E}(t)\ \psi_E(t)\ d\mu(E) \tag{6.1.21}$$

satisfying the initial conditions

$$\Psi_{E'}(t_0) = \psi_{E'}(t_0). \tag{6.1.22}$$

It leads to

$$a_{E'E}(t_1) = U_{EE'}, \tag{6.1.23}$$

i.e. all matrix elements of U are calculated in a single numerical run[1].

The limit of infinite times $t_0 \to -\infty$ and $t_1 \to \infty$ will, in general, not exist for the evolution operator, as we have it mentioned before, because of complex phases which do not reach any limit. Therefore, to consider the infinite limit, we have to go to the scattering operator S, defined by

$$S \equiv \underset{\substack{t_0\to-\infty\\ t_1\to+\infty}}{\text{s-lim}}\ e^{it_1H_0}\ U(t_1,t_0)\ e^{-it_0H_0}. \tag{6.1.24}$$

The exponents cancel the complex oscillating factors in U and S as well as its matrix elements exist in the limit. Next, we use the fact that the potential vanishes asymptotically and hence $H(t) \to H_0$ as $t \to \pm\infty$. In consequence, the generalized eigenvectors reach the limits: $\lim_{t\to\pm\infty} \psi_E(t) = \varphi_E$, but the initial condition for the extended amplitudes must be modified by a corresponding phase factor: $\lim_{t\to-\infty} e^{iEt} a_{E'E}(t) = \tilde{\delta}(E' - E)$, which follows from the initial condition for the wave functions

$$\lim_{t\to-\infty} \left(\Psi_E(t) - e^{-iEt}\varphi_E\right) = 0, \tag{6.1.25}$$

because φ_E evolve asymptotically according to $\exp(-itH_0)$. Then, the matrix elements of

[1] which is of course computationally more involved, yet in all saves some steps which are repeated for every channel in the standard procedure

S can be defined and calculated as follows

$$\begin{aligned} S_{E'E} \equiv \langle \varphi_{E'} | S\ \varphi_E \rangle &= \lim_{\substack{t_0\to-\infty \\ t_1\to+\infty}} \left\langle e^{-it_1H_0}\varphi_{E'} \,\middle|\, U(t_1,t_0)\ e^{-it_0H_0}\ \varphi_E \right\rangle \\ &= \lim_{\substack{t_0\to-\infty \\ t_1\to+\infty}} \left\langle e^{-it_1E'}\varphi_{E'} \,\middle|\, U(t_1,t_0)\ e^{-it_0E}\ \varphi_E \right\rangle \\ &= \lim_{\substack{t_0\to-\infty \\ t_1\to+\infty}} e^{it_1E'} \langle \varphi_{E'} \mid U(t_1,t_0)\ \Psi_E(t_0) \rangle \\ &= \lim_{\substack{t_0\to-\infty \\ t_1\to+\infty}} e^{it_1E'} \langle \varphi_{E'} \mid \Psi_E(t_1) \rangle \\ &= \lim_{t_1\to\infty} e^{it_1E'} a_{EE'}(t_1). \end{aligned} \tag{6.1.26}$$

Define, for convenience,

$$c_{EE'}(t) \equiv e^{itE'} a_{EE'}(t). \tag{6.1.27}$$

It satisfies the simple initial condition $\lim_{t\to-\infty} c_{E'E}(t) = \tilde{\delta}(E'-E)$ and gives rise to the decomposition

$$\Psi_{E'}(t) \equiv \int_{\sigma(t)} e^{-iEt} c_{E'E}(t)\ \psi_E(t)\ d\mu(E). \tag{6.1.28}$$

The matrix elements of the scattering operator are obtained as a simple limit

$$\boxed{S_{E'E} = \lim_{t\to\infty} c_{EE'}(t).} \tag{6.1.29}$$

Summarizing, we compare all introduced amplitude types

$$\boxed{a_{E'E}(t) = e^{-i\chi_E(t)} b_{E'E}(t) = e^{-itE} c_{E'E}(t),} \tag{6.1.30}$$

where $a_{E'E}$ construct the matrix elements of the evolution operator U, $c_{E'E}$ construct in the limit the scattering operator S and $b_{E'E}$ fulfill the coupled channel equations having the simplest form. We want to mention that these types are often confused in the literature, e.g. in the series of papers by Reinhardt *et al.* [RMG81, RMMG81], etc. as well as in the book of Eichler [EM95], where $b_{E'E}$ and $c_{E'E}$ are mixed up. Fortunately, the error is only up to the complex phase factor which disappears in many observables of interest, like the number of particles created in a scattering process, but may influence more complicated results involving interference of the phase factors.

At the end, note that in the static basis the amplitudes $a_{E'E}$ also construct the evolution operator U, while $c_{E'E}$ construct the scattering operator S, too.

6.1.2 Continuum discretization and cut-off

Numerical calculations cannot be performed in an infinite basis with a continuous parameter (E). There is even no way to remember (encode) all coefficients $a_E(t)$ when $E \in \sigma_{cont}(t)$. Therefore, $\sigma_{cont}(t)$ must be discretized and cut-off so that the resulting set $\tilde{\sigma}_{cont}(t)$ is finite. One way is to base on an integration approximation scheme, replacing the integral by a

sum, picking a discrete set of points where the integrand should be evaluated, and keeping the gaps ΔE_n between them small[2]

$$\begin{aligned}\Psi(t,\mathbf{x}) &\approx \sum_{E\in\tilde{\sigma}_{cont}(t)} a_E(t)\ \psi_E(t,\mathbf{x})\ \Delta E + \sum_{E_n\in\sigma_{disc}(t)} a_{E_n}(t)\ \psi_{E_n}(t,\mathbf{x}) \\ &\equiv \sum_n \tilde{a}_n(t)\ \tilde{\psi}_n(t,\mathbf{x})\ \Delta E_n + \sum_n a_n(t)\ \psi_n(t,\mathbf{x})\end{aligned} \tag{6.1.31}$$

where $E_n \in \tilde{\sigma}_{cont}(t)$. The simplest choice is to pick equidistant points within the continuum, $\Delta E_n = \Delta E$, and choose start points $E_0^{\pm}$ what gives

$$\tilde{\sigma}_{cont} \ni E_n = \begin{cases} E_0^+ + (n-1)\Delta E, & n > 0, \\ E_0^- - (n-1)\Delta E, & n < 0. \end{cases} \tag{6.1.32}$$

Optimal choice of $E_0^{\pm}$, giving best approximation of the integral, is $E_0^{\pm} = \pm 1 \pm \Delta E/2$. Then

$$\Psi(t,\mathbf{x}) \approx \sum_{n=1}^{\infty} \tilde{a}_n(t)\ \tilde{\psi}_n(t,\mathbf{x})\ \Delta E + \sum_{n=-\infty}^{-1} \tilde{a}_n(t)\ \tilde{\psi}_n(t,\mathbf{x})\ \Delta E + \sum_n a_n(t)\ \psi_n(t,\mathbf{x}). \tag{6.1.33}$$

This system is still infinite, hence as next one has to cut-off the infinite sums to finite, introducing the numbers $N_{\pm}$ of (numerical) states in the positive and negative discretized continua. Finally,

$$\Psi(t,\mathbf{x}) \approx \sum_{n=1}^{N_+} \tilde{a}_n(t)\ \tilde{\psi}_n(t,\mathbf{x})\ \Delta E + \sum_{n=-N_-}^{-1} \tilde{a}_n(t)\ \tilde{\psi}_n(t,\mathbf{x})\ \Delta E + \sum_n a_n(t)\ \psi_n(t,\mathbf{x}). \tag{6.1.34}$$

Here, the argument for the approximation is more involved and concerns the quantities to be calculated. Namely, it is expected that the matrix elements of the discretized evolution or scattering operator, which will be calculated by this method, are small for big absolute values of the index $|n|$. This condition must be carefully checked, since it is not obvious at all and is not always fulfilled.

Fano formalism: extraction of the resonance state

When a resonance is present in the continuum there is a method, called sometimes the Fano formalism, to treat it as a separate state. One defines a projector on the resonance state and by its help redefines all states in the continuum to make them orthogonal to the resonance state (in a sense, one subtracts the resonance from the continuum) [WS70], so that the new continuum does not "contain" the resonance any more, what can be observed in a phase-shift analysis (mentioned in section 3.3.2) of the new continuum wave functions [RMG81]. Such new basis does not diagonalize the Hamiltonian what leads to

[2]Some other methods are based upon stationary or Weyl time-dependent wave packets, but their calculation is much more involved numerically. For their definition and comparison we refer to [Bru01], [GGS03] and [BS85].

a nontrivial free evolution of the states, in particular, the resonance gets "coupled" to the new continuum and its amplitude decays in time.

There are two problems with this method, which cause that we do not adopt it in our calculations. First, the resonance eigenfunction corresponding to a complex pole of the resolvent (cf. section 3.3) is not normalizable in Hilbert space. Therefore one has to use some other, similar function to represent the resonance, but such choice is always arbitrary, like e.g. in [RMG81], where a phase-shift analysis with a cut-off at big distances has been performed. Second, the problem of "no decay" of a resonance in a discretized finite continuum for long evolution times, which we discussed in section 4.4.1 under "Problems in the numerics", remains, because it is a consequence of a finite-dimensionality of the Hilbert space spanned by a discretized finite continuum and not of a choice of the basis.

6.2 Time-dependence: sudden switch on

First, we consider the simplest time-dependent process, which we called in the previous chapter *quasi-static*, where the potential is almost all the time static, except a single moment when its value changes discontinuously. Here, time-dependent will be the strength of the spherically symmetric square well, i.e.

$$V(t,\mathbf{x}) = V(t,r) = U(t)\cdot v(r) = U(t)\cdot\Theta(a-r) = \begin{cases} U(t), & r<a, \\ 0, & r>a \end{cases} \tag{6.2.1}$$

and

$$U(t) = -U - (U'-U)\cdot\Theta(T-|t|) = \begin{cases} -U, & t<0, \\ -U', & t>0, \end{cases} \tag{6.2.2}$$

with $U' > U > 0$. It gives

$$V(t,\mathbf{x}) = V(t,r) \equiv \begin{cases} V_1(r), & t<0, \\ V_2(r), & t>0 \end{cases}, \qquad H(t) \equiv \begin{cases} H_1, & t<0, \\ H_2, & t>0. \end{cases} \tag{6.2.3}$$

From theorem 9 or 10 with $a = 0$ and $b = U'$ follows that $H(t) = H_0 + V(t)$ is self-adjoint on $\mathcal{D}(H_0)$ for every time t. Because $H(t)$ is constant for $t < 0$ and $t > 0$ there exists a unitary propagator (cf. section 3.4)

$$U(t_2,t_1) = \begin{cases} e^{-iH_1(t_2-t_1)} & \text{for } t_1,t_2<0, \\ e^{-iH_2(t_2-t_1)} & \text{for } t_1,t_2>0, \\ e^{-iH_2t_2}e^{iH_1t_1} & \text{for } t_1<0<t_2. \end{cases} \tag{6.2.4}$$

Since $V(t)$ is of short-range the wave-operators (3.5.3) exist and are complete (e.g. because $V(t) \in L^p(\mathbb{R}^3)$ with any $p > 0$ – cf. section 3.5.1). Consequently, there exists a unitary scattering operator S in $\mathcal{H}$ (3.5.10). According to considerations in section 4.2.4 and equation (4.2.47) this scattering operator S is implementable when the switched potential

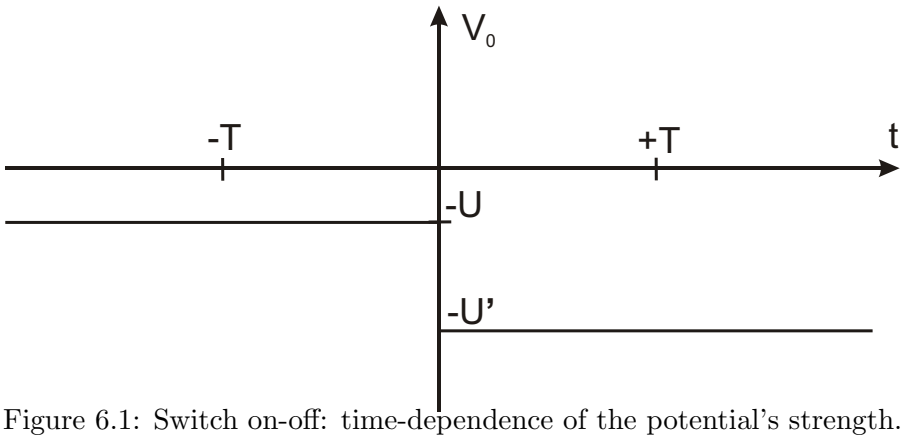


Figure 6.1: Switch on-off: time-dependence of the potential's strength.

is regular (in the sense of theorem 6). Though the still do not know whether the square well potential is regular, we have shown in section 5.4 that it can be easily regularized by making it continuous what hardly modifies the solutions. We will be able to check the regularity and thereby the implementability of S for the exact square well when we find the operator S explicitly.

The scattering operator in $\mathcal{H}$ can be calculated, as discussed in the previous section, from the coupled channel equations (inserting the discontinuously varying potential), however we can easily solve the evolution in two bases ϕ_E and χ_E consisting of generalized eigenvectors to the Hamiltonians H_1 and H_2, respectively, and make a projection at $t = 0$ to find

$$\boxed{S^{U'U}_{E'E} = \langle \chi_{E'}, \phi_E \rangle.} \tag{6.2.5}$$

It means that to calculate $S^{U'U}_{E'E}$ we only need to evaluate the scalar products $(\chi_{E'}, \phi_E)$, what we do below.

6.2.1 Projections – scalar products

From now on, we go over to dimensionless variables introduced in (5.2.3). Consider the bases ϕ_ε and χ_ε as special cases of a more general family of bases $\psi_{\varepsilon,U}$ formed by the generalized eigenvectors of $H_U \equiv H_0 - Uv(r)$. In this section we will calculate the scalar products $\langle \psi_{\varepsilon,U} | \psi_{\varepsilon',U'} \rangle$.

Let $F_{\varepsilon,U}$ and $G_{\varepsilon,U}$ denote the functions $F_{\varepsilon,U}(R)$ and $G_{\varepsilon,U}(R)$ solving the Dirac equations (5.2.11)-(5.2.12). First, using these equations, transform the following expression

$$
\begin{aligned}
&\big((\varepsilon+U)-(\varepsilon'+U')\big)\int_0^A \left[\overline{G_{\varepsilon,U}}\,G_{\varepsilon',U'}+\overline{F_{\varepsilon,U}}\,F_{\varepsilon',U'}\right]R\,dR\\
&\qquad=\int_0^A \left[(\varepsilon+U)\,\overline{G_{\varepsilon,U}}\,G_{\varepsilon',U'}+(\varepsilon+U)\,\overline{F_{\varepsilon,U}}\,F_{\varepsilon',U'}\right]R\,dR\\
&\qquad\quad-\int_0^A \left[\overline{G_{\varepsilon,U}}\,(\varepsilon'+U')\,G_{\varepsilon',U'}+\overline{F_{\varepsilon,U}}\,(\varepsilon'+U')\,F_{\varepsilon',U'}\right]R\,dR\\
&\qquad\overset{\substack{(5.2.11)\\(5.2.12)}}{=}\int_0^A \left[\left(\overline{F'_{\varepsilon,U}}+\frac{\kappa+\frac12}{R}\,\overline{F_{\varepsilon,U}}-\overline{G_{\varepsilon,U}}\right)G_{\varepsilon',U'}\right.\\
&\qquad\qquad\left.+\left(-\overline{G'_{\varepsilon,U}}+\frac{\kappa-\frac12}{R}\,\overline{G_{\varepsilon,U}}+\overline{F_{\varepsilon,U}}\right)F_{\varepsilon',U'}\right]R\,dR\\
&\qquad\quad-\int_0^A \left[\overline{G_{\varepsilon,U}}\left(F'_{\varepsilon',U'}+\frac{\kappa+\frac12}{R}\,F_{\varepsilon',U'}-G_{\varepsilon',U'}\right)\right.\\
&\qquad\qquad\left.+\overline{F_{\varepsilon,U}}\left(-G'_{\varepsilon',U'}+\frac{\kappa-\frac12}{R}\,G_{\varepsilon',U'}+F_{\varepsilon',U'}\right)\right]R\,dR\\
&\qquad=\int_0^A \left[\overline{F'_{\varepsilon,U}}\,G_{\varepsilon',U'}+\overline{F_{\varepsilon,U}}\,G'_{\varepsilon',U'}+\frac{1}{R}\,\overline{F_{\varepsilon,U}}\,G_{\varepsilon',U'}\right.\\
&\qquad\qquad\left.-\overline{G'_{\varepsilon,U}}\,F_{\varepsilon',U'}-\overline{G_{\varepsilon,U}}\,F'_{\varepsilon',U'}-\frac{1}{R}\,\overline{G_{\varepsilon,U}}\,F_{\varepsilon',U'}\right]R\,dR\\
&\qquad=\int_0^A \left[R\left(\overline{F_{\varepsilon,U}}\,G_{\varepsilon',U'}-\overline{G_{\varepsilon,U}}\,F_{\varepsilon',U'}\right)\right]'dR\\
&\qquad=A\left[\overline{F_{\varepsilon,U}(A)}\,G_{\varepsilon',U'}(A)-\overline{G_{\varepsilon,U}(A)}\,F_{\varepsilon',U'}(A)\right].
\end{aligned}
\tag{6.2.6}
$$

Analogously, we can transform

$$
\begin{aligned}
&\big(\varepsilon-\varepsilon'\big)\int_A^\infty \left[\overline{G_{\varepsilon,U}}\,G_{\varepsilon',U'}+\overline{F_{\varepsilon,U}}\,F_{\varepsilon',U'}\right]R\,dR\overset{\substack{(5.2.11)\\(5.2.12)}}{=}\int_A^\infty \left[R\left(\overline{F_{\varepsilon,U}}\,G_{\varepsilon',U'}-\overline{G_{\varepsilon,U}}\,F_{\varepsilon',U'}\right)\right]'dR\\
&=-A\left[\overline{F_{\varepsilon,U}(A)}\,G_{\varepsilon',U'}(A)-\overline{G_{\varepsilon,U}(A)}\,F_{\varepsilon',U'}(A)\right]\\
&\quad+\lim_{R\to\infty}R\left[\overline{F_{\varepsilon,U}(R)}\,G_{\varepsilon',U'}(R)-\overline{G_{\varepsilon,U}(R)}\,F_{\varepsilon',U'}(R)\right].
\end{aligned}
\tag{6.2.7}
$$

By a similar technique, using (5.2.11)-(5.2.12), we can show

$$
\big(\varepsilon+\varepsilon'\big)\left[\overline{F_{\varepsilon,U}}\,G_{\varepsilon',U'}-\overline{G_{\varepsilon,U}}\,F_{\varepsilon',U'}\right]\overset{\substack{(5.2.11)\\(5.2.12)}}{=}W\left[\overline{G_{\varepsilon,U}},G_{\varepsilon',U'}\right]+W\left[\overline{F_{\varepsilon,U}},F_{\varepsilon',U'}\right],
\tag{6.2.8}
$$

with W denoting the Wronskian of two functions. Using the last three relations, we can

express the scalar product as

$$\begin{aligned}\langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle &\equiv \int_0^\infty \left[\overline{G_{\varepsilon,U}}\, G_{\varepsilon',U'} + \overline{F_{\varepsilon,U}}\, F_{\varepsilon',U'}\right] R\, dR \\ &= \int_0^A \left[\overline{G_{\varepsilon,U}}\, G_{\varepsilon',U'} + \overline{F_{\varepsilon,U}}\, F_{\varepsilon',U'}\right] R\, dR + \int_A^\infty \left[\overline{G_{\varepsilon,U}}\, G_{\varepsilon',U'} + \overline{F_{\varepsilon,U}}\, F_{\varepsilon',U'}\right] R\, dR \\ &= \left[\frac{1}{(\varepsilon+U)-(\varepsilon'+U')} - \frac{1}{(\varepsilon-\varepsilon')}\right] A\left[\overline{F_{\varepsilon,U}(A)}\, G_{\varepsilon',U'}(A) - \overline{G_{\varepsilon,U}(A)}\, F_{\varepsilon',U'}(A)\right] \\ &\quad + \frac{1}{\varepsilon^2-\varepsilon'^2}\lim_{R\to\infty} R\left(W\left[\overline{G_{\varepsilon,U}}, G_{\varepsilon',U'}\right] + W\left[\overline{F_{\varepsilon,U}}, F_{\varepsilon',U'}\right]\right) \\ &= \frac{A(U-U')}{[(\varepsilon-\varepsilon')+(U-U')](\varepsilon-\varepsilon')}\left[\overline{G_{\varepsilon,U}(A)}\, F_{\varepsilon',U'}(A) - \overline{F_{\varepsilon,U}(A)}\, G_{\varepsilon',U'}(A)\right] \\ &\quad + \frac{1}{\varepsilon^2-\varepsilon'^2}\lim_{R\to\infty} R\left(W\left[\overline{G_{\varepsilon,U}}, G_{\varepsilon',U'}\right] + W\left[\overline{F_{\varepsilon,U}}, F_{\varepsilon',U'}\right]\right)\end{aligned} \tag{6.2.9}$$

It remains to evaluate the limit $R\to\infty$ in the last expression. The functions F and G tend to zero exponentially for bound states and oscillate with a very slow $\sim R^{-1/2}$ decay in the continuum. Therefore we immediately get zero in the case when at least one of the functions describes a bound state, i.e. one of the energies ε or ε' is in $(-1,1)$. If both are in the continuum then we must insert the explicit form of the solutions (5.2.38)-(5.2.39), use the asymptotic expansion of the Bessel functions (5.5.23) and utilize the distributional identities

$$\lim_{R\to\infty}\frac{\sin(kR)}{k} = \pi\delta(k), \qquad \lim_{R\to\infty}\frac{\cos(kR)}{k} = 0 \tag{6.2.10}$$

to obtain

$$\begin{aligned}&\frac{1}{\varepsilon^2-\varepsilon'^2}\lim_{R\to\infty} R\left(W\left[\overline{G_{\varepsilon,U}}, G_{\varepsilon',U'}\right] + W\left[\overline{F_{\varepsilon,U}}, F_{\varepsilon',U'}\right]\right) \\ &\qquad = \left[\overline{A_2(\varepsilon,U)}A_2(\varepsilon,U') + \overline{B_2(\varepsilon,U)}B_2(\varepsilon,U')\right]\frac{2}{|\varepsilon-1|}\,\delta(\varepsilon-\varepsilon').\end{aligned} \tag{6.2.11}$$

Finally, we have

$$\boxed{\begin{aligned}\langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle &= \frac{A(U-U')}{[(\varepsilon-\varepsilon')+(U-U')](\varepsilon-\varepsilon')}\left[\overline{G_{\varepsilon,U}(A)}\, F_{\varepsilon',U'}(A) - \overline{F_{\varepsilon,U}(A)}\, G_{\varepsilon',U'}(A)\right] \\ &\quad + \begin{cases}\left[\overline{A_2(\varepsilon,U)}A_2(\varepsilon,U') + \overline{B_2(\varepsilon,U)}B_2(\varepsilon,U')\right]\frac{2}{|\varepsilon-1|}\,\delta(\varepsilon-\varepsilon'), & |\varepsilon|,|\varepsilon'|>1, \\ 0, & \text{otherwise.}\end{cases}\end{aligned}} \tag{6.2.12}$$

It satisfies explicitly the complex conjugation property

$$\langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle = \overline{\langle\psi_{\varepsilon',U'}|\psi_{\varepsilon,U}\rangle}. \tag{6.2.13}$$

Below we analyze some special values of $\varepsilon, \varepsilon', U$ and U' in this formula.

Singular point $\varepsilon = \varepsilon'$

For energies $\varepsilon, \varepsilon'$ such that $\varepsilon - \varepsilon' \to 0$ the denominator of the first term in the scalar product (6.2.12) becomes zero. The terms $(U - U')/[(\varepsilon - \varepsilon') + (U - U')]$ cancel to 1 and the behaviour of the term $\left[\overline{G_{\varepsilon,U}}\, F_{\varepsilon',U'} - \overline{F_{\varepsilon,U}}\, G_{\varepsilon',U'}\right]\big|_A$ depends on whether the energies are in the continuous or discrete spectrum. In continuum, $\left[\overline{G_{\varepsilon,U}}\, F_{\varepsilon,U'} - \overline{F_{\varepsilon,U}}\, G_{\varepsilon,U'}\right]\big|_A$ is finite and non-zero, in general. Therefore, the first term becomes singular at $\varepsilon = \varepsilon'$, having a pole of the first order. The second term contains $\delta(\varepsilon - \varepsilon')$ and is also singular at $\varepsilon = \varepsilon'$. Later, to integrate the scalar product (6.2.12) over the continuum, the principal value will have to be taken.

In the bound state situation, there are again two cases. In the first, it may happen that the potential strengths are different $U \neq U'$, but both have a bound state with the same energy $\varepsilon = \varepsilon'$. Because the functions $G_{\varepsilon,U}(A), F_{\varepsilon,U}(A)$ depend on U only by the normalization constants, which can be taken in front of the difference $\left[\overline{G_{\varepsilon,U}}\, F_{\varepsilon,U'} - \overline{F_{\varepsilon,U}}\, G_{\varepsilon,U'}\right]\big|_A$, the rest depends only on the energies $\varepsilon, \varepsilon'$, which we put equal and get zero. To deal with the result $0/0$ we have to differentiate this expression with respect to ε at the point $\varepsilon = \varepsilon'$. A rather lengthy calculation gives finally a finite result, which we do not cite here, because it is very rarely used.

The second case, when the bound state energies $\varepsilon' \to \varepsilon$ together with $U' \to U$, i.e. $\varepsilon = \varepsilon_n(U)$ and $\varepsilon' = \varepsilon'_n(U')$ correspond to the same bound state, will be treated below as a limit $U' \to U$.

Singular point $\varepsilon + U = \varepsilon' + U'$

Again, for $\varepsilon + U = \varepsilon' + U'$ the denominator of the first term in the scalar product (6.2.12) becomes zero and $(U - U')/(\varepsilon - \varepsilon')$ cancel to -1, yet the term $\left[\overline{G_{\varepsilon,U}}\, F_{\varepsilon',U'} - \overline{F_{\varepsilon,U}}\, G_{\varepsilon',U'}\right]\big|_A$ becomes zero, too, what can be deduced from (6.2.6)

$$\big((\varepsilon + U) - (\varepsilon' + U')\big) \int_0^A \left[\overline{G_{\varepsilon,U}}\, G_{\varepsilon',U'} + \overline{F_{\varepsilon,U}}\, F_{\varepsilon',U'}\right] R\, dR = A\left[\overline{F_{\varepsilon,U}(A)}\, G_{\varepsilon',U'}(A) - \overline{G_{\varepsilon,U}(A)}\, F_{\varepsilon',U'}(A)\right]. \quad (6.2.14)$$

The integral on the l.h.s. is bounded, hence the r.h.s. must vanish when $(\varepsilon+U)-(\varepsilon'+U') \to 0$. Therefore, the whole first term in the scalar product is of type $0/0$ and we again must differentiate it with respect to ε to find the limit which is finite. The second term of the scalar product (6.2.12), containing $\delta(\varepsilon - \varepsilon')$, vanishes, because we consider here only $\varepsilon \neq \varepsilon'$ and $U \neq U'$.

Limit $U' \to U$

For completeness we add a short analysis of the limit $U' \to U$ in the scalar product formula (6.2.12). If both energies ε and ε' belong to the continuum, the first term vanishes and the

second term becomes $1 \cdot \delta(\varepsilon - \varepsilon')$ therefore reproducing the orthonormality of the basis

$$\langle \psi_{\varepsilon,U} | \psi_{\varepsilon',U} \rangle = \delta(\varepsilon - \varepsilon'). \tag{6.2.15}$$

If one of the energies belongs to the discrete and the other to the continuous spectrum then the limit $U' \to U$ in (6.2.12) gives trivially zero. If both energies $\varepsilon, \varepsilon'$ are from the discrete spectrum (i.e. correspond to bound states) then they are functions of U, U', respectively. Enumerating the bound states with n, m we have $\varepsilon = \varepsilon_n(U)$ and $\varepsilon' = \varepsilon_m(U')$. The first (and only) term of (6.2.12) vanishes when $U = U'$ and $\varepsilon_n(U) \neq \lim_{U' \to U} \varepsilon_m(U') = \varepsilon_m(U)$, i.e. for $n \neq m$. In the case $n = m$ we get again $0/0$ and must differentiate with respect to U, including the dependence of $\varepsilon_n(U)$ and $\varepsilon_m(U)$. A lengthy calculation gives 1, hence

$$\langle \psi_{\varepsilon_n,U} | \psi_{\varepsilon_m,U} \rangle = \delta_{nm}, \tag{6.2.16}$$

confirming orthonormality of bound states.

Asymptotic behaviour for $|\varepsilon|, |\varepsilon'| \gg 1$

For the purpose of numerical error estimation, we need to find the asymptotic behaviour of the scalar product (6.2.12) for big values of one or both values of $|\varepsilon|, |\varepsilon'|$. Since we consider only continuum wave functions, we use the definitions (5.2.36)-(5.2.37)

$$G_{\varepsilon,U}(A) = A_1(\varepsilon, U)\ J_{|\kappa - \frac{1}{2}|}(\omega_1 A), \tag{6.2.17}$$

$$F_{\varepsilon,U}(A) = C_1(\varepsilon, U)\ J_{|\kappa + \frac{1}{2}|}(\omega_1 A) \tag{6.2.18}$$

and $C_1(\varepsilon, U) = \text{sign}\,(\kappa)\, \frac{\sqrt{(\varepsilon+U)^2 - 1}}{\varepsilon + U - 1} A_1(\varepsilon, U)$ with $A_1(\varepsilon, U)$ being the normalization constant. The asymptotic analysis gives

$$A_1(\varepsilon, U) \cong \sqrt{\frac{|\varepsilon|}{2}}, \qquad C_1(\varepsilon, U) \cong \text{sign}\,(\kappa)\, \text{sign}\,(\varepsilon)\, A_1(\varepsilon, U) \tag{6.2.19}$$

and

$$J_{|\kappa \pm \frac{1}{2}|}(\omega_1 A) \cong \sqrt{\frac{2}{\pi A |\varepsilon|}}\ \cos\left(|\varepsilon + U| A - \frac{\pi}{2} \left| \kappa \pm \frac{1}{2} \right| - \frac{\pi}{4} \right). \tag{6.2.20}$$

Combined together we obtain

$$|G_{\varepsilon,U}(A)| \lesssim \frac{1}{\sqrt{\pi A}}, \qquad |F_{\varepsilon,U}(A)| \lesssim \frac{1}{\sqrt{\pi A}}. \tag{6.2.21}$$

Hence, for $|\varepsilon| \gg 1$ and ε' arbitrary, we find the estimate

$$\left| \langle \psi_{\varepsilon,U} | \psi_{\varepsilon',U'} \rangle \right| \lesssim \frac{\sqrt{A}\ |U - U'|}{\sqrt{\pi}\ \varepsilon^2} \left(|F_{\varepsilon',U'}(A)| + |G_{\varepsilon',U'}(A)| \right), \tag{6.2.22}$$

which shows that the absolute value of the scalar product vanishes for big energies like $\sim |\varepsilon|^{-2}$ for a constant value of ε'.

For both $|\varepsilon|, |\varepsilon'|$ being big we find

$$\overline{G_{\varepsilon,U}(A)}\ F_{\varepsilon',U'}(A) - \overline{F_{\varepsilon,U}(A)}\ G_{\varepsilon',U'}(A) \cong -\frac{1}{\pi A}\ \sin\left[(\varepsilon - \varepsilon' + U - U')A\right]. \tag{6.2.23}$$

Because $\varepsilon - \varepsilon'$ may be small, we must keep the second term in the scalar product (6.2.12), approximating only the factor multiplying the delta-function

$$\overline{A_2(\varepsilon,U)}\ A_2(\varepsilon,U') + \overline{B_2(\varepsilon,U)}\ B_2(\varepsilon,U')\frac{2}{|\varepsilon-1|} \cong \frac{2}{|\varepsilon|}\ \cos\left[(U-U')A\right]. \tag{6.2.24}$$

Finally, we get

$$\boxed{\langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle \cong -\frac{(U-U')\ \sin\left[(\varepsilon-\varepsilon'+U-U')A\right]}{\pi(\varepsilon-\varepsilon'+U-U')(\varepsilon-\varepsilon')} + \frac{2}{|\varepsilon|}\ \cos\left[(U-U')A\right]\ \delta(\varepsilon-\varepsilon')}, \tag{6.2.25}$$

which approximates also cases with $\varepsilon \approx \varepsilon'$ and $\varepsilon + U \approx \varepsilon' + U'$. For $\mathrm{sign}\,(\varepsilon) = -\mathrm{sign}\,(\varepsilon')$ it reduces to

$$\left|\langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle\right| \lesssim \frac{|U-U'|}{\pi|\varepsilon-\varepsilon'|^2}. \tag{6.2.26}$$

Implementability of S

Now, having

$$\begin{aligned} S^{U'U}_{E'E} &= \langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle \\ &= \frac{A(U-U')}{[(\varepsilon-\varepsilon')+(U-U')](\varepsilon-\varepsilon')}\left[\overline{G_{\varepsilon,U}(A)}\ F_{\varepsilon',U'}(A) - \overline{F_{\varepsilon,U}(A)}\ G_{\varepsilon',U'}(A)\right] \\ &+ \begin{cases} \left[\overline{A_2(\varepsilon,U)}A_2(\varepsilon,U') + \overline{B_2(\varepsilon,U)}B_2(\varepsilon,U')\right]\frac{2}{|\varepsilon-1|}\ \delta(\varepsilon-\varepsilon'), & |\varepsilon|,|\varepsilon'|>1, \\ 0, & \text{otherwise} \end{cases} \end{aligned} \tag{6.2.27}$$

we can explicitly investigate the implementability of S.

Theorem 18 *The above defined unitary operator S is implementable in Fock space, i.e. $S_{\pm\mp}$ are Hilbert-Schmidt.*

Proof:
Since for $t_2 > 0 > t_1$ holds (4.2.47)

$$||[U(t_2,t_1)]_{\pm\mp}||_{HS} = ||S_{\pm\mp}||_{HS}, \tag{6.2.28}$$

it is enough to show that $[U_T]_{\pm\mp}$ are Hilbert-Schmidt (and hence implementable in $\mathcal{F}$).

$$\begin{aligned} ||U(t_2,t_1)_{-+}||^2_{HS} &= \int_0^\infty d\mu(\varepsilon)\int_{-\infty}^0 d\mu(\varepsilon')\ |(\chi_{\varepsilon'},\phi_\varepsilon)|^2 \\ &= \int_1^\infty d\varepsilon\int_{-\infty}^{-1} d\varepsilon'\ \frac{A^2(U-U')^2\left|\overline{G_{\varepsilon,U}(A)}\ F_{\varepsilon',U'}(A) - \overline{F_{\varepsilon,U}(A)}\ G_{\varepsilon',U'}(A)\right|^2}{[(\varepsilon+U)-(\varepsilon'+U')]^2(\varepsilon-\varepsilon')^2} \\ &+ \sum_{\text{bound states}}(...) \end{aligned} \tag{6.2.29}$$

The sum over the bound states is finite hence we do not need to consider it any more. The double-integral, call it I_1, can be split using the asymptotic form of the integrand by the scheme

$$I_1 = \int X = \underbrace{\int (X - X_{asympt})}_{I_2} + \underbrace{\int X_{asympt}}_{I_3}. \tag{6.2.30}$$

Again I_2 must be finite, so we need to consider further only I_3. Using (6.2.25) we have

$$I_3 = \int_1^\infty d\varepsilon \int_{-\infty}^{-1} d\varepsilon' \; \frac{(U-U')^2 \sin^2((\varepsilon + U - \varepsilon' - U')A)}{\pi^2(\varepsilon + U - \varepsilon' - U')^2(\varepsilon - \varepsilon')^2}. \tag{6.2.31}$$

By substitution $v \equiv \varepsilon - \varepsilon'$, $w \equiv \varepsilon + \varepsilon'$ and introducing $\Delta U \equiv U - U'$ we obtain

$$\begin{aligned} I_3 &= \frac{\Delta U^2}{\pi^2} \int_2^\infty dv \int_{2-v}^{v-2} dw \; \frac{\sin^2((v+\Delta U)A)(v-2)}{(v+\Delta U)^2 v^2} \\ &\leq \frac{\Delta U^2}{\pi^2} \underbrace{\sup_{v \geq 2} \frac{v-2}{v^2}}_{\leq 1/2} \cdot \underbrace{\int_{(2+\Delta U)A}^\infty \frac{\sin^2(x)}{x^2} \, dx}_{\leq \pi} \\ &\leq \frac{\Delta U^2}{2\pi} < \infty. \end{aligned} \tag{6.2.32}$$

So we have shown finiteness of $||U(t_2,t_1)_{-+}||_{HS}$. The case $||U(t_2,t_1)_{+-}||_{HS}$ can be treated analogously. Finally, $U(t_2,t_1)$ and hence S are implementable in the Fock space $\mathcal{F}$. □

Moreover, it follows immediately

Theorem 19 *The spherically symmetric square well potential defined in (5.2.1) is regular (in the sense of theorem 6).*

Proof:
By (4.2.47) we have

$$||P_\pm(\lambda_1^+) \; P_\mp^0||_{HS} = ||[U(t_2,t_1)]_{\pm\mp}||_{HS} = ||S_{\pm\mp}||_{HS}, \tag{6.2.33}$$

and according to the theorem 18 these norms are finite. Hence, by theorem 6 the potential is regular. □

This result falsifies the conjecture of Nenciu and Scharf [NS78] that the condition (2.7.27) decides about regularity of the potential. The square well does not satisfy this condition, but is regular.

Particle production and continuum cut-off problem

The numerical problems with the infinite set of continuum states, mentioned above, appear in this very simple setting of a sudden switch on of the potential first at the level of a particle production, where a first integral over the continuum must be evaluated. The

numbers of particles and antiparticles created from vacuum are (4.2.37)

$$N_\varepsilon^+ = \int_{\sigma^-} |S^{U'U}_{\varepsilon\varepsilon'}|^2 d\varepsilon' = \int_{{\sigma_{cont}}^-} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' + \sum_{\sigma^-_{disc}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon'_n,U}\rangle\right|^2 \Delta\varepsilon'_n \quad (6.2.34)$$

$$N_\varepsilon^- = \int_{\sigma^+} |S^{U'U}_{\varepsilon\varepsilon'}|^2 d\varepsilon' = \int_{{\sigma_{cont}}^+} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' + \sum_{\sigma^+_{disc}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon'_n,U}\rangle\right|^2 \Delta\varepsilon'_n. \quad (6.2.35)$$

Introducing cut-offs in both continua ${\sigma_{cont}}^\pm$ at the values $\varepsilon^\pm_{cut}$ we get

$$N_\varepsilon^+ = \int_{\varepsilon^-_{cut}}^{-1} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' + \sum_{\sigma^-_{disc}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon'_n,U}\rangle\right|^2 \Delta\varepsilon'_n + \delta N_\varepsilon^+ \quad (6.2.36)$$

$$N_\varepsilon^- = \int_{1}^{\varepsilon^+_{cut}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' + \sum_{\sigma^+_{disc}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon'_n,U}\rangle\right|^2 \Delta\varepsilon'_n + \delta N_\varepsilon^-, \quad (6.2.37)$$

where $\delta N_\varepsilon^\pm$ are errors due to the neglected tails of the integrals, which can be estimated with the help of (6.2.26) to

$$|\delta N_\varepsilon^+| = \int_{-\infty}^{\varepsilon^-_{cut}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' \lesssim \int_{-\infty}^{\varepsilon^-_{cut}} \frac{|U-U'|^2}{\pi^2|\varepsilon-\varepsilon'|^4}\, d\varepsilon' = \frac{|U-U'|^2}{3\pi^2(\varepsilon-\varepsilon^-_{cut})^3} \le \frac{|U-U'|^2}{3\pi^2|\varepsilon^-_{cut}|^3}, \quad (6.2.38)$$

$$|\delta N_\varepsilon^-| = \int_{\varepsilon^+_{cut}}^{\infty} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' \lesssim \int_{\varepsilon^-_{cut}}^{\infty} \frac{|U-U'|^2}{\pi^2|\varepsilon-\varepsilon'|^4}\, d\varepsilon' = \frac{|U-U'|^2}{3\pi^2(\varepsilon^+_{cut}-\varepsilon)^3} \le \frac{|U-U'|^2}{3\pi^2|\varepsilon^+_{cut}|^3}. \quad (6.2.39)$$

The cut-offs $\varepsilon^\pm_{cut}$ must be chosen so that the errors are small relative to the interesting quantities, i.e.

$$|\delta N_\varepsilon^\pm| \ll |N_\varepsilon^\pm|. \quad (6.2.40)$$

6.2.2 Particle production spectra – numerical results

In all calculations below we assume $A = 1$. In most cases, stable numerical results have been obtained from $\varepsilon_{cut} = 6$ and 50 states in the discretized continuum, if not stated otherwise below.

Weakly subcritical → strongly overcritical

Consider a switch on process from a weakly subcritical $U = 2$ with a bound state at $\varepsilon_1 \approx 0.641$ to a strongly overcritical $U' = 5$ with no bound states. In that case

$$N_\varepsilon^+ = \int_{\varepsilon^-_{cut}}^{-1} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon', \quad (6.2.41)$$

$$N_\varepsilon^- = \int_{1}^{\varepsilon^+_{cut}} \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon',U}\rangle\right|^2 d\varepsilon' + \left|\langle\psi_{\varepsilon,U'}|\psi_{\varepsilon_1,U}\rangle\right|^2. \quad (6.2.42)$$

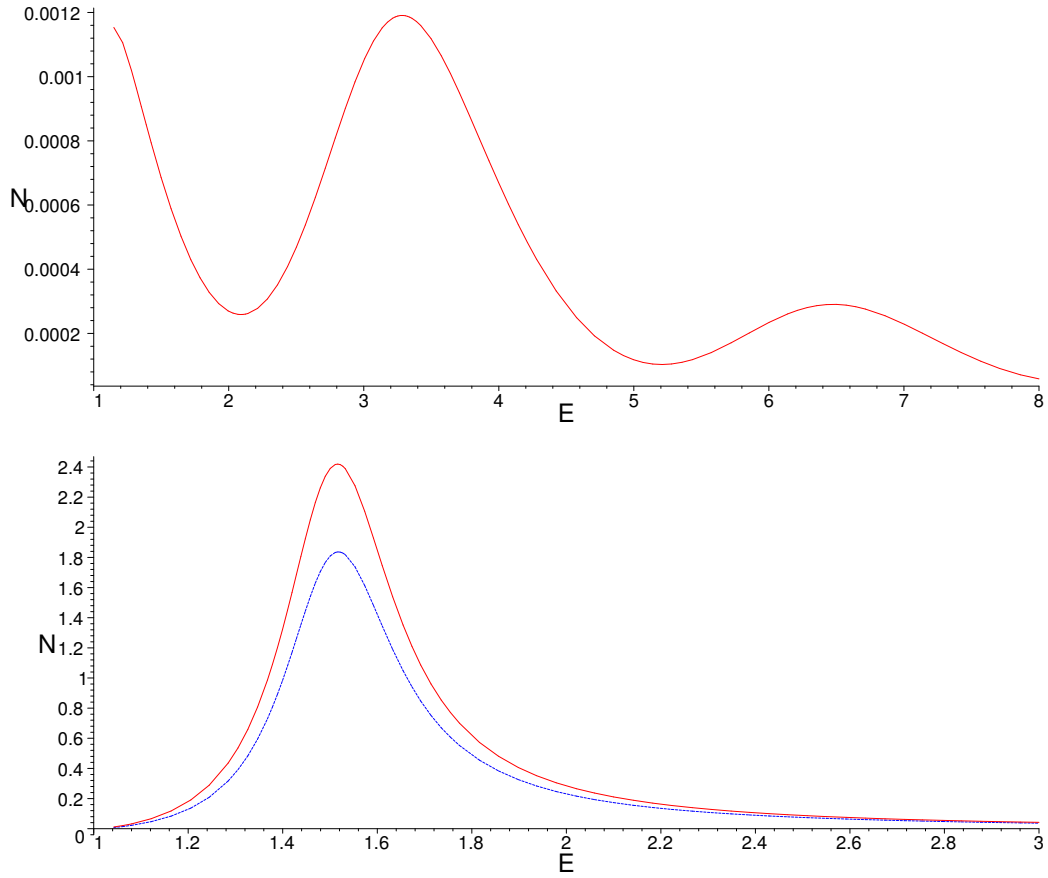


Figure 6.2: Switch on: weakly subcritical $\rightarrow$ strongly overcritical. Particle (up) and antiparticle (down) production. The (blue) dashed line shows contribution from the diving bound state only.

On figure 6.2 we see that production of antiparticles is strongly peaked around $\varepsilon_{peak} \approx -1.5$. The diving bound state itself makes the strongest contribution. The bumps in the particle production spectrum, weaker than the antiparticle peak by more then 3 orders of magnitude, are due to interference effects at the finite size of the potential well and have period π/A. In the positive spectrum stable numerical results have been obtained first from $\varepsilon_{cut} = 21$ due to its non-local distribution.

Weak (no bound states) $\rightarrow$ strongly overcritical

The existence of the peak in the antiparticle production spectrum is related to the overcriticality of the final potential, where a bound state dives into the continuum and becomes a resonance. In order to check if the existence of the peak is related to the existence of a bound state in the initial potential, we consider a weak initial potential $U = 1$ which has no bound states. On figure 6.3 we clearly see the peak, which is only slightly weaker than the one from the case above, i.e. with a bound state $\varepsilon_1 \approx 0.641$.

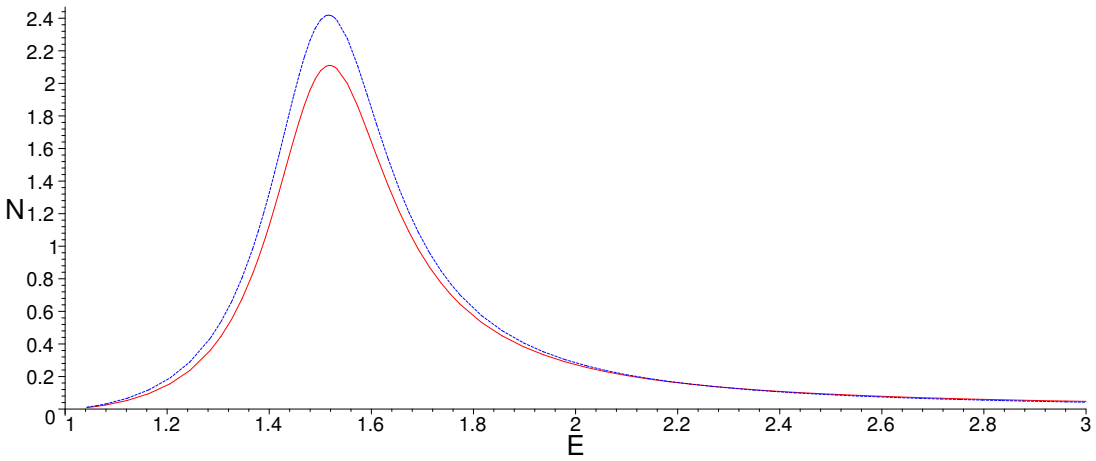


Figure 6.3: Switch on: weak (no bound states) → strongly overcritical. Antiparticle production from the initial weak potential with no bound states (red solid line) compared to slightly higher production from initial potential with a bound state (blue dashed line).

Weakly overcritical → strongly overcritical

– initial ground state

Now, consider a switch on from a weakly overcritical $U = 4$ with a bound state at $\varepsilon_1 \approx -0.794$ to a strongly overcritical $U' = 5$ with no bound states. Here,

$$N_\varepsilon^+ = \int_{\varepsilon_{cut}^-}^{-1} \left|\langle \psi_{\varepsilon,U'} | \psi_{\varepsilon',U} \rangle\right|^2 d\varepsilon' + \left|\langle \psi_{\varepsilon,U'} | \psi_{\varepsilon_1,U} \rangle\right|^2, \tag{6.2.43}$$

$$N_\varepsilon^- = \int_{1}^{\varepsilon_{cut}^+} \left|\langle \psi_{\varepsilon,U'} | \psi_{\varepsilon',U} \rangle\right|^2 d\varepsilon', \tag{6.2.44}$$

what differs essentially from the previous case with an initial subcritical potential. Now, since $\varepsilon_1 < 0$, there is no contribution from that initial state to the spectrum of antiparticles, because it is already in the antiparticle subspace, what in the Dirac language means that in the initial vacuum (ground state) it is initially occupied like the negative continuum.

– initial vacancy

Therefore, we consider also an initial state different from a vacuum Ω_0, but corresponding to an unoccupied state $\varepsilon_1 < 0$ in the Dirac language. It gives an initial state $\Phi_0 \equiv \hat{d}^*(\psi_{\varepsilon_1,U})\ \Omega_0$. The remaining parameters are the same as above, namely $U = 4$ and $U' = 5$. Now, the particle production expectation values change due to $\Phi_0 \neq \Omega_0$

$$N_\varepsilon^+ = \left(\hat{S}\ \Phi_0, \hat{b}_\varepsilon'^*\ \hat{b}_\varepsilon'\ \hat{S}\ \Phi_0\right), \qquad N_\varepsilon^- = \left(\hat{S}\ \Phi_0, \hat{d}_\varepsilon'^*\ \hat{d}_\varepsilon'\ \hat{S}\ \Phi_0\right). \tag{6.2.45}$$

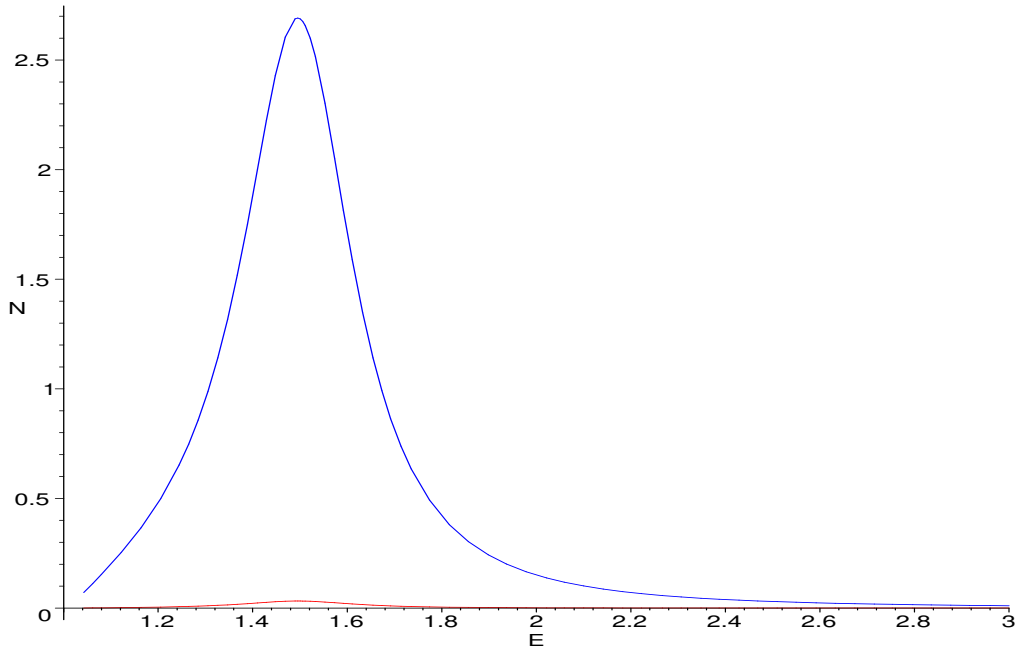


Figure 6.4: Switch on: weakly overcritical $\rightarrow$ strongly overcritical. Antiparticle production from initial empty bound state – big (blue) peak and from initial filled bound state (ground state) – flat (red) peak.

A short calculation gives

$$N_{\varepsilon}^{+} = \int_{\varepsilon_{cut}^{-}}^{-1} \left|\langle \psi_{\varepsilon,U'} | \psi_{\varepsilon',U} \rangle\right|^2 d\varepsilon', \tag{6.2.46}$$

$$N_{\varepsilon}^{-} = \int_{1}^{\varepsilon_{cut}^{+}} \left|\langle \psi_{\varepsilon,U'} | \psi_{\varepsilon',U} \rangle\right|^2 d\varepsilon' + \left|\langle \psi_{\varepsilon,U'} | \psi_{\varepsilon_1,U} \rangle\right|^2. \tag{6.2.47}$$

what is again of the same form as the initial weakly subcritical case and the bound state with $\varepsilon_1 < 0$ contributes again strongly to the spectrum of antiparticles. Both situations are compared on figure 6.4.

Almost strongly overcritical $\rightarrow$ slightly strongly overcritical

In this case we consider a small jump in the potential's strength through the critical value $U_1^- \approx 4.29$. As a result we obtain a distribution dominantly localized in the negative continuum of energies, corresponding to antiparticle creation spectrum with (positive) energies $|\varepsilon|$. We can compare the position of the complex resonance with the position and width of the peak. On figures 6.5 we see the peaks for several values of the final potential's strength U' together with listed complex values of the resonance ε_1. The qualitative expectation is confirmed that peaks laying near to the edge of the continuum are narrow, because the corresponding resonances' imaginary part is small. Since the

peaks are normalized almost to 1 (only a tiny part of the distribution is localized in the positive continuum), the narrow peaks are high.

On figure 6.6 we have a quantitative comparison between the (minus) real part of the resonance position $-\varepsilon_R(U)$ with the position of the antiparticle production peak ε_{res} and the imaginary part of the resonance position $\varepsilon_I(U)$ with the width of the antiparticle production peak Γ. The parameters ε_{res} and Γ are obtained by fitting a Lorentz-type resonance curve to the antiparticle production spectrum

$$\frac{A}{2\pi}\frac{\Gamma}{(\varepsilon-\varepsilon_{res})^2+\Gamma^2}. \tag{6.2.48}$$

We can see that the parameters of the peaks fit very precisely to the parameters of the complex resonances for slightly overcritical potentials $4.3 \lesssim U \lesssim 4.5$, while for stronger final potentials $U \gtrsim 4.5$ some small discrepancy appears and becomes bigger with increasing value of U, or in other words, as the peak moves away from the edge of the continuum and becomes wider. Several fits are shown on figure 6.7. Exact numerical values are presented in the table 6.1, where $\Delta\varepsilon_{res}$ and $\Delta\Gamma$ represent the fitting errors, which for $U' = 5.00$ exceed the values of 1% and 3%, respectively. Again the scaling $\varepsilon_I \sim (-\varepsilon_R - 1)^{3/2}$ confirms the theoretical prediction (3.3.13) and agrees with the results obtained in [AB65] and [Kla85], and disagrees with the result in [GMR85].

U'	ε_R	ε_{res}	$\Delta\varepsilon_{res}$	$\lvert\varepsilon_R-\varepsilon_{res}\rvert$	ε_I	$\Gamma/2$	$\Delta\Gamma/2$	$\lvert\varepsilon_I-\Gamma/2\rvert$
4.32	1.01368	1.01370	1.7E-6	1.9E-5	9.238E-4	9.2E-4	2.4E-6	3.8E-6
4.34	1.02565	1.02566	1.4E-6	1.3E-5	0.00236	0.00234	2.1E-6	1.5E-5
4.36	1.03773	1.03769	1.8E-6	3.6E-5	0.00418	0.00417	3.1E-6	1.0E-5
4.38	1.04992	1.04980	6.8E-6	1.2E-4	0.00633	0.00632	1.0E-5	1.0E-5
4.46	1.09994	1.09893	6.0E-5	0.001	0.017	0.018	9.0E-5	1.1E-4
4.61	1.19969	1.19449	3.7E-4	0.005	0.046	0.047	5.6E-4	9.0E-4
4.75	1.30060	1.28943	7.1E-4	0.011	0.079	0.082	0.001	0.003
4.88	1.40133	1.38386	7.3E-4	0.017	0.112	0.117	0.001	0.004
5.00	1.49999	1.47515	0.0011	0.025	0.143	0.148	0.002	0.004

Table 6.1: Antiparticle production spectra with Lorentz peak-curve fits.

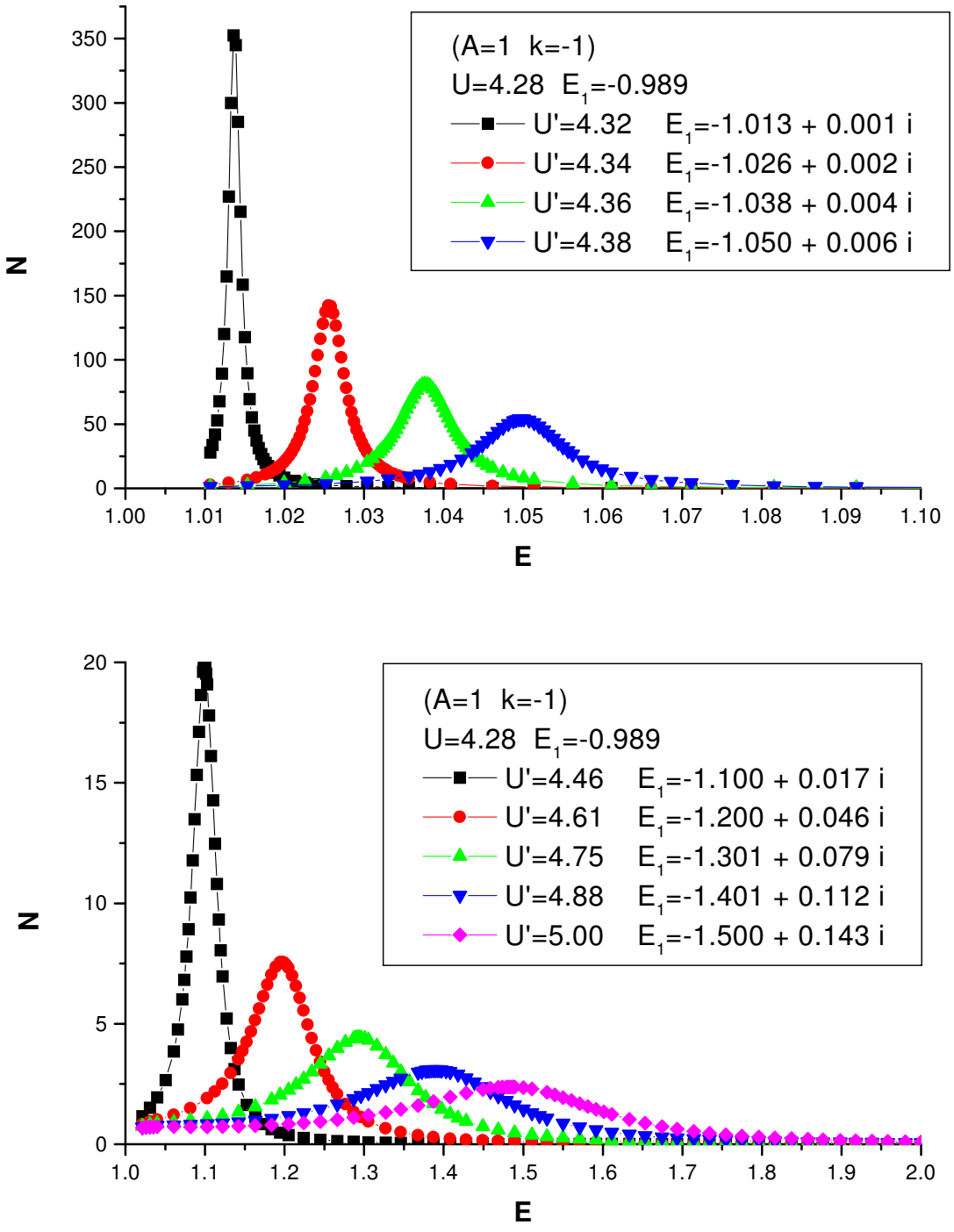


Figure 6.5: Switch on: almost strongly overcritical → strongly overcritical with various final potential strengths. Position and width of the peaks in the antiparticle production spectra agree well with the position of the complex resonances.

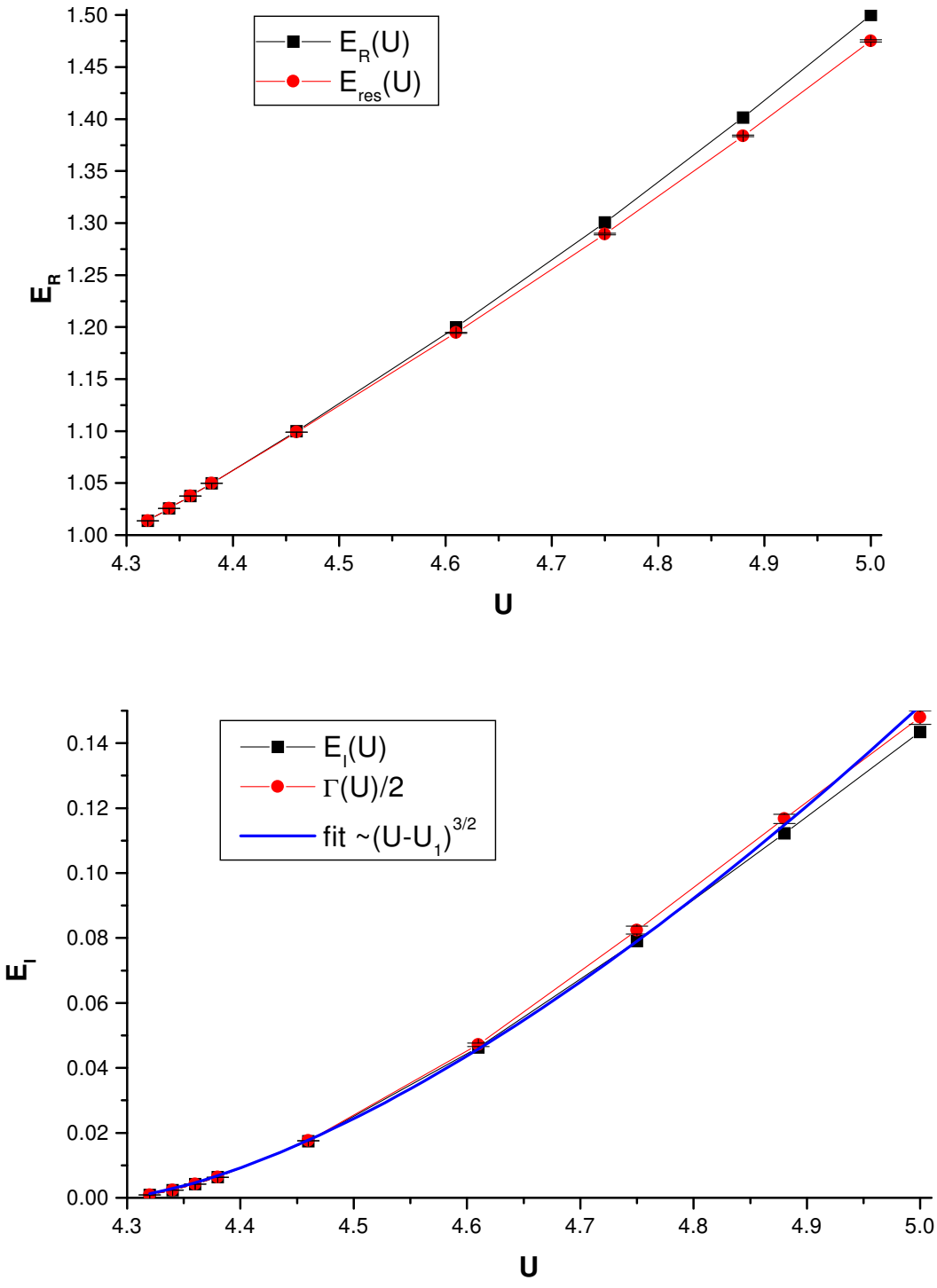


Figure 6.6: Switch on: almost strongly overcritical → strongly overcritical. Comparison between the position and width of the antiparticle production peak and the position of the complex resonance in the final potential. A $\sim (U - U_1^-)^{3/2}$ curve is fitted to the width $\Gamma(U)$.

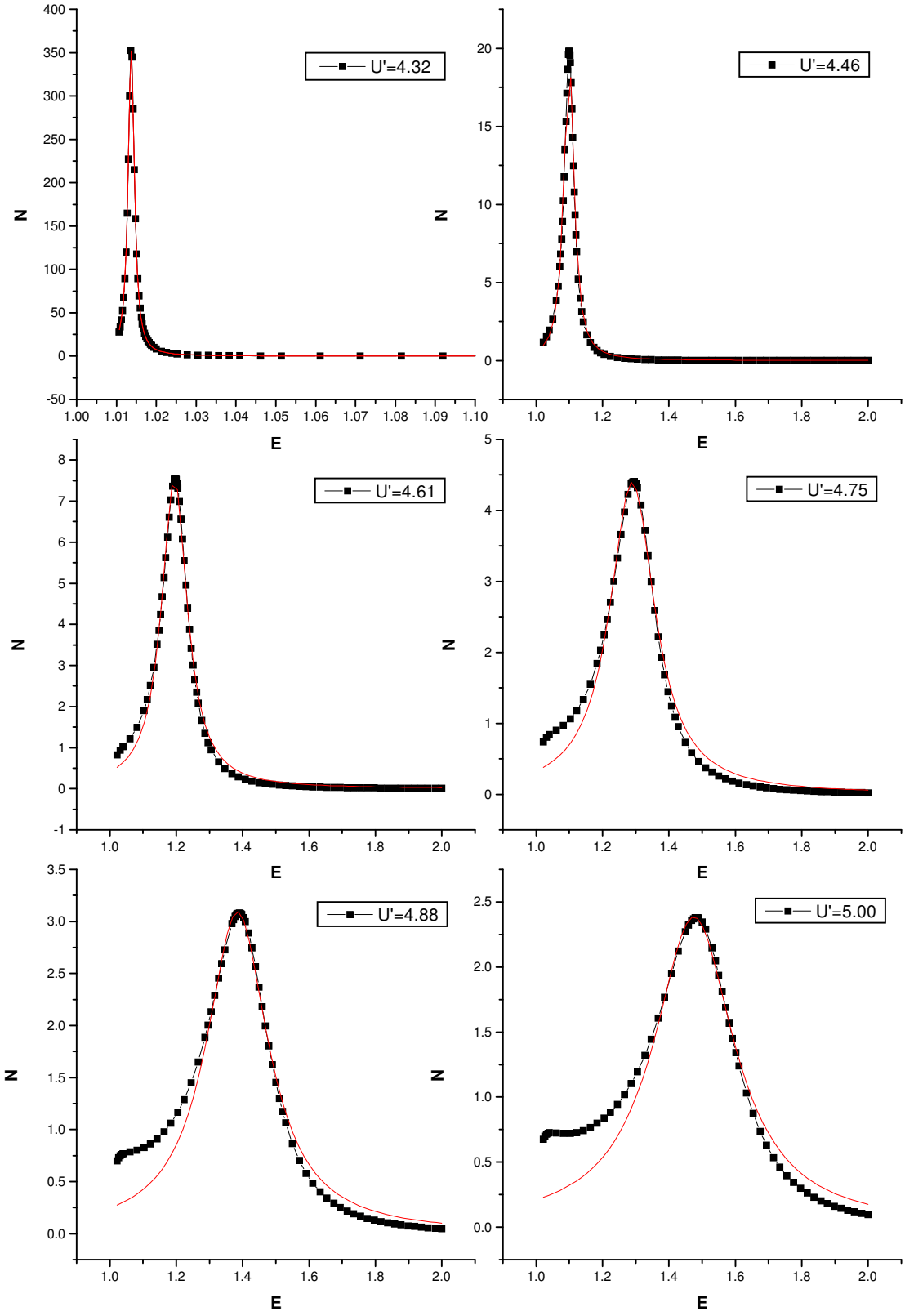


Figure 6.7: Switch on: almost strongly overcritical → strongly overcritical. Numerical values of the complex resonance and parameters of the fitted Lorentz-type peaks to the antiparticle production spectra.

6.3 Time-dependence: sudden switch on and off

First, we consider the simplest time-dependent processes, which we called in the previous chapter *quasi-static*, where the potential is almost all the time static, except single moments when its value changes discontinuously. Here, time-dependent will be the strength of the spherically symmetric square well, i.e.

$$V(t,\mathbf{x}) = V(t,r) = U(t)\cdot v(r) = U(t)\cdot\Theta(a-r) = \begin{cases} U(t), & r<a, \\ 0, & r>a \end{cases} \tag{6.3.1}$$

and

$$U(t) = -U - (U'-U)\cdot\Theta(T-|t|) = \begin{cases} -U, & -T<t<T, \\ -U', & |t|>T, \end{cases} \tag{6.3.2}$$

with $U' > U > 0$. It gives

$$V(t,\mathbf{x}) = V(t,r) \equiv \begin{cases} V_1(r), & |t|>T, \\ V_2(r), & -T<t<T \end{cases} \tag{6.3.3}$$

and correspondingly

$$H(t) \equiv \begin{cases} H_1, & |t|>T, \\ H_2, & -T<t<T \end{cases} \tag{6.3.4}$$

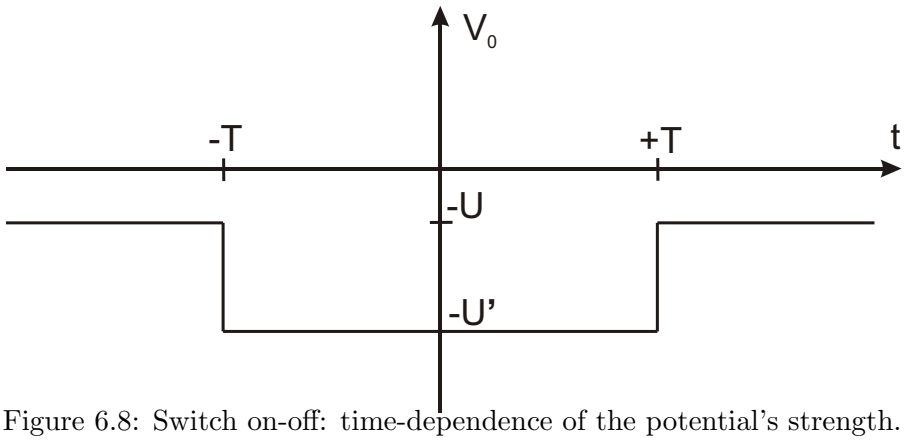


Figure 6.8: Switch on-off: time-dependence of the potential's strength.

Analogously to the previous section, theorem 9 or 10 with $a = 0$ and $b = U'$ says that $H(t) = H_0 + V(t)$ is self-adjoint on $\mathcal{D}(H_0)$ for every time t. Because $H(t)$ is constant for $|t| < T$ and $|t| > T$ there exists a unitary propagator (cf. section 3.4)

$$U(t_2,t_1) = \begin{cases} e^{-iH_1(t_2-t_1)} & \text{for } t_1,t_2<-T \text{ or } t_1,t_2>T, \\ e^{-iH_2(t_2-t_1)} & \text{for } |t_1|,|t_2|<T, \\ e^{-iH_2t_2}e^{iH_1t_1} & \text{for } t_1<-T<t_2<T, \\ e^{-iH_1t_2}e^{iH_2t_1} & \text{for } -T<t_1<T<t_2, \\ e^{-iH_1t_2}e^{-2iH_2T}e^{iH_1t_1} & \text{for } t_1<-T \text{ and } t_2>T. \end{cases} \tag{6.3.5}$$

Since $V(t)$ is of short-range the wave-operators (3.5.3) exist and are complete (e.g. because $V(t) \in L^p(\mathbb{R}^3)$ with any $p > 0$ – cf. section 3.5.1). Consequently, there exists a unitary scattering operator S in $\mathcal{H}$ (3.5.10). This scattering operator is implementable, according to section 4.2.3 and equation (4.2.22), if and only if the unitary evolution operator $U(t_2, t_1)$ with $t_1 < -T$, $t_2 > T$ is. The implementability of both, S and $U(t_2, t_1)$, has been shown in theorem 13.

Now, the scattering operator in $\mathcal{H}$ can be calculated, as discussed in the previous section, from the coupled channel equations (inserting the discontinuously varying potential), however we can easily solve the evolution in only two bases ϕ_ε and χ_ε consisting of generalized eigenvectors to the Hamiltonians H_1 and H_2, respectively, and make two consecutive projections at $t = \pm T$ to find

$$\boxed{S^{U,U'}_{\varepsilon'\varepsilon} = \int_{\sigma'} (\phi_{\varepsilon'}, \chi_{\varepsilon''}) e^{i(\varepsilon+\varepsilon'-2\varepsilon'')T} (\chi_{\varepsilon''}, \phi_\varepsilon)\, d\mu'(\varepsilon''),} \tag{6.3.6}$$

where $\sigma' \equiv \sigma(H_2)$ and $\hat{d}\mu'$ is the corresponding spectral measure. It turns out that the only quantity to be calculated to obtain $S^{U,U'}_{\varepsilon'\varepsilon}$ are the scalar products $(\chi_{\varepsilon'}, \phi_\varepsilon)$. Obviously, for $T = 0$ the scattering operator reduces

$$S^{U,U'}_{\varepsilon'\varepsilon} = \int_{\sigma'} (\phi_{\varepsilon'}, \chi_{\varepsilon''})(\chi_{\varepsilon''}, \phi_\varepsilon)\, d\mu'(\varepsilon'') = (\phi_{\varepsilon'}, \phi_\varepsilon) = \tilde{\delta}(\varepsilon' - \varepsilon). \tag{6.3.7}$$

Asymptotic behaviour for $|\varepsilon|, |\varepsilon'| \gg 1$ and continuum cut-off

Since the integral in (6.3.6) runs over an unbounded spectrum σ' we are forced to introduce numerical cut-offs at some finite energies $\varepsilon^\pm_{cut}$ (as in the previous section 6.2.1) which introduce the error

$$\delta S^{U,U'}_{\varepsilon'\varepsilon} = \left(\int_{-\infty}^{\varepsilon^-_{cut}} + \int_{\varepsilon^+_{cut}}^{+\infty} \right) (\phi_{\varepsilon'}, \chi_{\varepsilon''}) e^{i(\varepsilon+\varepsilon'-2\varepsilon'')T} (\chi_{\varepsilon''}, \phi_\varepsilon)\, d\varepsilon''. \tag{6.3.8}$$

For the energies $|\varepsilon|, |\varepsilon'| \ll |\varepsilon^\pm_{cut}|$ we can use the approximative formula (6.2.22) and obtain

$$\begin{aligned}
&\left| \delta S^{U,U'}_{\varepsilon'\varepsilon} \right| \\
&\cong \frac{A|U-U'|^2}{\pi} \left(\int_{-\infty}^{\varepsilon^-_{cut}} + \int_{\varepsilon^+_{cut}}^{+\infty} \right) \frac{|F_{\varepsilon,U}(A)| + |G_{\varepsilon,U}(A)|}{|\varepsilon''|^2} \, \frac{|F_{\varepsilon',U}(A)| + |G_{\varepsilon',U}(A)|}{|\varepsilon''|^2} \, d\varepsilon'' \\
&\lesssim \frac{2A|U-U'|^2}{3\pi} \frac{(|F_{\varepsilon,U}(A)| + |G_{\varepsilon,U}(A)|)\ (|F_{\varepsilon',U}(A)| + |G_{\varepsilon',U}(A)|)}{|\varepsilon_{cut}|^3} \\
&= \mathcal{O}\left(\frac{1}{|\varepsilon_{cut}|^3} \right),
\end{aligned} \tag{6.3.9}$$

where we have chosen $\pm\varepsilon^\pm_{cut} \equiv \varepsilon_{cut}$. Thus the error of numerically calculated $S^{U,U'}_{\varepsilon'\varepsilon}$ is small when the cut-offs $\varepsilon^\pm_{cut}$ are chosen big enough. The total particle production

$$N^+_\varepsilon \equiv \int_{\sigma^-} \left| S^{U,U'}_{\varepsilon\varepsilon'} \right|^2 \, d\mu(\varepsilon') \tag{6.3.10}$$

with energy $|\varepsilon| \ll \varepsilon_{cut}$ has two sources of error, namely due to the error in $\widetilde{S}^{U,U'}_{\varepsilon'\varepsilon}$ (calculated with cut-offs) and due to the cut-off introduced directly in

$$\widetilde{N}^+_\varepsilon \equiv \int_{\sigma^- > \varepsilon^-_{cut}} \left|\widetilde{S}^{U,U'}_{\varepsilon\varepsilon'}\right|^2 \, d\mu(\varepsilon'). \tag{6.3.11}$$

The error is

$$\delta N^+_\varepsilon \equiv N^+_\varepsilon - \widetilde{N}^+_\varepsilon = \int_{-\varepsilon_{cut}}^0 \left(\left|\widetilde{S}^{U,U'}_{\varepsilon\varepsilon'}\right|^2 - \left|S^{U,U'}_{\varepsilon\varepsilon'}\right|^2\right) \, d\mu(\varepsilon') + \int_{-\infty}^{-\varepsilon_{cut}} \left|S^{U,U'}_{\varepsilon\varepsilon'}\right|^2 \, d\mu(\varepsilon'). \tag{6.3.12}$$

Using

$$S^{U,U'}_{\varepsilon\varepsilon'} = \widetilde{S}^{U,U'}_{\varepsilon\varepsilon'} + \delta S^{U,U'}_{\varepsilon\varepsilon'} \tag{6.3.13}$$

we estimate the first integral in (6.3.12)

$$\begin{aligned}
&\left|\int_{-\varepsilon_{cut}}^0 \left(\left|\widetilde{S}^{U,U'}_{\varepsilon\varepsilon'}\right|^2 - \left|S^{U,U'}_{\varepsilon\varepsilon'}\right|^2\right) \, d\mu(\varepsilon')\right| \\
&\le \int_{-\varepsilon_{cut}}^0 \left(\left|\widetilde{S}^{U,U'}_{\varepsilon\varepsilon'}\,\delta S^{U,U'}_{\varepsilon\varepsilon'}\right| + \left|\delta S^{U,U'}_{\varepsilon\varepsilon'}\right|^2\right) \, d\mu(\varepsilon') \\
&\le \sqrt{\int_{-\varepsilon_{cut}}^0 \left|\widetilde{S}^{U,U'}_{\varepsilon\varepsilon'}\right|^2 \, d\mu(\varepsilon')} \cdot \sqrt{\int_{-\varepsilon_{cut}}^0 \left|\delta S^{U,U'}_{\varepsilon\varepsilon'}\right|^2 \, d\mu(\varepsilon')} + \mathcal{O}(|\varepsilon_{cut}|^{-6}) \cdot |\varepsilon_{cut}| \\
&\le \widetilde{N}^+_\varepsilon \cdot \mathcal{O}(|\varepsilon_{cut}|^{-5/2}) + \mathcal{O}(|\varepsilon_{cut}|^{-5}),
\end{aligned} \tag{6.3.14}$$

where we have used $\delta S^{U,U'}_{\varepsilon'\varepsilon} = \mathcal{O}(|\varepsilon_{cut}|^{-3})$ and the Cauchy-Schwarz inequality. In order to estimate the second integral in (6.3.12) we must first estimate $S^{U,U'}_{\varepsilon\varepsilon'}$ for $|\varepsilon| < \varepsilon_{cut}$ and $\varepsilon' < -\varepsilon_{cut}$. In the case $\varepsilon' < -2\varepsilon_{cut}$ using (6.2.22), (6.2.25) and (6.2.26) we find

$$\begin{aligned}
\left|S^{U,U'}_{\varepsilon\varepsilon'}\right| \le{}& \left|\int_{-\varepsilon_{cut}}^{+\varepsilon_{cut}} (\phi_\varepsilon, \chi_{\varepsilon''}) e^{i(\varepsilon+\varepsilon'-2\varepsilon'')T} (\chi_{\varepsilon''}, \phi_{\varepsilon'}) \, d\varepsilon''\right| \\
&+ \left|\left(\int_{-\infty}^{-\varepsilon_{cut}} + \int_{+\varepsilon_{cut}}^{+\infty}\right) (\phi_\varepsilon, \chi_{\varepsilon''}) e^{i(\varepsilon+\varepsilon'-2\varepsilon'')T} (\chi_{\varepsilon''}, \phi_{\varepsilon'}) \, d\varepsilon''\right| \\
\lesssim{}& \sqrt{\int_{-\varepsilon_{cut}}^{+\varepsilon_{cut}} |(\phi_\varepsilon, \chi_{\varepsilon''})|^2 \, d\mu(\varepsilon'')} \\
&\cdot \sqrt{\int_{-\varepsilon_{cut}}^{+\varepsilon_{cut}} \left(\frac{\sqrt{A}|U-U'|}{\sqrt{\pi}\varepsilon'^2}\right)^2 (|F_{\varepsilon'',U'}(A)| + |G_{\varepsilon'',U'}(A)|)^2 \, d\mu(\varepsilon'')} \\
&+ \left|\int_{-\infty}^{-\varepsilon_{cut}} (|F_{\varepsilon,U}(A)| + |G_{\varepsilon,U}(A)|) \frac{\sqrt{A}|U-U'|^2 \sin((\varepsilon''-\varepsilon'+U'-U)A)}{\pi^{3/2}\varepsilon''^2 \, (\varepsilon''-\varepsilon')(\varepsilon''-\varepsilon'+U'-U)} \, d\mu(\varepsilon'')\right| \\
&+ \int_{+\varepsilon_{cut}}^{+\infty} \frac{\sqrt{A}|U-U'|}{\sqrt{\pi}\varepsilon''^2} (|F_{\varepsilon,U}(A)| + |G_{\varepsilon,U}(A)|) \frac{|U-U'|}{\pi(\varepsilon''-\varepsilon')^2} \, d\mu(\varepsilon'')
\end{aligned} \tag{6.3.15}$$

$$\begin{aligned}\left|S^{U,U'}_{\varepsilon\varepsilon'}\right| \lesssim 1\cdot\frac{\sqrt{A}|U-U'|}{\sqrt{\pi}\varepsilon'^2}\sqrt{\int_{-\varepsilon_{cut}}^{+\varepsilon_{cut}}(|F_{\varepsilon'',U'}(A)|+|G_{\varepsilon'',U'}(A)|)^2\ d\mu(\varepsilon'')}\\ +(|F_{\varepsilon,U}(A)|+|G_{\varepsilon,U}(A)|)\frac{\sqrt{A}|U-U'|^2}{\pi^{3/2}}\left|\int_{-\infty}^{-\varepsilon_{cut}}\frac{\sin((\varepsilon''-\varepsilon'+U'-U)A)}{\varepsilon''^2\ (\varepsilon''-\varepsilon')(\varepsilon''-\varepsilon'+U'-U)}\ d\varepsilon''\right|\\ +\frac{\sqrt{A}|U-U'|^2}{\pi^{3/2}}(|F_{\varepsilon,U}(A)|+|G_{\varepsilon,U}(A)|)\int_{+\varepsilon_{cut}}^{+\infty}\frac{1}{\varepsilon''^2(\varepsilon''-\varepsilon')^2}\ d\varepsilon''.\end{aligned} \tag{6.3.16}$$

The integral in the second line must be calculated in the principal-value sense. A rather lengthy calculation leads to the estimation

$$\frac{1}{|\varepsilon'|}\left[\frac{1}{\varepsilon_{cut}}+\frac{1}{|\varepsilon'|}\ln\left(\frac{|\varepsilon'+\varepsilon_{cut}|}{\varepsilon_{cut}}\right)\right]\le\frac{1}{|\varepsilon'|\varepsilon_{cut}}\quad\text{for}\quad\varepsilon'<-2\varepsilon_{cut}. \tag{6.3.17}$$

The integral in the third line can be estimated by $1/(\varepsilon_{cut}\ |\varepsilon'|^2)$. It gives

$$\left|S^{U,U'}_{\varepsilon\varepsilon'}\right|\lesssim\ \mathcal{O}\left(\frac{1}{|\varepsilon'|^2}\right)+\mathcal{O}\left(\frac{1}{|\varepsilon'|\varepsilon_{cut}}\right)+\mathcal{O}\left(\frac{1}{\varepsilon_{cut}\ |\varepsilon'|^2}\right). \tag{6.3.18}$$

In the case when $-2\varepsilon_{cut}\le\varepsilon'<-\varepsilon_{cut}$ the estimation (6.3.17) for the principal-value integral cannot be used and we must slightly change the above method and estimate

$$\begin{aligned}&\left|\int_{-\infty}^{-\varepsilon_{cut}}(\phi_\varepsilon,\chi_{\varepsilon''})e^{i(\varepsilon+\varepsilon'-2\varepsilon'')T}(\chi_{\varepsilon''},\phi_{\varepsilon'})\ d\varepsilon''\right|\\ \le&\sqrt{\int_{-\infty}^{-\varepsilon_{cut}}\left(\frac{\sqrt{A}|U-U'|}{\sqrt{\pi}\varepsilon''^2}\right)^2(|F_{\varepsilon,U}(A)|+|G_{\varepsilon,U}(A)|)^2\ d\mu(\varepsilon'')}\\ &\cdot\sqrt{\int_{-\infty}^{-\varepsilon_{cut}}|(\chi_{\varepsilon''},\phi_{\varepsilon'})|^2\ d\mu(\varepsilon'')}\\ \le&\frac{\sqrt{A}|U-U'|}{\sqrt{\pi}}(|F_{\varepsilon,U}(A)|+|G_{\varepsilon,U}(A)|)\sqrt{\int_{-2\infty}^{-\varepsilon_{cut}}\frac{1}{\varepsilon''^4}\ d\varepsilon''}\cdot 1\end{aligned} \tag{6.3.19}$$

We estimate the integral by

$$\int_{-2\infty}^{-\varepsilon_{cut}}\frac{1}{\varepsilon''^4}\ d\varepsilon''=\frac{1}{3\varepsilon_{cut}^3}\le\frac{8}{3|\varepsilon'|^3}. \tag{6.3.20}$$

So we get (for $-2\varepsilon_{cut}\le\varepsilon'<-\varepsilon_{cut}$)

$$\left|S^{U,U'}_{\varepsilon\varepsilon'}\right|\lesssim\ \mathcal{O}\left(\frac{1}{|\varepsilon'|^2}\right)+\mathcal{O}\left(\frac{1}{|\varepsilon'|^3}\right)+\mathcal{O}\left(\frac{1}{\varepsilon_{cut}\ |\varepsilon'|^2}\right). \tag{6.3.21}$$

Finally, we can write

$$\left|S^{U,U'}_{\varepsilon\varepsilon'}\right|\lesssim\begin{cases}\mathcal{O}\left(\frac{1}{|\varepsilon'|^2}\right)+\mathcal{O}\left(\frac{1}{|\varepsilon'|\varepsilon_{cut}}\right) & \text{for } \varepsilon'<-2\varepsilon_{cut},\\ \mathcal{O}\left(\frac{1}{|\varepsilon'|^2}\right) & \text{for } -2\varepsilon_{cut}\le\varepsilon'<-\varepsilon_{cut}.\end{cases} \tag{6.3.22}$$

Now we can estimate the second integral in (6.3.12)

$$\begin{aligned}\left|\int_{-\infty}^{-\varepsilon_{cut}}\left|S^{U,U'}_{\varepsilon\varepsilon'}\right|^2\,d\mu(\varepsilon')\right| &\le \left|\int_{-\infty}^{-2\varepsilon_{cut}}\left|S^{U,U'}_{\varepsilon\varepsilon'}\right|^2\,d\mu(\varepsilon')\right| + \left|\int_{-2\varepsilon_{cut}}^{-\varepsilon_{cut}}\left|S^{U,U'}_{\varepsilon\varepsilon'}\right|^2\,d\mu(\varepsilon')\right| \\ &\lesssim \int_{-\infty}^{-2\varepsilon_{cut}}\left[\mathcal{O}\left(\frac{1}{|\varepsilon'|^2}\right)+\mathcal{O}\left(\frac{1}{|\varepsilon'|\varepsilon_{cut}}\right)\right]^2 d\varepsilon' \\ &+ \int_{-2\varepsilon_{cut}}^{-\varepsilon_{cut}}\left[\mathcal{O}\left(\frac{1}{|\varepsilon'|^2}\right)\right]^2 d\varepsilon' \\ &= \mathcal{O}\left(\frac{1}{\varepsilon^3_{cut}}\right)+\mathcal{O}\left(\frac{1}{\varepsilon^3_{cut}}\right)=\mathcal{O}\left(\frac{1}{\varepsilon^3_{cut}}\right).\end{aligned} \tag{6.3.23}$$

So we have shown

$$\delta N^+_\varepsilon = \widetilde{N}^+_\varepsilon\cdot\mathcal{O}\left(\frac{1}{\varepsilon^{5/2}_{cut}}\right)+\mathcal{O}\left(\frac{1}{\varepsilon^3_{cut}}\right), \tag{6.3.24}$$

what means that the (relative) error in calculation of the particle production due to the introduction of cut-offs can be made arbitrarily small by choosing appropriate ε_{cut}.

6.3.1 Positron spectra – switch on and off

The most interesting question is if the antiparticle production spectra for the switch on-off processes differ essentially from those of the only switch on processes discussed in the previous section. For several reasons it can be expected that they should be similar. First (mathematical), because the scalar product formula $\langle\psi_{\varepsilon,U}|\psi_{\varepsilon',U'}\rangle$ contains a $\sim\delta(\varepsilon-\varepsilon')$ term, which keeps the distribution of the wave function in the energy unchanged, up to the other term, singular as $\sim(\varepsilon-\varepsilon')^{-1}$, whose role is more difficult to estimate. Second (physical), a wave packet which decayed in the switched-on potential U' is localized spatially outside of the potential well, where the wave functions $\psi_{\varepsilon,U'}$ and $\psi_{\varepsilon,U}$ do not differ at all, therefore a projection of one on the other should not change the distribution in the energy scale of the wave packet. Of course, for not decayed wave packets the above should not hold and the peak-like distribution of the wave function in the negative continuum should build-up back giving finally again the bound state of U. The decay time for the Lorentzian wave packet is Γ^{-1}.

Buildup of the peak in time

In contrast to the switch on processes, the switch on-off processes have a characteristic time scale, namely the time T between switch on and off of the stronger potential. In the overcritical period the wave packets in the negative continuum (obtained numerically in the previous section) decay (approximately exponentially) and give rise to a peak in the negative continuum after the potential is eventually switched off. So the (exponential) decay of the wave packet leads to an (exponential) dependence of the amplitude of the peak on time $\mathcal{A}(T)\sim(1-e^{-\Gamma T/2})$, where Γ is the width of the peak. Figures 6.9-6.10 present the antiparticle production spectra for different duration times T of the switched

on potential U'. For $T = 50$ the wave packet is (almost) fully decayed, because $\Gamma/2 \approx 0.143$ and hence it reaches $1 - e^{-\Gamma T/2} \approx 0.999$ of its maximal amplitude.

Position, width and the buildup of the peaks

As next we show the different buildup rates of peaks with different widths (and thus at different positions). Figure 6.11 shows that for $T = 10$ the wider (right) peak around $\varepsilon \approx 1.5$ is higher, while for $T = 20$ figure 6.12 shows the narrower (left) peak around $\varepsilon \approx 1.1$ gets higher and remains so for all bigger values of T. The latter is natural, since narrower wave packets must be higher to have the same norm. The reason for the opposite situation at $T = 10$ is that wider wave packets decay quicker and the right peak decayed nearly fully, while the left peak decayed roughly to half of its maximal height.

Moreover, figures 6.11-6.12 show a qualitative difference in the antiparticle production spectra between strongly overcritical and subcritical intermediate potentials U'. For overcritical we always have a clear peak, while for subcritical there is only a small universal periodic structure (also seen in the overcritical cases) with period π/T. Yet, this quantitative difference is only observable for delay times T sufficiently long for the wave packets to decay (at leas partially), but vanishes at short times T. On figure 6.13 there is no essential difference between the sub- and overcritical spectra, the subcritical with $U' = 4.2$ differs by about 20% from the overcritical with $U' = 4.4$, which differs much more (by about 45%) from another overcritical with $U' = 5.0$.

Peak vs. resonance

Here we want to check how the shape of the peak depends on the energy of the bound state in the initial potential. In other words, it is clear that the resonance in the overcritical potential does not depend on the initial potential, but it is not clear how it is "excited" in the process of sudden diving of different initial bound states. On figures 6.14 we can see that the final peak is nearly identical for various initial potentials $U = 2, 3, 4$ with bound states $\varepsilon_1 = 0.641, -0.048, -0.794$, respectively, independent of the overcritical period ($T = 5, 20$). However, the little differences show some regularity, namely the deeper the initial bound state lies the more left shifted and higher the corresponding peak is. This difference, although not big, is very interesting, if we want to compare the shapes of the peaks with the position of the complex resonance, which depends uniquely on the overcritical potential. Table 6.2 shows the results of fitting of the Lorentz peak curves to the antiparticle production spectra. It is clear that: (a) for longer overcritical periods T the peaks fit better to the resonance parameters (due to the complete decay) and (b) peaks generated in processes with deeper lying initial bound state fit better to the resonance parameters, what means that higher lying bound states (further from the negative continuum) due to stronger jump of the potential's strength $U - U'$ excite more states in the negative continuum than only those corresponding to the shape of the resonance.

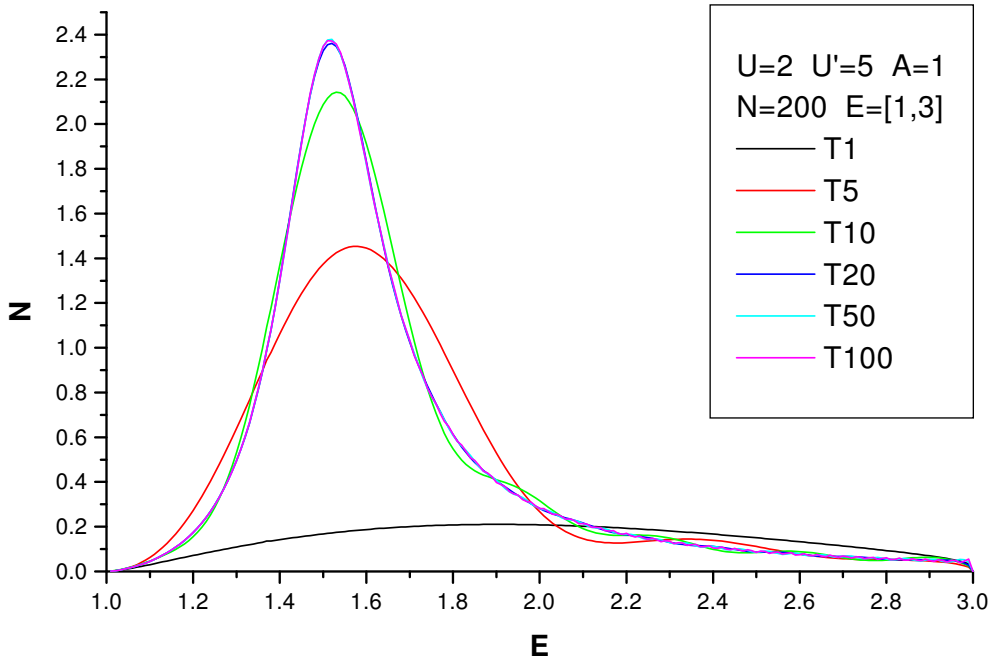


Figure 6.9: Switch on-off: weakly subcritical → strongly overcritical. Antiparticle production spectra for different duration times T of the switched on potential U'.

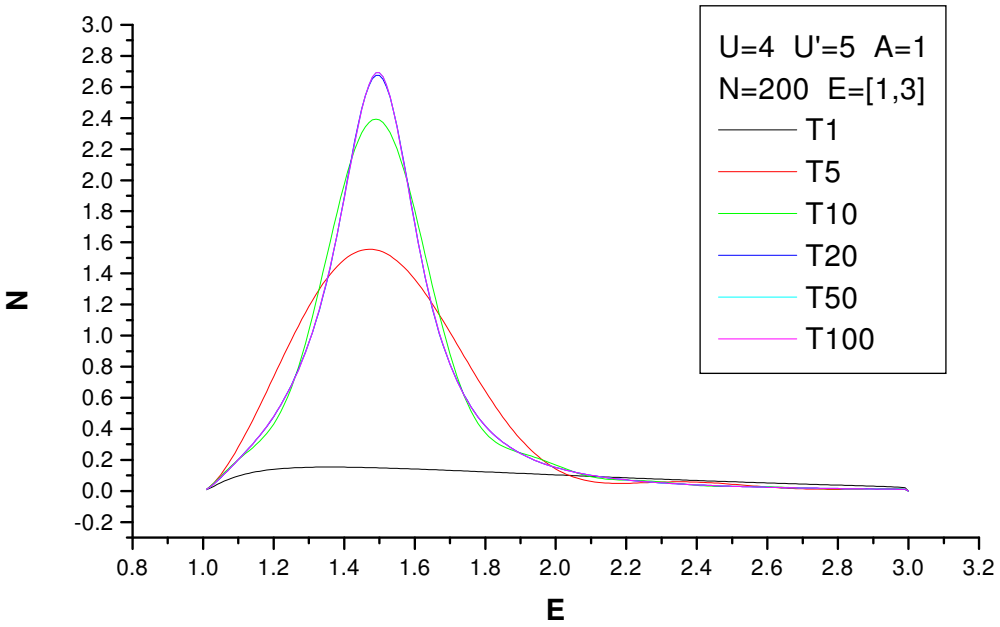


Figure 6.10: Switch on-off: weakly overcritical → strongly overcritical. Antiparticle production spectra for different duration times T of the switched on potential U'.

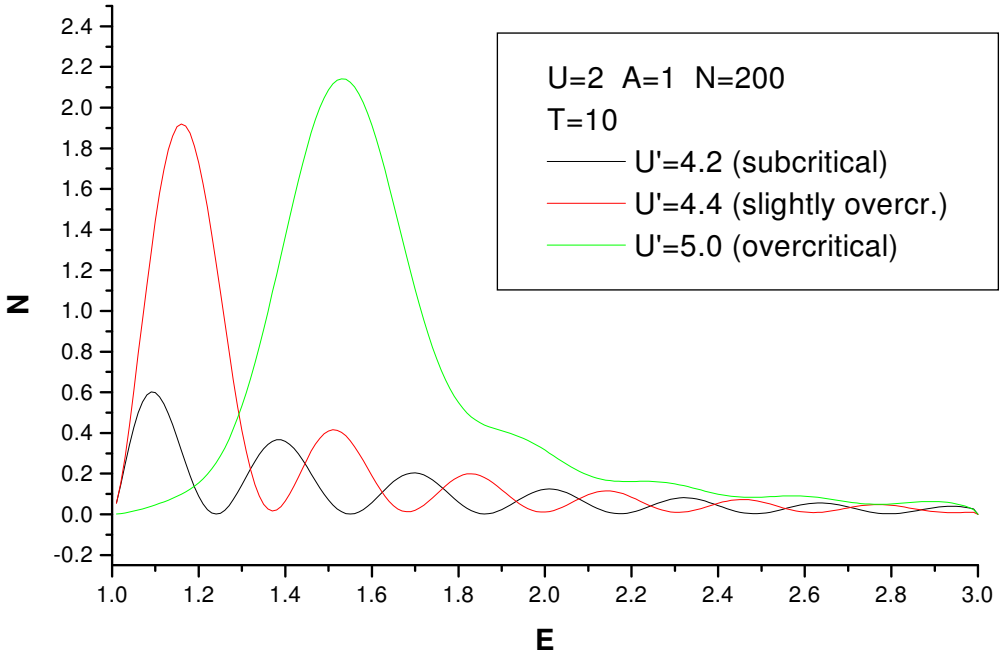


Figure 6.11: Switch on-off: buildup of the peaks in overcritical vs. no peaks in subcritical potential for the duration time $T = 10$ of the switched-on phase. Wider peak appears quicker and is wider at intermediate times T.

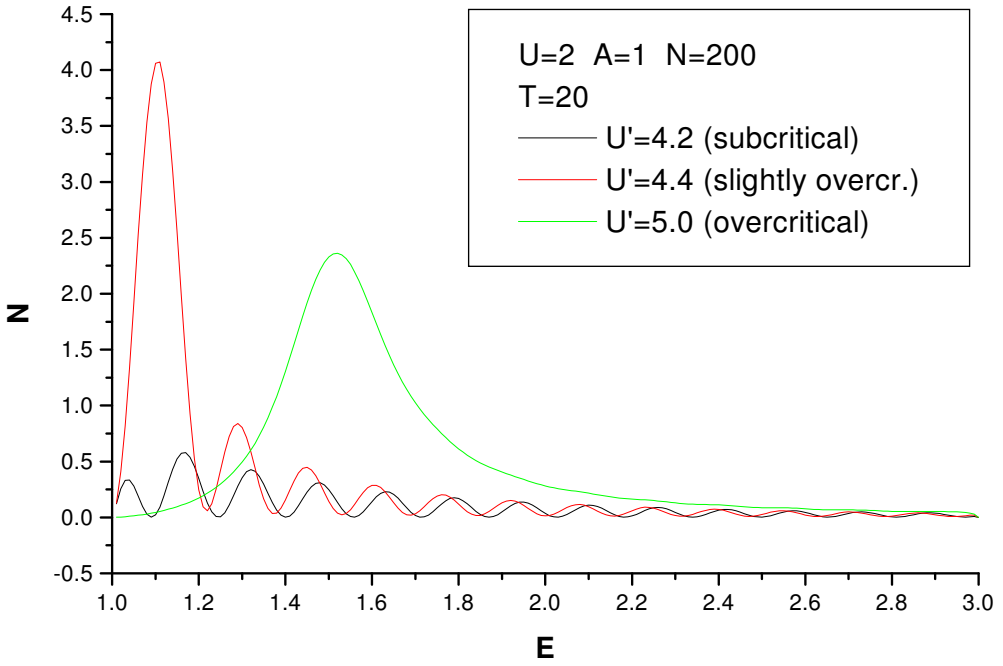


Figure 6.12: Switch on-off: buildup of the peaks in overcritical vs. no peaks in subcritical potential for the duration time $T = 20$ of the switched-on phase. Narrow peak becomes eventually higher for long times T.

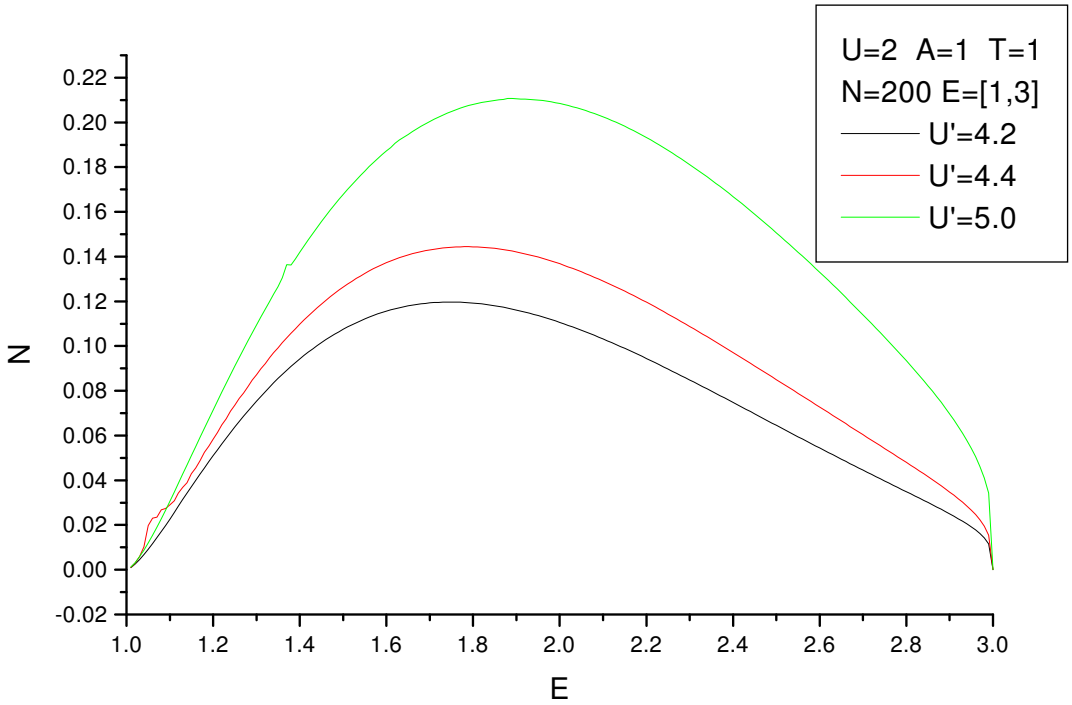


Figure 6.13: Switch on-off: no quantitative difference between subcritical and overcritical potentials in the switched-on phase for short times ($T = 1$).

T	U	ε_{res}	$\Delta\varepsilon_{res}$	$\lvert\varepsilon_{res} - \varepsilon_R\rvert$	Γ	$\Delta\Gamma$	$\lvert\Gamma - \varepsilon_I\rvert$
5	2	1.580	1.5E-3	0.079	0.267	3.1E-3	0.123
5	3	1.557	1.0E-3	0.057	0.284	2.6E-3	0.141
5	4	1.477	1.0E-3	0.023	0.303	2.7E-3	0.159
20	2	1.524	8.7E-4	0.024	0.144	1.9E-3	0.001
20	3	1.516	6.7E-4	0.016	0.140	1.4E-3	0.003
20	4	1.493	6.4E-4	0.007	0.135	9.2E-4	0.008

Table 6.2: Fitted (by Lorentz curves) position ε_{res} and half-width Γ of the peaks vs complex resonance position $|\varepsilon_R| \approx 1.5$ and $|\varepsilon_I| \approx 0.143$.

Concluding, the resonance in the negative continuum for switched on overcritical potentials gets strongly and dominantly excited and the shape of the peak in the antiparticle production spectrum (position and width) fits well to the parameters of the corresponding resonance, although the sudden switch processes are far from being adiabatic and it is in principle unclear how strong the rest of both continua will get excited. In the following sections we will analyze smooth switch on and on-off processes up to the adiabatic situation and compare the excitation of the resonance to the results obtained in this section.

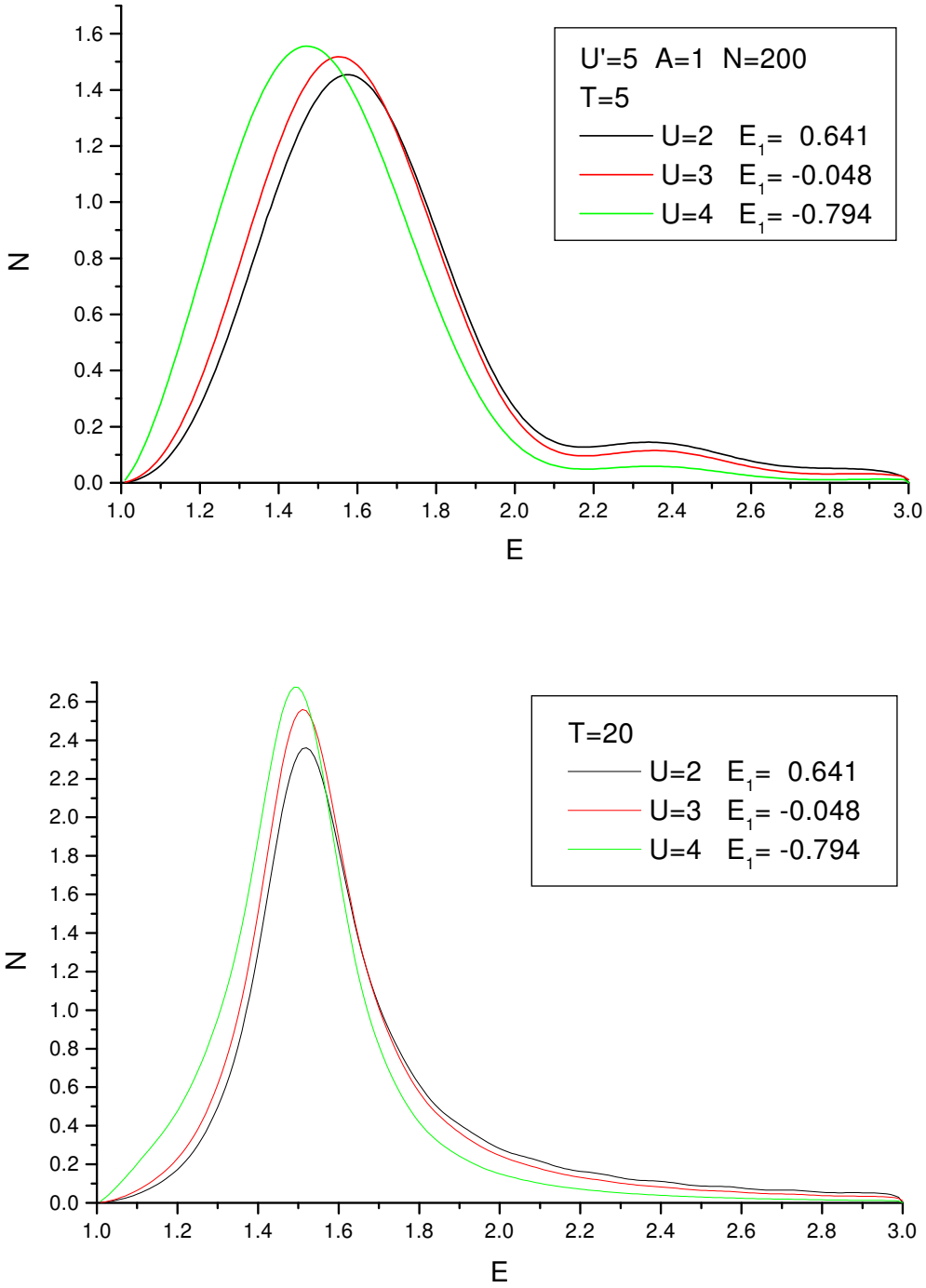


Figure 6.14: Switch on-off: peaks in the antiparticle production spectrum for various initial potentials U (i.e. bound state energies ε_1) and duration times T of the overcritical phase.

Appendix: numerical tests (discretization density and cut-off)

Figure 6.15 shows the same physical situation with different continuum discretization parameters N and $\Delta\varepsilon$. In a wide range of parameters the results remain stable.

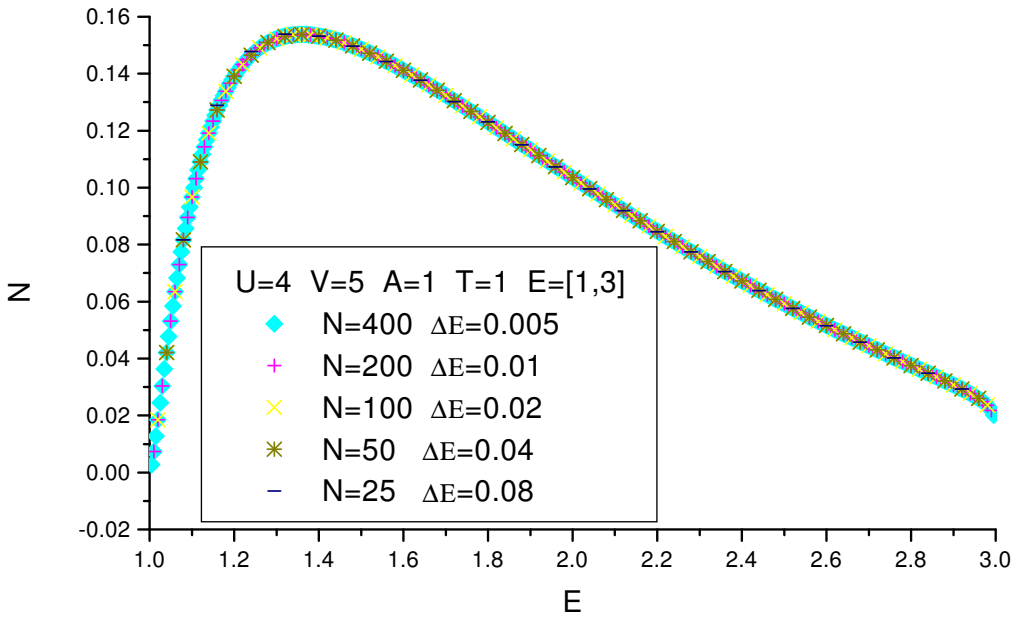


Figure 6.15: Switch on-off: numerical tests with different continuum discretization parameters N and $\Delta\varepsilon$. In the chosen range of parameters the results remain stable.

Figures 6.16 show that in the discretized continuum no true decay of wave packets occurs. The numerical results give some approximation to the continuous case, but at times T such that the phases of the neighbouring points become equal, i.e. $(\varepsilon + \Delta\varepsilon)T - \varepsilon T = \Delta\varepsilon T = 2\pi$, the wave packet builds up again to its original shape and the peak in the antiparticle production spectrum vanishes. Therefore the numerical approximation works for $T \ll 2\pi/\Delta\varepsilon$. We see that for $T \leq 100$ the peak builds up, while for $T = 1000$ it shrinks, what is a numerical artefact.

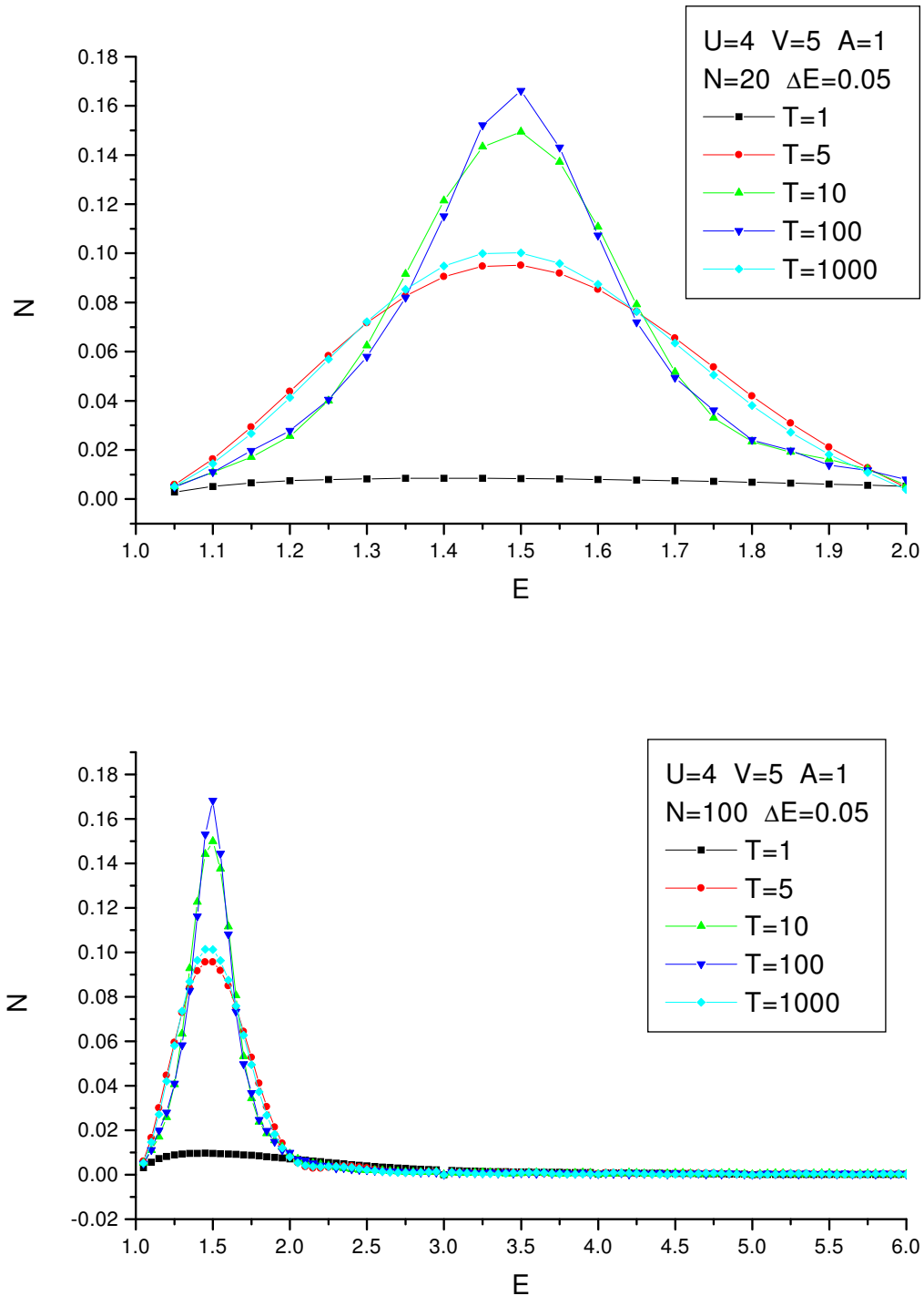


Figure 6.16: Switch on-off: numerical tests with different duration times T of the overcritical phase for given continuum discretization parameters. Good approximation is obtained only for $T \ll 2\pi/\Delta\varepsilon \approx 126$. For $T = 1000$ the peak decreases again, what is wrong.

6.4 Time-dependence: continuous in time

6.4.1 Adiabatic basis – coupled channel equations

We start with the coupled channel equations (6.1.8) for the adiabatic basis and need to evaluate the scalar products $\langle\psi_E|\dot{\psi}_{E'}\rangle$. To this end we differentiate the formula defining the generalized eigenvectors

$$H(t)\psi_E(t) = E(t)\psi_E(t) \tag{6.4.1}$$

with respect to time, keeping in mind that in our convention the bound state energies $E(t) = E_n(t)$ are time-dependent, but continuum energies $E(t) = E$ not. After some manipulations, we arrive at

$$\langle\psi_E|\dot{\psi}_{E'}\rangle = -\frac{\langle\psi_E|\dot{V}(t)\psi_{E'}\rangle}{E(t) - E'(t)}, \quad \text{where} \quad E(t) \neq E'(t). \tag{6.4.2}$$

For bound states it can be shown, that the scalar products $\langle\psi_n|\dot{\psi}_n\rangle \equiv \langle\psi_{E_n}|\dot{\psi}_{E_n}\rangle$ must be purely imaginary. If the basis vectors $\psi_k(t, \mathbf{x})$ are chosen real for all times, what has been done, these scalar products must vanish. Finally,

$$\boxed{\dot{b}_E(t) = \int_{\tilde{\sigma}(t)} e^{-i(\chi_E(t) - \chi_{E'}(t))} \frac{\langle\psi_E|\dot{V}(t)\psi_{E'}\rangle}{E(t) - E'(t)}\, b_{E'}(t)\, d\mu(E').} \tag{6.4.3}$$

where the integration goes over the whole spectrum of $H(t)$ except the value $E(t)$ appearing on the l.h.s, i.e. over the whole spectrum for $E(t)$ in the continuum (practically no difference, since $E(t)$ is of measure zero), but over all $E' \neq E_n(t)$ for $E(t) = E_n(t)$ in the point spectrum.

For numerical calculations we utilize the dimensionless variables, introducing in addition to (5.2.3)

$$\tau = \frac{mc^2}{\hbar}t, \tag{6.4.4}$$

and get

$$\dot{b}_\varepsilon(\tau) = \int_{\tilde{\sigma}(\tau)} e^{-i(\chi_\varepsilon(\tau) - \chi_{\varepsilon'}(\tau))} \frac{\langle\psi_\varepsilon|\dot{\upsilon}(\tau)\psi_{\varepsilon'}\rangle}{\varepsilon(\tau) - \varepsilon'(\tau)}\, b_{\varepsilon'}(\tau)\, d\mu(\varepsilon'). \tag{6.4.5}$$

Calculation of the scalar products $\langle\psi_\varepsilon|\dot{\upsilon}(\tau)\psi_{\varepsilon'}\rangle$

The time-dependent potential is

$$\upsilon(\tau, R) = U(\tau)\, \Theta(A - R), \tag{6.4.6}$$

so its time-derivative is

$$\dot{\upsilon}(\tau, R) = \dot{U}(\tau)\, \Theta(A - R). \tag{6.4.7}$$

Let $G_{\varepsilon,U}(R)$ and $F_{\varepsilon,U}(R)$ be the components of the wave functions $\psi_{\varepsilon,U}(R)$ with the energy ε in the potential parameterized by U (ε may belong to the point as well as the continuous spectrum). The scalar product can be calculated as follows

$$\begin{aligned}\langle\psi_{\varepsilon,U}|\dot{v}(\tau)\psi_{\varepsilon',U}\rangle &= \dot{U}(\tau)\int_0^A R\left[\overline{G_{\varepsilon,U}(R)}G_{\varepsilon',U}(R)+\overline{F_{\varepsilon,U}(R)}F_{\varepsilon',U}(R)\right]dR \\ &= \dot{U}(\tau)\frac{R\left[\overline{F_{\varepsilon,U}(R)}G_{\varepsilon',U}(R)-\overline{G_{\varepsilon,U}(R)}F_{\varepsilon',U}(R)\right]\Big|_0^A}{\varepsilon-\varepsilon'} \\ &= \dot{U}(\tau)\frac{A\left[\overline{F_{\varepsilon,U}(A)}G_{\varepsilon',U}(A)-\overline{G_{\varepsilon,U}(A)}F_{\varepsilon',U}(A)\right]}{\varepsilon-\varepsilon'},\end{aligned} \tag{6.4.8}$$

where we skipped explicit dependence on τ in U acting as index. Finally the system of coupled evolution equations becomes

$$\boxed{\dot{b}_\varepsilon(\tau)=A\dot{U}(\tau)\int_{\tilde{\sigma}(\tau)}e^{-i(\chi_\varepsilon(\tau)-\chi_{\varepsilon'}(\tau))}\frac{\left[\overline{F_{\varepsilon,U}(A)}\;G_{\varepsilon',U}(A)-\overline{G_{\varepsilon,U}(A)}\;F_{\varepsilon',U}(A)\right]}{(\varepsilon-\varepsilon')^2}\;b_{\varepsilon'}(\tau)\;d\mu(\varepsilon')}. \tag{6.4.9}$$

Explicit form of the coupling "matrix" elements

Now we can make use of the explicit form of the wave functions. Because $F(R)$ and $G(R)$ are continuous at $R=A$ we can choose any of the two solutions, which are defined respectively for $R<A$ and $R>A$. The first choice has the advantage that both, the continuum and the bound-state wave functions, have the same form

$$G(R) = A_1 J_{|\kappa-\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \tag{6.4.10}$$

$$F(R) = C_1 J_{|\kappa+\frac{1}{2}|}(\sqrt{(\varepsilon+U)^2-1}R) \tag{6.4.11}$$

$$C_1 = \mathrm{sign}\,(\kappa)\,\frac{\sqrt{(\varepsilon+U)^2-1}}{\varepsilon+U-1}A_1 \tag{6.4.12}$$

and can further be treated together. The term in the square brackets in (6.4.9) can be evaluated to

$$\begin{aligned}&\overline{F_{\varepsilon,U}(A)}\;G_{\varepsilon',U}(A)-\overline{G_{\varepsilon,U}(A)}\;F_{\varepsilon',U}(A)= \\ &=\mathrm{sign}\,(\kappa)\,\overline{A_1(\varepsilon,U)}A_1(\varepsilon',U) \\ &\quad\cdot\left[\frac{\overline{\omega_1}}{\varepsilon+u-1}\overline{J_{|\kappa+\frac{1}{2}|}(\omega_1 A)}J_{|\kappa-\frac{1}{2}|}(\omega_1' A)-\frac{\omega_1'}{\varepsilon'+U-1}\overline{J_{|\kappa-\frac{1}{2}|}(\omega_1 A)}J_{|\kappa+\frac{1}{2}|}(\omega_1' A)\right]\end{aligned} \tag{6.4.13}$$

The second order pole at $\varepsilon=\varepsilon'$ in (6.4.9) is indeed a first order pole, because

$$\overline{F_{\varepsilon,U}(A)}\;G_{\varepsilon',U}(A)-\overline{G_{\varepsilon,U}(A)}\;F_{\varepsilon',U}(A)\approx(\varepsilon'-\varepsilon)\cdot H(\varepsilon,U)\quad\text{for}\quad\varepsilon\approx\varepsilon' \tag{6.4.14}$$

and

$$H(\varepsilon,U)\equiv\frac{|A_1(\varepsilon,U)|^2}{\omega_1(\varepsilon+U-1)}\left[\mathrm{sign}\,(\kappa)\,\frac{2\kappa(\varepsilon+U)+1}{\omega_1}\overline{\omega_1}\overline{J_{|\kappa+\frac{1}{2}|}(\omega_1 A)}J_{|\kappa-\frac{1}{2}|}(\omega_1 A)\right.$$
$$\left.-A(\varepsilon+U)\left(\overline{\omega_1}|J_{|\kappa+\frac{1}{2}|}(\omega_1 A)|^2+\omega_1|J_{|\kappa-\frac{1}{2}|}(\omega_1 A)|^2\right)\right] \quad (6.4.15)$$

is finite. The integral in (6.4.9) containing the (actual) first order pole at $\varepsilon=\varepsilon'$ is to be calculated in a principal-value sense. Yet, it causes some difficulties in our numerical integration procedure.

Asymptotic behaviour for $|\varepsilon|,|\varepsilon'|\gg 1$

For the purpose of numerical error estimation we find the asymptotic behaviour of the integrand in (6.4.9) at big values of $|\varepsilon|$ and $|\varepsilon'|$. We have

$$\omega_2=\sqrt{\varepsilon^2-1}\cong|\varepsilon|+\mathcal{O}\left(\frac{1}{\varepsilon}\right),\qquad \omega_1=\sqrt{(\varepsilon+U)^2-1}\cong|\varepsilon+U|+\mathcal{O}\left(\frac{1}{\varepsilon}\right). \quad (6.4.16)$$

Using the asymptotic forms of the Bessel functions (5.5.23), we find first

$$\widetilde{A_2}(\varepsilon,U)\cong\cos((|\varepsilon+U|-|\varepsilon|)A),\qquad \widetilde{B_2}(\varepsilon,U)\cong-\sin((|\varepsilon+U|-|\varepsilon|)A), \quad (6.4.17)$$

then

$$\widetilde{A_1}(\varepsilon,U)\cong\sqrt{\frac{|\varepsilon|}{2}}, \quad (6.4.18)$$

and finally

$$\begin{aligned}&\overline{F_{\varepsilon,U}(A)}\,G_{\varepsilon',U}(A)-\overline{G_{\varepsilon,U}(A)}\,F_{\varepsilon',U}(A)\\&\quad\cong\frac{1}{\pi A}\sin\left[(\varepsilon-\varepsilon')A-\frac{\pi}{2}\left(\left|\kappa-\frac{1}{2}\right|+\frac{1}{2}\right)\left(\mathrm{sign}\,(\varepsilon)-\mathrm{sign}\,(\varepsilon')\right)\right]\\&\quad=\begin{cases}\frac{1}{\pi A}\sin\left[(\varepsilon-\varepsilon')A\right], & \text{for sign}\,(\varepsilon)=\text{sign}\,(\varepsilon'),\\ \frac{1}{\pi A}(-1)^{|\kappa-\frac{1}{2}|+\frac{1}{2}}\sin\left[(\varepsilon-\varepsilon')A\right], & \text{for sign}\,(\varepsilon)=-\text{sign}\,(\varepsilon')\end{cases}\end{aligned} \quad (6.4.19)$$

with the above defined regular function

$$H(\varepsilon,U)\cong\begin{cases}\frac{1}{\pi A}, & \text{for sign}\,(\varepsilon)=\text{sign}\,(\varepsilon'),\\ \frac{1}{\pi A}(-1)^{|\kappa-\frac{1}{2}|+\frac{1}{2}}, & \text{for sign}\,(\varepsilon)=-\text{sign}\,(\varepsilon'),\end{cases} \quad (6.4.20)$$

which becomes asymptotically constant for $|\varepsilon|,|\varepsilon'|\gg 1$.

Numerical coupled channel equations

Combining the coupled channel equations (6.4.9) with considerations about the calculation of the scattering operator in section 6.1.1 we arrive at the following numerical procedure. We solve numerically the system of differential equations

$$\dot{b}_{\varepsilon\varepsilon'}(\tau)=-\int_{\tilde{\sigma}(\tau)\setminus\{\varepsilon'\}}b_{\varepsilon\varepsilon''}(\tau)\;M_{\varepsilon'\varepsilon''}(\tau)\;d\mu(\varepsilon'') \quad (6.4.21)$$

where $\tilde{\sigma}(\tau)$ is the discretized spectrum of $H(\tau)$ defined in section 6.1.2 and the coupling matrix elements are

$$M_{\varepsilon\varepsilon'}(\tau) = -A\dot{U}(\tau)e^{-i(\chi_\varepsilon(\tau)-\chi_{\varepsilon'}(\tau))}\frac{\left[\overline{F_{\varepsilon,U}(A)}\; G_{\varepsilon',U}(A) - \overline{G_{\varepsilon,U}(A)}\; F_{\varepsilon',U}(A)\right]}{(\varepsilon-\varepsilon')^2}. \tag{6.4.22}$$

From (6.1.29) and (6.1.30) it follows that the scattering operator is obtained by

$$S_{\varepsilon\varepsilon'} = \lim_{\tau\to\infty} e^{i\tau\varepsilon}e^{-i\chi_\varepsilon(\tau)}b_{\varepsilon'\varepsilon}(\tau) \tag{6.4.23}$$

when the initial condition is chosen as

$$\lim_{\tau\to\infty} b_{\varepsilon'\varepsilon}(\tau) = \tilde{\delta}(\varepsilon'-\varepsilon). \tag{6.4.24}$$

In the numerical integration of (6.4.21) the time τ must be discretized to τ_n such that $\tau_{n+1} = \tau_n + \Delta\tau$. Then the equations take the form

$$b_{\varepsilon\varepsilon'}(\tau_{n+1}) = b_{\varepsilon\varepsilon'}(\tau_n) - \int_{\tilde{\sigma}(\tau)\setminus\{\varepsilon'\}} b_{\varepsilon\varepsilon''}(\tau_n)\; M_{\varepsilon'\varepsilon''}(\tau_n)\; d\mu(\varepsilon'')\; \Delta\tau. \tag{6.4.25}$$

Replacing $M_{\varepsilon'\varepsilon''}(\tau_n)$ with $M_{\varepsilon'\varepsilon''}((\tau_n+\tau_{n+1})/2)$ slightly improves the convergence rate as $\Delta\tau \to 0$.

Singularity problem at $\varepsilon = \varepsilon'$

As already mentioned, the singularity at $\varepsilon = \varepsilon'$ in $M_{\varepsilon\varepsilon'}(\tau)$, being actually a first order pole, causes that the integral in (6.4.21) must be calculated in a principal-value sense. Therefore one must be especially careful when discretizing the continuum and transforming the integral into a sum. (This problem is absent in the numerical scheme with continuum discretization based upon wave packets like in [BS85].) The correct procedure for integration of a function $f(\varepsilon,\varepsilon')$ having a first order pole at $\varepsilon = \varepsilon'$ is

$$\mathrm{PV}-\int f(\varepsilon,\varepsilon_0)\; d\varepsilon \equiv \mathrm{PV}-\int \frac{g(\varepsilon,\varepsilon_0)}{\varepsilon-\varepsilon_0}\; d\varepsilon \approx \sum_{n\neq 0}\frac{g(\varepsilon_n,\varepsilon_0)}{\varepsilon_n-\varepsilon_0}\;\Delta\varepsilon + g'(\varepsilon_0)\Delta\varepsilon \tag{6.4.26}$$

with $g(\varepsilon,\varepsilon')$ regular at $\varepsilon = \varepsilon'$ and

$$\begin{aligned} g'(\varepsilon_0) &\equiv \frac{\partial}{\partial\varepsilon}\; g(\varepsilon,\varepsilon_0)\bigg|_{\varepsilon=\varepsilon_0} = \lim_{\delta\to 0}\frac{g(\varepsilon_0+\delta,\varepsilon_0)-g(\varepsilon_0-\delta,\varepsilon_0)}{2\delta} \\ &= \lim_{\delta\to 0}\frac{f(\varepsilon_0+\delta,\varepsilon_0)+f(\varepsilon_0-\delta,\varepsilon_0)}{2} \approx \frac{f(\varepsilon_0+\Delta\varepsilon,\varepsilon_0)+f(\varepsilon_0-\Delta\varepsilon,\varepsilon_0)}{2}. \end{aligned} \tag{6.4.27}$$

This scheme must be applied to (6.4.21) by replacing $f(\varepsilon',\varepsilon'')$ with $-b_{\varepsilon\varepsilon''}(\tau)\; M_{\varepsilon'\varepsilon''}(\tau)$. It is important to note that not only the singular term $M_{\varepsilon'\varepsilon''}(\tau)$ but the full function $-b_{\varepsilon\varepsilon''}(\tau)\; M_{\varepsilon'\varepsilon''}(\tau)$ must be differentiated at $\varepsilon = \varepsilon'$, what is not easy because we know only discrete numerical values of $b_{\varepsilon\varepsilon''}(\tau)$

$$\tilde{b}_{ij}(\tau) \equiv b_{\varepsilon_i,\varepsilon_j}(\tau). \tag{6.4.28}$$

Writing $M_{\varepsilon'\varepsilon''}(\tau) \equiv g_{\varepsilon'\varepsilon''}(\tau)/(\varepsilon' - \varepsilon'')$ we obtain

$$\begin{aligned}\dot{\tilde{b}}_{ij}(\tau) &\cong -\sum_{k\neq j} \tilde{b}_{ik}(\tau)\ M_{jk}(\tau)\ \Delta\varepsilon_k + \frac{d}{d\varepsilon} b_{\varepsilon_i\varepsilon}(\tau)\ M_{\varepsilon_j\varepsilon}(\tau)\Big|_{\varepsilon=E_j} \Delta\varepsilon_j \\ &\cong -\sum_{k\neq j} \tilde{b}_{ik}(\tau)\ M_{jk}(\tau)\ \Delta\varepsilon_k + \frac{b_{\varepsilon_i\varepsilon_{j+1}}(\tau) - b_{\varepsilon_i\varepsilon_{j-1}}(\tau)}{2\Delta\varepsilon_j}\ g_{\varepsilon_j\varepsilon_j}(\tau)\Delta\varepsilon_j \\ &\qquad + b_{\varepsilon_i\varepsilon_j}(\tau)\ \frac{g_{\varepsilon_j\varepsilon_{j+1}}(\tau) - g_{\varepsilon_j\varepsilon_{j-1}}(\tau)}{2\Delta\varepsilon_j}\ \Delta\varepsilon_j.\end{aligned} \tag{6.4.29}$$

In order to find the function $g_{\varepsilon\varepsilon'}$ one has to differentiate twice

$$g_{\varepsilon\varepsilon'} \equiv \frac{\partial^2}{\partial\varepsilon'^2}\left[\overline{F_{\varepsilon,U}(A)}\ G_{\varepsilon',U}(A) - \overline{G_{\varepsilon,U}(A)}\ F_{\varepsilon',U}(A)\right]\Big|_{\varepsilon'=\varepsilon}. \tag{6.4.30}$$

The result is quite a long expression and we do not give it here.

Continuum cut-off

Error control due to the introduction of cut-offs in the continuum is much more complicated in the system described by coupled channel equations with a continuously changing potential than in the previously studied cases with quasi-static potentials. Therefore we only sketch the ideas of the estimations needed to show that the error can be made arbitrarily small when the cut-offs are chosen appropriately. First, we argue that the amplitudes $b_{\varepsilon\varepsilon'}(\tau)$ satisfying the system of equations (6.4.21) and the initial conditions (6.4.24) stay uniformly bounded during the evolution by

$$|b_{\varepsilon\varepsilon'}(\tau)| \leq \mathcal{O}\left(\frac{1}{(\varepsilon - \varepsilon')^2}\right) \quad \text{for} \quad |\varepsilon - \varepsilon'| \gg 1. \tag{6.4.31}$$

This is a consequence of the asymptotic form of the coupling matrix elements $M_{\varepsilon\varepsilon'}$ derived in (6.4.19). We do not have a rigorous proof of this fact, but numerical evidence confirms that behaviour. Moreover, considering discretized time one can show that $b_{\varepsilon\varepsilon'}(\tau_n)$ has that form at every $\tau_n = n\Delta\tau$. Next, we estimate how much of the amplitude $b_{\varepsilon\varepsilon'}(\tau)$ "flows" to the region outside the cut-offs, i.e. for $|\varepsilon_0| < \varepsilon_{cut}$

$$||b_{\varepsilon_0}.||_{out} \equiv \sqrt{\left(\int_{-\infty}^{-\varepsilon_{cut}} + \int_{\varepsilon_{cut}}^{\infty}\right)|b_{\varepsilon_0\varepsilon}|^2\ d\mu(\varepsilon)} \leq \mathcal{O}\left(\frac{1}{(\varepsilon_0 - \varepsilon_{cut})^{3/2}}\right) + \mathcal{O}\left(\frac{1}{(\varepsilon_0 + \varepsilon_{cut})^{3/2}}\right). \tag{6.4.32}$$

The amplitudes $b_{\varepsilon\varepsilon'}(\tau)$ calculated with cut-offs have two sources of error: due to neglect of the amplitudes outside the cut-offs (new error introduced at every time) and due to the evolution of the approximate quantity (propagation of the error). It becomes transparent when we write the time-derivative of a difference between the exact $b_{\varepsilon\varepsilon'}(\tau)$ and the

approximated $\widetilde{b}_{\varepsilon\varepsilon'}(\tau)$ amplitude

$$\begin{aligned}|\dot{b}_{\varepsilon_0\varepsilon} - \dot{\widetilde{b}}_{\varepsilon_0\varepsilon}| &= \left| \int_{-\infty}^{+\infty} b_{\varepsilon_0\varepsilon'} M_{\varepsilon\varepsilon'}\ d\mu(\varepsilon') - \int_{-\varepsilon_{cut}}^{+\varepsilon_{cut}} \widetilde{b}_{\varepsilon_0\varepsilon'} M_{\varepsilon\varepsilon'}\ d\mu(\varepsilon') \right| \\ &\leq \underbrace{\left| \left(\int_{-\infty}^{-\varepsilon_{cut}} + \int_{\varepsilon_{cut}}^{\infty} \right) b_{\varepsilon_0\varepsilon'} M_{\varepsilon\varepsilon'}\ d\mu(\varepsilon') \right|}_{I_1(\varepsilon_0,\varepsilon)} + \underbrace{\left| \int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} (b_{\varepsilon_0\varepsilon'} - \widetilde{b}_{\varepsilon_0\varepsilon'}) M_{\varepsilon\varepsilon'}\ d\mu(\varepsilon') \right|}_{I_2(\varepsilon_0,\varepsilon)}\end{aligned} \tag{6.4.33}$$

The second integral $I_2(\varepsilon_0, \varepsilon)$ can be estimated by use of the Cauchy-Schwarz inequality

$$\begin{aligned}I_2(\varepsilon_0,\varepsilon) &\leq \sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon'} - \widetilde{b}_{\varepsilon_0\varepsilon'}|^2\ d\mu(\varepsilon')} \cdot \sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |M_{\varepsilon\varepsilon'}|^2\ d\mu(\varepsilon')} \\ &\equiv ||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in} \cdot ||M_{\varepsilon\cdot}||_{in},\end{aligned} \tag{6.4.34}$$

where we have introduced a new norm $||...||_{in}$ which will be useful later. The estimation of the first integral $I_1(\varepsilon_0, \varepsilon)$ is more involved and requires information on the behaviour of $b_{\varepsilon_0\varepsilon'}$, namely the bound (6.4.31). One can show that

$$\begin{aligned}I_1(\varepsilon_0,\varepsilon) &\leq \left| \left(\int_{-\infty}^{-\varepsilon_{cut}} + \int_{\varepsilon_{cut}}^{\infty} \right) \frac{C}{(\varepsilon_0 - \varepsilon')^2} \frac{\sin((\varepsilon - \varepsilon')A)}{(\varepsilon - \varepsilon')^2}\ d\mu(\varepsilon') \right| \\ &\leq \mathcal{O}\left(\frac{1}{(\varepsilon_0 - \varepsilon_{cut})^2 (\varepsilon - \varepsilon_{cut})^2} \right) + \mathcal{O}\left(\frac{1}{(\varepsilon_0 + \varepsilon_{cut})^2 (\varepsilon + \varepsilon_{cut})^2} \right),\end{aligned} \tag{6.4.35}$$

for big $\varepsilon_0, \varepsilon$ or ε_{cut}, but it behaves less singular at the ends of the cut-off interval

$$I_1(\varepsilon_0,\varepsilon) \leq \mathcal{O}\left(\frac{\log(\varepsilon \pm \varepsilon_{cut})}{(\varepsilon_0 - \varepsilon_{cut})^2} \right) \quad \text{for} \quad \varepsilon \pm \varepsilon_{cut} \approx 0. \tag{6.4.36}$$

Now, we can estimate the total error in the amplitudes due to the cut-offs

$$||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in} = \sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon'} - \widetilde{b}_{\varepsilon_0\varepsilon'}|^2\ d\mu(\varepsilon')}. \tag{6.4.37}$$

We find its time-derivative using the above estimations

$$\begin{aligned}\frac{d}{d\tau}||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in} &= \frac{1}{||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in}} \int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon} - \widetilde{b}_{\varepsilon_0\varepsilon}|\, |\dot{b}_{\varepsilon_0\varepsilon} - \dot{\widetilde{b}}_{\varepsilon_0\varepsilon}|\ d\mu(\varepsilon) \\ &\leq \int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon} - \widetilde{b}_{\varepsilon_0\varepsilon}|\, ||M_{\varepsilon\cdot}||_{in}\ d\mu(\varepsilon) + \frac{1}{||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in}} \int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon} - \widetilde{b}_{\varepsilon_0\varepsilon}|\, I_1\ d\mu(\varepsilon) \\ &\leq \underbrace{\sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon} - \widetilde{b}_{\varepsilon_0\varepsilon}|^2\ d\mu(\varepsilon)}}_{||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in}} \cdot \underbrace{\sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} ||M_{\varepsilon\cdot}||_{in}^2\ d\mu(\varepsilon)}}_{\equiv ||M_{\cdot\cdot}||_{in}} \\ &\quad + \frac{1}{||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in}} \underbrace{\sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |b_{\varepsilon_0\varepsilon} - \widetilde{b}_{\varepsilon_0\varepsilon}|^2\ d\mu(\varepsilon)}}_{||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in}} \cdot \sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |I_1(\varepsilon_0,\varepsilon)|^2\ d\mu(\varepsilon)} \\ &\leq ||b_{\varepsilon_0\cdot} - \widetilde{b}_{\varepsilon_0\cdot}||_{in} \cdot ||M_{\cdot\cdot}||_{in} + \sqrt{\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |I_1(\varepsilon_0,\varepsilon)|^2\ d\mu(\varepsilon)}\end{aligned} \tag{6.4.38}$$

The last integral to estimate is finite, because its (quadratic) logarithmic singularities at $\varepsilon \pm \varepsilon_{cut} \approx 0$ are integrable. It can be shown that it behaves like

$$\begin{aligned}&\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |I_1(\varepsilon_0,\varepsilon)|^2 \, d\mu(\varepsilon) \\ &\leq \mathcal{O}\left(\frac{1}{(\varepsilon_{cut})^3}\right)\left[\mathcal{O}\left(\frac{1}{(\varepsilon_0-\varepsilon_{cut})^4}\right)+\mathcal{O}\left(\frac{1}{(\varepsilon_0+\varepsilon_{cut})^4}\right)+\mathcal{O}\left(\frac{1}{(\varepsilon_0-\varepsilon_{cut})^2(\varepsilon_0+\varepsilon_{cut})^2}\right)\right]\end{aligned} \tag{6.4.39}$$

for big ε_0 or ε_{cut}, but for $\varepsilon_0 \pm \varepsilon_{cut} \approx 0$ it behaves like

$$\begin{aligned}&\int_{-\varepsilon_{cut}}^{\varepsilon_{cut}} |I_1(\varepsilon_0,\varepsilon)|^2 \, d\mu(\varepsilon) \\ &\qquad \leq \mathcal{O}\left(\frac{1}{(\varepsilon_{cut})^3}\right)\left[\mathcal{O}\left(\log(\varepsilon_0 \pm \varepsilon_{cut})^2\right)+\mathcal{O}\left(\frac{\log(\varepsilon_0 \pm \varepsilon_{cut})}{\varepsilon_{cut}^2}\right)+\mathcal{O}\left(\frac{1}{\varepsilon_{cut}^4}\right)\right]\end{aligned} \tag{6.4.40}$$

So, finally we have

$$\frac{d}{d\tau}||b_{\varepsilon_0\cdot}-\widetilde{b}_{\varepsilon_0\cdot}||_{in}(\tau) \leq ||b_{\varepsilon_0\cdot}-\widetilde{b}_{\varepsilon_0\cdot}||_{in}(\tau)\cdot||M_{\cdot\cdot}||_{in}(\tau)+\mathcal{O}\left(\frac{1}{(\varepsilon_{cut})^{7/2}}\right) \tag{6.4.41}$$

when ε_0 is not too near the cut-off at $\pm\varepsilon_{cut}$. Having this estimate, we can show a uniform bound (in ε_{cut}) on the error in the whole evolution

$$||b_{\varepsilon_0\cdot}-\widetilde{b}_{\varepsilon_0\cdot}||_{in}(\tau) \leq \mathcal{O}\left(\frac{1}{(\varepsilon_{cut})^{7/2}\,\widehat{||M_{\cdot\cdot}||}_{in}}\right)\left(e^{\widehat{||M_{\cdot\cdot}||}_{in}\cdot\tau}-1\right), \tag{6.4.42}$$

where $\widehat{||M_{\cdot\cdot}||}_{in} \equiv \sup_{\tau'\in(0,\tau)}||M_{\cdot\cdot}||_{in}(\tau')$. We see that the error can be made arbitrarily small by an appropriate choice of the cut-off value ε_{cut}. In an analogous way one can show an estimate for the particle production $N_\varepsilon^\pm$, but we do not cite here these long calculations.

Unitarity control

The operator $b(\tau)$ giving in the limit $\tau \to \infty$ the scattering operator S is unitary for every τ, i.e. it holds $b(\tau)^* b(\tau) = \mathbf{1}$. While the exact coupled channel equations (6.4.21) preserve unitarity of $b(\tau)$, the numerical equations do not keep $\tilde{b}(\tau)$ exactly unitary, i.e. the condition $b(\tau)^* b(\tau) = \mathbf{1}$ gets violated. The difference $b(\tau)^* b(\tau) - \mathbf{1}$ can be used as an error estimator for the numerical result. In a single time step $\tau_n \to \tau_{n+1}$ we have symbolically

$$\tilde{b}_{ij}(\tau_{n+1}) = \tilde{b}_{ij}(\tau_n) + \sum_k \tilde{b}_{ik}(\tau_n)\; H_{jk}(\tau_n) \tag{6.4.43}$$

where

$$H_{jk}(\tau_n) \equiv -M_{jk}(\tau_n)\Delta\varepsilon_k\Delta\tau. \tag{6.4.44}$$

It gives

$$[b(\tau_{n+1})^* b(\tau_{n+1})]_{ij} = [b(\tau_n)^* b(\tau_n)]_{ij} + \sum_k H_{ki}(\tau)^* H_{kj}(\tau) \tag{6.4.45}$$

or in short

$$b(\tau_{n+1})^* b(\tau_{n+1}) - b(\tau_n)^* b(\tau_n) = H(\tau)^* H(\tau) = \mathcal{O}(H^2). \tag{6.4.46}$$

If we define the error as $\mathrm{Err}(\tau) \equiv ||b(\tau)^* b(\tau) - \mathbf{1}||$, where the norm can be an absolute value of the trace, Hilbert-Schmidt or any other matrix norm, we find by starting with τ_0 where $\mathrm{Err}(\tau_0) = 0$

$$\begin{aligned} \mathrm{Err}(\tau_N) &= ||b(\tau_N)^* b(\tau_N) - b(\tau_0)^* b(\tau_0)|| \\ &= \left|\left| \sum_{k=0}^{N-1} b(\tau_{k+1})^* b(\tau_{k+1}) - b(\tau_k)^* b(\tau_k) \right|\right| \\ &= \left|\left| \sum_{k=0}^{N-1} H(\tau_k)^* H(\tau_k) \right|\right|. \end{aligned} \tag{6.4.47}$$

Taking into account (6.4.44), the fact that $M(\tau)$ has the form $\dot{U}(\tau)\widetilde{M}(\tau)$ and the norm is proportional to the number of states N_E in the discretized spectrum we can estimate

$$\mathrm{Err}(\tau_N) \lesssim N\ \Delta\tau^2\ ||\dot{U}||^2\ \Delta\varepsilon^2\ N_E^2\ ||\widetilde{M}||^2 \tag{6.4.48}$$

where $||\dot{U}|| \equiv \sup_k |\dot{U}(\tau_k)|$, $\Delta\varepsilon \equiv \sup_m \Delta\varepsilon_m$ and $||\widetilde{M}|| \equiv \sup_k \sqrt{||M(\tau_k)^* M(\tau_k)||}/N_E$. Finally it can be written as

$$\mathrm{Err}(\tau_N) \lesssim \frac{T^2}{N}\ ||\dot{U}||^2\ |\varepsilon_{max} - \varepsilon_{min}|^2\ ||\widetilde{M}||^2, \tag{6.4.49}$$

where $T \equiv N\Delta\tau$ and $|\varepsilon_{max} - \varepsilon_{min}|$ is the range of the discretized energy spectrum. It shows that when the number of time-discretization steps N grows while the total time T is kept constant, hence $\Delta\tau \to 0$, the error $\mathrm{Err}(\tau_N)$ decreases like $1/N$. It proves convergence of the numerical scheme to a one giving in the limit a unitary b and thus unitary scattering matrix S.

6.4.2 Continuous switch on and off

We want to consider processes where the potential is continuously switched on and off. The interesting parameters are the time rate of the switch on-off and duration of the overcritical phase. Therefore we choose a simple function describing the time-dependence of the potential's strength, which allows us to control easily both parameters

$$U(t) = \begin{cases} -U_0, & t < -T_0/2 - T_1, \\ -U_1 + \frac{t+T_0/2}{T_1}(U_0 - U_1), & -T_0/2 - T_1 < t < -T_0/2, \\ -U_1, & -T_0/2 < t < T_0/2, \\ -U_1 - \frac{t-T_0/2}{T_2}(U_0 - U_1), & T_0/2 < t < T_0/2 + T_2, \\ -U_0, & T_0/2 + T_2 < t, \end{cases} \tag{6.4.50}$$

with $U_1 > U_0 > 0$. The full potential is

$$V(t,\mathbf{x}) = V(t,r) = U(t)\cdot v(r) = U(t)\cdot\Theta(a-r) = \begin{cases} U(t), & r<a, \\ 0, & r>a \end{cases}. \tag{6.4.51}$$

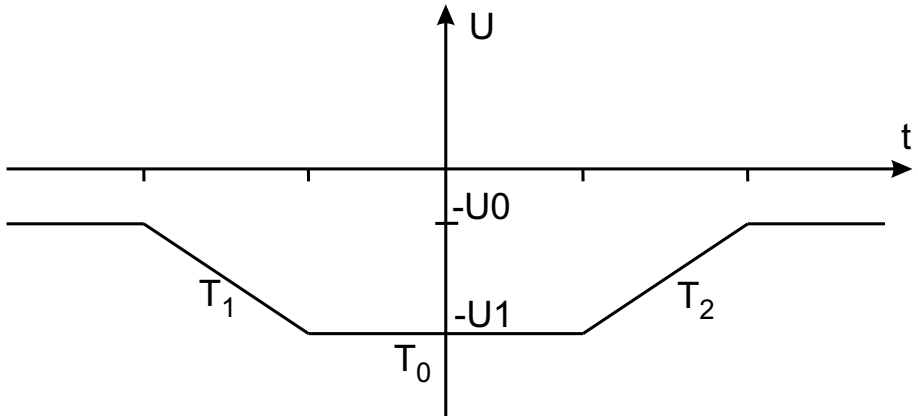


Figure 6.17: Smooth switch on-off: time-dependence of the potential's strength.

Once again we use the theorem 9 or 10 with $a = 0$ and $b = U'$ to find that $H(t) = H_0 + V(t)$ is self-adjoint on $\mathcal{D}(H_0)$ for every time t. Since $V(t)$ is bounded, self-adjoint and continuous (cf. section 3.4 there exists a unitary propagator $U(t_2,t_1)$ [Tha92, Th. 4.10]. If we treat

$$\tilde{H}_0 \equiv \lim_{t\to\pm\infty} H(t) = H_0 - U_0\cdot v(r) \tag{6.4.52}$$

as an asymptotic Hamiltonian and

$$\tilde{V}(t,r) = (U(t)+U_0)\cdot v(r) \tag{6.4.53}$$

as its perturbation then it has a switching factor

$$\varphi(t) = \frac{U(t)+U_0}{U_1-U_0}, \tag{6.4.54}$$

what together gives

$$H(t) = \tilde{H}_0 + \tilde{V}(t,r) = \tilde{H}_0 + (U_1-U_0)\ \varphi(t)\ v(r). \tag{6.4.55}$$

Since the spatial part of the potential $v(\mathbf{x})$ is short-range and belongs to $L^p(\mathbb{R}^3)$ with any $p > 0$ and the switching factor $\varphi(t)$ satisfies (3.5.16)-(3.5.17) the wave-operators (3.5.12) exist and are complete (cf. section 3.5.2). Consequently, there exists a unitary scattering operator S in $\mathcal{H}$ (3.5.18). It is implementable in $\mathcal{F}$, because such $\tilde{V}(t,r)$ satisfies conditions of theorem 8 (it satisfies (2.8.28)-(2.8.29) in the example below the theorem).

6.4.3 Particle production spectra – subcritical

First, we study potentials which stay subcritical during the whole evolution (it is enough to choose U_0 and U_1 subcritical). We can observe how the total (dynamical) particle production depends on the time rate of change of the potential as well as application (and numerical precision) of the adiabatic theorem in slow processes.

Dynamical production and the adiabatic limit

Figure 6.18 shows antiparticle production for a series of processes with different speeds of switching, i.e. different values of T_1 and T_2 (here $T_1 = T_2$). There is no doubt that for slower processes (bigger value of $T_{1,2}$) particle production decreases. As one can deduce from the proof of the adiabatic theorem, which we sketched in section 4.5, the vanishing of the amplitude distribution in the negative continuum in adiabatic limit is reached via a multiplicative factor quickly oscillating in energy. Therefore we can see oscillations in the spectrum with period $\sim 1/T$. Simultaneously, the amplitudes decrease for longer times.

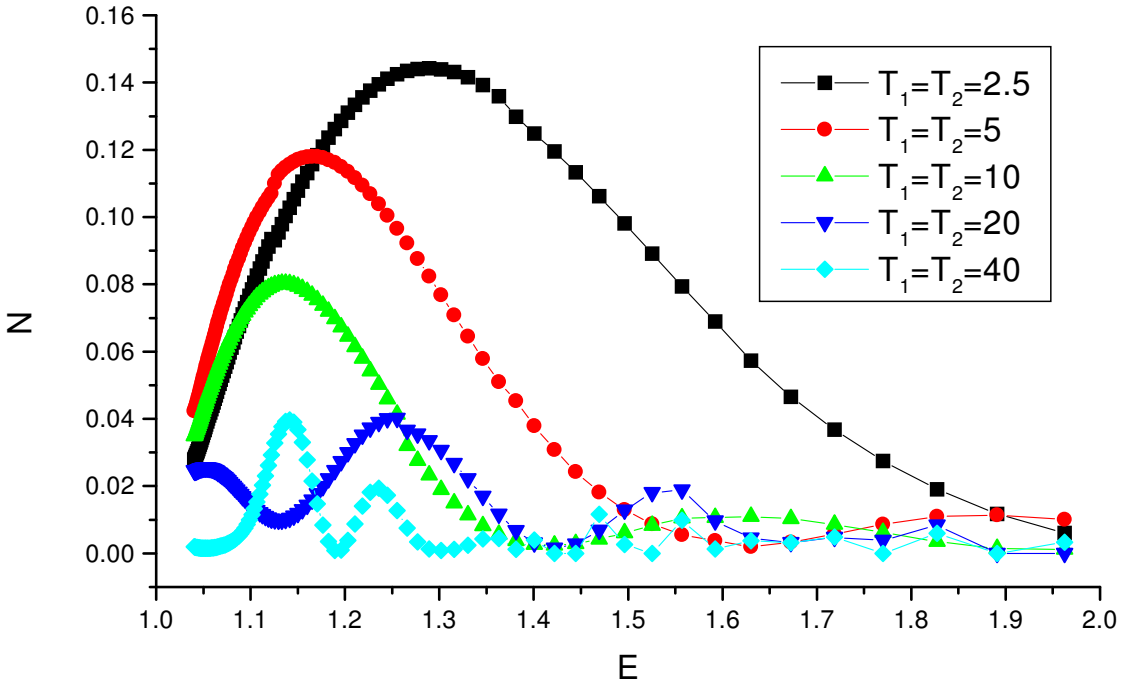


Figure 6.18: Antiparticle production spectra for a series of processes with different speeds of potential switching.

The next figure 6.19 shows the total production (the integrated spectrum) of antiparticles (which is equal to the total number of particles) as a function of the time-rate of the switching process. It scales as $1/T$ and slowly reaches zero in the adiabatic limit.

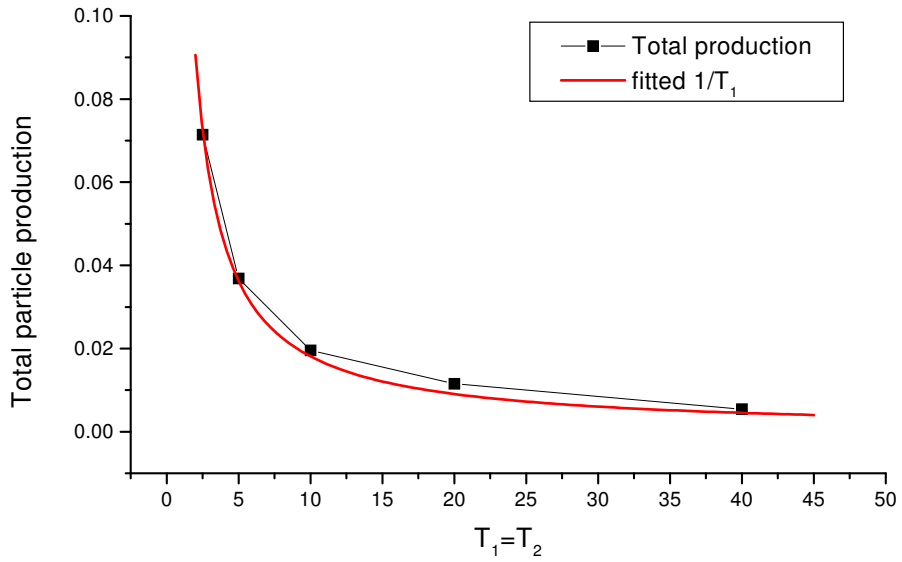


Figure 6.19: Total production of antiparticles (=particles) as a function of the time-rate of the switching process. Fitted curve $0.18/T_1$.

6.4.4 Particle production spectra – overcritical

Here, the initial and final potential U_0 will be subcritical, while the intermediate U_1 will be overcritical. We expect a bound state diving into the negative continuum, turning into a resonance which can decay, depending on the duration of the overcritical period. Finally, the bound state reappears, but the amplitude of the wave function (which previously was identical with the initial bound state) in this state will be decreased by the amount which decayed in the continuum and has been trapped there. As we have discussed in section 4.5 and have observed in the previous numerical section, it is clear that a resonance decays in a static potential. Yet, it is unclear, what really happens to a moving resonance in presence of a time-dependent potential. In section 4.5 we reached the conclusion that in quick processes the peak (i.e. peak-shape energy distribution of the wave function in the continuum) should roughly follow the position of the resonance, because the situation is similar to consecutive projections from one to the next basis in continuum, corresponding to changing Hamiltonian $H(t)$. Of course, part of the wave function gets dispersed (into both continua) due to the quick time-dependence. On the other hand, in slow processes the peak additionally decays at every stage of the evolution. As we have seen in section 4.5, the dispersion due to the time-change of the basis gets small, but the loss of the amplitude due to the continuous decay becomes essential. However, the resonance near the edge of the continuum is very narrow and decays slower than as it gets deeper and becomes wider. Therefore, the decay in time-dependent overcritical potentials is quite complicated with different phenomena occurring simultaneously, of which one does not know theoretically which will dominate. In order to understand their interplay, we need to perform numerical simulations.

Narrow peaks – non-uniform continuum discretization

One of the most difficult problems in numerical simulations of moving resonances is the fact that their width tends to zero as their position approaches the edge of the continuum. As we have estimated in previous sections, it behaves like $\Gamma \sim (-\varepsilon_{res}+1)^{3/2}$, where ε_{res} is the position of the peak near the continuum's edge at $\varepsilon = -1$. Numerics with uniform continuum discretization by $\Delta\varepsilon_n = \Delta\varepsilon$ cannot handle this problem, because some peaks (near the edge) have width $\Gamma < \Delta\varepsilon$. On figure 6.20 (presenting an antiparticle creation spectrum in slow switch on/off process) we see problems at the edge of the continuum: consecutive refinements of the discretization step do not converge and the curve behaves unstable – there are big jumps between the values of the neighbouring points near the maximum. Further refinement of the discretization step (figure 6.21) still behaves unstable and shows no convergence.

In order to successfully treat peaks numerically, one always has to have several points within every peak. It suggests to choose a non-uniform discretization with $\Delta\varepsilon_n$ smaller for $\varepsilon_n \approx -1$, where the peaks are narrower. To find the optimal distribution of discretization points ε_n and intervals $\Delta\varepsilon_n$, let's first consider approximation of an abstract integral over a peak. Divide the real axis into the intervals (x_n^-, x_n^+) with $\Delta x_n \equiv x_n^+ - x_n^-$ and take the values of the function $f(x)$ at discrete points $x_n \in (x_n^-, x_n^+)$. Then

$$\begin{aligned}\int f(x)\,dx - \sum_n f(x_n)\,\Delta x_n \cong \sum_n f'(x_n)\left(\frac{x_n^+ + x_n^-}{2} - x_n\right)\Delta x_n \\ + \sum_n \frac{1}{3} f''(x_n)\left[(x_n^+)^2 + (x_n^-)^2 + x_n^+ x_n^- + 3x_n^2 - 3x_n^+ x_n - 3x_n^- x_n\right]\Delta x_n\end{aligned} \tag{6.4.56}$$

The first sum vanishes when we choose $x_n = (x_n^+ + x_n^-)(2)$, i.e. in the middle of the intervals, whatever their distribution is. Then, the second term becomes

$$\sum_n \frac{4}{3} f''(x_n)\,\Delta x_n^3. \tag{6.4.57}$$

It can be shown that the next term is of order $\sim \Delta x_n^5$, so much smaller. In order to minimize the above sum at given number of discretization points, we must choose

$$\Delta x_n \sim \frac{\Delta x}{\sqrt[3]{|f''(x_n)|}}. \tag{6.4.58}$$

Consider now $f(x)$ being resonance shapes

$$f(x) \equiv f_{x_R,\Gamma}(x) \equiv \frac{\Gamma}{(x-x_R)^2 + \Gamma^2}. \tag{6.4.59}$$

Their second derivative have maxima at $x = x_R$ and

$$\max_x |f''(x)| = \frac{2}{\Gamma^3}. \tag{6.4.60}$$

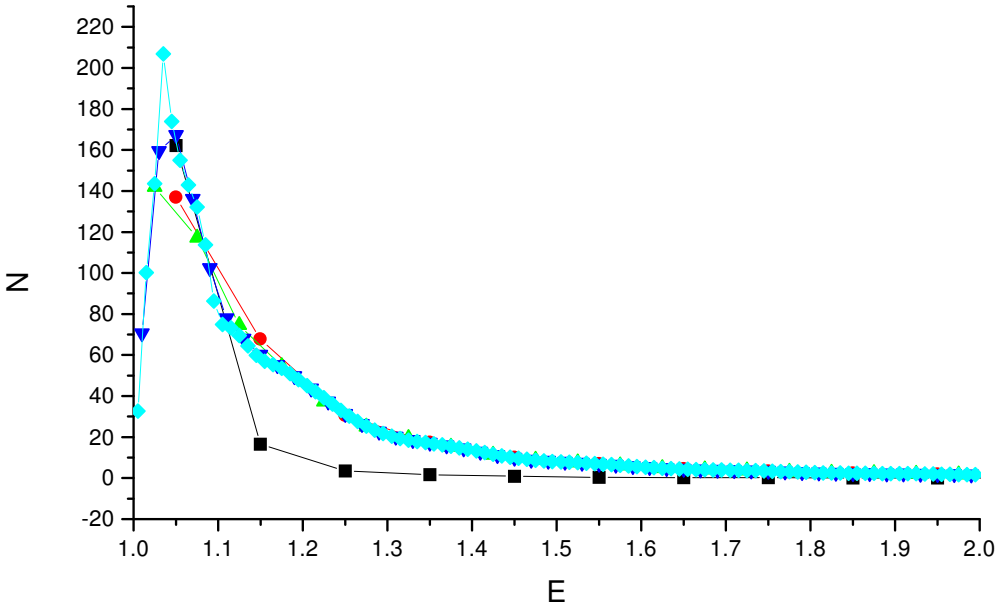


Figure 6.20: Slow switch on-off process: decay of the wave packet occurs during the whole overcritical phase, starting near the continuum's edge, where the peak is very narrow. There are no enough points in the discretized continuum to represent the peak and the numerical resolution becomes insufficient.

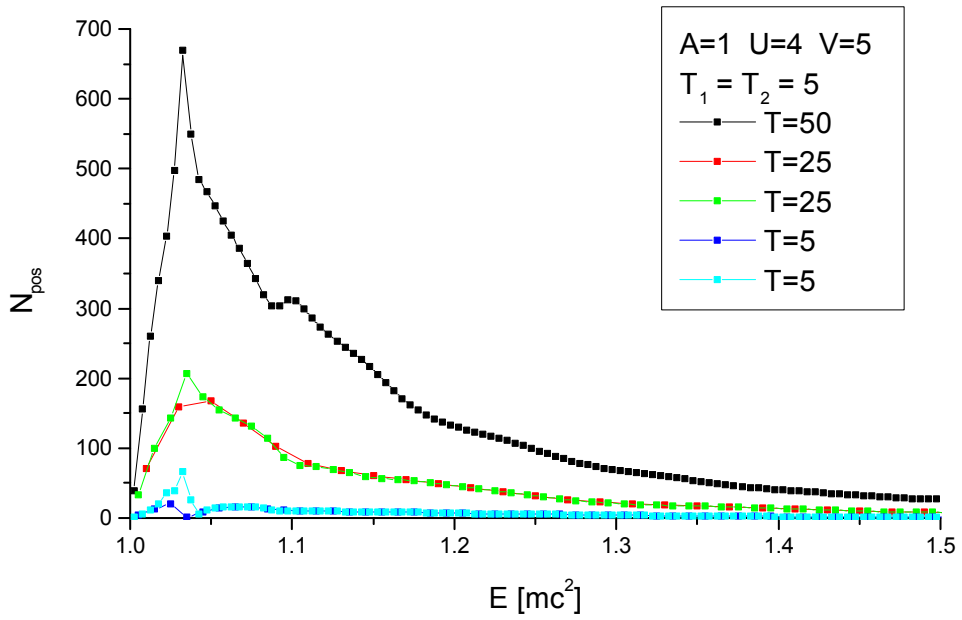


Figure 6.21: Slow switch on-off: refining the continuum's discretization step does not help, because the peak is arbitrary narrow near the continuum's edge and therefore cannot be handled by this method.

Further, we know that there is a scaling between the position and width of the resonance $\Gamma \approx \alpha\ x^{3/2}$, where we use x for $-\varepsilon - 1$. Hence, we can estimate the terms

$$|f''(x_n)\ \Delta x_n^3| \leq \frac{2\ \Delta x_n^3}{\alpha^3\ x_n^{9/2}} = 2\left(\frac{\Delta x_n}{\alpha\ x_n^{3/2}}\right)^3. \tag{6.4.61}$$

Therefore we should choose $\Delta x_n \sim x_n^{3/2} \cdot \Delta x$ what agrees with the intuition that $\Delta x_n \sim \Gamma \sim x_n^{3/2}$ should be optimal. The last step is to determine such x_n. It turns out (by solving a simple differential equation) that these points must be placed at

$$x_n = \frac{x_{max}}{(1+\alpha(n-1))^2} \tag{6.4.62}$$

with $x_1 = x_{max}$ and the inverse order $x_{n+1} < x_n$, i.e. x_n tending to 0. Figure 6.22 shows the distribution of Δx_n vs. x_n. Since the number of points is finite, there is a last point, x_N, nearest $x = 0$ with smallest interval Δx_N and there are no more points between x_N and 0. Hence, we can only consider peaks which entirely lie above x_N. Roughly, a peak centered at x_R with width Γ is localized in 70% (in the sense of an integral) in the interval $(x_R - 2\,\Gamma, x_R + 2\,\Gamma)$ and its amplitude outside this interval is less than 1/5 of its maximum. Figure 6.23 shows how many discretization points lie "within" the peak (i.e. within this interval) at every value of x under the assumption that $\Gamma = \Gamma(x) = \alpha\ x^{3/2}$ as we have found for resonances in section 5.3 and is shown on figure 5.3. We can see clearly that the number of points within every peak is approximately constant 16 ± 1 for $x \gtrsim 0.05$. Below this value this discretization scheme is not reliable, what is confirmed on figure 6.24 presenting exact value of the integral of the peak on the interval $(0, 1)$ against the approximation based on discretization x_n.

Concluding, **this discretization scheme treats all peaks laying between $x_{min} = x_N$ and $x_{max} = x_1$ with the same accuracy**, but it does not allow for treating peaks laying near and below x_N, what is a problem of all discretization schemes, because of arbitrarily narrow peaks near the edge of the continuum. We want to argue now, that it is not a real problem for the evolution processes. Assume $U(t)$ starts from a subcritical value $U(t_0) = U_0$ and tends to overcritical $U(t_1) = U_1$. In between, at $t = t_{cr}$, it reaches the critical value $U(t_{cr}) = U_{cr}$ such that the deepest bound state energy reaches $\varepsilon = -1$. Then, for $t > t_{cr}$ we have a resonance, which lies very near the continuum edge and is very narrow for $t \approx t_{cr}$. However, the time-dependent process must be discretized in time to be numerically applicable, i.e. divided into time-steps t_n. Then, there exists a step, say n', such that $U(t_{n'-1}) < U_{cr}$ is subcritical, while $U(t_{n'}) > U_{cr}$ is overcritical (we must avoid situation with $U(t_n)$ exactly critical, because many formulas become singular at that point and are numerically inapplicable). So, the resonance appears first at position, say $x_R(t_{n'}) > 0$, which is well separated from the edge of continuum (although it may be very near). We have only to choose the discretization in such a way, that $x_N \ll x_R(t_{n'})$, i.e. (nearly) the whole peak is well approximated by the discretization points.

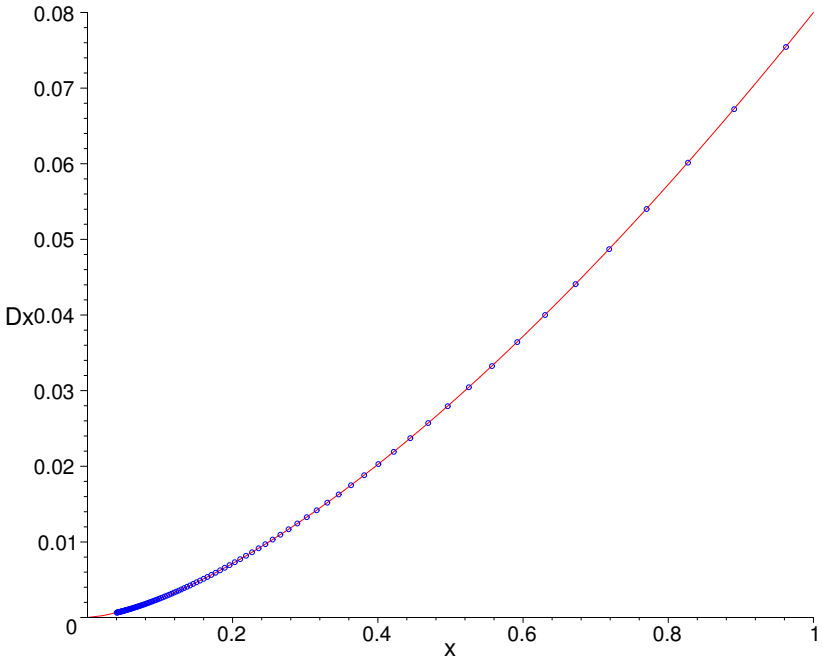


Figure 6.22: Distribution of the discretization points in the negative continuum: Δx_n vs. x_n with $x \equiv -\varepsilon - 1$ and line $\Delta x \sim x^{3/2}$.

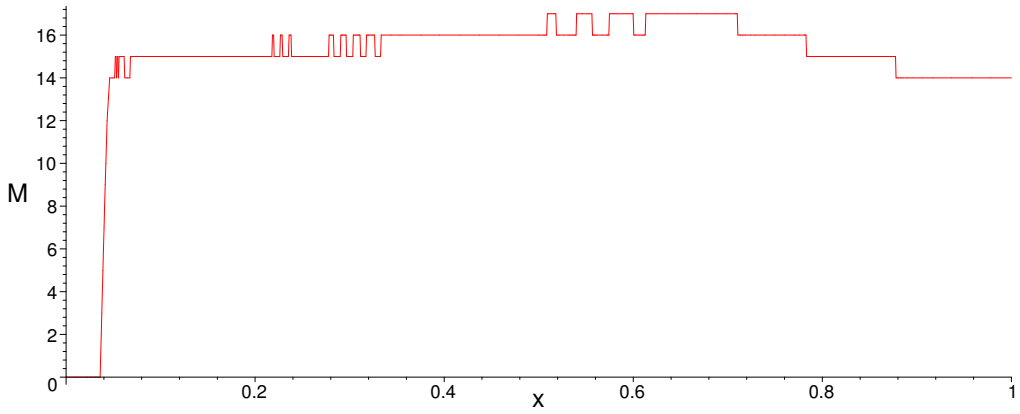


Figure 6.23: Number of points M in the discretized continuum laying "within" a peak centered around x having width $\Gamma = \alpha\ x^{3/2}$.

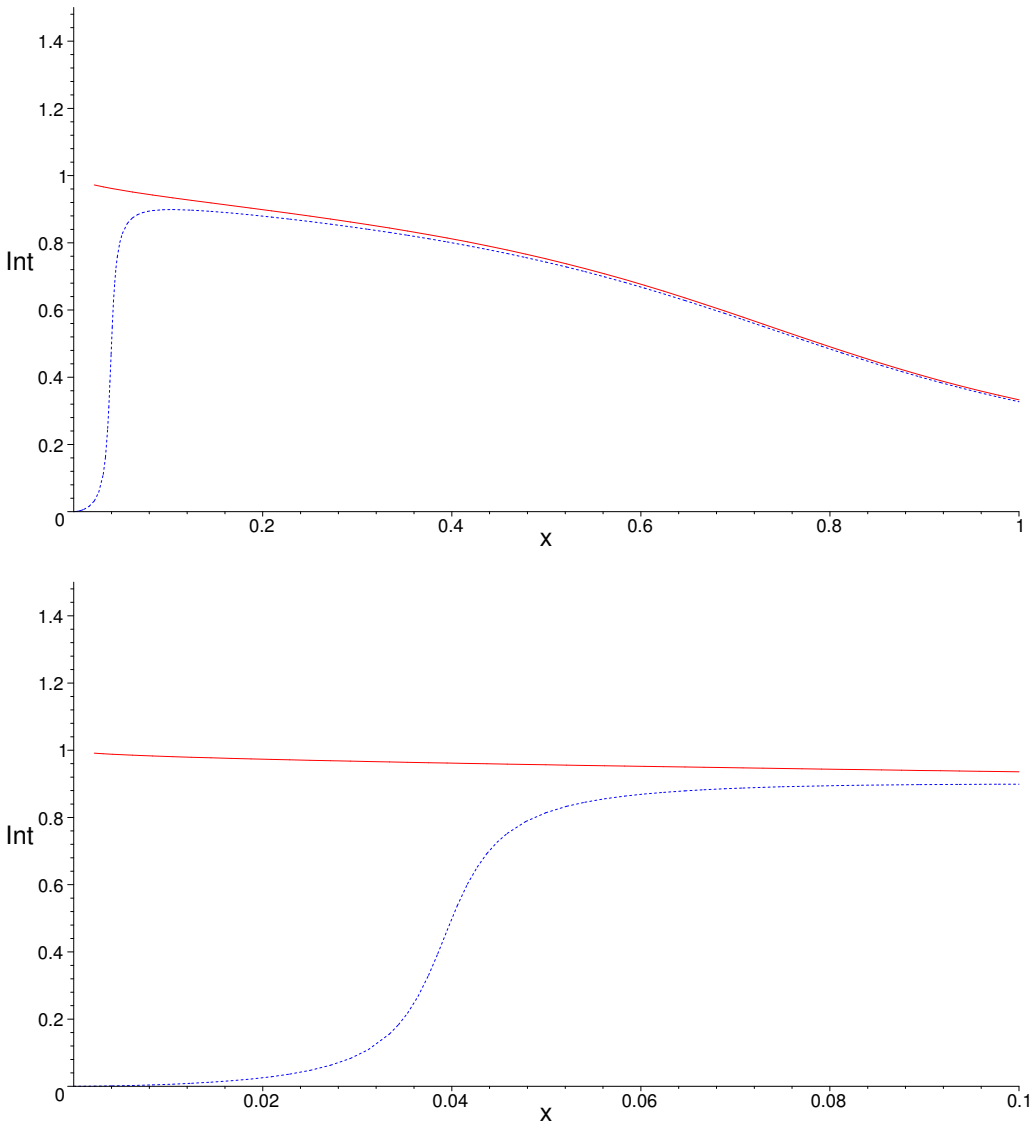


Figure 6.24: Exact value of the integral of the peak on the interval $(0, 1)$ (solid red line) against the approximation based on discretization x_n (dashed blue line).

Quick processes with no overcritical delay

Consider first processes with quick switch on and off of the potential with no overcritical delay phase. We obtain nearly no particle creation, also nearly no dynamical, even if the time-variation of the potential is big. The reason is that the whole process is very short and the wave function gets nearly projected from one to another basis (corresponding to changing Hamiltonian $H(t)$) and finally gets projected onto the initial basis with no loss due to the evolution (of phases), what results in (nearly) no particle production.

The main contribution to the antiparticle production spectrum in the overcritical processes has the bound state, which dives into the negative continuum during the evolutions. More precisely, the antiparticle production distribution

$$N_\varepsilon^- = \int_{\sigma^+} |S_{\varepsilon\varepsilon'}|^2 d\varepsilon' = \int_{{\sigma_{cont}}^+} |S_{\varepsilon\varepsilon'}|^2 d\varepsilon' + \sum_{\sigma^+_{disc}} |S_{\varepsilon\varepsilon'_n}|^2 \Delta\varepsilon'_n. \tag{6.4.63}$$

is dominated by the last term, which corresponds to the energy distribution ε in the negative continuum of an amplitude of a wave function evolving from the initial bound state with energy ε'_n and diving into the continuum during the evolution, when it assumes a peak shape around the resonance position. If this amplitude distribution goes back to the final bound state, no antiparticle production occurs. If (some part of) it remains in the negative continuum, it contributes to the antiparticle production. Therefore, it is interesting to observe how this distribution changes during the evolution. Figure 6.25 shows the final particle production, which is nearly zero (≈ 0.001), as well as consecutive distributions of the discussed amplitude. Clearly, it moves along the moving resonance as the strength of the potential increases and then moves back as the strength of the potential decreases. Finally, it rebuilds the bound state wave function, whose amplitude just after the dive-out amounts 0.978.

Quick processes with overcritical delay

If we allow for a delay in the overcritical phase, causing the potential value to freeze for some time $T > 0$, the situation changes completely. The amplitude of the dived bound state forming a peak in the continuum decays[3] during the delay and remains trapped there in the switch-off phase. Finally, it contributes dominantly to the antiparticle production distribution. The same effect has been observed in numerical calculations in the case of heavy ion collisions with delay [RMMG81].

Figure 6.26 shows the distribution of the wave packet representing the dived bound state moving along the moving resonance up to the deepest position, when the potential is strongest. Then the delay $T = 50$ causes the peak around $\varepsilon \approx 1.469$ with a half-width $\Gamma \approx 0.177$ to decay completely. Consequently the peak stays there in the dive out phase

[3]The "decay" means here a dephasing of different energy contributions such that the wave packet becomes orthogonal to its initial value in the sense of a scalar product.

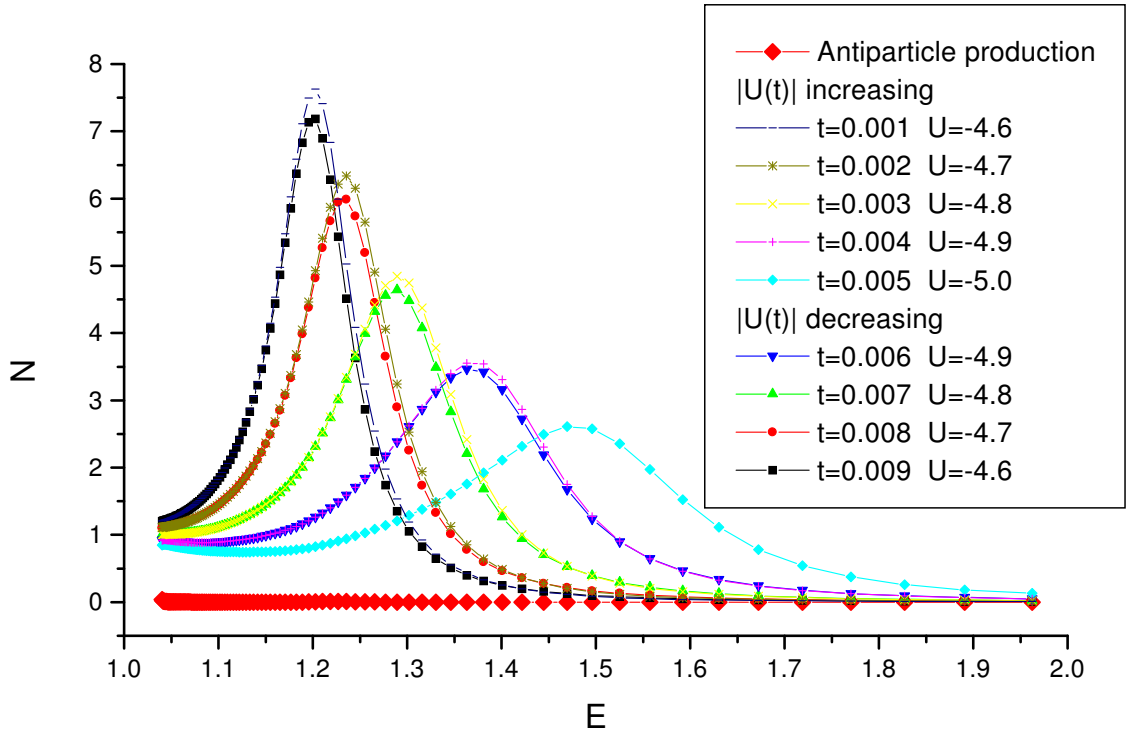


Figure 6.25: Quick switch on-off process with no overcritical delay: the antiparticle production, which is nearly zero (red diamonds on bottom) and the amplitude of the wave packet representing the dived bound state at several time instants (1-5 diving in, 6-9 diving out).

and does not follow the resonance moving back left. The final amplitude in the dived-out bound state is tiny and amounts about 0.015. Figure 6.26 shows also the total particle production, whose profile is identical with those of the decayed peak and its integral, i.e. the total probability of antiparticle production is nearly 1.

Intermediate and slow processes

Now, we analyze slower processes and allow the wave packet to decay during the switch on and off phase. First, to show the idea of the continuous decay but avoid complications at the edge of the continuum, we consider situation, where the initial subcritical potential U_0 is suddenly switched to some overcritical value U_1, then changes continuously to a stronger value U_2, stays for some time $T > 0$ constant, goes back to the value U_1, and eventually jumps back to U_0. It has the advantage that we start at U_1 with a relatively wide peak well separated from the continuum's edge. We have chosen

$$U_0 = 4.00 \qquad \text{subcritical,} \tag{6.4.64}$$

$$U_1 = 4.90 \qquad \text{resonance: } \varepsilon_R = -1.417,\ \varepsilon_I = 0.117, \tag{6.4.65}$$

$$U_2 = 5.00 \qquad \text{resonance: } \varepsilon_R = -1.500,\ \varepsilon_I = 0.143 \tag{6.4.66}$$

and choose the switch-in T_1 and switch-out T_2 phase duration to be in the range from $T_1 = T_2 = 0.005$ to $T_1 = T_2 = 250$. Figure 6.27 shows the resulting antiparticle production spectra. For diving-times below $T_1 \leq 0.5$ the peak is completely transported near the resonance position in the strongest potential U_2 (fitted $\varepsilon_{res} \approx 1.505$, $\Gamma \approx 0.155$) and decays fully in the delay phase with $T = 25$. For $T_1 = 5$ which is of order of magnitude of the characteristic decay time (between 6.99 and 8.55 depending on the position of the resonance) there appears a slight deviation in the antiparticle production spectrum. For slower dive-in processes, i.e. for $T_1 \geq 25$ the spectrum changes essentially. It moves towards lower energies, what means that the peak decays earlier during the switch-on phase. In the extremely slow switch-on with $T_1 = 250$ the whole peak decays already at $U = U_1$ (fitted $\varepsilon_{res} \approx 1.375$, $\Gamma \approx 0.160$).

Now, we can make the same comparison eliminating the initial jump in the potential's strength and start with wave packets localized near the continuum's edge. However, as we discussed at the begin of this section, simulation of a truly continuous switch on process in numerically impossible and the discretization of time always introduces small jumps in the switch on and off phases, including a jump from some slightly subcritical potential U_0 to slightly overcritical U_1. So we choose $U_0 = 4.29$ (bound state energy $\varepsilon_1 = -.996$), $U_1 = 4.40$ (resonance $\varepsilon_R = -1.062$, $\Gamma = 0.0087$) and $U_2 = 5.00$ (resonance: $\varepsilon_R = -1.500$, $\varepsilon_I = 0.143$). Since the results for this choice of parameters are clear enough, there is no point to force the value U_1 against the critical value $U_{cr} = 4.297$, what induces tremendous increase of the computational expense due to the extremely narrow peaks which require very dense discretization of the continuum. The results, the antiparticle

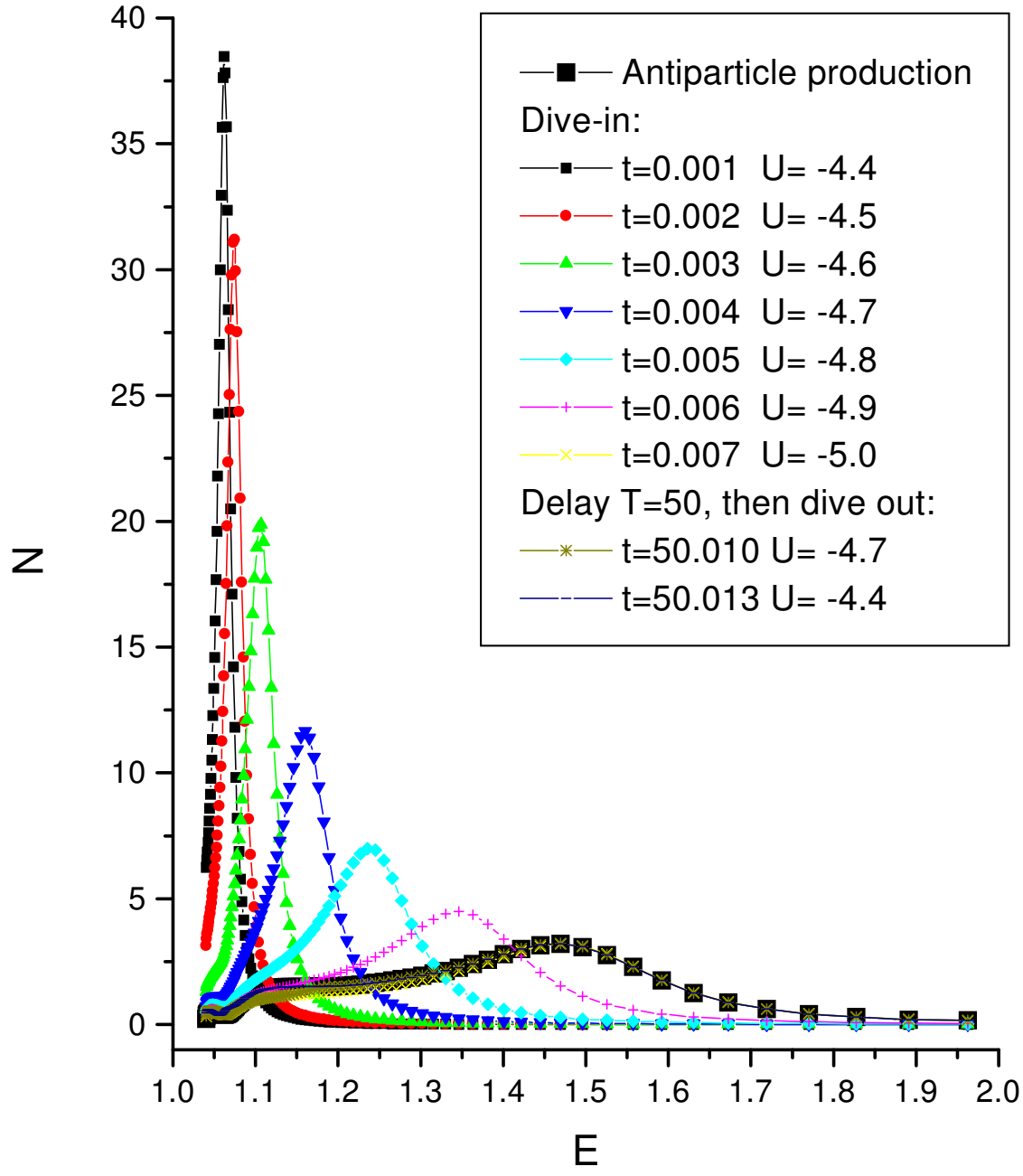


Figure 6.26: Quick switch on-off process with overcritical delay $T = 50$: the amplitude of the wave packet representing the dived bound state at several time instants: 1-7 diving in, 8-9 diving out after the delay and decay (peak shape remains constant) and the antiparticle production, which is identical with the decayed peak's shape (red filled squares).

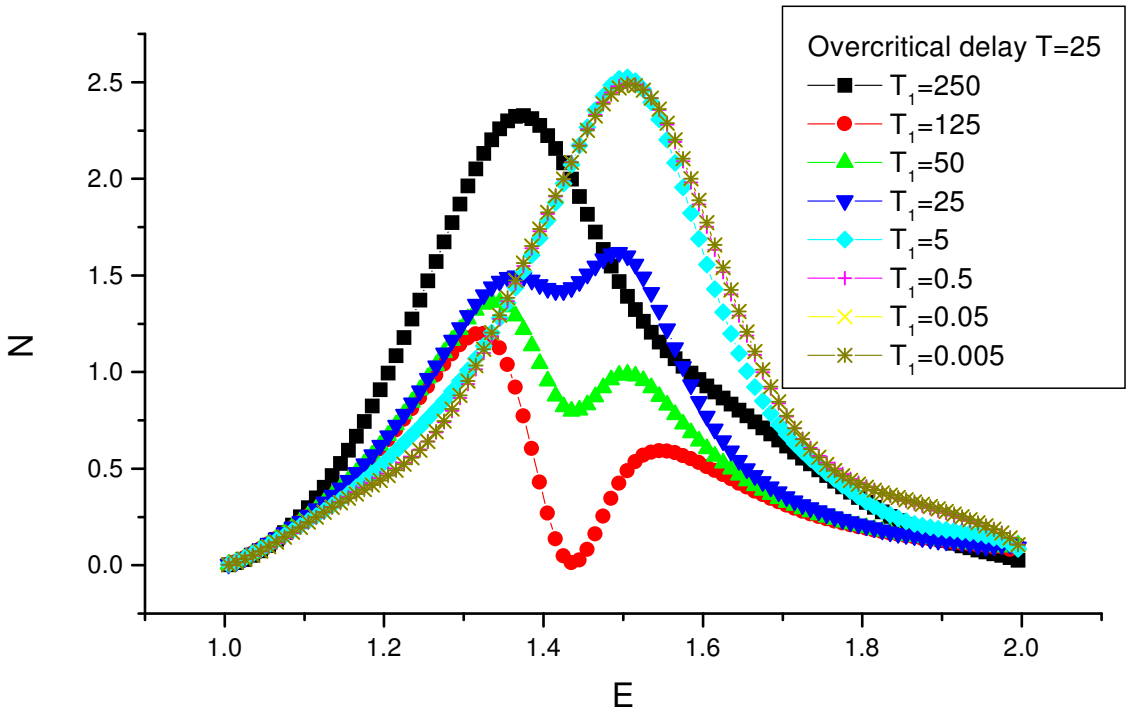


Figure 6.27: Slow switch on-off process with initial and final jump and overcritical delay $T = 25$: antiparticle production spectra for different time rates of the switch on and switch off phase. The slower is the switch phase the earlier (shifted to lower energies) decays the wave packet representing the dived bound state.

production spectra, for these parameters and switch on/off duration times in the range between $T_1 = T_2 = 0.006$ and $T_1 = T_2 = 300$ are presented on figure 6.28. Again, for short switch on/off times $T_1 \ll 1$ the wave packet is transported near the position of the resonance in the deepest potential U_2 (fitted $\varepsilon_{res} \approx 1.469$, $\Gamma \approx 0.197$) where it decays during the delay phase with $T = 50$. For slower switch on processes the decay occurs continuously during the switch on, when the resonance moves right. The wave packet partially decays and partially follows the resonance, what results in a distributed spectrum of antiparticle production (like e.g. for $T_1 = 24$). For extremely slow processes, which approach the adiabatic limit, the peak decays almost fully as soon as it appears in the continuum, what in our case occurs for $U = U_1$ (fitted $\varepsilon_{res} \approx 1.101$, $\Gamma \approx 0.0742$).

Concluding, the wave packet in the negative continuum representing the dived bound state in presence of an overcritical potential partially follows a moving resonance and partially decays continuously in the whole overcritical period, what, in general, results in an antiparticle production spectrum distributed over all positions of the resonance during the overcritical phase. The slower the overcritical potential varies the more intensive the continuous decay is. In contrast, the quicker the overcritical potential varies the more accurately the peak follows the position of the resonance.

Optimal resonance excitation

Figure 6.29 presents comparison between the antiparticle creation spectra for a sudden switch on and off ($T_1 = T_2 = 0$) from slightly subcritical $U_0 = 4.29$ (bound state $\varepsilon_1 = -0.996$) with overcritical delay $T = 50$, continuous switch on and off with $T_1 = T_2 = 0.006$ and overcritical delay $T = 50$, and the theoretical shape of the (Lorentz) resonance for the final potential $U_1 = 5$. Due to the quick time-dependence the spectrum for the sudden switch on-off differs slightly from the ideal resonance shape. Yet, the spectrum for the continuous switch on-off differs more and is shifted to lower energies, what is the property of all continuous processes, where the peak decays continuously during the evolution. From figure 6.28 we know that for slower processes the spectrum is even more shifted to lower energies. Therefore the optimal time-rate for switching on/off to obtain maximal production corresponding to the resonance is reached in the sudden switch case. In contrast, when we start from an initial potential which is far from being critical and choose $U_0 = 1.5$ (bound state $\varepsilon_1 = +0.905$), the antiparticle production spectrum shown on figure 6.30 differs more from the theoretical resonance shape and is shifted slightly to higher energies (what is the effect of a stronger contribution from the dynamical production). Since slower processes give shift to lower energies, there should theoretically exist an optimal time-rate such that the maximum of the spectrum agrees with those of the theoretical resonance. However, this time-rate must be extremely quick, because for $T_1 = T_2 = 0.006$ we get the spectrum shown on the figure 6.30, which is essentially shifted to lower energies. Our numerical methods do not allow us for successful consideration of shorter switch times and to reach

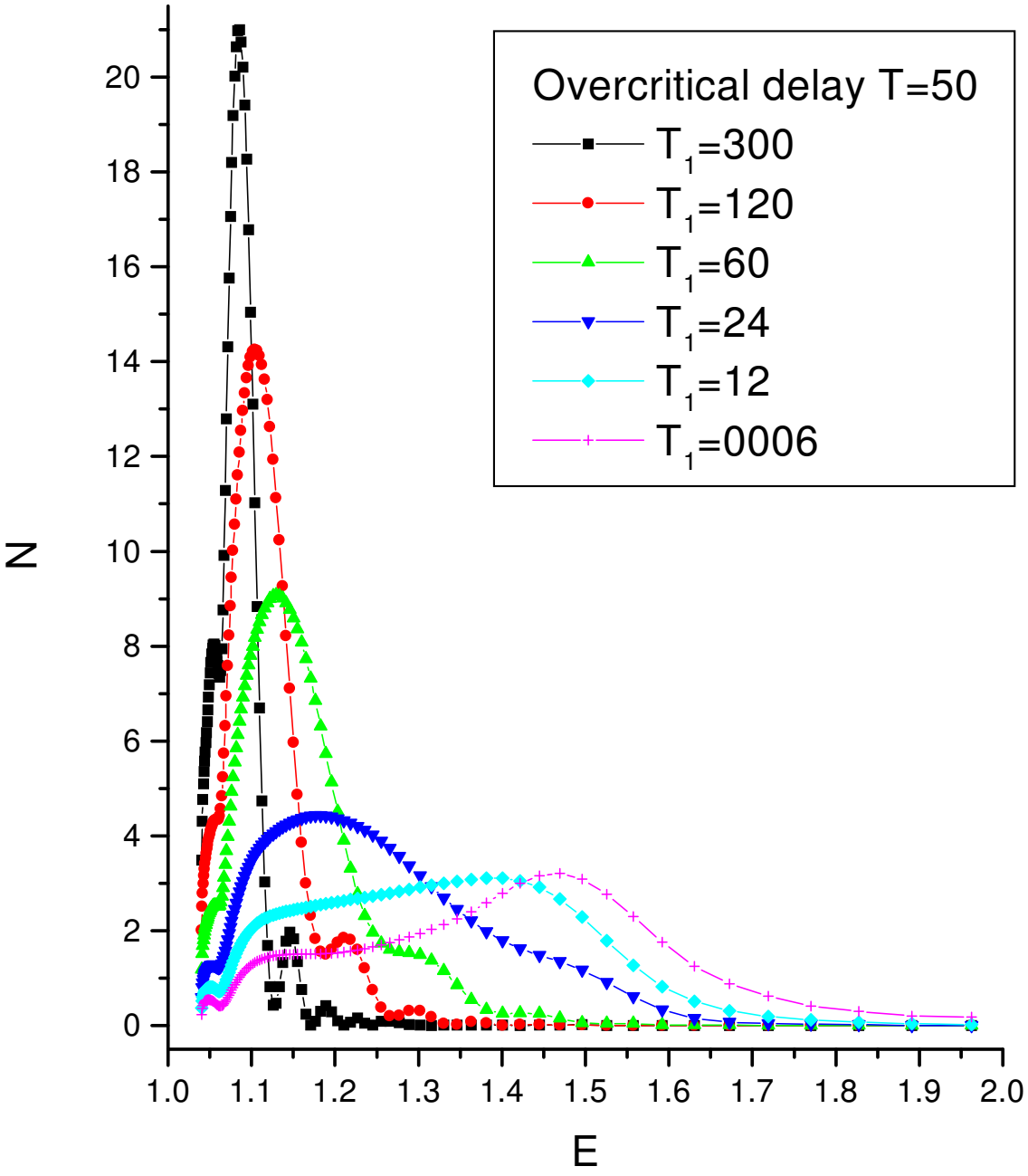


Figure 6.28: Slow switch on-off process with overcritical delay $T = 50$: antiparticle production spectra for different time rates of the switch on and switch off phase. The slower is the switch phase the earlier (shifted to lower energies) decays the wave packet representing the dived bound state.

the discontinuous sudden switch limit. Yet, it does not seem essential, because this time scale is physically already tremendously short (10^{-24} s.).

We can conclude, that the optimal time-rate for switch on and off processes with a long overcritical delay to obtain maximally peaked spectrum of created antiparticles agreeing with the shape of the resonance in the overcritical potential is reached for (almost) suddenly switched on and off potentials. Slower and adiabatic switching, due to the continuous decay of the wave packet in the negative continuum (representing the dived bound state), lead to spectra peaked at lower energies, with the position $\varepsilon_{max} \to 1^+$ in the adiabatic limit.

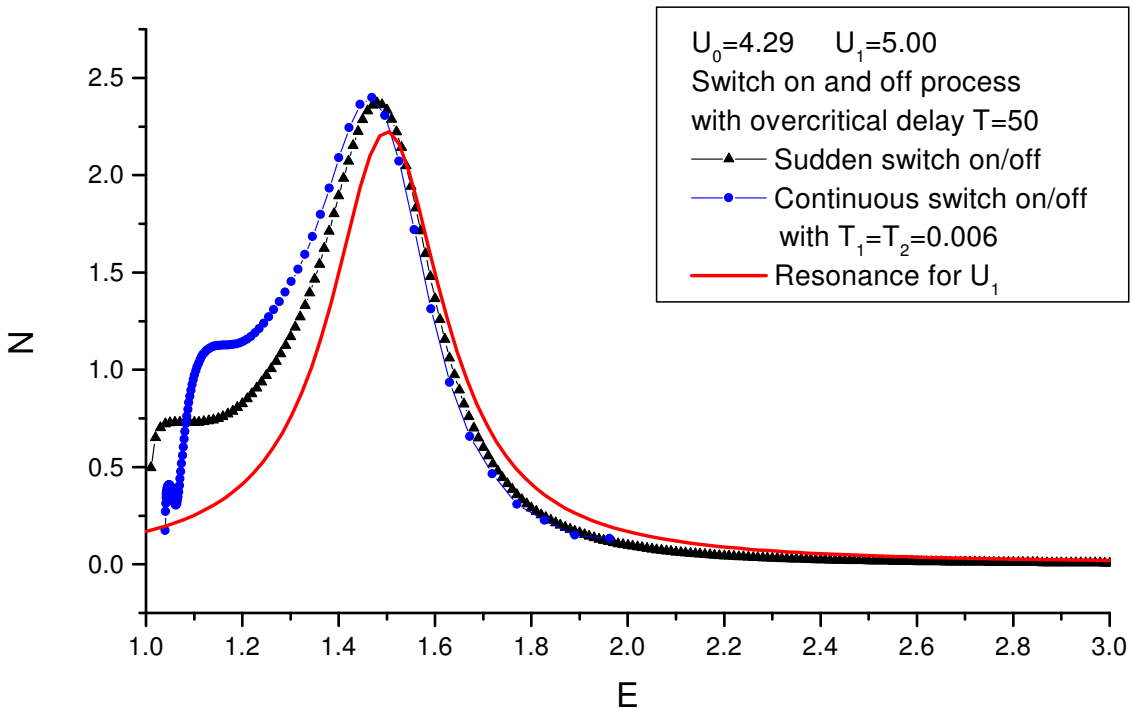


Figure 6.29: Antiparticle creation spectra for a sudden switch on and off ($T_1 = T_2 = 0$) from slightly subcritical $U_0 = 4.29$ with overcritical delay $T = 50$ and continuous switch on and off with $T_1 = T_2 = 0.006$ with overcritical delay $T = 50$ compared to the theoretical shape of the (Lorentz) resonance for the final potential $U_1 = 5$.

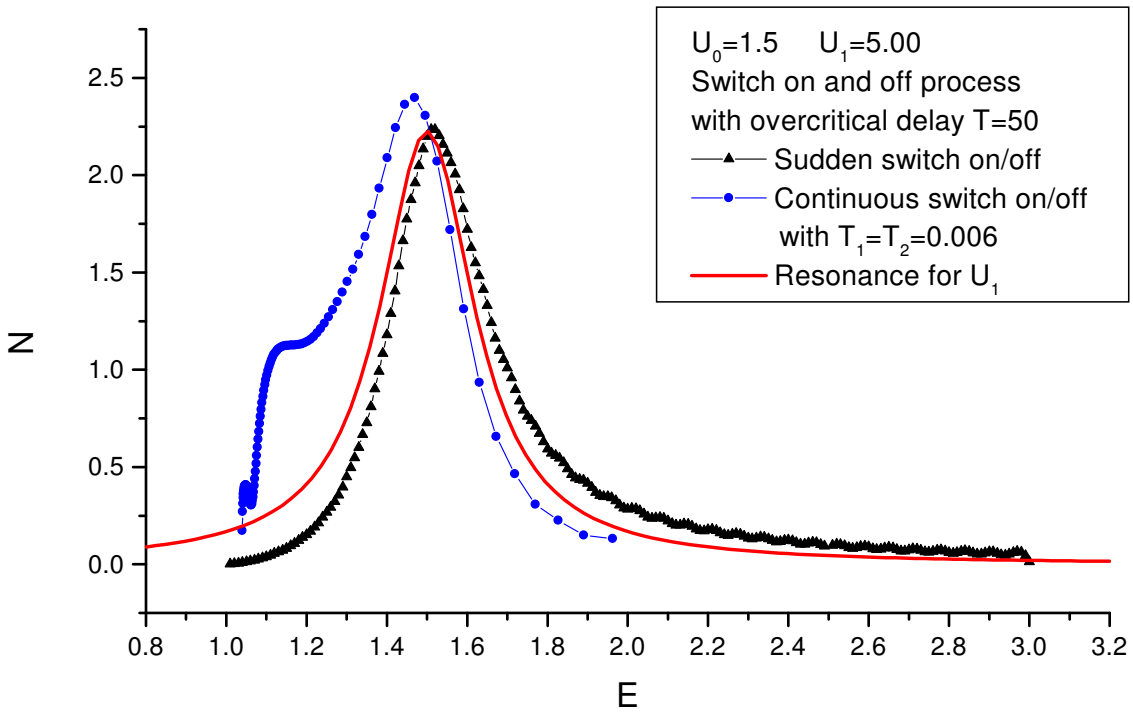


Figure 6.30: Antiparticle creation spectra for a sudden switch on and off ($T_1 = T_2 = 0$) from a weak potential $U_0 = 1.5$ with overcritical delay $T = 50$ and continuous switch on and off with $T_1 = T_2 = 0.006$ with overcritical delay $T = 50$ compared to the theoretical shape of the (Lorentz) resonance for the final potential $U_1 = 5$.

Chapter 7

The inverse problem

In this chapter we want to ask the question how much information about the time-dependent potential can be reconstructed from the scattering data, represented by the scattering operator or the particle production spectrum. Being aware that such procedure is far from being unique, we consider several simplified cases, where only few degrees of freedom of the potential are to be guessed. Using results from the previous chapter we give some answers to what extent information about the potential's parameters can be successfully obtained. Finally, we propose a simple approximation method (master equation) basing on exponential, decoherent decay of time-dependent resonances for prediction of particle creation spectra. Despite its simplicity we obtain relatively good agreement with the results of full numerical calculations from the previous chapter. This method can be relatively easily applied to the inverse problem.

7.1 Time-dependent inverse scattering

The problem of reconstructing the Hamiltonian or potential from the scattering data is know in the literature as an inverse (scattering) problem. In general (for the Dirac equation) it is already impossible to solve the inverse problem for static potentials. Only in some cases, where the form of the potential is further restricted (e.g. spherical symmetry) there is a chance for a unique result. The last possibility is to treat the potential as belonging to a n-parameter family of functions and fit the n parameters to obtain the scattering data nearest to those which are given. In case of time-dependent potentials the situation regarding general methods is hopeless. Only parameter fitting can be tried.

7.2 Overcriticality

It is interesting, if unique signs of overcriticality can be found in the scattering data. Of course, overcriticality implies spontaneous particle creation. Yet, as we have shown in part I, the spontaneous particle creation defined rigorously is practically useless and extremely

rare (i.e. unstable with respect to tiny perturbations of the potential). On the other hand, the spontaneous particle creation in a weaker sense, discussed in section 4.5, is not unique. As long as the resulting peak in the antiparticle production is narrow and high, there is no doubt regarding overcriticality, but for wide and small peaks, which are of order of the dynamical production, the uniqueness is lost. Let's consider several cases, when this question can be answered.

7.2.1 Short duration processes

As we have seen in section 6.3.1, there is no quantitative difference between subcritical and overcritical potentials when the overcritical period is short. Figure 7.1 shows the situation for a sudden switch on and off with delay $T = 1$. The difference between the sub- and overcritical spectra is not more than 20% in amplitude and both have the same shape.

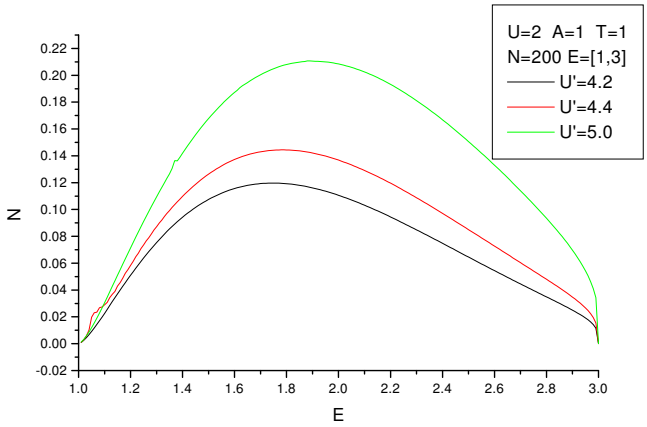


Figure 7.1: Switch on-off: no quantitative difference between subcritical and overcritical potentials in the switched-on phase for short times ($T = 1$). $U' = 4.2$ (black) is subcritical, while $U' = 4.4$ (red) and $U' = 5$ (green) are overcritical.

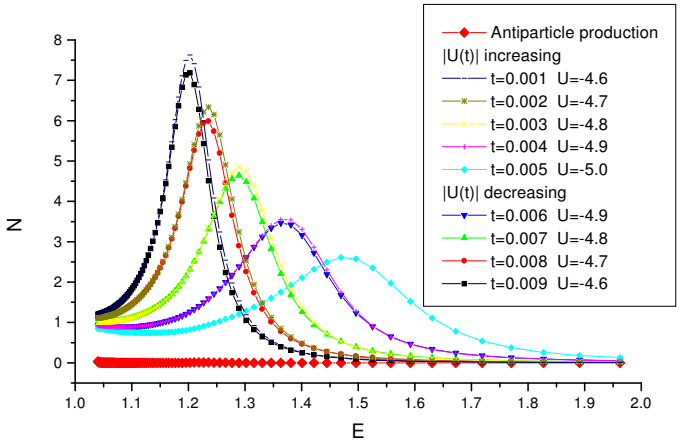


Figure 7.2: Quick switch on-off process with no overcritical delay: the antiparticle production, which is nearly zero (red diamonds on bottom) and the amplitude of the wave packet representing the dived bound state at several time instants (1-5 diving in, 6-9 diving out).

The reason is that although a wave packet appears in the overcritical continuum, it has not enough time to decay and dives out forming a reappearing bound state again. It can be clearly seen on figure 7.2 which presents a process with continuous switch on/off ($T_1 = T_2 = 0.01$) and no delay. The wave packet moves right and then back left, what results in nearly no particle production.

7.2.2 Quick processes with delay

The situation changes dramatically, when the overcritical phase has a delay of order of the decay time of the resonance. Whether for sudden switch on-off (figure 7.3) or for continuous (figure 7.4), the wave packet always decays at the position of the resonance in the overcritical potential and clearly contributes to the antiparticle creation spectrum. Here the inverse problem is trivial.

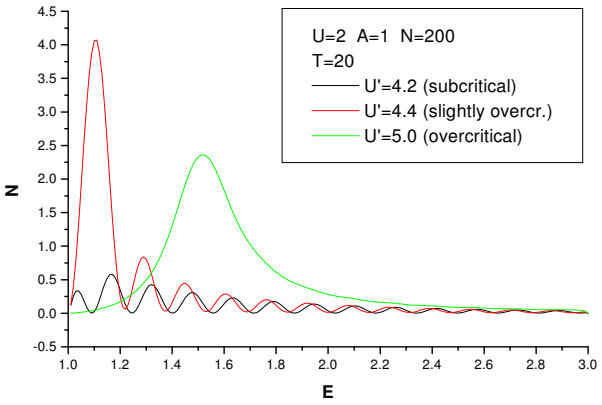


Figure 7.3: Switch on-off: the peaks in overcritical vs. no peaks in subcritical potential for the duration time $T = 20$ of the switched-on phase.

The position of the resonance allows for a unique determination of the value of the overcritical potential. The only open question is the duration of the overcritical delay. We know (cf. figure 7.5) that the maximal amplitude of the peak in the particle production spectrum is reached like $\sim (1 - e^{-2\Gamma T})$. Times T, which are of order of $1/\Gamma$ can be uniquely determined, but for very long times the uniqueness gets lost.

7.2.3 Slow continuous switching processes

The most complicated are slow continuous switch on/off processes, during which the wave packet decays continuously and contributes to the particle production spectrum at many positions, corresponding to the moving position of the resonance. Here, there is no doubt that the wave packet decays hence the overcriticality is proved, but it is by no means obvious how to deduce the time-dependence of the potential (figure 7.6). In the following section we propose an approximative method to deal with this problem.

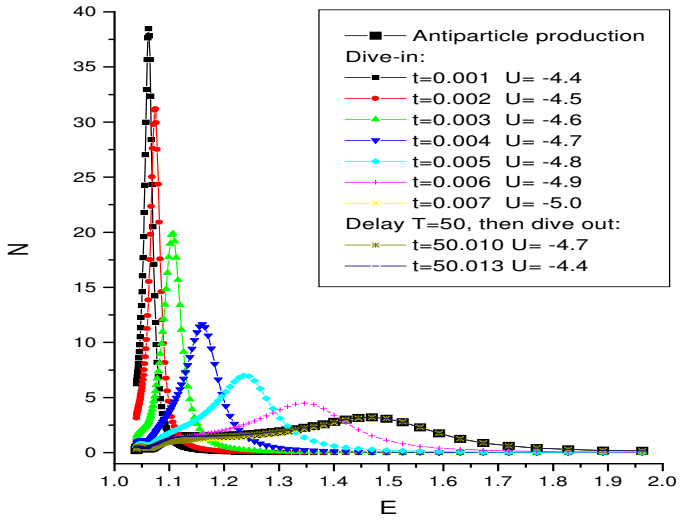


Figure 7.4: Quick switch on-off process with overcritical delay $T = 50$: the amplitude of the wave packet representing the dived bound state at several time instants: 1-7 diving in, 8-9 diving out after the delay and decay (peak shape remains constant) and the antiparticle production, which is identical with the decayed peak's shape (red filled squares).

7.3 Master equation

Using time-dependent perturbation theory one can try to predict the particle production spectra, but this is not easy, as discussed in [MRG83] and references therein. Alternatively, one can try to find analytical results in some limiting situations, like very quick processes considered in [BM98]. But we want to concentrate on the contribution to the particle production spectrum from the dynamically decaying resonance in an overcritical potential.

7.3.1 Particle production from the position of the resonance

The approximation technique, which we want to develop in this section, bases on the observation of the decay of a wave packet in continuum. A decay is possible because the wave packet is spread over a range of energies, or more exactly, over a set of continuum wave functions being generalized eigenvectors to different eigenvalues (energies). These energies act as frequencies in a free evolution so that every component changes its complex phase in a different rate. Just the dephasing of all components leads to the decay – the wave packet stays localized in energy, but disperses spatially and therefore projected on its initial value gives a number smaller than one. It can be shown that a Lorentz-type peak with a half-width Γ

$$\phi_R = \int a_E \phi_E \, dE = \int \frac{\sqrt{\Gamma}}{\sqrt{\pi}\sqrt{(E-E_R)^2+\Gamma^2}} \phi_E \, dE \tag{7.3.1}$$

decays exponentially in free evolution

$$a_R(t) \equiv \langle \phi_E | e^{-iHt} \phi_R \rangle = e^{(-iE_R - \Gamma)t}, \tag{7.3.2}$$

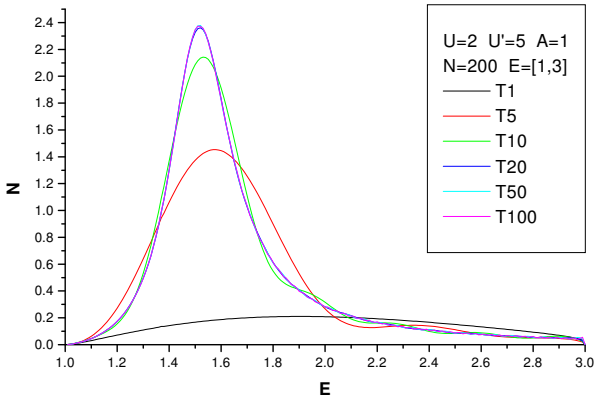


Figure 7.5: Switch on-off: weakly subcritical → strongly overcritical. Antiparticle production spectra for different duration times T of the switched on potential U'.

or

$$|a_R(t)|^2 = e^{-2\Gamma t}. \tag{7.3.3}$$

In other words, the part of the wave packet with the amplitude $|a_R(t)| < 1$ still corresponds to the initial wave packet and forms a spatially localized part of the wave function, while the rest corresponds to the spatially spread out function of vanishing amplitude. Yet, it is still well localized in the energy spectrum and will stay localized forever, giving rise to the particle creation spectrum (because it is just this part of the wave packet, which gets trapped in the continuum). For a time-dependent Hamiltonian, when the resonance moves, one can approximately assume that only the non-decayed ($\sim |a_R(t)|$) part of the wave packet will follow the resonance, while the decayed part remains untouched in the continuum and does not interact (one can argue that after dephasing or decoherence the part of the wave packet behaves "classically" showing no more interference). We suggest a simplified picture (cf. figure 7.7) that the wave packet during evolution in a time-dependent Hamiltonian partially follows the resonance shape and partially decays, and the part which has decayed immediately decouples from the system only contributing to the final particle production spectrum.

The technique of the approximation bases on two relations: first describes the contribution of the decaying wave packet to the particle production spectrum and second describes the loss of amplitude of the wave packet which follows a moving (time-dependent) resonance. The above argumentation leads to the following equation

$$dN(E,t) = -d|a_R(t)|^2 f^2(E, E_R(t), \Gamma(t)), \tag{7.3.4}$$

where $N(E,t)$ is the sum of contributions to the distribution of produced particles until time t and

$$f(E, E_R(t), \Gamma(t)) \equiv \frac{\sqrt{\Gamma}}{\sqrt{\pi}\sqrt{(E-E_R)^2+\Gamma^2}} \tag{7.3.5}$$

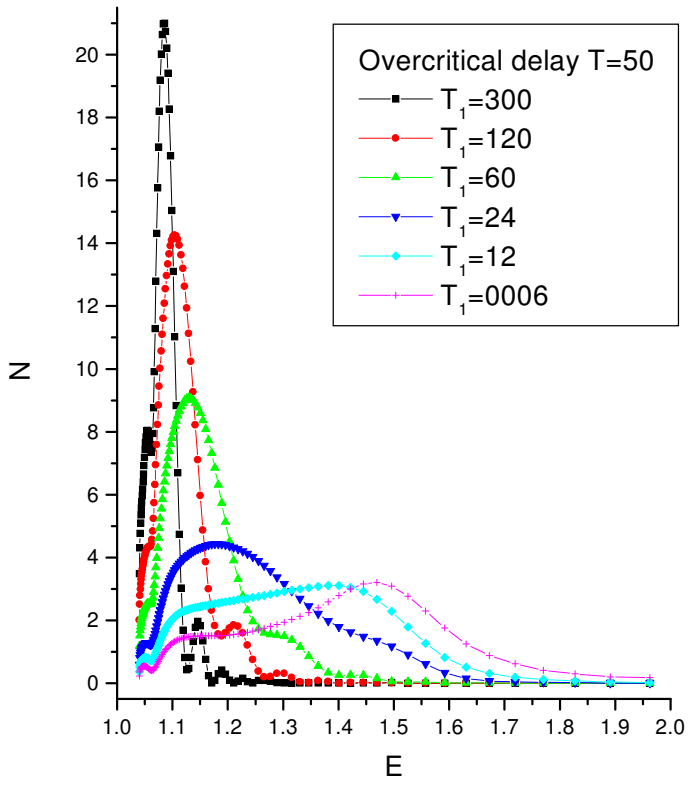


Figure 7.6: Slow switch on-off process with overcritical delay $T = 50$: antiparticle production spectra for different time rates of the switch on and switch off phase. The slower is the switch phase the earlier (shifted to lower energies) decays the wave packet representing the dived bound state.

is the idealized shape of a resonance. This equation can be integrated over time

$$N(E,t) = -\int_{t_0}^{t} \frac{d|a_R(t)|^2}{dt} f^2(E, E_R(t), \Gamma(t))\ dt, \tag{7.3.6}$$

assuming initially $N(E,t_0) = 0$. Following the technique presented in the proof of adiabatic theorem (section 4.5) we assume (what however does not have to be true for resonances) that the evolution of a wave packet splits into decay and follow of the resonance position. Therefore we assume that the resonance decays at every instant of time as if it were evolving freely, i.e.

$$\frac{d\ |a_R(t)|^2}{dt} = -2\ \Gamma(t)\ |a_R(t)|^2. \tag{7.3.7}$$

Now, this equation can be inserted into the previous one and we obtain

$$N(E,t) = \int_{t_0}^{t} 2\ \Gamma(t)\ |a_R(t)|^2 f^2(E, E_R(t), \Gamma(t))\ dt. \tag{7.3.8}$$

The last two equations form a closed system, if the parameters of the resonance $E_R(t), \Gamma(t)$ are known. They depend uniquely on the potential $U(t)$, whose dependence on time remains the last free parameter in the system. Its solution, the final particle production

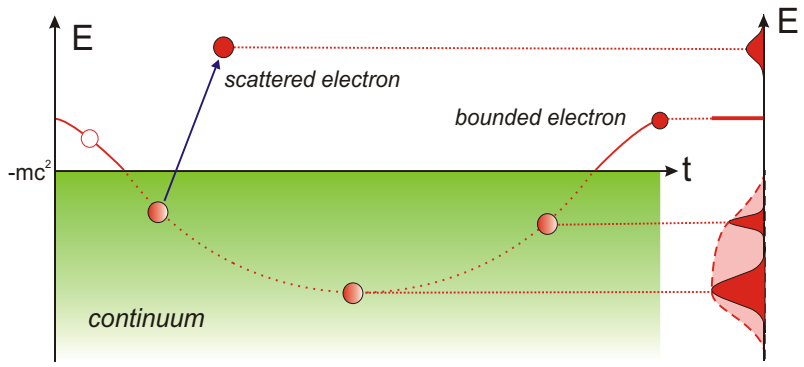


Figure 7.7: Decay of the wave packet in the negative continuum following the position of the resonance and contributing to the spectrum of created antiparticles.

spectrum $N(E, t_1)$ is to be compared with the exact particle production. When the approximation woks well, the time-dependent position of the resonance or the time-dependence of the potential can be found by a simple fitting.

For extremely narrow peaks a further approximation can be made. When $\Gamma \approx 0$ then

$$f(E, E_R, \Gamma) \approx \delta(E_R - E) \tag{7.3.9}$$

and

$$N(E,t) = \int_{t_0}^{t} 2\ \Gamma(t)\ |a_R(t)|^2 f^2(E, E_R(t), \Gamma(t))\ dt = \sum_{\substack{t_0 \le t_i \le t: \\ E_R(t_i)=E}} \frac{2\ \Gamma(t_i)\ |a_R(t_i)|^2}{|E_R'(t_i)|} \tag{7.3.10}$$

Knowing $E_R(t)$ and $\Gamma(t)$ the particle production $N(E, t_1)$ can be calculated analytically. By the same, the inverse problem can be solved analytically.

7.3.2 Square well potential

We apply this technique to the time-dependent square well potential considered in the previous chapter. We consider decay of a wave packet during a continuous switch on process from $U_1 = 4.40$ to $U_2 = 5$ at different time-rates, after which a long delay phase occurs with $T_0 = 50$. We consider switch times in the range from $T = 0.006$ to $T = 60$. The results, "exact" numerically calculated particle production spectra and approximated by the presently discussed method, are shown on figure 7.8.

We see a quite good agreement for the intermediate values $T = 12, 24$, but some discrepancy for very quick as well as for very slow switch on processes. Unfortunately, these are regimes, where we are not certain that the "exact" spectra are correct. For extremely slow processes there appear big numerical errors due to slowly evolving (and decaying) very narrow peaks near the continuum's edge. On the contrary, for very quick processes, the wave packet is transported far from the edge, but this transport occurs in many numerical steps during which small errors add up. Finally, the numerical uncertainty does not allow us to draw conclusions in these extreme situations, and actually did not allow us to work

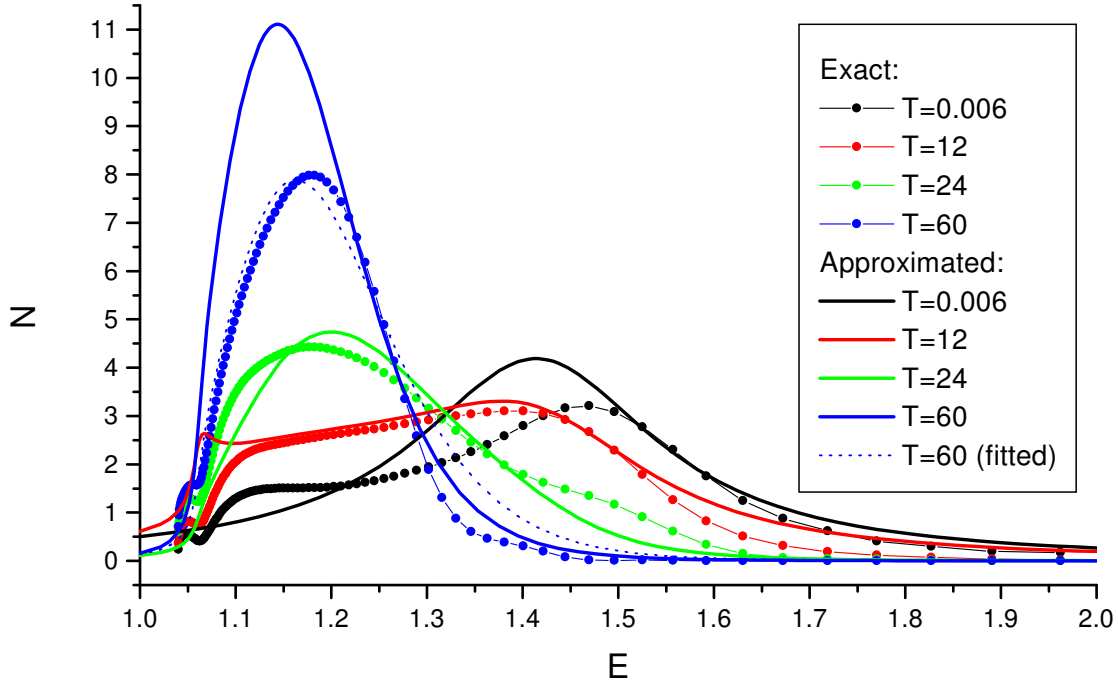


Figure 7.8: "Exact" numerically calculated particle production spectra and approximated by the presently discussed method.

further on this method until the full numerical code does not reach a better precision. Only to show the flexibility of this technique we have fitted a different amplitude time-development $|a_R(t)|$ in order to match the given particle production spectrum for $T = 60$. By a simple modification in the decay rate (which can be further improved) we have obtained quite good agreement (dotted blue line on figure 7.8). It seems that for nearly any particle production spectrum there exists a function $|a_R(t)|$ such that the generated $N(E, t_1)$ approximates the given spectrum. The question how good this approximation is open and worth further work, because its numerical simplicity and possibility of application to the inverse problem are very tempting.

"Das Problem zu erkennen ist wichtiger, als die Lösung zu erkennen,
denn die genaue Darstellung des Problems führt zur Lösung."
A. Einstein

Chapter 8

Conclusions

We solve a longstanding open problem of definition and existence of the spontaneous particle creation. We accept the demand (Scharf *et al.*) that the definition of the effect must be formulated in Fock space as well as that the information on particle creation is contained in the structure of the implemented scattering operator $\hat{S}$. Hence, we treat it as a part of the definition and a necessary condition. However, we show that the change in the structure of $\hat{S}$ does not have to lead to stable, observable effects. On the other hand, we show that the condition (Greiner *et al.*) for a classical Dirac Hamiltonian having of a bound state dived into the continuum is a necessary condition for the existence of stable, physically observable spontaneous particle creation.

In order to treat this problem rigorously, we carefully develop the theory of QED in external fields. In particular, we implement in Fock space and discuss for the first time the evolution of time-dependent Hamiltonians with unequal initial and final external fields, what is necessary to understand spontaneous creation of a single (anti-)particle.

We show that the spontaneous particle creation exists only in a weaker sense (defined in section 4.5), i.e. overcritical fields lead to a vacuum decay and spontaneous particle creation, but there are no processes in which one can observe exclusively the spontaneous antiparticle with the energy corresponding to the resonance position in the overcritical field. Either there are other particles created confusing the picture (dynamical pairs in quick processes) or the spontaneous antiparticle does not fit to the parameters of the resonance (much smaller momentum and kinetic energy) independent on the strength of the overcritical field and position of the resonance (adiabatic limit).

Moreover, we demonstrate numerically how a wave packet in the negative continuum representing the dived bound state in presence of an overcritical potential partially follows a moving resonance and partially decays continuously during the whole overcritical period, what in general results in an antiparticle production spectrum distributed over all positions of the resonance during the overcritical phase. The slower the overcritical potential varies the more intensive the continuous decay is. In contrast, the quicker the overcritical potential varies the more accurately the peak follows the position of the resonance.

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Publications - Articles & Conference contribiutions

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- "'Spontaneous pair creation' in strong electric fields of Highly Charged Ions", NIMB, Vol: 205, May, 2003, pp: 30-35
- "Spontaneous emission of light from atoms: the model" with P. Marecki - Ann. d. Phys. 14 (No. 7), pp. 428-437 (2005); quant-ph/0407186
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- Contributed talk presented at the International Conference of Physics Students (ICPS), Helsinki, 1999:
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- My Master Thesis (Jagellonian University Cracow, Poland, 1999):
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- Invited talk presented at the International Conference on "Informatics Systems", Bielsko-Biala (Poland), 1999:
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Spontaneous emission of light in atoms:

- "Spontaneous emission of light from atoms: the model" with P. Marecki - Ann. d. Phys. 14 (No. 7), pp. 428-437 (2005); quant-ph/0407186

Spectral decompositon of the gravitational radiation:

- Invited talk at the Institute of Physics, General Relativity Department, Jagellonian University, Cracow (Poland), October 2003
  "Rozklad rozwiazan rownan falowych z potencjalem na mody quasi-normalne" (in polish)

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