

Reformulation of Bohmian mechanics

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ZUSAMMENFASSUNG

Die Bohmsche Mechanik hat seit ihrer Einführung durch David Bohm im Jahr 1952 die Entwicklung leistungsfähiger Simulationsmethoden zur Lösung komplizierter quantenmechanischer Probleme inspiriert. Trotz seiner Vorteile stand dieser Ansatz auch im Zentrum von Kontroversen, die bis ins Jahr 1952 zurückreichen und bis heute anhalten.

Der Ursprung der Diskreditierung von Bohms Ansatz rührt von der Kritik her, die Heisenberg und Pauli im selben Jahr erhoben, als Bohm seine beiden berühmten Arbeiten über die Theorie der verborgenen Variablen (heutzutage als Bohmsche Mechanik bekannt) veröffentlichte. Heisenberg und Pauli wiesen unabhängig voneinander auf die mangelnde Symmetrie des von Bohm vorgeschlagenen Modells hin. In der Tat beschränkt sich die Bohmsche Mechanik allein auf die Behandlung jeglicher Probleme im Konfigurationsraum. Das bedeutet, dass, zusätzlich zu den prinzipiellen Problemen des Trajektorienkonzepts, die Theorie selbst einer Darstellung eine bevorzugte Rolle einräumt. Dies steht im Widerspruch zu den konzeptuellen Säulen der Quantenmechanik: Wie in der linearen Algebra gibt es keine bevorzugte Basis; die Beschreibung von Quantensystemen darf nicht an eine bestimmte Darstellung gebunden sein, hingegen kann die Wahl einer solchen die Berechnungen erleichtern. In diesem Sinne ist beispielsweise die fehlende Formulierung der Bohmschen Mechanik im Impulsraum ein schwerwiegender konzeptioneller Nachteil. Wegen der andererseits ansprechenden Idee einer kausalen Interpretation der Quantenmechanik führte dies schon gleich nach der Veröffentlichung von Bohms Arbeiten zu einer Polarisierung der „Scientific Community“. Daher gab es seitdem Versuche, die Bohmsche Mechanik zumindest im Impulsraum zu formulieren. Das Hauptproblem bei diesen liegt darin, dass sie auf der Einführung von ad hoc definierten Operatoren oder der Wahl spezieller Zustände basieren.

Als weiterer Punkt kommt hinzu, dass bei der Behandlung atomarer Phänomene das lokale Konzept der Trajektorie bereits aufgegeben wurde, als Schrödinger 1926 seine bahnbrechenden Arbeiten veröffentlichte. Eines der unmittelbaren Probleme beim Konzept von Trajektorien ist die Implikation der Instabilität von Atomen, was aber experimentell nicht beobachtet wird. Daher ist die Zurückhaltung der Wissenschaftler, einen alternativen Ansatz, der auf dem Konzept von Trajektorien basiert zu akzeptieren, verständlich. Ferner wurde

schon frühzeitig darauf hingewiesen, dass es bedeutungslos sei zu sagen, dass die Trajektorien das Problem lösen können, wenn diese zunächst die Kenntnis der Wellenfunktion erfordern, die ihrerseits bereits die Lösung des Problems darstellt. Darüber hinaus gab es keine neuen Vorhersagen, die die konventionelle Theorie nicht auch machen konnte. Das Konzept der Trajektorien schien daher in jener Zeit eher dekorativ als praktisch zu sein.

Ein dritter Nachteil der Bohmschen Theorie ist die eigentliche Einführung neuer Postulate. Eines davon ist die Existenz eines surrealen Objekts, das auch als Bohmsche Trajektorie bekannt ist. Was die anderen Postulate betrifft, so wären die Gleichgewichtshypothese und die „Bewegungsgleichung“ (guidance law) für die Trajektorien zu nennen. Erstere besagt, dass die lokale Dichte von Trajektorien als die Meßwahrscheinlichkeit für das Auffinden des atomaren Systems in der Nähe des Punktes interpretiert werden muß. Letztere legt andererseits fest, dass das Geschwindigkeitsfeld der Trajektorien ein rotationsfreies Feld ist, dessen Potential mit der Phase der komplexen Wellenfunktion übereinstimmt. Das Problem der zusätzlichen Postulate ist deren Begründung. In der Tat wurden die Postulate der konventionellen Quantenmechanik durch die zahlreichen experimentellen Befunden an atomaren Systemen inspiriert; man könnte den Formalismus als positivistisch einordnen. Andererseits wurden die Bohmschen Postulate, wie Bohm selbst in seinem ersten Artikel von 1952 feststellt, in der Hoffnung eingeführt, dass letztendlich der technologische Fortschritt den Nachweis der postulierten Trajektorien ermöglichen und diese dadurch rechtfertigen würde.

„Letztendlich wurden jedoch Effekte gefunden, die den Vorhersagen widersprachen, die durch Extrapolation bestimmter rein makrophysikalischer Theorien in den Bereich des sehr Kleinen erhalten wurden und die unter der Annahme, dass Materie aus Atomen besteht, richtig verstanden werden konnten. In ähnlicher Weise schlagen wir vor, dass, wenn verborgene Variable der vorliegenden Quantentheorie zugrunde liegen, diese höchstwahrscheinlich im atomaren Bereich zu Effekten führen werden, die auch mit den üblichen quantenmechanischen Konzepten angemessen beschrieben werden können.“

Bis zu diesem Punkt sind die drei Hauptnachteile der Bohmschen Theorie im Wesentlichen: die Asymmetrie der Formulierung bezüglich Orts- und Impulsdarstellung, die Interpretation der Trajektorien und die Notwendigkeit zusätzlicher Postulate. Bezüglich des ersten Kritikpunkts lieferten Heisenberg und Pauli 1952 eine fundierte Argumentation. Die Interpretation von Trajektorien als lokale Beschreibung atomarer Systeme wurde 1976 mittels des optischen Experiments von A. Aspect durch die Verletzung der Bellschen

Ungleichung als falsch erwiesen. Der Aspekt betreffend die Konsistenz der zusätzlichen Postulate wurde ebenfalls in einem Experiment von M. O. Scully im Jahr 1998 mit einer Stern-Gerlach-Apparatur in Kombination mit einem optischen Hohlraum analysiert. Er zeigte, dass die Bohmschen Trajektorien (als reelle Teilchenpfade interpretiert) im oben genannten Experiment falsche Vorhersagen liefern würden. Diese dynamische Kontroverse um die Bohmsche Mechanik scheint bereits beigelegt zu sein. Dennoch ist es erwähnenswert, dass die oben erwähnten Experimente die Interpretation der Bohmschen Trajektorien als Teilchenpfade verworfen, aber nicht deren Verwendung. Daher besteht immer noch die Notwendigkeit, eine korrekte physikalische Interpretation für diese Trajektorien zu finden. Trotzdem gibt es immer noch ein loses Ende in der Geschichte. Trotz der schwerwiegenden Nachteile der Bohmschen Formulierung liefert sie dennoch ein funktionierendes Werkzeug für Simulationen in der Quantenmechanik, die ansonsten übermäßig zeitaufwändig wären. Daher ist die Bohmsche Mechanik gegenwärtig zwar eine schlecht definierte Theorie, aber ein leistungsfähiges Rechenwerkzeug. Es besteht somit ein begründetes Interesse daran, diese Diskrepanz aufzuklären und den Bohmschen Formalismus aus der Perspektive der konventionellen Theorie neu zu formulieren, überflüssige Postulate zu vermeiden und gerade die angemessene mathematische Behandlung zu finden.

In diesem Zusammenhang will diese Arbeit einen vermittelnden Standpunkt zwischen der Bohmschen Mechanik und der konventionellen Quantenmechanik einnehmen, erstere ausgehend von letzterer neu formulieren und ihr ihren angemessenen Platz im quantenmechanischen Formalismus, ohne zusätzliche Postulate, Interpretationen oder philosophische Argumente zuordnen. Zu diesem Zweck basiert diese Arbeit auf drei Grundpfeilern: eine von der gewählten Darstellung unabhängige Formulierung, eine rationale Kritik der Bohmschen Trajektorie und nicht zuletzt die Struktur der lokalen Transportgleichungen, die den Bohmschen Trajektorien zugeordnet sind.

Kapitel 2 dient der Neuformulierung der Bohmschen Mechanik. In Abschnitt 2.1 wird gezeigt, dass die Kontroverse über die Formulierung der Bohmschen Mechanik in der Impulsdarstellung immer noch von Interesse ist; siehe Tabelle 2.2 für die mit der Kontroverse verbundenen Argumente. In Abschnitt 2.2 werden mittels der Polardarstellung (2.6) der Wellenfunktion gemäß der Vorschrift (2.9) komplexen Bohmsche Größen wie Ort, Impuls, kinetische und potenzielle Energien für die Orts- (2.12-2.15) und Impulsdarstellung (2.22-2.25) definiert. Die bemerkenswerteste Eigenschaft der Bohmschen Größen ist, dass sie in allgemeinen komplex sind. Eine Ausnahme betrifft Ort und Impuls, diese sind in ihren jeweiligen Darstellungen reelle

Großen, ansonsten aber auch komplex. Ferner enthalten quadratische Größen wie kinetische und potenzielle Energien nicht nur die Quadrate von Real- und Imaginärteil der entsprechenden komplexen Größen, sondern auch einen zusätzlichen imaginären Beitrag, der die ursprünglichen Real- und Imaginärteile koppelt.

Vorteile durch die Verwendung der Bohmschen Formulierung in der Impulsdarstellung werden anhand eines linearen Potentials für stationäre Zustände illustriert. Arbeitet man im Ortsraum ergibt sich die Schwierigkeit bei der Lösung eines Problems aus der quadratischen Struktur der kinetischen Energie und des daraus resultierenden Quantenbeitrags in der modifizierten Hamilton--Jacobi-Gleichung. Verwendet man hingegen die in dieser Arbeit eingeführte Formulierung der Bohmschen Mechanik im Impulsraum, resultiert der Quantenbeitrag aus den quadratischen Termen des Potentials. Beim linearen Potential gibt es aber gar keinen quadratischen Beitrag. Dies bedeutet, dass die Komplikation infolge des Quantenbeitrags in der Impulsdarstellung der Bohmschen Methode gar nicht auftritt.

In Abschnitt 2.3 wird festgestellt, dass selbst wenn die modifizierte Hamilton--Jacobi-Gleichung in der Bohmschen Mechanik eine Hamiltonsche Struktur nahelegt, diese aufgrund des Fehlens kanonisch konjugierter Variablen jedoch nicht vorliegt. Dennoch ähneln die komplexen dynamischen Gleichungen den Newtonschen Gegenstücken, siehe zum Beispiel (2.60-2.62) für die Orts- und (2.70-2.72) für die Impulsdarstellung. Ferner erweisen sich diese Gleichungen als nützlich beim Auffinden von Konstanten der Bewegung, wie z.B. der Ermakov Invarianten für zeitabhängige Zustände wie die generalisierten kohärenten Zustände.

In Abschnitt 2.4 erweist es sich, dass das Quantenpotential, im Rahmen der in dieser Arbeit eingeführten Formulierung, mit dem Quantenbeiträgen zur Orts- und Impulsbestimmtheit zusammenhängt, siehe (2.159-2.160) und (2.162-2.163). In der Tat erlaubt die vorgeschlagene Formulierung des Bohmschen Ansatzes die Unbestimmtheiten in zwei Arten von Beiträgen zu trennen, wobei einer von den klassischen Größen herrührt, während der andere seinen Ursprung im sogenannten „Quantenpotential“ hat. In diesem Sinne macht die vorgeschlagene Formulierung deutlich, dass das Quantenpotential, auch wenn der Begriff es nahelegt, kein Potential ist, sondern ein kinetischer Term, der sich aus den Unbestimmtheiten ergibt, die den klassisch konjugierten Variablen zugeordnet sind. Außerdem ist es nun möglich, das Heisenbergsche Unbestimmtheitsprodukt in der Form (2.164) darzustellen, da nun die Orts- und

Impulsversionen der Bohmschen Mechanik vorliegen. Dies wird am Beispiel der generalisierten kohärenten Zustände demonstriert.

Kapitel 3 befasst sich mit einer Neudefinition und Neuinterpretation der Bohmschen Trajektorien. Zu diesem Zweck wird in Abschnitt 3.1 auf die Unzulänglichkeit der zusätzlichen Postulate bei der Definition und Einführung der Bohmschen Trajektorien hingewiesen. Insbesondere ist die mathematische (und physikalische) Begründung des „Führungsgesetzes“ (guidance law) (3.4) inkonsistent.

In Abschnitt 3.2 werden Bohmsche Trajektorien ohne zusätzliche Postulate hergeleitet. Dies ist das Ergebnis einer spezifischen Parametrisierung der jeweiligen Kontinuitätsgleichungen, im Fall des Ortsraums durch (3.19) mit der Definition (3.23) der zugehörigen Bohmfunktion und im Impulsraum durch (3.49) mit der Bohmfunktion (3.48).

Dies wird durch die Verwendung eines einfachen thermodynamischen Verfahrens erreicht, das Maxwell-Beziehungen beinhaltet (siehe Kasten 3.2.1). Davon ausgehend werden nach Durchführung eines Linienintegrals im (x,t) -Raum die für die Bohmschen Trajektorien charakteristische Nichtkreuzungsregel und die Erhaltung der Wahrscheinlichkeit bewiesen. Dies deutet natürlich darauf hin, Bohmsche Trajektorien, nicht wie allgemein angenommen wird, als (reale) Pfade zu interpretieren, sondern als Begrenzung von „Wahrscheinlichkeitsbahnen“. Diese Idee wird mit Hilfe generalisierter kohärenter Zustände veranschaulicht. Es wird auch vorgeschlagen, dass dies die Grenzen der Anwendbarkeit der Bohmschen Mechanik einschränkt. Diese Interpretation zeigt, dass die Stärke der Trajektorien in deskriptiver Statistik liegt, d.h. in der Bestimmung von Perzentilbereichen. Dies bedeutet, dass die Verwendung von Trajektorien bei all jenen Problem angeraten ist, bei denen man daran interessiert ist, wie die Nachweiswahrscheinlichkeit in einem bestimmten Gebiet verteilt ist, wie z.B. bei Tunnel- oder Streuproblemen. Ist das Ziel jedoch die Berechnung von Mittelwerten (oder höheren Momenten), ist die Bohmsche Mechanik recht umständlich, und generell die Anwendung des konventionellen Formalismus ratsam.

In Abschnitt 3.3 wird ein Zusammenhang zwischen konventioneller Quantenmechanik und Bohmscher Mechanik durch den Wignerformalismus gefunden. Der Bohmsche Formalismus kann als projizierter Aspekt der Wignerfunktion betrachtet werden, siehe z.B. (3.75) und (3.76). Dies bekräftigt die in Kapitel 2 eingeführte Idee komplexer Bohmscher Größen, da sie

Projektionen von Observablen auf eine kontinuierliche Darstellung repräsentieren.

In Abschnitt 3.4 wird die neue Interpretation angewandt, um eine Ionenfalle, charakterisiert durch einen parametrischen Oszillator mit der Frequenz $1/(at+b)$, zu analysieren. Im Gegensatz zu den üblichen Frequenzen bei Ionenfallen ist diese offensichtlich aperiodisch, aber dennoch kann dank der neuen Interpretation und Anwendung Bohmscher Trajektorien gezeigt werden, dass eine solche Falle zum Einfang eines Systems für Zeitintervalle in einer Größenordnung von Mikrosekunden nützlich wäre. Wenn längere „Trappingzeiten“ benötigt werden, ist diese Frequenz natürlich nicht adäquat. Immerhin kann die „Trappingzeit“ durch Veränderung des Parameters dieses Oszillators variiert werden (siehe Abbildungen 3.6-3.8).

Als dritter Aspekt wird in Kapitel 4 eine systematische Behandlung der hydrodynamischen Betrachtungsweise der Bohmschen Mechanik vorgestellt. In Abschnitt 4.1 wird das Fehlen konsistenter hydrodynamischer Gleichungen für die Orts- und Impulsdarstellung zusammengefasst. Die lokalen Bohmschen Gleichungen für Impuls und Energie besitzen nicht die Struktur von Transportgleichungen.

In Abschnitt 4.2 werden die komplexen hydrodynamischen Gleichungen erhalten. Im Gegensatz zu dem, was in der aktuellen Literatur zu finden ist, haben sie alle dieselbe Struktur: es sind Transportgleichungen. Man muß jedoch vorsichtig sein hinsichtlich Spekulationen über mögliche Transportphänomene, da die involvierten Größen nicht reelle sondern komplexe sind (für die Ortsdarstellung siehe (4.26) für die Impulsdarstellung (4.83)).

Mit all den oben genannten Resultaten versucht diese Arbeit die losen Enden der Bohmschen Mechanik zu verknüpfen, sodass sie als echt kompatibler und wertvoller Teil der konventionellen quantenmechanischen Theorie betrachtet werden kann.

SUMMARY

Since its introduction by David Bohm in 1952, Bohmian mechanics has inspired the development of performant simulation methods for solving complicated quantum mechanical problems. Despite its benefits though, this approach has also been at the center of a controversy that dates back to 1952 and continues to the present day.

The origin of the discrediting of Bohm's proposal originates from the criticism Heisenberg and Pauli made in the same year Bohm published his two famous papers on the theory of hidden variables (nowadays known as Bohmian mechanics). Heisenberg and Pauli independently pointed out the lack of symmetry in the proposed scheme by Bohm. Indeed, Bohmian mechanics is limited to the treatment of any problem in the configuration space. This means that, in addition to the fundamental problems of the trajectory concept, the theory itself gives a preferential role to the coordinate representation. This contradicts the conceptual pillars of quantum mechanics: Likewise in linear algebra, there is no preferred basis; the description of quantum systems must not be tied to a specific representation, however the choice of such a representation can facilitate the calculations. In this sense, for example, the lack of a formulation of Bohmian mechanics in momentum space is a serious conceptual disadvantage. On the other hand, because of the appealing idea of a causal interpretation of quantum mechanics, this led to a polarization of the scientific community immediately after the publication of Bohm's papers. Therefore, since then there have been attempts to formulate Bohmian mechanics at least in momentum space. The main problem with these is that they are based on the introduction of ad hoc defined operators or the choice of special states.

Another point is that in the treatment of atomic phenomena, the local concept of the trajectory had already been abandoned when Schrödinger published his pioneering papers in 1926. One of the immediate problems with the concept of trajectories is the implication of the instability of the atom, which is not observed experimentally. Hence the reluctance of scientists to accept an alternative approach based on the concept of trajectories is understandable. Furthermore,

it was pointed out early on that it is meaningless to say that the trajectories can solve the problem if they first require the knowledge of the wavefunction, which in turn already represents the solution to the problem. Furthermore, there were no new predictions that the conventional theory could not also make. The concept of trajectories therefore seemed more ornamental than practical at the time.

A third disadvantage of the Bohmian theory is the actual introduction of new postulates. One of them is the existence of a surreal object, also known as Bohmian trajectory. As far as the other postulates are concerned, the equilibrium hypothesis and the guidance law for the trajectories should be mentioned. The former states that the local density of trajectories must be interpreted as the detection probability for finding the atomic system in the vicinity of the point. The latter, on the other hand, establishes that the velocity field of the trajectories is an irrotational field whose potential corresponds to the phase of the complex wavefunction. The problem with the additional postulates is their justification. Indeed, the postulates of conventional quantum mechanics were inspired by the abundant experimental results on atomic systems; one could classify the formalism as positivistic; on the other hand, as Bohm himself states in his first article from 1952, the Bohmian postulates were introduced in the hope that in the end technological progress would make it possible to prove the existence of the postulated trajectories and thereby justify them:

“Ultimately, however, effects were found which contradicted the predictions obtained by extrapolating certain purely macrophysical theories to the domain of the very small, and which could be understood correctly in terms of the assumption that matter is composed of atoms. Similarly, we suggest that if there are hidden variables underlying the present quantum theory, it is quite likely that in the atomic domain, they will lead to effects that can also be described adequately in the terms of the usual quantum-mechanical concepts”.

Up to this point, the three main disadvantages of the Bohmian theory are essentially: the asymmetry of the formulation with regard to position and momentum representation, the interpretation of the trajectories and the need for additional postulates. Concerning the first point of criticism, Heisenberg and Pauli provided sound arguments in 1952. The interpretation of trajectories as a local description of atomic systems was proven wrong in 1976 by means of the optical experiment of A. Aspect by violating Bell's inequality. The aspect concerning the consistency of the additional postulates was also analyzed in an experiment by M. O. Scully in 1998 with a Stern--Gerlach apparatus, in combination with an optical cavity. He showed that the Bohmian trajectories

(when interpreted as real paths of particles) in the above experiment provide false predictions. This dynamic controversy around Bohmian mechanics seems to have already been settled; nevertheless, it is worth noticing that the above-mentioned experiments discarded the interpretation of Bohmian trajectories as paths of particles, but not the use of them. Therefore, there is still a need to find a properly physical interpretation for those trajectories. Even so, there is still a loose end in the story. Despite the serious drawbacks of the Bohmian formulation, it still provides a performant tool for simulations in quantum mechanics that would otherwise be excessively time-consuming. Therefore, currently Bohmian mechanics constitutes an ill-defined theory, but a powerful computational tool. There is therefore a justified interest in clearing up this discrepancy and reformulating the Bohmian framework from the perspective of the conventional theory, avoiding superfluous postulates and precisely finding the appropriate mathematical treatment.

In this context, this thesis aims to take a mediating standpoint between Bohmian mechanics and conventional quantum mechanics, reformulate the former based on the latter and assign it its appropriate place in the quantum mechanical formalism, without additional postulates, interpretations or philosophical arguments. For this purpose, this work is based on three major pillars: a formulation that is independent of the chosen representation, a rational criticism of the Bohmian trajectory and, last but not least, the structure of the local transport equations that are assigned to the Bohmian trajectories.

Chapter 2 serves to reformulate Bohmian mechanics. Section 2.1 shows that the controversy over the formulation of Bohmian mechanics in momentum representation is still of interest; see Table 2.2 for the arguments related to the controversy. In Section 2.2, using the polar decomposition (2.6) of the wave function according to (2.9), complex Bohmian quantities such as position, momentum, kinetic and potential energies for the position (2.12-2.15) and momentum representation (2.22-2.25) are defined. The most remarkable property of these Bohmian quantities is that they are generally complex. One exception concerns the position and momentum, these are real quantities in their respective representations, but otherwise they are also complex. Furthermore, quadratic quantities such as kinetic and potential energies contain not only the squares of the real and imaginary parts of the corresponding complex quantities, but also an additional imaginary contribution that couples the original real and imaginary parts.

Advantages of using the Bohmian formulation in the momentum representation are illustrated using a linear potential for stationary states. Working in position

space, the difficulty in solving a problem arises from the quadratic structure of the kinetic energy and the resulting quantum contribution in the modified Hamilton--Jacobi equation. Using, on the other hand, the Bohmian formulation in momentum space introduced in this work, the quantum contribution originates from the quadratic terms of the potential. For the linear potential, however, there is no quadratic contribution at all. This means that the complication due to the quantum contribution is absent in the momentum representation for the Bohmian framework.

In Section 2.3, it is stated that even if the modified Hamilton--Jacobi equation in Bohmian mechanics suggests a Hamiltonian structure, this is not the case due to the lack of canonically conjugated variables. Nevertheless, the complex dynamical equations are similar to the Newtonian counterparts, see for example (2.60-2.62) for the position and (2.70-2.72) for the momentum representation. Furthermore, these equations prove to be useful in finding constants of motion, such as the Ermakov invariant for time-dependent states like the general coherent states.

In Section 2.4 it turns out that the quantum potential, within the scheme of the formulation introduced in this work, is related to the quantum contribution to the position and momentum uncertainties, see (2.159-2.160) and (2.162-2.163). Indeed, the proposed formulation of Bohm's approach allows the uncertainties to be separated into two types of contributions, one originating from the classical quantities, while the other arises from the so-called "quantum potential". In this sense, the proposed formulation makes it clear that the quantum potential, even if the term suggests it, is not a potential, but a kinetic term that results from the uncertainties associated with the classically conjugated variables. In addition, it is now possible to represent Heisenberg's uncertainty product in the form (2.164) since the position and momentum versions of Bohmian mechanics are now available. This is demonstrated using the example of the general coherent states.

Chapter 3 deals with a redefinition and reinterpretation of the Bohmian trajectories. For this purpose, Section 3.1 points out the inadequacy of the additional postulates in the definition and introduction of the Bohmian trajectories. In particular, the mathematical (and physical) justification of the "guidance law" (3.4) is inconsistent.

In Section 3.2, Bohmian trajectories are derived without additional postulates. This is the result of a specific parametrization of the respective continuity equations, in the case of the position space by (3.19) with the definition (3.23)

of the associated Bohm function and in the momentum space (3.49) with the Bohm function (3.48).

This is achieved through the use of a simple thermodynamic procedure that involves Maxwell relations (see Box 3.2.1). Starting from this, after performing a contour integral in the $(x; t)$ -space, the non-crossing rule, characteristic of Bohmian trajectories, and the conservation of the probability are proven. Of course, this indicates that Bohmian trajectories should not be interpreted as (real) paths, as is generally assumed, but rather as the borders of “probability lanes”. This idea is illustrated using general coherent states. It is also suggested that this limits the applicability of Bohmian mechanics. This interpretation shows that the strength of the trajectories lies in the descriptive statistics, i.e., in the determination of percentile regions. This means that the use of trajectories is advisable for all those problems where one is interested in how the dection probability is distributed in a certain region, such as in tunneling or scattering problems. However, if the goal is to calculate mean values (or higher moments), Bohmian mechanics is rather cumbersome and the use of the conventional formalism is generally advisable.

In Section 3.3 a connection between conventional quantum mechanics and Bohmian mechanics is found through the Wigner formalism. The Bohmian framework can be viewed as a projected aspect of the Wigner function, see e.g. (3.75) and (3.76). This confirms the idea of complex Bohmian quantities introduced in Chapter 2, since they represent projections of observables onto continuous representations.

In Section 3.4 the new interpretation is used to analyze an ion trap, characterized by a parametric oscillator with the frequency $1/(at+b)$. In contrast to usual frequencies for ion traps, this one is obviously aperiodic, but thanks to the new interpretation and the application of Bohmian trajectories it can be shown that such a trap would be useful for trapping a system for time intervals in the range of microseconds. If longer trapping times are required, this frequency is of course not adequate. At least the trapping times can be varied by changing the parameter of this oscillator (see Figures 3.6-3.8).

As a third aspect, a systematic treatment of the hydrodynamic viewpoint of Bohmian mechanics is presented in Chapter 4. Section 4.1 summarizes the lack of consistent hydrodynamical equations for position and momentum representation. The local Bohmian equations for momentum and energy do not have the structure of transport equations.

The complex hydrodynamical equations are obtained in Section 4.2. Contrary to what can be found in the current literature, they all have the same structure: they are transport equations. However, one must be careful with regard to speculations about possible transport phenomena, since the quantities involved are not real but complex (for the position representation see (4.26) and for the momentum representation (4.83)).

With all the above results, this thesis seeks to connect the loose ends of Bohmian mechanics, so that it can be viewed as a genuinely compatible and valuable part of the conventional quantum mechanical theory.

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List of symbols

- m : mass of the system.
- e : electric charge of the electron.
- \hbar : Planck's quantum of action.
- m : mass of the system.
- t : time variable.
- x, p : position and momentum representation variables.
- $\frac{\partial}{\partial t}, \frac{d}{dt}$: partial and total time derivatives.
- u, t', t'' : integration dumm variables.
- $\int dt', \int_0^t dt'$: indefinite integral and definite integral over the time interval $[0, t]$.
- i : imaginary complex number.
- $|\psi(t)\rangle$: quantum state.
- $\Psi(x, t) = \langle x | \psi(t) \rangle$: wave function.
- U, V, S, P, T, n, R : thermodynamic properties; internal energy, volume, entropy, pressure, temperature, mole number, universal gas constant, respectively.
- $\frac{\partial}{\partial x}, \frac{\partial}{\partial p}$: partial derivative with respect to position and momentum.
- $\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial p^2}$: Laplacian with respect to position and momentum.

- a, b, γ, f : generic scalars.
- ρ_x, ρ_p, ρ_a : probability density in configuration, momentum space and a -space .
- j_x, j_p, j_a : probability current in configuration, momentum space and a -space.
- S_x, S_p, S_a : wave function's phase in configuration, momentum space and a -space .
- ε : energy eigenvalue.
- ω : frequency of a (parametric) oscillator.
- E_0 : Strength of the electrostatic field.
- m : mass of the system.
- q, π : Bohmian trajectory in configuration and momentum space.
- v : Bohmian velocity of the trajectories in configuration space.
- $|\cdot|$: magnitude of a complex number.
- Ai : Airy function.
- W : Wigner function.
- B_x, B_p : Bohm function in configuration and momentum space.
- $\eta, \langle p \rangle = m\dot{\eta}$: position and momentum mean value.
- I_{Ermakov} : Ermakov invariant.
- F, F_R, F_I : generic complex Bohmian quantity, and its real and imaginary parts.
- E, E_R, E_I : complex Bohmian energy, and its real and imaginary parts.
- X, X_R, X_I : complex Bohmian position, and its real and imaginary parts.
- P, P_R, P_I : complex Bohmian momentum, and its real and imaginary parts.
- T, T_R, T_I : complex Bohmian kinetic energy, and its real and imaginary parts.
- V, V_R, V_I : complex Bohmian potential energy, and its real and imaginary parts.

- $V_{qu,x}, V_{qu,p}$: Quantum potential in configuration and momentum representation.
- $\sigma_x, \sigma_p; \sigma_{cl,x}, \sigma_{cl,p}$: position and momentum uncertainties; “classical” position and momentum uncertainties.
- $\mathcal{C}, \mathcal{C}_R, \mathcal{C}_I$: complex Riccati variable, and its real and imaginary parts.
- $\alpha = \sqrt{\frac{2m}{\hbar}} \sigma_x$
- \mathcal{C}_p : particular solution of the Riccati equation

Chapter 1

Introduction

Undoubtedly, in quantum mechanics no other topic than Bohmian mechanics has been the reason of so much ink in publications: as criticism to discredit Bohm's proposal, or as an argument in favor of the theory. The reason for such a controversy dates back to 1952, when Bohm claimed that his proposal was a causal alternative to the conventional approach to quantum mechanical phenomena. Nevertheless, in doing so, Bohm had to introduce three postulates; one of which is a surreal object, also known as Bohmian trajectories. Regarding the other postulates, we can take into account the equilibrium hypothesis and the guidance law; both of them basically establish the structure and interpretation of the above mentioned trajectories which cannot be measured. Hence, Bohm's approach violates the quantum paradigm established with the Copenhagen interpretation, *i.e.*, the building blocks of the theory must be related to a feasible measurement. Shortly after the introduction of Bohmian mechanics, the criticisms did not take long to wait for. Indeed, the arguments of Heisenberg and Pauli were sufficient for the community to discredit Bohm's proposal.

Ever since, the Bohmian community has undertaken the task of exploiting the benefits of the Bohmian trajectories to solve numerically complicated quantum problems in a more efficient way than other conventional approaches. With this pragmatic scope for the rehabilitation of Bohm's proposal, the roots of the initial controversy have been ignored though. Indeed, most of the publications of Bohmian supporters since 1952 only restate how reasonable is the introduction of Bohmian trajectories, even though counter experiments have been already presented against the real existence of Bohmian trajectories. The absence of a critical revision of the Bohmian postulates rises the question how is it possible that a powerful simulation tool as Bohmian mechanics results from postulates already proven incorrect?

Regarding this problematic situation, three major flaws can be found in Bohmian mechanics as it is currently formulated. First of all, there is no systematic treatment of other representations than configuration space (this was already pointed out by Heisenberg and Pauli, back in 1952). Second, the Bohmian trajectories are inadequately defined and inconsistently used. Third, the Bohmian hydrodynamic treatment seems to be composed of unrelated dynamical equations.

In this context, this thesis presents a conciliating standpoint of Bohmian mechanics, reformulates it from the conventional quantum mechanical framework, and finds its right place in this formalism, without introducing additional postulates, interpretations or philosophical arguments. To accomplish that goal the thesis is organized around three major pillars: the basic formulation, a rational criticism of the Bohmian trajectory and last but not least, the structure of the local transport equations associated to the Bohmian trajectories is studied.

Chapter 2 starts treating the basic formulation of Bohmian mechanics. In Section 2.1, the controversy of Bohmian mechanics is revisited, regarding its lack of a systematic formulation in other representations. Next, in Section 2.2 new complex Bohmian quantities are defined, what allows the formulation of Bohmian mechanics in any arbitrary continuous representation, for instance, the momentum representation. Concerning Section 2.3, it is shown that contrary to common belief, Bohmian mechanics has no Hamiltonian structure, despite the presence of a modified Hamilton–Jacobi (mHJ) equation. Still it is found that the Bohmian dynamical equations ease the search for new constants of motion like the Ermakov invariant for generalized coherent states. In Section 2.4 it is analysed how to express the Heisenberg principle in Bohmian mechanics, and the possibility to interpret the quantum potential as a quantum contribution to the uncertainties is found as well. Section 2.5 provides a brief summary of the results obtained in this Chapter.

Concerning the second aspect, Chapter 3 deals with a redefinition and reinterpretation of the Bohmian trajectories. For that purpose, in Section 3.1 a brief account of the status quo of the Bohmian trajectories is given. Next, Section 3.2 offers a new definition of the Bohmian trajectories from the handling of the continuity equation, without any need of additional postulates or interpretations. Further, in Section 3.3 it is found that the Wigner formalism is the connection between conventional quantum mechanics and Bohmian mechanics. Bohmian mechanics can be considered as a projective aspect of the Wigner function. Regarding Section 3.4, the proposed definition and interpretation of Bohmian trajectories is illustrated through an ion trap, characterized by a parametric oscillator with a non periodic frequency. In Section 3.5 the results of the Chapter are summarized.

As a third point, Chapter 4 presents a systematic treatment of the hydrodynamic scheme of Bohmian mechanics. In Section 4.1 a brief summary of the transport equations in Bohmian mechanics is given. Next, in Sections 4.2 and 4.3 a unified hydrodynamic treatment is found for Bohmian mechanics in position and momentum representation.

In Chapter 5 conclusions of this thesis are drawn.

Chapter 2

Theoretical framework

Objective

Since its introduction in 1952, Bohmian mechanics [Bohm(1952a), Bohm(1952b)] claims to be a deterministic and self-consistent alternative to the conventional paradigm of quantum mechanics. Nevertheless, shortly after the publication of Bohm's first paper, the scientific community rejected it as an alternative on the same level as the Heisenberg picture or the von Neumann formalism. This was due mainly to the absence of a formulation of Bohmian mechanics in arbitrary representations [Pauli(1952)]; because every result is centered upon the position representation. Apart from this drawback, difficulties appeared when applying the framework even to simple systems that were already solved in the 1920's. Finally, concerning the conceptual field, Bohmian mechanics introduces new postulates that are not based on experimental facts and going against the positivism of quantum mechanics, it assigns an inherent reality to unmeasurable objects, named Bohmian trajectories.

In this chapter it is shown how to circumvent all the criticisms mentioned above by reformulating Bohmian mechanics, not from the rhetorical stand point, but from the conventional framework of quantum mechanics and reveal the link between both formulations, so that Bohmian mechanics can be put in its right place. Therefore, as a start, in Section 2.1 a concise summary of the typical Bohmian mechanics formulation is given. In Section 2.2, it is proven how to extend the Bohmian framework to other representations, for instance, momentum representation, by extending the original idea of David Bohm. Next, in Section 2.3 a complex formulation of Bohmian mechanics is obtained that allows to find dynamical invariants for time-dependent Hamiltonians. This is considered for both, the position and momentum representations. Finally, the important concept of the Heisenberg uncertainty principle is obtained in 2.4, for the Bohmian mechanics approach.

keywords

Quantum state projection, complex Bohmian quantities, Ermakov invariant, Heisenberg uncertainty product, quantum potential.

2.1 Overview

2.1.1 *Conventional Bohmian mechanics*

The realism of the system as an existing object with well defined properties independently of the observer can be traced back to the Newtonian formalism. In the first Scholium of the Principia [Newton(1687)] it is stated: “*Place is a part of space which a body takes up, and, is according to the space, either absolute or relative*”. Namely, the object occupies a well defined place in space independently of the observer and therefrom, the mechanical properties that depend on the position of the system are always simultaneously well defined. Their precise value depends on the relationship between object and observer. All the mechanical information in classical mechanics is contained in the trajectory followed by the object.

Experimentally the position can vary from measurement to measurement, due to experimental uncertainties though; nevertheless, the introduction of statistical tools in mechanics during the XIXth century in metrology and notably in statistical mechanics, related the position of a system to a probability distribution, thereby the other dynamical variables are also described by probability distributions. It is worth noticing that classically, all the probability distributions of the dynamical variables may shrink simultaneously in an indefinite way, leading again to the Newtonian realism even for small sized systems as the molecules in a gas.

During the crisis of physics in the beginning of the XXth century, two approaches for the study of physical systems appear: Relativity does not require that distances are independent to the observer. It is the speed of light that must be taken as an independent quantity though; still every object occupies a well defined place in space-time. Quantum mechanics, on the other hand, states that the measurement performed by the observer on a microscopic system introduces uncontrollable perturbations, such that individual detections cannot be predicted, but only statistical patterns that in turn cannot be simultaneously precise [Bohr(1948)], this is depicted in Figure 2.1. Even if the relativity alters the way of studying the object, quantum mechanics genuinely renounces to the realism of the object. The identity of the object strongly depends on the statistical patterns obtained once a measurement apparatus is used: not every dynamical property can be simultaneously well defined. This is known as the Copenhagen interpretation, which up to date is the conventional paradigm of quantum mechanics.

In this context, the two papers of David Bohm [Bohm(1952a), Bohm(1952b)] challenged the standpoint of the Copenhagen interpretation. He suggested in a

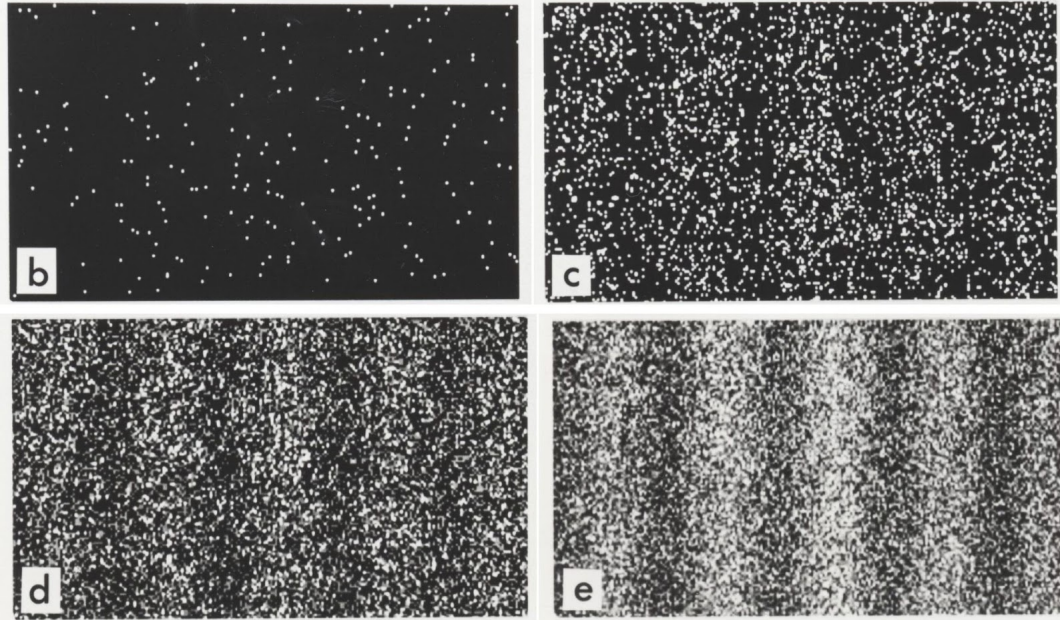


Fig. 2.1 Statistical patterns from single electron detection, once the electron is sent out through a double slit, for (b) 100, (c) 3000, (d) 20000 and (e) 70000 electrons [Tonomura(1989)].

reverse logic, that the assumption of a system with simultaneously well defined properties (hidden variables), at that time, was similar to the proposal of the atomic hypothesis in the XIXth century:

“Now it may be asked why these hidden variables should have so long remained undetected. To answer this question, it is helpful to consider as an analogy the early forms of the atomic theory, in which the existence of atoms was postulated in order to explain certain large-scale effects, such as the laws of chemical combination, the gas laws, etc. On the other hand, these same effects could also be described directly in terms of existing macrophysical concepts (such as pressure, volume, temperature, mass, etc.); and a correct description in these terms did not require any reference to atoms. Ultimately, however, effects were found which contradicted the predictions obtained by extrapolating certain purely macrophysical theories to the domain of the very small, and which could be understood correctly in terms of the assumption that matter is composed of atoms. Similarly, we suggest that if there are hidden variables underlying the present quantum theory, it is quite likely that in the atomic domain, they will lead to

effects that can also be described adequately in the terms of the usual quantum-mechanical concepts; while in a domain associated with much smaller dimensions, such as the level associated with the “fundamental length” of the order of 10^{-13} cm, the hidden variables may lead to completely new sects not consistent with the extrapolation of the present quantum theory down to this level.” [Bohm(1952a)].

He postulated that the subatomic systems: electrons, protons, etc. do possess well defined mechanical properties and therefore, the individual detections are indeed predictable (see Figure 2.2). The name of the paths that he claimed particles would follow are nowadays known as Bohmian trajectories $q = q(t)$. Every hidden variable would depend on those trajectories in analogy to classical mechanics; therefore, Bohmian mechanics, since 1952 was restricted conceptually to the position representation. The main difference with the quantum mechanical approach is that Bohmian mechanics claimed to be able to express any prediction in terms of such trajectories, while quantum mechanics simply expresses the predictions in terms of the experimental preparation of the system, *i.e.*, the quantum state of the system $|\psi(t)\rangle$.

Bohmian mechanics is based on two main postulates (see Box 2.2.1): **the equilibrium hypothesis** states the relationship of the realism of the hidden variables and the statistical outcomes in the experiment; regarding the second postulate, **the guidance law** establishes the structure of the velocity field¹ $v(x, t)$ of Bohmian trajectories.

Box 2.1.1

Guidance law [Holland(1995)]

The particle motion is obtained as solution $q = q(t)$ to the equation,

$$\frac{d}{dt}q(t) \triangleq \frac{1}{m} \frac{\partial}{\partial x} S_x(x, t) \Big|_{x=q(t)}, \quad (2.1)$$

¹ Without loss of generality, one dimensional systems are considered hereafter.

where S_x is the phase of the complex wave function $\psi(x, t)$. To solve this equation it is required to specify the initial condition $q_0 \triangleq q(0)$. This specification constitutes the only extra information introduced by the theory that is not contained in $\psi(x, t)$ (the initial velocity is fixed once we know S). An ensemble of possible motions associated with the same wave is generated by varying q_0 .

Equilibrium hypothesis [Holland(1995)]

The probability that a particle in the ensemble lies between the points x and $x + dx$ at time t is given by

$$\rho_x(x, t)dx \triangleq |\psi(x, t)|^2 dx. \quad (2.2)$$

This postulate has the effect of selecting, from all the possible motions implied by the guidance law (2.1), those that are compatible with an initial distribution $|\psi(x, 0)|^2 dx$.

In this sense, for Bohmian mechanics the wave function is just a convenient way to condense all the information of the hidden variables into a single complex function, as follows:

$$\psi(x, t) = \underbrace{\sqrt{|\psi|^2}}_{\text{spatial density}} \exp \left[\underbrace{\frac{i}{\hbar} S_x}_{\text{velocity field}} \right]. \quad (2.3)$$

The dynamics of Bohmian mechanics is given by a system of coupled differential equations: The **continuity equation** (CE) (2.5) describes the spatial distribution of the Bohmian trajectories, while the **modified Hamilton–Jacobi equation** (mHJE) (2.4) rules the dynamics of the phase S_x , related to the velocity field.

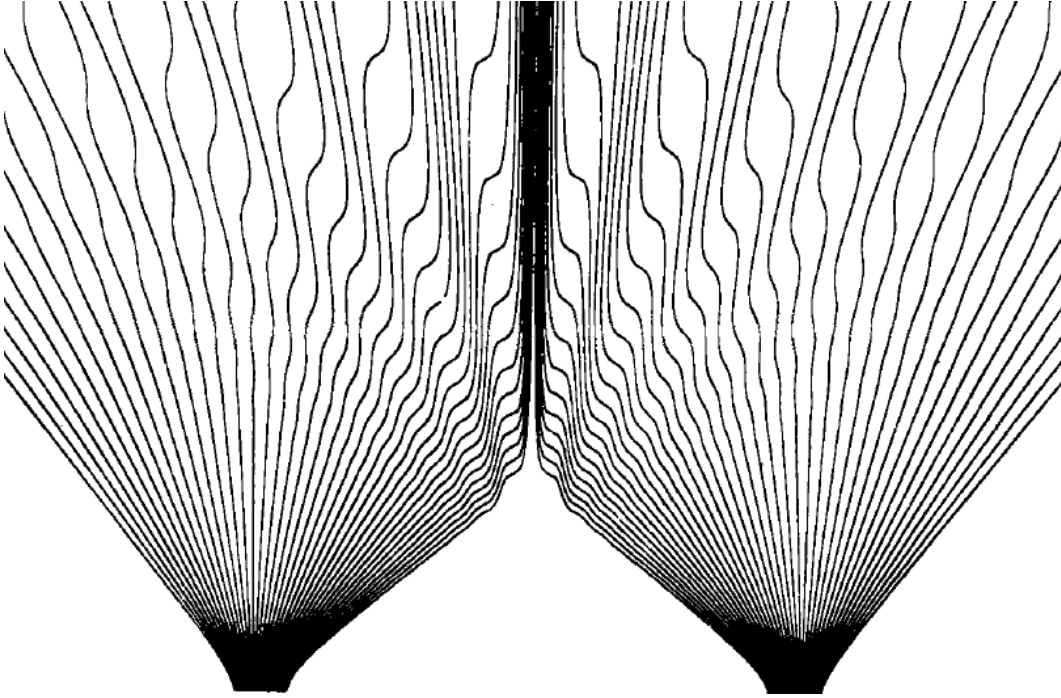


Fig. 2.2 Bohmian trajectories through two Gaussian slits [Philippidis(1979)]. The spatial density ρ is expressed through the shrinking or spreading of the fan of trajectories. The velocity field is related to the local slopes of the trajectories.

$$\frac{\partial}{\partial t} S_x + \frac{(\frac{\partial}{\partial x} S_x)^2}{2m} + V - \underbrace{\hbar^2 \frac{1}{2m} \frac{\frac{\partial^2 \sqrt{\rho_x}}{\partial x^2}}{\sqrt{\rho_x}}}_{\text{quantum contribution}} = 0, \quad (2.4)$$

$$\frac{\partial}{\partial t} \rho_x + \frac{\partial}{\partial x} \cdot \left(\rho_x \frac{\partial}{\partial x} S_x \right) = 0. \quad (2.5)$$

The conceptual core of Bohmian mechanics arises from this system of equations. The CE (2.5) justifies the interpretation of ρ_x as a probability density and $\frac{\partial}{\partial x} S_x$ as the momentum field. The latter being associated to streamlines known as Bohmian trajectories. Regarding equation (2.4), it shows that those streamlines follow a classical-like dynamics (except for the presence of the term $-\hbar^2 \frac{1}{2m} \frac{\frac{\partial^2 \sqrt{\rho_x}}{\partial x^2}}{\sqrt{\rho_x}}$ which is called “quantum potential”) with S_x the associated action. The Bohmian idea can be summarized as follows: Every quantum system, described by a pure

state, is associated to a fluid whose density corresponds to the probability of detecting the system in a position. The streamlines are derived from a potential flow that is associated with action S_x . The dynamics of the fluid under consideration is ruled by classical mechanics with the additional term of the quantum potential.

2.1.2 Problems with Bohmian mechanics

As it was mentioned in Section 2.1.1, the scope of Bohmian mechanics at the beginning [Bohm(1952a), Bohm(1952b)] was to ease the understanding of individual events in quantum dynamics through the use of trajectories and the non-local concept of a “quantum potential” in the configuration space. Even if appealing, shortly after the publication of Bohm’s papers, his proposed idea clashed with a criticism concerning the asymmetry of his formulation [Passon(2005)]. The main objections arose from Pauli [Pauli(1952)] and Heisenberg [Passon(2005), Bacciagaluppi(2009)]. Pauli and Heisenberg stressed that, besides the lack of experimental evidence of the hidden variables, the asymmetric role of the canonical variables in Bohm’s theory was a fundamental drawback. While conventional quantum mechanics is formulated independently of a particular representation, Bohmian mechanics is solely expressed in terms of the position representation with no traces of other possible representations, for instance, momentum representation. Basically, the criticism against Bohmian mechanics during the 50’s is summarized in the idea that the the absence of a description in terms of momentum and its unique description in terms of the position was a contradiction to the claimed generality of the theory proposed by Bohm. Not to mention that the physical meaning of his trajectories was not proven at the time. A brief summary of the chronology of the criticisms on the absence of other representations in Bohmian mechanics as shown in Table 2.1.

From the side of the Bohmian community, shortly after the criticism of Bohm’s papers [Bohm(1952a), Bohm(1952b)], Epstein suggested in a note [Epstein(1953a)] the possibility of expressing Bohm’s approach in the momentum representation by a polar decomposition. The same year Bohm himself [Bohm(1953)] objected to the idea by evoking the Coulomb potential and a supposed misconception on the canonical transformation within his hidden variables framework. Not long after Epstein illustrated this possibility in another note [Epstein(1953b)]. He did not write down the associated continuity equation though and was unable to deter-

Supporters	Detractors
Epstein [Epstein(1953a), Epstein(1953b)]	Pauli [Pauli(1952)] Heisenberg [Passon(2005), Bacciagaluppi(2009)] Bohm [Bohm(1953)] Freistadt [Freistadt(1957)]
Polavieja [Polavieja(1996a), Polavieja(1996b)] Hiley [Hiley(2000)]	

Table 2.1 Summary of the timeline of the controversy about Bohmian mechanics in momentum representation.

mine the form of the quantum contribution in the Hamilton–Jacobi equation. He expressed the potential term as a convolution integral and did not specify for what kind of potential an analogous quantum term is obtained for the momentum representation.

Years later, Freistadt criticized concisely that polar decomposition in a review about the causal description of quantum mechanics [Freistadt(1957)]. Freistadt argued that the unspecified form of the potential prevents the dynamical equations in momentum representation from presenting a causal form as in the case of the position representation. It should also be mentioned that, to our knowledge, Polavieja [Polavieja(1996a), Polavieja(1996b)] was the first to go beyond Bohmian mechanics in configuration space by means of a projection technique similar to the one used in this thesis. He obtained a phase space description by performing a polar decomposition of the Husimi function in the basis of generalized coherent states (that are elements of a nonlinear submanifold of the Hilbert space, as a superposition of two coherent states no longer belongs to this space), not on a basis of the momentum space wave functions (that span the whole Hilbert space).

As a matter of fact, Struyve published a possible method to express Bohmian mechanics causally in momentum representation [Struyve(2010)]. Nevertheless, all along the paper he was not able to write down explicitly for specific systems neither the CE nor the HJE in momentum representation. Therefore, since the works of Epstein [Epstein(1953a), Epstein(1953b)] there have been no explicit dynamical equations in a causal form for the momentum representation.

Recently an extension of the Bohmian formulation [Hiley(2000)] has been implemented to a free representation framework through the introduction of a phase operator. Nevertheless, its major drawback is the *ad hoc* introduction of the phase operator. This means, the missing symmetry between position and momentum representation argued by Pauli [Pauli(1952)] was formally established. The

dynamics was shown to be gauge invariant and every representation has its own associated phase space. It is also worth pointing out the attempt for formulating Bohmian mechanics in terms of the density matrix [Maroney(2005)]. An outline of the main arguments involved in the controversy of Bohmian mechanics in momentum representation is shown in Table 2.2.

Now in this present work, the extension of Bohmian mechanics to momentum representation is achieved without the need of any *ad hoc* introduction of new operators. The original idea of Bohm is simply used and extended. This is shown in the next Section.

2.2 Continuous representation

2.2.1 Extension principle

The main feature and limitation of Bohm's proposal [Bohm(1952a), Bohm(1952b)] are its foundation exclusively in the position representation $\{|x\rangle\}$. As it was mentioned in Section 2.1.2, in [Hiley(2000)] a formulation of Bohmian mechanics for any representation was achieved through the use of the Quantum Liouville equation and the introduction of a quantum phase operator in an *ad hoc* way. However, as will be seen in the following, the extension of Bohmian mechanics to any continuous representation $\{|a\rangle\}$ can be based on the most basic concept: The projection of the state, formulated using the polar form of the complex wave function.

In quantum mechanics [Dirac(1931), Newton(2004)] all measurable information is embedded in the quantum state $|\psi(t)\rangle$ that can be given in different representations, depending on the chosen independent variable a . That variable can be, *e.g.*, position, momentum, energy, etc., leading to the projection $\langle a|\psi(t)\rangle \in \mathbb{C}$. Instead of introducing a quantum phase operator as a new concept, we will use the original method of Bohm (the polar decomposition) in a broader sense. As the projection of the state is a complex quantity for any representation, we can express it always in polar form:

$$\langle a|\psi(t)\rangle = \sqrt{\rho_a(a,t)} \exp\left(i\frac{S_a(a,t)}{\hbar}\right) \quad (2.6)$$

with $\rho_a = |\langle a|\psi(t)\rangle|^2$ associated with the probability density function of the experimental detections. We have to bear in mind that the bricks of the Bohmian

Supporters	Detractors
	<p>Pauli [Pauli(1952)]</p> <p>Heisenberg [Passon(2005), Bacciagaluppi(2009)]</p> <p>Absence of experimental detections of hidden variables.</p> <p>Absence of a representation-free formulation.</p>
<p>Epstein [Epstein(1953a)]</p> <p>Suggestion of finding paths that satisfy both:</p> $\frac{d}{dt}q(t) \propto \frac{\partial}{\partial x}S(x,t) _{x=q(t)}$ $\frac{d}{dt}\pi(t) \propto \frac{\partial}{\partial p}S(p,t) _{p=\pi(t)} .$ <p>Schrödinger equation in momentum representation obtained for a general potential given explicitly.</p> <p>Neither CE nor mHJE is written down.</p>	<p>Bohm [Bohm(1953)]</p> <p>There cannot be trajectories in momentum space, since a non convergent series expansion would arise for the Coulomb potential.</p>
	<p>Freistadt [Freistadt(1957)]</p> <p>The impossibility comes from the potential form. As long as its form is not stated; then in the momentum representation, the dynamical equations remain just as an integral expression. Therefore there is neither continuity nor mHJ equation.</p>
<p>Polavieja [Polavieja(1996a), Polavieja(1996b)]</p> <p>Projection of the Husimi function with help of generalized coherent states (state dependent representation)</p>	
<p>Hiley [Hiley(2000)]</p> <p>Momentum representation for Bohmian mechanics, as long as a “Phase operator” is introduced in an <i>ad hoc</i> way.</p>	
<p>Struyve [Struyve(2010)]</p> <p>Conditions for the form of the potential to ensure the existence of a continuity equation.</p>	

Table 2.2 Summary of the arguments in the controversy about Bohmian mechanics in momentum representation.

formulation are the norm ρ and the phase S , because **Bohmian mechanics is a quantum formulation of the projected state**, as it will be proven in what follows. For this purpose, the dynamics of these elements for every continuous representation must be established. To reach this goal, we take the time derivative of (2.6), take into account Schrödinger's equation and separate it into real and imaginary parts:

$$-\rho_a \frac{\partial}{\partial t} S_a = \frac{1}{2} \langle a | [\hat{H}, \hat{\rho}(t)]_+ | a \rangle = \frac{1}{2} \langle a | (\hat{H} \hat{\rho}(t) + \hat{\rho}(t) \hat{H}) | a \rangle, \quad (2.7)$$

$$\frac{\hbar}{2} \frac{\partial}{\partial t} \rho_a = \frac{1}{2i} \langle a | [\hat{H}, \hat{\rho}(t)]_- | a \rangle = \frac{1}{2i} \langle a | (\hat{H} \hat{\rho}(t) - \hat{\rho}(t) \hat{H}) | a \rangle, \quad (2.8)$$

where $\hat{\rho}(t)$, in Dirac notation, correspond to the density operator of a pure state, $\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|$, and is different from the density function $\rho_a = \psi_a^*(a, t) \psi_a(a, t)$.

It is important to note that the dynamics of the density ρ_a and the phase S_a depends on the complex quantity $\langle a | \hat{H} \hat{\rho} | a \rangle$, with \hat{H} being the Hamiltonian operator in the respective representation. Indeed the real part $\frac{1}{2} \langle a | [\hat{H}, \hat{\rho}(t)]_+ | a \rangle$ and imaginary part $\frac{1}{2i} \langle a | [\hat{H}, \hat{\rho}(t)]_- | a \rangle$ determine the time dependence of the density ρ_a and the phase S_a , respectively.

Let us consider an arbitrary observable with the corresponding operator \hat{F} . We will define a *complex Bohmian quantity* $F_{Bo} \doteq F \in \mathbb{C}$ as follows:

$$\boxed{F(a, t) \doteq \frac{\langle a | \hat{F} | \psi \rangle}{\langle a | \psi \rangle} = F_R + iF_I.} \quad (2.9)$$

In other words, our complex Bohmian quantities are nothing more than the action of the operator \hat{F} on the quantum state, $\langle a | \hat{F} | \psi \rangle$, divided by the projected quantum state $\langle a | \psi \rangle$. From now on, for the sake of simplicity, the difference between a Bohmian quantity F and an operator \hat{F} will be indicated by a hat on the latter.

Box 2.2.1**On the notation of the complex Bohmian quantities [Bonilla(2020a)]**

As we will see in future Sections, the introduced notation (2.9) allows a simplification of the analysis of quantum systems and, particularly, of time-dependent systems. To avoid any misunderstanding though, it is necessary to clarify an important point regarding this new notation. At first glance it would seem inconvenient the use of $F(a, t)$ because it does not indicate the involved representation. One could argue that, for instance, a complex Bohmian quantity in position and momentum representation, according to (2.9) should be written, respectively, $F(x, t)$ and $F(p, t)$, causing then the impression that the relation between both quantities is a mere substitution of the type $x \leftrightarrow p$, which is not the case. One solution could be indicating the representation as a subscript $F_a(a, t)$.

Nevertheless, on one hand, $F_p(x, t)$ and $F_x(p, t)$ do not exist based on (2.9) and, on the other hand, stating every time $F_x(x, t)$ and $F_p(p, t)$ is redundant and slows down the reading (this goes against the initial reason for the notation (2.9) which is the simplification of the Bohmian expressions). Therefore, in order to ease the notation the representation subscript was drop in (2.9), and we will only indicate $F(x, t)$ and $F(p, t)$ instead of $F_x(x, t)$ and $F_p(p, t)$.

Besides, Bohmian mechanics is a projective aspect of quantum mechanics, as we will see in Section 3.3; that means that the choice of a representation **must** always be previously stated. For that reason it is always clear in which representation we are working. Also, to ease the reading, the involved representation is contained in the headings of the correspondent Sections. In this sense, hereafter we will not indicate the representation subscript because the context is clear enough to avoid a misunderstanding.

Going back to (2.8-2.7), the Bohmian dynamical equations may be rewritten as

$$-\rho_a \frac{\partial}{\partial t} S_a = \rho_a H_R(a, t), \quad (2.10)$$

$$\frac{\hbar}{2} \frac{\partial}{\partial t} \rho_a = \rho_a H_I(a, t), \quad (2.11)$$

where the first corresponds to the CE (2.5) and the second to the mHJE (2.4), but now in **any** continuous representation.

The latter system of equations is more fundamental than the usual Bohm's equations, because it is expressed in an arbitrary representation (and not restricted to the position representation). Further, the advantages of working in representations other than position, for instance, momentum representation will be illustrated, *e.g.* in Section 2.2.2.3. Equations (2.10-2.11) were obtained in [Hiley(2000)] by using the quantum Liouville equation and the introduction of a so called quantum phase operator. The method proposed in this thesis is simpler, since it is based on the general idea that the projection of a state $|\psi(t)\rangle$ on a representation $\{|a\rangle\}$ is a complex number, that can always be expressed in polar form.

2.2.2 Position and momentum representations

2.2.2.1 Position representation

Let us review the derivation of Bohm's equations to point out the key element of the Bohmian formulation. A non-relativistic system with zero spin, under the influence of a real potential $\hat{V} = f(\hat{X})$ in the coordinate representation shall be considered. Bearing in mind the polar decomposition of the projection of the state (2.6), the following Bohmian quantities can be computed according to definition (2.9)

$$\boxed{X = x \quad \text{real}} \quad (2.12)$$

$$\boxed{P = \frac{\partial}{\partial x} S_x - i \frac{\hbar}{2} \frac{\partial}{\partial x} \frac{\rho_x}{\rho_x} = P_R + iP_I \quad \text{complex}} \quad (2.13)$$

$$\boxed{V = f(x)} \quad (2.14)$$

$$\boxed{\begin{aligned} T &= \frac{1}{2m} [P^2] = \frac{1}{2m} \left((P)^2 - i\hbar \frac{\partial}{\partial x} P \right) \\ &= \frac{1}{2m} \left[\left(P_R^2 - P_I^2 + \hbar \frac{\partial}{\partial x} \cdot P_I \right) + i \left(2P_R P_I - \hbar \frac{\partial}{\partial x} P_R \right) \right], \end{aligned}} \quad (2.15)$$

i.e., $[P^2] \neq (P)^2$, what reflects the non-locality of the theory, as in general $(\frac{\partial}{\partial x} P) \neq 0$.

Like the Bohmian momentum, also the corresponding kinetic energy is a complex quantity. The real part can be rewritten as

$$T_R = \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V_{qu} \quad (2.16)$$

where the quantum potential V_{qu} is completely determined by the imaginary part of the Bohmian momentum (2.13) according to

$$\begin{aligned} V_{qu} &= -\frac{1}{2m} \left[P_I^2 - \hbar \frac{\partial}{\partial x} P_I \right] \\ &= \frac{\hbar^2}{8m} \left(\frac{\partial}{\partial x} \frac{\rho_x}{\rho_x} \right)^2 - \frac{\hbar^2}{4m} \frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \frac{\rho_x}{\rho_x} \right) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \sqrt{\rho_x}. \end{aligned} \quad (2.17)$$

The complex Bohmian Hamiltonian takes then the form

$$H_x = \left[\frac{P_R^2}{2m} + V(x,t) - \frac{P_I^2}{2m} + \frac{\hbar}{2m} \frac{\partial}{\partial x} P_I \right] - i \frac{\hbar}{2\rho_x} \frac{\partial}{\partial x} \left(\rho_x \frac{P_R}{m} \right). \quad (2.18)$$

The real part is essentially the real part of the kinetic energy supplemented by the real potential $V(x,t)$, where the time-dependence may, *e.g.*, arise from a time-dependent frequency of a parametric oscillator, *i.e.*, $V = \frac{m}{2} \omega^2(t) x^2$. The imaginary part of the Hamiltonian is identical with the imaginary part of the kinetic energy and can be written as

$$\begin{aligned}
T_I &= \frac{1}{2m} \left(2P_R P_I - \hbar \frac{\partial}{\partial x} P_R \right) \\
&= -\frac{1}{2m} \left[\hbar \left(\frac{\partial_x \rho_x}{\rho_x} \right) \frac{\partial}{\partial x} S_x + \hbar \frac{\partial^2}{\partial x^2} S_x \right] \\
&= -\frac{\hbar}{2} \frac{1}{\rho_x} \frac{\partial}{\partial x} \left(\rho_x \frac{\partial_x S_x}{m} \right). \tag{2.19}
\end{aligned}$$

From the real part of the Hamiltonian follows according to (2.10)

$$\begin{aligned}
-\frac{\partial}{\partial t} S_x &= T_R + V(x, t) \\
&= \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V_{qu} + V(x, t), \tag{2.20}
\end{aligned}$$

i.e., the mHJE (2.4).

In agreement with (2.11), this leads to

$$\begin{aligned}
\frac{\hbar}{2} \frac{\partial}{\partial t} \rho_x &= \rho_x T_I = \rho_x H_I \\
&= -\frac{\hbar}{2} \frac{\partial}{\partial x} \left(\rho_x \frac{\partial_x S_x}{m} \right), \tag{2.21}
\end{aligned}$$

what is, apart from a constant factor $\frac{\hbar}{2}$, just the CE (2.5).

2.2.2.2 Momentum representation

In the following the momentum space representation will be developed in analogy to the preceding position space representation. A general quadratic potential $\widehat{V}(\widehat{X}) = a + b\widehat{X} + \frac{1}{2}m\omega^2(t)\widehat{X}^2$ will be considered, particularly as the quadratic term represents the counterpart of the quadratic form of the kinetic energy and also provides a term corresponding to the quantum potential in position space. For that purpose, again the polar form of the state and the definition (2.9) of the Bohmian quantities are considered. Hence, in the momentum representation one obtains for a given wave function $\psi_p(p, t) = \sqrt{\rho_p(p, t)} \exp \left[\frac{i}{\hbar} S_p(p, t) \right]$

$$X = -\frac{\partial}{\partial p} S_p + i \frac{\hbar}{2} \frac{\frac{\partial}{\partial p} \rho_p}{\rho_p} = X_R + iX_I \quad \text{complex} \quad (2.22)$$

$$P = p \quad \text{real} \quad (2.23)$$

$$T = \frac{p^2}{2m} \quad (2.24)$$

$$\begin{aligned} [X^2] &= (X)^2 + i\hbar \frac{\partial}{\partial p} X \\ &= \left(X_R^2 - X_I^2 - \hbar \frac{\partial}{\partial p} \cdot X_I \right) + i \left(2X_R X_I + \hbar \frac{\partial}{\partial p} \cdot X_R \right). \end{aligned} \quad (2.25)$$

Also in momentum space, the non-locality is expressed by the fact that $[X^2] \neq (X)^2$, but differs by the term $i\hbar(\frac{\partial}{\partial p} X)$. The real part of $[X^2]$ is given by the square of X_R (like in position space the real part of P^2 is given by P_R^2), but supplemented by a term that is formally equivalent to the quantum potential V_{qu} in position space, *i.e.*,

$$\begin{aligned} [X^2]_R &= \left(-\frac{\partial}{\partial p} S_p \right)^2 - \frac{\hbar^2}{2} \left[\frac{\frac{\partial^2}{\partial p^2} \rho_p}{\rho_p} - \frac{1}{2} \left(\frac{\frac{\partial}{\partial p} \rho_p}{\rho_p} \right)^2 \right] \\ &= (X_R)^2 - \hbar^2 \frac{\frac{\partial^2}{\partial p^2} \sqrt{\rho_p}}{\sqrt{\rho_p}}. \end{aligned} \quad (2.26)$$

Therefore, the Hamiltonian for the above mentioned potential can, in Bohmian form, be written as

$$\begin{aligned} H_p &= \frac{p^2}{2m} + a + b \left(-\frac{\partial}{\partial p} S_p \right) + \frac{m}{2} \omega^2 \left[\left(-\frac{\partial}{\partial p} S_p \right)^2 - \hbar^2 \frac{\frac{\partial^2}{\partial p^2} \sqrt{\rho_p}}{\sqrt{\rho_p}} \right] \\ &\quad + i \left[b \frac{\hbar}{2} \frac{\frac{\partial}{\partial p} \rho_p}{\rho_p} + \frac{m}{2} \omega^2 \left(-\frac{\hbar}{\rho_p} \frac{\partial}{\partial p} (\rho_p \frac{\partial}{\partial p} S_p) \right) \right]. \end{aligned} \quad (2.27)$$

According to (2.11), from the imaginary part follows

$$\frac{\partial}{\partial t} \rho_p = -\frac{\partial}{\partial p} (-b\rho_p) - m\omega^2 \frac{\partial}{\partial p} \left(\rho_p \frac{\partial}{\partial p} S_p \right) \quad (2.28)$$

or, with the definition of X_R ,

$$\frac{\partial}{\partial t}\rho_p + \frac{\partial}{\partial p}\left[\rho_p(-b - m\omega^2 X_R)\right] = 0. \quad (2.29)$$

The second term on the lhs corresponds to the momentum contribution to the flux in phase space according to $\rho_p \dot{P}$, if \dot{P} is given by the Bohmian quantity

$$\dot{P} = -b - m\omega^2 X_R = \left(-\frac{\partial}{\partial x}V(x)\right)\Bigg|_{x=X_R}. \quad (2.30)$$

From the real part of the Hamiltonian follows:

$$\frac{\partial}{\partial t}S_p + \frac{p^2}{2m} + a + b\left(-\frac{\partial}{\partial p}S_p\right) + \frac{m}{2}\omega^2\left[\left(\frac{\partial}{\partial p}S_p\right)^2 - \hbar^2\frac{\frac{\partial^2\sqrt{\rho_p}}{\partial p^2}}{\sqrt{\rho_p}}\right] = 0, \quad (2.31)$$

or with the definition of X_R ,

$$\frac{\partial}{\partial t}S_p + \frac{p^2}{2m} + V(X_R) - \frac{m}{2}\omega^2\hbar^2\frac{\frac{\partial^2\sqrt{\rho_p}}{\partial p^2}}{\sqrt{\rho_p}} = 0, \quad (2.32)$$

in summary

$$\frac{\partial}{\partial t}S_p + \frac{p^2}{2m} + V(X_R) - \underbrace{\frac{m}{2}\omega^2\hbar^2\frac{\frac{\partial^2\sqrt{\rho_p}}{\partial p^2}}{\sqrt{\rho_p}}}_{\text{quantum contribution}} = 0, \quad (2.33)$$

$$\frac{\partial}{\partial t}\rho_p + \frac{\partial}{\partial p}\left[\rho_p(-b - m\omega^2 X_R)\right] = 0. \quad (2.34)$$

These equations are the momentum space versions of the CE (2.5) or (2.21) and the mHJE (2.4) or (2.20) valid in position space.

2.2.2.3 Example of application: Linear potential in momentum space

As an example, let us consider an electron of mass m and charge e acted upon by a linear potential, *e.g.*, a uniform, homogeneous and isotropic electric field in the x

direction, represented by the potential $V(x) = eEx$, where we will exclusively consider stationary states. In this case the probability density ρ_p does not explicitly depend on time, thus according to (2.9) and (2.11), the Bohmian Hamiltonian is a real quantity, $H = \varepsilon \in \mathbb{R}$, with ε an energy of the spectrum. The conventional treatment in coordinate representation through the Schrödinger equation is already known [Schiff(1970)]. To solve it by means of the Bohmian mechanics in momentum representation $\{|p\rangle\}$, the Bohmian dynamical equations (2.11-2.10) must be written down, taking into account the real character of the Bohmian Hamiltonian for the stationary states:

$$\frac{\partial}{\partial t}\rho_p = 0 = eE \frac{\partial}{\partial p}\rho_p, \quad (2.35)$$

$$-\frac{\partial}{\partial t}S_p = \varepsilon = -eE \frac{\partial}{\partial p}S_p + \frac{p^2}{2m}. \quad (2.36)$$

The probability density not depending explicitly on time, $\frac{\partial}{\partial t}\rho_p = 0$, and $\frac{\partial}{\partial t}S_p = -\varepsilon$, is leading to

$$\frac{\partial}{\partial p}\rho_p = 0, \quad (2.37)$$

$$\varepsilon = -eE \frac{\partial}{\partial p}S_p + \frac{p^2}{2m}. \quad (2.38)$$

As the probability density does not depend explicitly neither on time nor on momentum, the probability density is constant, $\rho_p = \text{const}$. Regarding the phase, from (2.38) follows:

$$\frac{\partial}{\partial p}S_p = \frac{p^2}{2meE} - \frac{\varepsilon}{eE}. \quad (2.39)$$

Therefore, this problem has as solution:

$$\rho_p = \text{const}, \quad (2.40)$$

$$S_p = \frac{1}{2meE} \frac{p^3}{3} - \frac{\varepsilon}{eE} p - \varepsilon t. \quad (2.41)$$

Applying the inverse Fourier transform to the wave function, *i.e.* the transformation to the position representation

$$\begin{aligned}\sqrt{\rho_x(x,t)} \exp\left[i\frac{S_x(x,t)}{\hbar}\right] &= \int dp \exp\left[\frac{i}{\hbar}\left\{\frac{1}{2meE}\frac{p^3}{3} - \frac{\varepsilon}{eE}p - \varepsilon t + xp\right\}\right] \\ &= \exp\left[-i\frac{\varepsilon t}{\hbar}\right] \int dp \exp\left[i\left(\frac{1}{2m\hbar eE}\frac{p^3}{3} + \left(x - \frac{\varepsilon}{eE}\right)\frac{p}{\hbar}\right)\right]\end{aligned}\quad (2.42)$$

and introducing the following change of variable $u = \frac{1}{\sqrt[3]{2m\hbar eE}}p$ leads to

$$\sqrt{\rho_x(x,t)} \exp\left[i\frac{S_x(x,t)}{\hbar}\right] \propto \exp\left[-i\frac{\varepsilon t}{\hbar}\right] \int du \exp\left[i\left(\frac{u^3}{3} + \left(x - \frac{\varepsilon}{eE}\right)\sqrt[3]{\frac{2m\hbar eE}{\hbar^2}}u\right)\right]. \quad (2.43)$$

The integral on the right side of the equation turns out to be the integral representation of the Airy function (see equation (2.24) in [Vallee(2004)]), leading to

$$\sqrt{\rho_x(x,t)} \exp\left[i\frac{S_x(x,t)}{\hbar}\right] \propto Ai\left[\sqrt[3]{\frac{2m\hbar eE}{\hbar^2}}\left(x - \frac{\varepsilon}{eE}\right)\right] \exp\left[-i\frac{\varepsilon t}{\hbar}\right]. \quad (2.44)$$

The solution in the position representation can be identified as

$$\boxed{\rho_x(x,t) = \left(Ai\left[\sqrt[3]{\frac{2m\hbar eE}{\hbar^2}}\left(x - \frac{\varepsilon}{eE}\right)\right]\right)^2} \quad (2.45)$$

$$S_x(x,t) = -\varepsilon t, \quad (2.46)$$

where the energy spectrum will depend on the imposed boundary conditions. For instance, in a triangular well $V(x) = eEx, \forall x > 0$ and $V(x) = +\infty$ otherwise, the imposed boundary condition is $\rho_x(0,t) = 0$. This leads to

$$Ai\left[\sqrt[3]{\frac{2m\hbar eE}{\hbar^2}}\left(0 - \frac{\varepsilon}{eE}\right)\right] = 0, \quad (2.47)$$

$$\zeta_i = -\sqrt[3]{\frac{2m\hbar eE}{\hbar^2}} \frac{\varepsilon_i}{eE} \quad (2.48)$$

where ζ_i denotes the zeroes of the Airy function; the energy spectrum ε_i is then given by

$$\varepsilon_i = -eE \sqrt[3]{\frac{\hbar^2}{2meE}} \zeta_i. \quad (2.49)$$

With this brief example, we stress that Bohmian mechanics can ease significantly the treatment of some systems (for instance, in the case of a linear potential), just by changing the representation.

2.3 Complexification

2.3.1 *Complex Hamiltonian*

2.3.1.1 Complex Hamiltonian in position representation

In the remaining Sections of this chapter the structure of the proposed complex Bohmian quantities (2.9) is presented.

Since the first communication of Schrödinger [Schrödinger(1926a)] there was a search for formulating quantum mechanical behavior in a Hamiltonian way. This task was already achieved during the 20's with the works of Schrödinger [Schrödinger(1926a), Schrödinger(1926b), Schrödinger(1926c), Schrödinger(1926d)], Heisenberg, Born and Jordan [Heisenberg(1925), Born(1925), Born(1926)] and Dirac [Dirac(1931)], amongst others. During those times the Copenhagen interpretation set the conceptual structure of quantum mechanics, which was summed up in 1948 by Bohr:

“The entire formalism is to be considered as a tool for deriving predictions, of definite or statistical character, as regards information obtainable under experimental conditions described in classical terms and specified by means of parameters entering into the algebraic or differential equations of which the matrices or the wave-functions, respectively, are solutions. These symbols themselves, as is indicated already by the use of imaginary numbers, are not susceptible to pictorial interpretation.; and even derived real functions like densities and currents are only to be regarded as expressing the probabilities for the occurrence of individual events observable under well-defined experimental conditions.” [Bohr(1948)]

For that reason what has a Hamiltonian structure is the observable operator formalism, not the actual detections, *i.e.*, mean values, uncertainties, etc. As we saw in Section 2.1, in 1952, Bohm [Bohm(1952a), Bohm(1952b)] criticized that the involved entities (operators and states) were deprived of an objective reality and underlined the necessity of seeking for a law for predicting single detections and not just statistical ensembles of detections of systems with an equal initial preparation. He proposed therefore a causal interpretation of the individual objects, imposing thus the realism in quantum mechanics, by decoupling the Schrödinger equation into real and imaginary parts (2.5-2.4), by means of a polar decomposition of the wave function (2.3). This led to the revival of the causal interpretation

of de Broglie and Madelung [Madelung(1927)] in terms of hydrodynamical equations.

Despite the criticisms of Heisenberg and Pauli, among others (see Section 2.1), Bohmian mechanics continued being studied: The interpretation of the quantum potential by Philippidis [Philippidis(1979)] and Dewdney [Dewdney(1982)]; the attempts for a formulation of momentum space by Epstein [Epstein(1953a)], Freistadt [Freistadt(1957)], Hiley [Hiley(2000)] and Bonilla [Bonilla(2020a)]; among other contributions [Polavieja(1996a), Polavieja(1996b), Struyve(2010), Maroney(2005)]. The main lines of Bohmian mechanics were already summed up in [Holland(1995)]. Nevertheless, conceptually speaking, the realism proposed in the interpretation by Bohmian mechanics was already proven to be false when Alain Aspect violated Bell's inequalities [Bell(1964)] in 1980 with a quantum optical experiment [Aspect(1976)].

Besides the ontological interpretation of Bohmian mechanics (already proven wrong), the mathematical framework is still useful because of the intuition that it provides and the ease in computing simulations for quantum systems [Sanz(2014), Nassar(1993), Goldfarb(2006), Poirier(2008)]. This thesis adheres to this scheme and Bohmian mechanics is only considered as a convenient mathematical formulation for treating quantum mechanics, without any additional interpretations. That being said, the natural question that arises is, if our proposed Bohmian structure has a Newtonian or Hamiltonian structure, since non-relativistic quantum mechanics is naturally Hamiltonian in its structure.

As it was seen in Section 2.2.2, the proposed complex quantities (2.14-2.15) are given by

$$V = f(x), \quad (2.50)$$

$$T = \frac{1}{2m} [P^2] = \frac{1}{2m} \left((P)^2 - i\hbar \frac{\partial}{\partial x} P \right). \quad (2.51)$$

The Bohmian Hamiltonian is then naturally expressed as follows:

$$H_x = \frac{1}{2m} \left((P)^2 - i\hbar \frac{\partial}{\partial x} P \right) + V. \quad (2.52)$$

It is straight forward to compute the following derivatives:

$$\frac{\partial H_x}{\partial x} = \frac{1}{2m} \left(2P \frac{\partial P}{\partial x} - i\hbar \frac{\partial^2 P}{\partial x^2} \right) + \frac{\partial V}{\partial x}, \quad (2.53)$$

$$\frac{\partial H_x}{\partial P} = \frac{1}{m} P, \quad (2.54)$$

$$\frac{\partial H_x}{\partial t} = \frac{1}{2m} \left(2P \frac{\partial P}{\partial t} - i\hbar \frac{\partial^2 P}{\partial x \partial t} \right) + \frac{\partial V}{\partial t}. \quad (2.55)$$

Now, if time derivatives are taken individually of the Bohmian position, momentum and Hamiltonian, using (2.11), (2.10) and (2.13) one obtains

$$\frac{\partial X}{\partial t} = 0, \quad (2.56)$$

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial t} \left(\frac{\partial}{\partial x} S_x(x,t) - \frac{i\hbar}{2} \frac{\partial}{\partial x} \ln \rho_x(x,t) \right) = -\frac{\partial H_x}{\partial x}, \quad (2.57)$$

$$\frac{\partial H_x}{\partial t} = \frac{\partial}{\partial t} \left(-\frac{\partial}{\partial t} S_x(x,t) + \frac{i\hbar}{2} \frac{\partial}{\partial t} \ln \rho_x(x,t) \right). \quad (2.58)$$

Apparently, in the Bohmian framework the Hamiltonian formalism does not hold, due to the fact that the representation variable $x = X$ does not depend explicitly on time. This rises the question on how to express the Bohmian formalism in a Hamiltonian way, if possible. Within this framework one can introduce Q , the conjugate variable of the Bohmian momentum, in the following way:

$$Q(x,t) \doteq \frac{1}{m} \int P(x,t) dt. \quad (2.59)$$

In this way, we could compute again the respective derivatives and realize that now we dispose of two conjugate dynamical variables (Q, P), and when remembering the definition of the Bohmian quantities (2.9), apparently we have a Hamiltonian system of equations,

$$\begin{aligned} \frac{\partial P}{\partial t}(x,t) &= -\frac{\partial}{\partial x} V - \frac{P}{m} \frac{\partial}{\partial x} P - \frac{i\hbar}{2} \frac{\partial^2}{\partial x^2} P \\ &= -\frac{\partial H_x}{\partial x} \neq -\frac{\partial H_x}{\partial Q}, \end{aligned} \quad (2.60)$$

$$\frac{\partial Q}{\partial t}(x,t) = \frac{1}{m} P = \frac{\partial H_x}{\partial P}, \quad (2.61)$$

$$-\frac{\partial}{\partial t} \left(S_x(x,t) - \frac{i\hbar}{2} \ln \rho_x(x,t) \right) = H_x(P, \frac{\partial}{\partial x} P; x,t) \neq H_x(Q, P; x,t). \quad (2.62)$$

It should be mentioned that the real part of Eq. (2.61) with $P_R = \frac{\partial}{\partial x} S_x$ is identical with the guidance law (2.1) **postulated** in Bohmian mechanics, thus the real part of Q is just the Bohmian trajectory $q(t)$!

Nevertheless, the Hamiltonian structure is not really obvious, because a closer inspection reveals that, first of all the complex Hamiltonian is a function of P , $\frac{\partial}{\partial x} P$, x and t , but Q does not occur. Furthermore, in (2.60) the time derivative of the complex momentum is given by $\frac{\partial P}{\partial t} = \frac{\partial}{\partial x} H_x$, instead of $\frac{\partial P}{\partial t} = \frac{\partial}{\partial Q} H_x$. It is worth mentioning that the mHJ equation (2.4) in Bohmian mechanics served originally as an argument supporting the idea that the structure of Bohmian mechanics is Hamiltonian. Nonetheless, we have seen that this claim is not quite correct. That does not mean that the structure is useless though. On the contrary, it only means that Bohmian mechanics does not share the conventional Hamiltonian structure. This is partly due to the fact that Bohmian mechanics is a projective version of quantum mechanics, as it is shown in definition (2.9). But, still we have to emphasize that the dynamics of the system is contained in the following equation,

$$\boxed{\frac{\partial P}{\partial t} + \frac{P}{m} \frac{\partial}{\partial x} P = -\frac{\partial}{\partial x} V - \underbrace{\frac{i\hbar}{2} \frac{\partial^2}{\partial x^2} P}_{\text{quantum contribution}}}, \quad (2.63)$$

which reminds of the Newtonian equation. However, this analogy is not new in quantum mechanics. What is new is that it is proposed to rewrite the elements of Bohmian mechanics with complex functions (2.9) to form a **complex** Newton-like equation (2.63). The latter can be decoupled with help of (2.13) and (2.17) into real and imaginary parts, leading then to Bohm's original expressions:

$$\frac{\partial}{\partial t} S_x + \frac{(\frac{\partial}{\partial x} S_x)^2}{2m} + V + V_{qu,x} = 0, \quad (2.64)$$

$$\frac{\partial \rho_x}{\partial t} + \frac{\partial}{\partial x} \left[\rho_x \frac{P_R}{m} \right] = 0, \quad (2.65)$$

with $P_R = \frac{\partial}{\partial x} S_x$. This system of equations corresponds to the usual Hamilton–Jacobi-like equation in Bohmian mechanics and the associated continuity equation. That means that the structure of Bohmian mechanics is neither Newtonian

nor Hamiltonian², yet its dynamics is ruled by a complex Newtonian-like equation, provided complex quantities are used.

2.3.1.2 Complex Hamiltonian in momentum representation

In this Section, the results of Section 2.3.1.1 are taken to the momentum representation. For that purpose, the polar decomposition of the projection of the quantum state [Bonilla(2020a)] is performed for the case of a non-relativistic system with zero spin, under the influence of a general harmonic potential \widehat{V} in the momentum representation (see Eqs. (2.22-2.25)).

The Hamiltonian for the general quadratic potential considered in Section 2.2.2.2 has the form

$$H_p = \frac{p^2}{2m} + a + bX + \frac{m}{2}\omega^2(t)X^2 + i\frac{\hbar m}{2}\omega^2(t)\frac{\partial}{\partial p}X. \quad (2.66)$$

Like in the previous Section one can compute the time derivatives [Bonilla(2021a)],

$$\frac{\partial X}{\partial t} = +\frac{\partial}{\partial p}H_p = \frac{p}{m} + (b + m\omega^2 X)\frac{\partial}{\partial p}X + i\hbar\frac{m\omega^2}{2}\frac{\partial^2}{\partial p^2}X, \quad (2.67)$$

$$\frac{\partial P}{\partial t} = 0. \quad (2.68)$$

Like in Section 2.3.1.1, the Hamiltonian structure is apparently missing, since p is in this case the representation variable. Nevertheless, in a similar way one can define a function Π conjugated to the Bohmian position according to

$$\Pi(p, t) \doteq \int (-b - m\omega^2 X(p, t)) dt. \quad (2.69)$$

In this way, one could form a dynamical system with the two conjugate dynamical variables (X, Π) ,

² Even though a conjugate variable Q (2.59) can be introduced by hand.

$$\begin{aligned} \frac{\partial X}{\partial t} &= \frac{p}{m} + (b + m\omega^2 X) \frac{\partial X}{\partial p} + i\hbar \frac{m\omega^2}{2} \frac{\partial^2 X}{\partial p^2} \\ &= \frac{\partial H_p}{\partial p} \neq \frac{\partial H_p}{\partial \Pi}, \end{aligned} \quad (2.70)$$

$$\frac{\partial \Pi(p, t)}{\partial t} = -\frac{\partial}{\partial X} H_p = -b - m\omega^2 X \quad (2.71)$$

$$-\frac{\partial}{\partial t} \left(S_p(p, t) - \frac{i\hbar}{2} \ln \rho_p(p, t) \right) = H_p \left(X, \frac{\partial X}{\partial p}; p, t \right) \neq H_p(X, \Pi; p, t). \quad (2.72)$$

Notice that Π and $\frac{\partial X}{\partial p}$ are not the same quantity. Indeed, the definition (2.69) of Π shows that $-\frac{1}{m\omega^2} \frac{\partial^2 \Pi}{\partial t \partial p} = \frac{\partial X}{\partial p}$.

When defining the Bohmian force $F \doteq -\frac{\partial}{\partial X} V(X, t) = -b - m\omega^2 X = \frac{\partial \Pi}{\partial t}$, one obtains a **complex** dynamical equation equivalent to Eq. (2.63),

$$\frac{\partial X}{\partial t} + \underbrace{\Pi \frac{\partial}{\partial p}}_{\text{quantum contribution}} X = \frac{p}{m} + i\hbar \frac{m\omega^2}{2} \frac{\partial^2}{\partial p^2} X. \quad (2.73)$$

With the help of (2.22) and (2.26) this one can again be decoupled into real and imaginary parts leading to Eqs. (2.34) and (2.33).

Since the 50's Bohmian mechanics has provided an alternative to rethink quantum mechanical problems with the claim to be based on a classical Hamiltonian mathematical structure. Now it was shown that, on the contrary, this Hamiltonian structure of Bohmian mechanics is not apparent. This can be seen clearly from the dynamical system (2.60-2.62) in position representation and (2.70-2.72) in momentum representation. In both cases, it was found that the effect of the projection of the quantum state (2.9) prevents the Hamiltonian structure to manifest completely.

2.3.2 Constants of motion

In the previous Section it was proven that the Bohmian structure is not exactly Hamiltonian, but this is not a problem though. Indeed, the importance that a theory has a Hamiltonian structure is mainly due to the interest in searching for constants of motions. Nevertheless, even though Bohmian theory does not follow this

scheme, it is useful for finding other constants of motion, that are otherwise difficult to access.

In Section 2.2.1 it was shown how Bohmian mechanics can be formulated in terms of complex quantities that are obtained by applying a quantum mechanical operator \widehat{F} onto a quantum state or wave function $\langle a|\psi(t)\rangle$ in the $\{|a\rangle\}$ representation (bear in mind it can be either position x or momentum p representation) and dividing the result by $\langle a|\psi(t)\rangle$, see Eq. (2.9).

The result is in general complex, however, the mean value of the imaginary part always vanishes, $\langle A_I \rangle = 0$, *i.e.*, it cannot be observed directly. In order to obtain exact analytical expressions, in the following our discussion is restricted to generalized coherent states as quantum states $|\psi(t)\rangle$, *i.e.*, to Gaussian wave packets with time-dependent width (first in position space). These functions are solutions of the time-dependent Schrödinger equation with potentials that are at most quadratic in the position variable. Without loss of generality, we consider the one-dimensional case, *i.e.*,

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right\} \psi(x,t) \quad (2.74)$$

with $\psi(x,t) = \langle x|\psi(t)\rangle$, *i.e.* the quantum state $|\psi(t)\rangle$ in position representation; the momentum representation is discussed in the next Section. The time-dependence of the potential $V(x,t)$ originates from the time-dependence of the oscillator frequency $\omega(t)$ and has the form $V(x,t) = \frac{1}{2}m\omega^2(t)x^2$, describing the so-called parametric oscillator.

The Gaussian solution can be written in the form

$$\langle x|\psi(t)\rangle = N_x(t) \exp \left[\frac{i}{\hbar} \left(\frac{m}{2} \mathcal{C} \tilde{x}^2 + \langle p \rangle \tilde{x} + K(t) \right) \right], \quad (2.75)$$

where $\tilde{x} = x - \langle x \rangle = x - \eta(t)$, *i.e.*, the maximum of the wave function is at $\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)x\psi(x,t)dx$ in agreement with Ehrenfest's theorem that the mean value $\langle x \rangle$ follows the classical trajectory, here denoted as $\eta(t)$. The coefficient of the quadratic term, $\mathcal{C} = \mathcal{C}(t)$, is a complex function of time and $\langle p \rangle = m\dot{\eta}$, where the overdots denote time-derivatives. Inserting (2.75) into (2.74) provides two equations of motion for $\eta(t)$ and $\mathcal{C}(t)$,

$$\ddot{\eta} + \omega^2(t)\eta = 0 \quad (2.76)$$

and

$$\dot{\mathcal{C}} + \mathcal{C}^2 + \omega^2(t) = 0. \quad (2.77)$$

Equation (2.76) is just Newton's equation of motion for the trajectory, Eq. (2.77) is a complex nonlinear Riccati equation that is connected with the time-dependence of the wave packet width. This connection becomes clearer by introducing a new variable $\alpha(t)$ and expressing $\mathcal{C}(t)$ in terms of α and its time-derivative as

$$\mathcal{C} \doteq \frac{\dot{\alpha}}{\alpha} + i \frac{1}{\alpha^2}. \quad (2.78)$$

The real part $\mathcal{C}_R = \frac{\dot{\alpha}}{\alpha}$ follows from inserting $\mathcal{C}_I = \frac{1}{\alpha^2}$ into the imaginary part of the complex Riccati equation (2.77). With these expressions for \mathcal{C}_R and \mathcal{C}_I , the real part of this equations turns into

$$\ddot{\alpha} + \omega^2(t) = \frac{1}{\alpha^3}, \quad (2.79)$$

a real nonlinear differential equation known as Ermakov equation that is equivalent to the complex nonlinear Riccati equation.

The imaginary part of \mathcal{C} shows that $\alpha(t)$ is directly proportional to the wave packet width, as $\mathcal{C}_I = \frac{1}{\alpha^2} = \frac{\hbar}{2m} \frac{1}{\sigma_x^2}$ with $\sigma_x^2 = \langle \tilde{x}^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$ being the mean square deviation in position, so $\alpha(t)$ represents up to a constant factor the position uncertainty.

According to (2.9), the Bohmian quantities for position, momentum, potential energy and kinetic energy for the coherent state (2.75) are obtained as

$X = x$	real	(2.80)
$P = m\mathcal{C}\tilde{x} + \langle p \rangle$	complex	(2.81)
$V = \frac{m}{2}\omega^2(t)x^2$		(2.82)
$T = \frac{1}{2m} \left[(P)^2 + \frac{\hbar}{i} \frac{\partial}{\partial x} P \right] = \frac{1}{2m} \left[(P)^2 - i\hbar m \mathcal{C} \right]$		(2.83)

2.3.2.1 Dynamical invariant

In quantum mechanics a dynamical invariant \hat{I} , for a system with Hamiltonian operator \hat{H} has to satisfy the relation

$$\frac{d}{dt}\langle\hat{\mathbb{I}}\rangle = \frac{1}{i\hbar}\langle[\hat{\mathbb{I}},\hat{\mathbb{H}}]_-\rangle + \left\langle\frac{\partial}{\partial t}\hat{\mathbb{I}}\right\rangle = 0 \quad (2.84)$$

with $[\ , \]_-$ being the commutator.

Finding such an invariant is particularly difficult when the Hamiltonian is explicitly time-dependent, as in Eq. (2.74) where the time-dependence is introduced via the time-dependent frequency $\omega(t)$ in the potential. Already in 1880, Vladimir Ermakov solved this problem for the classical case [Ermakov(1880)] by eliminating $\omega(t)$ between Eqs. (2.76) and (2.79), leading to an invariant named after him in the literature.

In the following it is shown how to obtain the same invariant without the necessity of using the Newtonian equation of motion (2.76) and the Ermakov equation (2.79). This derivation is based on Hamiltonian equations for the complex Bohmian quantities and the complex Riccati equation.

As shown in (2.60), in position space the Hamiltonian equation for the complex momentum \mathbb{P} is given by

$$\frac{\partial}{\partial t}\mathbb{P} = -\frac{\partial}{\partial x}H_x. \quad (2.85)$$

With the expressions for \mathbb{P} as given for the generalized coherent states in (2.81) one obtains

$$\frac{\partial}{\partial t}\mathbb{P} = -\frac{\partial}{\partial x}\left(\frac{1}{2m}\mathbb{P}^2 - \frac{i\hbar}{2}\mathcal{C} + \frac{m}{2}\omega^2(t)x^2\right). \quad (2.86)$$

Taking into account that $\mathcal{C}(t)$ does not depend on position and replacing $\omega^2(t)$ using Riccati equation (2.77) leads to

$$\frac{\partial}{\partial t}\mathbb{P} = -\mathbb{P}\mathcal{C} + m\dot{\mathcal{C}}x + m\mathcal{C}^2x. \quad (2.87)$$

These terms can be rearranged to yield

$$\frac{\partial}{\partial t}\ln\left(\mathbb{P} - m\mathcal{C}x\right) = -\mathcal{C} = -\frac{\partial}{\partial t}\ln\alpha - i\frac{1}{\alpha^2}. \quad (2.88)$$

Recalling that the logarithm of a complex number $z = |z|\exp(i\phi)$ is given by $\ln z = \ln|z| + i\phi$, Eq. (2.88) can be rewritten as,

$$\boxed{\frac{\partial}{\partial t}\ln\left|\mathbb{P} - m\mathcal{C}x\right| + i\frac{\partial}{\partial t}\tan^{-1}\left(\frac{\mathbb{P}_I - m\mathcal{C}_I x}{\mathbb{P}_R - m\mathcal{C}_R x}\right) = -\frac{\partial}{\partial t}\ln\alpha - i\frac{1}{\alpha^2}.} \quad (2.89)$$

Equating real and imaginary parts leads to two relations that have to be fulfilled,

$$\frac{\partial}{\partial t} \ln |P - m\mathcal{C}x| = \frac{\partial}{\partial t} \ln \frac{1}{\alpha} \quad (2.90)$$

and

$$\frac{\partial}{\partial t} \tan^{-1} \left(\frac{P_I - m\mathcal{C}_I x}{P_R - m\mathcal{C}_R x} \right) = -\frac{1}{\alpha^2}. \quad (2.91)$$

After integration, the real part leads to

$$\frac{|P - m\mathcal{C}x|}{|P_0 - m\mathcal{C}_0 x|} = \frac{\alpha_0}{\alpha} \quad (2.92)$$

or

$$\boxed{\alpha |P - m\mathcal{C}x| = \alpha_0 |P_0 - m\mathcal{C}_0 x|}, \quad (2.93)$$

and the imaginary part to

$$\tan^{-1} \left(\frac{P_I - m\mathcal{C}_I x}{P_R - m\mathcal{C}_R x} \right) = -\int_0^t \frac{1}{\alpha^2} dt', \quad (2.94)$$

where the lhs corresponds to the phase angle ϕ of the complex quantity z . The physical meaning of this angle will be discussed in the next Subsection.

Squaring the expressions in Eq. (2.93) leads to the quadratic invariant

$$\alpha^2 |P - m\mathcal{C}x|^2 = \alpha_0^2 |P_0 - m\mathcal{C}_0 x|^2. \quad (2.95)$$

Bearing in mind that according to (2.81) $P - m\mathcal{C}x = -m\mathcal{C}\eta + m\dot{\eta}$, Eq. (2.95) can be written as

$$\alpha^2 \left[(-m\mathcal{C}_R \eta + m\dot{\eta})^2 + (-m\mathcal{C}_I \eta)^2 \right] = \alpha_0^2 \left[(-m\mathcal{C}_R(0)\eta_0 + m\dot{\eta}_0)^2 + (-m\mathcal{C}_I(0)\eta_0)^2 \right], \quad (2.96)$$

what can be reduced to

$$(\dot{\alpha}\eta - \alpha\dot{\eta})^2 + \left(\frac{\eta}{\alpha}\right)^2 = (\dot{\alpha}_0\eta_0 - \alpha_0\dot{\eta}_0)^2 + \left(\frac{\eta_0}{\alpha_0}\right)^2. \quad (2.97)$$

In most cases, the classical initial position η_0 can be taken equal to zero, $\eta_0 = 0$, and $\dot{\eta}_0$ can in our case be expressed via the initial momentum as $\dot{\eta}_0 = \frac{p_0}{m}$. Then the rhs of (2.97) can be simplified to yield

$$(\dot{\alpha}\eta - \alpha\dot{\eta})^2 + \left(\frac{\eta}{\alpha}\right)^2 = \left(\frac{\alpha_0 p_0}{m}\right)^2. \quad (2.98)$$

The lhs is, apart from a factor of $\frac{1}{2}$, identical to the invariant found by Ermakov, but here neither without making use of the Newtonian equation for η nor of the nonlinear equation for α .

Instead, the ingredients that were needed for the above derivation of this invariant are the Hamiltonian equation of motion (2.85) for the complex Bohmian quantities and the complex Riccati equation (2.77).

2.3.2.2 Phase angles of the complex quantities

In the last Subsection the quantity $P - m\mathcal{C}x$ was identified with a complex number $z = |z| \exp(i\phi)$ that can also be written in Cartesian coordinates as $z = z_R + iz_I = |z| \cos \phi + i|z| \sin \phi$ with $\frac{z_I}{z_R} = \tan \phi$. Therefore, the lhs of Eq. (2.94) is just the phase angle ϕ of the complex quantity. In order to get an idea what the meaning of this angle is, the corresponding angle $-\int_0^t \frac{1}{\alpha^2} dt'$ on the rhs of Eq. (2.94) is now considered. How can this be related to the quantities we already know?

To answer this question the fact is used that a nonlinear Riccati equation can always be linearized replacing the Riccati-variable by a logarithmic derivative. In this case, an ansatz

$$\mathcal{C} = \frac{\dot{\lambda}}{\lambda} \quad (2.99)$$

leads to the linear second order Newtonian-type differential equation

$$\ddot{\lambda} + \omega^2(t)\lambda = 0 \quad (2.100)$$

for the complex variable $\lambda = \alpha \exp(i\phi) = u + iv = \alpha \cos \phi + i\alpha \sin \phi$. The choice of α for the amplitude of λ is not by chance, as can be seen inserting the polar form of λ into (2.99), leading to

$$\mathcal{C} = \frac{\dot{\alpha}}{\alpha} + i\dot{\phi}, \quad (2.101)$$

what would be in agreement with (2.78) if the relation

$$\dot{\phi} = \frac{1}{\alpha^2} \quad (2.102)$$

is fulfilled. This can be proven easily by inserting (2.101) into the complex Riccati equation (2.77) and checking the imaginary part of this equation. Relation (2.102), written in the form $\alpha^2 \dot{\phi} = 1$ looks again like a conservation law, this time the conservation of angular momentum for the motion of $\lambda(t)$ in the **complex** plane (for further details, see [Schuch(2018a), Schuch(1989)]). Therefore, the rhs of (2.94) turns into $-\int_0^t \dot{\phi} dt' = -(\phi(t) - \phi_0)$, *i.e.*, up to a minus sign and a constant initial angle ϕ_0 , it is just the phase angle of $\lambda(t)$.

Also the lhs of (2.94) can be related to λ . For this purpose the fact is used that the wave packet (2.75) can also be obtained by applying a time-dependent Green function $G(x, x', t, t')$ on an initial Gaussian wave packet, *i.e.*, $\psi(x, t) = \int dx' G(x, x', t, t') \psi(x', t')$. The time-dependent parameters occurring in the Green function can entirely be expressed in terms of $u(t)$ and $v(t)$, the real and imaginary parts of $\lambda(t)$. Comparing the wave packet obtained in this way with the form in (2.75) shows that

$$v = \frac{m}{\alpha_0 p_0} \langle x \rangle = \frac{m}{\alpha_0 p_0} \eta(t) \quad (2.103)$$

is valid (for further details, see [Schuch(2018a), Schuch(1989)]).

Multiplying Eq. (2.98) by $(\frac{m}{\alpha_0 p_0})^2$ and using $v = \alpha \sin \phi$ yields

$$\left(\frac{m}{\alpha_0 p_0}\right)^2 (\dot{\alpha} \eta - \alpha \dot{\eta})^2 + \sin^2 \phi = 1. \quad (2.104)$$

Therefore, the first term on the lhs must be $\cos^2 \phi = (\frac{u}{\alpha})^2$, leading to (up to a \pm sign)

$$u = \frac{m}{\alpha_0 p_0} (\dot{\eta} \alpha^2 - \eta \dot{\alpha} \alpha) \quad (2.105)$$

and hence to

$$\tan \phi = \frac{v}{u} = \frac{\eta}{\dot{\eta} \alpha^2 - \eta \dot{\alpha} \alpha} \quad (2.106)$$

Returning now to the lhs of Eq. (2.94), using expression (2.81) for P and the form (2.78) for \mathcal{L} , one can write,

$$\begin{aligned}\tan^{-1}\left(\frac{P_I - m\mathcal{C}_{Ix}}{P_R - m\mathcal{C}_{Rx}}\right) &= \tan^{-1}\left(\frac{-m\mathcal{C}_I\eta}{-m\mathcal{C}_R\eta + m\dot{\eta}}\right) \\ &= -\tan^{-1}\left(\frac{\eta}{\dot{\eta}\alpha^2 - \eta\dot{\alpha}\alpha}\right) = -\varphi,\end{aligned}\quad (2.107)$$

in agreement with $-\int \frac{1}{\alpha^2} dt' = -\int \dot{\varphi} dt'$ on the rhs of (2.94).

To summarize, the phase angle ϕ of the complex quantity $P - m\mathcal{C}x = z = |z|\exp(i\phi)$ is identical with the phase angle φ of the complex quantity $\lambda = \alpha\exp(i\varphi)$ whose logarithmic time-derivative is the variable of the Riccati equation (2.77), whose amplitude is proportional to the wave packet width and whose motion in the complex plane has an ‘‘angular momentum’’-type invariant according to $\alpha^2\dot{\varphi} = 1$.

2.3.3 Momentum representation

In this Section it is shown how to recover the results in momentum space that were obtained in position space in the previous Section. This is important, as the validity of a constant of motion should be independent of the chosen representation.

The quantum state in momentum space corresponding to (2.75) in position space can be obtained by Fourier transformation and can be written in the form

$$\langle p|\Psi(t)\rangle = N_p(t)\exp\left[-\frac{i}{\hbar}\left(\frac{1}{2m}\mathcal{U}\tilde{p}^2 + \eta\tilde{p} + g(t)\right)\right],\quad (2.108)$$

where $\tilde{p} = p - \langle p \rangle = p - m\dot{\eta}$ and the complex coefficient of \tilde{p}^2 is the inverse of the quantity $\mathcal{C}(t)$, fulfilling the Riccati equation (2.77), *i.e.*, $\mathcal{U} = \mathcal{C}^{-1}(t)$; the new symbol is used just for convenience. Also the dynamics of \mathcal{U} is ruled by a complex Riccati equation,

$$-\dot{\mathcal{U}} + \omega^2(t)\mathcal{U}^2 + 1 = 0\quad (2.109)$$

that turns into Eq. (2.77) if \mathcal{U} is replaced by \mathcal{C}^{-1} .

The Bohmian quantities [Bonilla(2020a)] for position, momentum and potential energy for these states, obtained according to (2.9), are given by

$$\boxed{P = p \quad \text{real}} \quad (2.110)$$

$$\boxed{X = \frac{1}{m} \mathcal{U} \tilde{p} + \eta \quad \text{complex}} \quad (2.111)$$

$$\boxed{V = \frac{1}{2} m \omega^2(t) \left[(X)^2 - \frac{\hbar}{i} \frac{\partial}{\partial p} X \right] = \frac{1}{2} m \omega^2(t) \left[(X)^2 + \frac{i\hbar}{m} \mathcal{U} \right].} \quad (2.112)$$

2.3.3.1 Dynamical invariants

The procedure is repeated as in Section 2.3.2.1, only in momentum space. As shown in [Bonilla(2021a)], in this space the Hamiltonian equation for the complex position is

$$\frac{\partial}{\partial t} X = \frac{\partial}{\partial p} H_p, \quad (2.113)$$

i.e., like the classical Hamiltonian equation of motion, but with complex position X and Hamiltonian $H_p = \frac{p^2}{2m} + V(X, \frac{\partial}{\partial p} X)$. For the coherent state (2.108) this leads to

$$\begin{aligned} \frac{\partial}{\partial t} X &= \frac{\partial}{\partial p} \left[\frac{p^2}{2m} + \frac{1}{2} m \omega^2(t) \left(X^2 + \frac{i\hbar}{m} \mathcal{U}(t) \right) \right] \\ &= \frac{p}{m} + m \omega^2(t) X \frac{\partial}{\partial p} X = \frac{p}{m} + \omega^2(t) X \mathcal{U}. \end{aligned} \quad (2.114)$$

Using $\mathcal{U}\mathcal{C} = 1$ and eliminating $\omega^2(t)$ with the help of Riccati equation (2.109), one obtains

$$\begin{aligned} \frac{\partial}{\partial t} X &= \frac{p}{m} + \omega^2(t) \mathcal{U}^2 \mathcal{C} X \\ &= \frac{p}{m} + (\mathcal{U}\dot{\mathcal{C}} - 1) \mathcal{C} X. \end{aligned} \quad (2.115)$$

Using expression (2.111) for the Bohmian position and again $\mathcal{U}\mathcal{C} = 1$, yields

$$\frac{\partial}{\partial t} X = \frac{p}{m} + \mathcal{U} \left(\frac{1}{m} (p - m\dot{\eta}) + \mathcal{C}\dot{\eta} \right) - \mathcal{C} X, \quad (2.116)$$

what can be rearranged to

$$\frac{\partial}{\partial t} \left(X - \mathcal{U} \frac{P}{m} \right) = \frac{P}{m} + \mathcal{U} \dot{\mathcal{C}} (-\dot{\eta} + \mathcal{C}\eta) - \mathcal{C}X. \quad (2.117)$$

With $\dot{\eta} = \mathcal{U} \mathcal{C} \dot{\eta}$ and $\frac{P}{m} = \mathcal{U} \mathcal{C} \frac{P}{m}$ as well as adding and subtracting $\mathcal{U} \frac{P}{m}$ this turns into

$$\frac{\partial}{\partial t} \left(X - \mathcal{U} \frac{P}{m} \right) = \left(\frac{1}{m} \mathcal{U} (P - m\dot{\eta}) + \eta - \mathcal{U} \frac{P}{m} \right) \mathcal{C} \mathcal{U} - \left(X - \mathcal{U} \frac{P}{m} \right) \mathcal{C}. \quad (2.118)$$

Applying $\dot{\mathcal{U}} = -\frac{\mathcal{C}}{\mathcal{C}^2}$ and the expression (2.111) for X allows to write this as

$$\frac{\partial}{\partial t} \left(X - \mathcal{U} \frac{P}{m} \right) = - \left(X - \mathcal{U} \frac{P}{m} \right) \frac{\dot{\mathcal{C}}}{\mathcal{C}} - \left(X - \mathcal{U} \frac{P}{m} \right) \mathcal{C} \quad (2.119)$$

or

$$\frac{\partial}{\partial t} \ln \left(X - \mathcal{U} \frac{P}{m} \right) = - \frac{\partial}{\partial t} \ln \mathcal{C} - \mathcal{C} \quad (2.120)$$

and finally, as m is not time-dependent, this can be expressed in the form

$$\frac{\partial}{\partial t} \ln \left(m \mathcal{C} X - P \right) = -\mathcal{C}. \quad (2.121)$$

Comparing this result with the corresponding one in position space, Eq. (2.88), shows

$$\boxed{\frac{\partial}{\partial t} \ln \left(P - m \mathcal{C} x \right) = -\mathcal{C} \quad \text{for x-representation}} \quad (2.122)$$

$$\boxed{\frac{\partial}{\partial t} \ln \left(m \mathcal{C} X - P \right) = -\mathcal{C} \quad \text{for p-representation,}} \quad (2.123)$$

or, using the expressions for the Bohmian quantities X and P,

$$\boxed{\frac{\partial}{\partial t} \ln \left(-m \mathcal{C} \eta + m \dot{\eta} \right) = -\mathcal{C} \quad \text{for the x-representation}} \quad (2.124)$$

$$\boxed{\frac{\partial}{\partial t} \ln \left(-m \dot{\eta} + m \mathcal{C} \eta \right) = -\mathcal{C} \quad \text{for the p-representation.}} \quad (2.125)$$

This means that the argument of the logarithm on the lhs is, up to a $+/-$ sign identical. Therefore, the absolute values of these two complex expressions and

thus the dynamical invariants as well as the ratio of imaginary and real parts, and thus the phase angles are identical too. This confirms that the invariants we obtained are independent of the representation.

The relation to the invariant $\alpha^2 \dot{\phi} = 1$, connected with the phase angle of the complex quantities discussed in Section 2.3.2.2, becomes more obvious if the rhs of Eq. (2.124) is written with help of (2.99) in the form

$$-\mathcal{C} = -\frac{\dot{\lambda}}{\lambda} = -\frac{\partial}{\partial t} \ln \lambda. \quad (2.126)$$

Comparing this with the lhs where the constant m is replaced by the constant $\frac{\alpha_0 p_0}{m}$ and using $\frac{\alpha_0 p_0}{m} \eta = z$, Eq. (2.124) can be rewritten as

$$\frac{\dot{\lambda}}{\lambda} z - \dot{z} = \frac{1}{\lambda} \quad (2.127)$$

or

$$\dot{\lambda} z - \dot{z} \lambda = 1 = \dot{u} z - \dot{z} u + i(\dot{z} z - \dot{z} z). \quad (2.128)$$

Keeping in mind that $z = \alpha \sin \varphi$ and $u = \alpha \cos \varphi$ leads to

$$\dot{u} z - \dot{z} u = \alpha^2 \dot{\phi} = 1, \quad (2.129)$$

i.e., the conservation law (2.102) written in the “cartesian coordinates” z and u in the complex plane.

As relation (2.125) for the momentum representation differs from Eq. (2.124) only by a constant factor -1 , the same applies to this expression.

2.3.4 Linear potential

In this Section, the dynamical invariant associated with a linear potential $\hat{V} = -E\hat{X}$ along the x -axis is obtained. For that purpose, the quantities (2.12-2.15) for a general coherent state (2.75) are computed,

$$\boxed{X = x \quad \text{real}} \quad (2.130)$$

$$\boxed{P = m\mathcal{C}\tilde{x} + \langle p \rangle \quad \text{complex}} \quad (2.131)$$

$$\boxed{V = -Ex} \quad (2.132)$$

$$\boxed{T = \frac{1}{2m} \left((P)^2 - i\hbar m\mathcal{C} \right)}. \quad (2.133)$$

In analogy to Section 2.3.2.1 one can proceed by handling Eq. (2.63) taking into account these Bohmian quantities. Therefore,

$$\frac{\partial}{\partial t} P = -\frac{\partial}{\partial x} \left(\frac{1}{2m} P^2 - \frac{i\hbar}{2} \mathcal{C} - Ex \right), \quad (2.134)$$

$$\frac{\partial}{\partial t} P = -\frac{P}{m} \frac{\partial}{\partial x} P + E, \quad (2.135)$$

or

$$\frac{\partial}{\partial t} P = -P\mathcal{C} + E. \quad (2.136)$$

For the case of a linear potential, it is clear that as $\frac{\partial^2 V}{\partial x^2} = 0$, then the potential does not contribute to the Riccati equation; therefore, the Riccati equation imposes $\dot{\mathcal{C}} + \mathcal{C}^2 = 0$. This helps to simplify the previous equation by adding a zero:

$$\frac{\partial}{\partial t} P = -P\mathcal{C} + m(\dot{\mathcal{C}} + \mathcal{C}^2)x + E, \quad (2.137)$$

$$\frac{\partial}{\partial t} (P - m\mathcal{C}x) = -(P - m\mathcal{C}x)\mathcal{C} + E. \quad (2.138)$$

Due to the presence of E from the linear contribution of the potential, the differential equation is not separable anymore unlike in the case of the parametric oscillator. Indeed, expressing \mathcal{C} as a logarithmic derivative of a complex function λ , $\mathcal{C} = \frac{d}{dt} \ln \lambda$ (see Appendix A) allows us to write down

$$\frac{\partial}{\partial t} \left(\lambda (P - m\mathcal{C}x) \right) = E\lambda. \quad (2.139)$$

By direct integration and taking the absolute square

$$\left| \lambda (P - m\mathcal{C}x) \right|^2 = E^2 \left| \int_0^t \lambda dt' \right|^2, \quad (2.140)$$

one can see that the definite integral on the rhs cannot be evaluated until the magnitude and phase of $\lambda = \alpha \exp [i\varphi]$ are specified. This means, that the Ermakov quantity is not a constant of motion for the generalized coherent states under the influence of a **stationary linear potential**.

$$I_{\text{Ermakov}} = \frac{E^2}{2} \left| \int_0^t \lambda dt' \right|^2 \neq \text{const.} \quad (2.141)$$

Nevertheless, one may drop the assumption of stationarity of E , $E = \text{const}$, and assume, based on Eq. (2.139), the following form for the potential parameter E ,

$$E(t) = \kappa \frac{\phi}{\alpha}, \quad (2.142)$$

where $\phi = \frac{1}{\alpha^2}$ (see Appendix A) and κ represents the (constant) strength of the potential in the units $g \cdot cm \cdot s^{-2}$. With this expression, the integration of Eq. (2.139) turns into,

$$\frac{\partial}{\partial t} \left(\lambda (P - m\mathcal{E}x) \right) = \kappa \frac{\phi}{\alpha} \lambda, \quad (2.143)$$

where $\lambda = \alpha \exp \left[i \int \frac{1}{\alpha^2} dt' \right] = \alpha \exp [i\varphi]$. Therefore, it is straightforward to obtain the following expression,

$$\frac{\partial}{\partial t} \left(\lambda (P - m\mathcal{E}x) \right) = \kappa \phi \exp [i\varphi], \quad (2.144)$$

and after direct integration in time,

$$\lambda (P - m\mathcal{E}x) - \lambda_0 (P_0 - m\mathcal{E}_0x) = \frac{\kappa}{i} \exp [i\varphi] - \frac{\kappa}{i} \exp [i\varphi_0] \quad (2.145)$$

or

$$\lambda (P - m\mathcal{E}x) - \lambda_0 (P_0 - m\mathcal{E}_0x) = \frac{\kappa}{i\alpha} \lambda - \frac{\kappa}{i\alpha_0} \lambda_0, \quad (2.146)$$

leading to

$$\lambda \left(P - m\mathcal{E}x + i \frac{\kappa}{\alpha} \right) = \lambda_0 \left(P_0 - m\mathcal{E}_0x + i \frac{\kappa}{\alpha_0} \right). \quad (2.147)$$

Using, as before, $P - m\mathcal{C}x = m\dot{\eta} - m\mathcal{C}\eta$ and \mathcal{C} in the form (2.78), after taking the square of the magnitude, one obtains

$$\alpha^2 \left[(m\dot{\eta} - m\frac{\dot{\alpha}}{\alpha}\eta)^2 + \left(\frac{\kappa}{\alpha} - m\frac{1}{\alpha^2}\eta \right)^2 \right] = \text{const} \quad (2.148)$$

or

$$(m\alpha\dot{\eta} - m\dot{\alpha}\eta)^2 + \left(m\frac{\eta}{\alpha} \right)^2 + \kappa^2 - 2\kappa m\frac{\eta}{\alpha} = \text{const}. \quad (2.149)$$

Dividing by m^2 and taking into account that κ and m are constants, the equation might be rewritten directly as

$$(\alpha\dot{\eta} - \dot{\alpha}\eta)^2 + \left(\frac{\eta}{\alpha} \right)^2 - 2\frac{\kappa}{m}\frac{\eta}{\alpha} = \text{const}. \quad (2.150)$$

It is worth noticing that if the time-dependent linear potential has the form $V = -\kappa\phi\frac{1}{\alpha}\widehat{X}$, its associated Ermakov invariant $I_{\text{Ermakov, LP}}$ differs from the Ermakov invariant of the parametric oscillator (see Eq. (2.98)) $I_{\text{Ermakov, PO}}$ in the following way

$$I_{\text{Ermakov, LP}} = I_{\text{Ermakov, PO}} - \frac{\kappa}{m}\frac{\eta}{\alpha} = \text{const}. \quad (2.151)$$

This result depends clearly on the choice of the structure of E to ensure the integrability of Eq. (2.139). For further details see [Schuch(2018a)] page 61.

In a nutshell, for the generalized coherent states the Ermakov invariants can be obtain for the parametric oscillator in the form $I_{\text{Ermakov, PO}} = \frac{1}{2} \left((\dot{\alpha}\eta - \alpha\dot{\eta})^2 + \left(\frac{\eta}{\alpha} \right)^2 \right)$. For the case of a linear potential, the Ermakov invariant takes the form $I_{\text{Ermakov, LP}} = \frac{1}{2} \left((\dot{\alpha}\eta - \alpha\dot{\eta})^2 + \left(\frac{\eta}{\alpha} \right)^2 \right) - \frac{\kappa}{m}\frac{\eta}{\alpha}$, as long as the linear potential has the following structure: $V = -\kappa\phi\frac{1}{\alpha}\widehat{X}$.

2.4 Uncertainties

2.4.1 Quantum potential

Let us reinterpret the so called ‘‘quantum potential’’ within our approach. It is known [Holland(1995)], within the conventional Bohmian mechanics, that the

mHJE is written with help of the quantum potential $V_{qu,x}$, see for instance Eq. (2.4), as

$$-\frac{\partial}{\partial t}S_x = \frac{\left(\frac{\partial}{\partial x}S_x\right)^2}{2m} + V_{qu,x} + V. \quad (2.152)$$

This is basically Eq. (2.10) corresponding to the real part of the Bohmian Hamiltonian defined through (2.9). That means that the quantum potential is related to our Bohmian quantities, according to (2.15) via

$$\boxed{V_{qu,x} = T_R - \frac{\left(\frac{\partial}{\partial x}S_x\right)^2}{2m}}. \quad (2.153)$$

Let us now express the “quantum potential” via the momentum uncertainty. The momentum uncertainty σ_p^2 is given by

$$\sigma_p^2 = \langle \psi | \hat{P}^2 | \psi \rangle - \langle p \rangle^2, \quad (2.154)$$

what can be rearranged to,

$$\sigma_p^2 = \int \langle \psi | x \rangle \langle x | \psi \rangle \frac{\langle x | \hat{P}^2 | \psi \rangle}{\langle x | \psi \rangle} dx - \langle p \rangle^2, \quad (2.155)$$

and, bearing in mind the definition of the complex Bohmian quantities (2.9) $T = \frac{1}{2m} \frac{\langle x | \hat{P}^2 | \psi \rangle}{\langle x | \psi \rangle}$, expressed as

$$\sigma_p^2 = 2m \int \rho_x T dx - \langle p \rangle^2. \quad (2.156)$$

Besides, we must not forget that the mean value of the imaginary parts of the complex Bohmian quantities are zero. Therefore, the integral is simplified to

$$\sigma_p^2 = 2m \int \rho_x T dx - \langle p \rangle^2. \quad (2.157)$$

Let us now use expression (2.153),

$$\sigma_p^2 = \int \rho_x \left[\left(\frac{\partial}{\partial x} S_x \right)^2 - \langle p \rangle^2 + 2m V_{qu,x} \right] dx, \quad (2.158)$$

or

$$\sigma_p^2 = \sigma_{\text{cl},p}^2 + \underbrace{2m \int \rho_x V_{qu,x} dx}_{\text{quantum contribution}}, \quad (2.159)$$

where the “classical uncertainty” $\sigma_{\text{cl},p}^2$ is denoted by

$$\sigma_{\text{cl},p}^2 = \int \rho_x \left[\left(\frac{\partial}{\partial x} S_x \right)^2 - \langle p \rangle^2 \right] dx. \quad (2.160)$$

A similar argument can be used in the momentum space. In that case, the mHJ equation (2.33) contains again a term which is responsible for the deviation from the classical case. For symmetry purposes, we will refer to it as “quantum potential in momentum space” $V_{qu,p}$,

$$V_{qu,p} = \frac{1}{2} m \omega^2(t) [X^2]_R - \frac{1}{2} m \omega^2(t) \left(\frac{\partial}{\partial p} S_p \right)^2. \quad (2.161)$$

In analogy to the position space, for the momentum space we have to recall also the complex Bohmian quantities (2.9) when computing the position uncertainty. Then, the position uncertainty σ_x , calculated in momentum space, is given by

$$\sigma_x^2 = \sigma_{\text{cl},x}^2 + \underbrace{\frac{2}{m\omega^2} \int \rho_p V_{qu,p} dp}_{\text{quantum contribution}}, \quad (2.162)$$

where the position uncertainty σ_x exhibits a structure similar to the momentum uncertainty σ_p : there is a “classical” term and a contribution from quantum nature. The “classical uncertainty” $\sigma_{\text{cl},x}$ is given by,

$$\sigma_{\text{cl},x}^2 = \int \rho_p \left(\left(\frac{\partial}{\partial p} S_p \right)^2 - \langle x \rangle^2 \right) dp. \quad (2.163)$$

Up to this point, it is worth noticing that, for both the position and momentum spaces, the so-called “quantum potentials” in Bohmian mechanics are not interactions with the system as Bohm suggested in his first publications about the topic

[Bohm(1952a), Bohm(1952b)]. On the contrary, according to (2.159) and (2.162) it is clear that those terms are the manifestation of the quantum fluctuations for the kinetic and potential energy respectively. Notice that the conventional Bohmian mechanics is able to split the structure of the position uncertainty into two parts as it is shown in Eq. (2.162). It gives though the impression that that structure is only possible in the position space due to the lack of a formulation in the momentum space. Nevertheless, the Bohmian extension proposed in this thesis is useful to show that there is a structural symmetry between the position and the momentum spaces as it can be seen in the expressions of the momentum (2.159) and the position (2.162) uncertainties. Furthermore, it shows that the quantum contributions of the mHJ equations are responsible for the difference between the “classical” and quantum expression of the uncertainties.

2.4.2 Heisenberg principle

Up to date there is no treatment of the Heisenberg principle within Bohmian mechanics. This is due to the fixation with the trajectories in position space. This makes it more difficult or even prevents to approach such a simple and fundamental relation as the Heisenberg uncertainty principle. Now, with the proposed Bohmian scheme in this thesis, that relation is, according to (2.159) and (2.162), easily expressed as follows,

$$\sigma_x^2 \sigma_p^2 = \left(\sigma_{\text{cl},x}^2 + \frac{2}{m\omega^2} \int \rho_p V_{qu,p} dp \right) \left(\sigma_{\text{cl},p}^2 + 2m \int \rho_x V_{qu,x} dx \right) \geq \frac{\hbar^2}{4}.$$

(2.164)

Let us illustrate this relation by considering a general coherent state in position space (A.1) as well as in momentum space (A.21). For those states, the phase is given by

$$S_x = \frac{m}{2} \mathcal{C}_R \tilde{x}^2 + \langle p \rangle \tilde{x} + K(t), \quad (2.165)$$

$$S_p = -\frac{1}{2m} \mathcal{U}_R \tilde{p}^2 - \langle x \rangle \tilde{p} + L(t), \quad (2.166)$$

with the \mathcal{C}_R and \mathcal{U}_R being the real parts of the Riccati variable associated to the position and momentum space, respectively. Bear in mind that they are related by $\mathcal{U} = \frac{1}{\mathcal{C}}$. Now, after taking the derivatives, their squares are

$$\left(\frac{\partial}{\partial x} S_x\right)^2 = m^2 \mathcal{C}_R^2 \tilde{x}^2 + 2m \mathcal{C}_R \langle p \rangle \tilde{x} + \langle p \rangle^2, \quad (2.167)$$

$$\left(\frac{\partial}{\partial p} S_p\right)^2 = \frac{1}{m^2} \mathcal{U}_R^2 \tilde{p}^2 + \frac{2}{m} \mathcal{U}_R \langle x \rangle \tilde{p} + \langle x \rangle^2. \quad (2.168)$$

Considering that the uncertainties are defined as $\sigma_x^2 \doteq \langle \tilde{x}^2 \rangle$ and $\sigma_p^2 \doteq \langle \tilde{p}^2 \rangle$ and $\langle \tilde{x} \rangle = \langle \tilde{p} \rangle = 0$, one can directly compute the ‘‘classical uncertainties’’, taking into account the expressions (2.160) and (2.163),

$$\sigma_{\text{cl},p}^2 = m^2 \mathcal{C}_R^2 \sigma_x^2 = \frac{\mathcal{C}_R^2}{|\mathcal{C}|^2} \sigma_p^2 = \mathcal{C}_R \mathcal{U}_R \sigma_p^2, \quad (2.169)$$

$$\sigma_{\text{cl},x}^2 = \frac{1}{m^2} \mathcal{U}_R^2 \sigma_p^2 = \mathcal{U}_R^2 |\mathcal{C}|^2 \sigma_x^2 = \mathcal{C}_R \mathcal{U}_R \sigma_x^2. \quad (2.170)$$

Notice that the relation between the position and momentum uncertainties $\sigma_p^2 = m^2 |\mathcal{C}|^2 \sigma_x^2$ was used (see Appendix A, Eq. (A.8)).

Regarding the position space, Eq. (2.159) and (2.169) allow to compute the quantum contribution of the fluctuations of kinetic energy according to (2.171). Concerning the momentum space, similarly, Eq. (2.162) together with Eq. (2.170) yield the quantum contribution for the fluctuation of potential energy, (2.172),

$$2m \int \rho_x V_{qu,x} dx = m^2 \mathcal{C}_I^2 \sigma_x^2 = \frac{\mathcal{C}_I^2}{|\mathcal{C}|^2} \sigma_p^2 = \mathcal{C}_I \mathcal{U}_I \sigma_p^2, \quad (2.171)$$

$$\frac{2}{m\omega^2} \int \rho_p V_{qu,p} dp = \frac{1}{m^2} \mathcal{U}_I^2 \sigma_p^2 = \mathcal{U}_I^2 |\mathcal{C}|^2 \sigma_x^2 = \mathcal{C}_I \mathcal{U}_I \sigma_x^2. \quad (2.172)$$

In this way we can easily identify that the quantum effect in the uncertainty is related not only with the spreadings σ_x and σ_p , but also with their spreading speed $\dot{\sigma}_x$ and $\dot{\sigma}_p$ through the real part $\mathcal{C}_R = \frac{\dot{\sigma}_x}{\sigma_x}$ occurring in $|\mathcal{C}|^2 = \mathcal{C}_R^2 + \mathcal{C}_I^2$.

Besides, with the proposed scheme we can fully identify the contribution to the spreadings. For instance, in the case of a **stationary bound state under the action**

of a symmetrical potential, the classical contributions cancel out, *i.e.*, $\sigma_{x,cl} = 0$ and $\sigma_{p,cl} = 0$; hence the spreadings are due to quantum effects via the “quantum potentials”. That is why the study of the quantum potentials allows the access to the information of the spreading of the bound stationary states under the action of symmetrical potentials. It is not related though, as conventional Bohmian mechanics suggests, to a “special kind of force”; but rather comes from fluctuations of the kinetic and potential energies.

2.5 Summary

■ In Section 2.1, it was shown that the controversy regarding the formulation of Bohmian mechanics in momentum representation is still of interest, see Table 2.2.

■ In Section 2.2, by means of the polar decomposition (2.6), complex Bohmian quantities were defined according to (2.9) for position and momentum representation:

Observable	Position representation	Momentum representation
X	x	$-\frac{\partial}{\partial p}S_p + i\frac{\hbar}{2}\frac{\partial}{\partial p}\frac{\rho_p}{\rho_x}$
P	$\frac{\partial}{\partial x}S_x - i\frac{\hbar}{2}\frac{\partial}{\partial x}\frac{\rho_x}{\rho_p}$	p
V	$a + bx + \frac{1}{2}m\omega^2x^2$	$a + bX + \frac{1}{2}m\omega^2\left((X)^2 + i\hbar\frac{\partial}{\partial p}X\right)$
T	$\frac{1}{2m}\left((P)^2 - i\hbar\frac{\partial}{\partial x}P\right)$	$\frac{p^2}{2m}$

Advantages for using the Bohmian formulation in the momentum representation were illustrated with a linear potential for stationary states.

■ In Section 2.3, it was found that even if the mHJE in Bohmian mechanics suggest a Hamiltonian structure, it is not the case due to the absence of canonical conjugate variables. However, the complex dynamical equations are similar to the Newtonian counterparts,

$$\underbrace{\left\{\frac{\partial}{\partial t} + \dot{Q}\frac{\partial}{\partial x}\right\}}_{=\frac{D}{Dt}}P = -\frac{\partial}{\partial x}V - \underbrace{\frac{i\hbar}{2}\frac{\partial^2}{\partial x^2}P}_{\text{quantum contribution}} \quad \text{in the } x\text{-space,} \quad (2.173)$$

$$\underbrace{\left\{\frac{\partial}{\partial t} + \dot{P}\frac{\partial}{\partial p}\right\}}_{=\frac{D}{Dt}}X = \frac{p}{m} + \underbrace{i\hbar\frac{m\omega^2}{2}\frac{\partial^2}{\partial p^2}X}_{\text{quantum contribution}} \quad \text{in the } p\text{-space,} \quad (2.174)$$

These equations reveal to be useful to find constants of motion, *e.g.* the Ermakov invariant, for time dependent states such as the generalized coherent states.

■ In Section 2.4 the quantum potential, within our scheme, occurred to be related with the quantum contribution to the position and momentum uncertainties,

	Position uncertainty	Momentum uncertainty
Classical contribution	$\int \rho_p \left(\left(\frac{\partial}{\partial p} S_p \right)^2 - \langle x \rangle^2 \right) dp$	$\int \rho_x \left(\left(\frac{\partial}{\partial x} S_x \right)^2 - \langle p \rangle^2 \right) dx$
Quantum contribution	$2m \int \rho_x V_{qu,x} dx$	$\frac{2}{m\omega^2} \int \rho_p V_{qu,p} dp$
Quantum potential	$T_R - \frac{\left(\frac{\partial}{\partial x} S_x \right)^2}{2m}$	$\frac{1}{2} m \omega^2(t) [X^2]_R - \frac{1}{2} m \omega^2(t) \left(\frac{\partial}{\partial p} S_p \right)^2$

Besides, the Heisenberg principle was stated in Eq. (2.164) and illustrated through the consideration of a general coherent state.

Chapter 3

Bohmian trajectories

Objective

As stated in Chapter 1, Bohmian mechanics can be formulated save and sound through the conventional quantum mechanics using simple and useful mathematical tools. Regarding the Bohmian trajectories (the milestone of Bohmian mechanics), there has been a lot of reluctance and suspicion towards it because it presents (according to the typical Bohmian mechanics) a two fold inconvenience: Using the Bohmian trajectories would imply accepting two additional postulates, *i.e.*, the guidance law and the equilibrium hypothesis; furthermore they need to be regarded as real objects. Nevertheless, they have proven to be very useful in numerical simulations for hard problems, what otherwise would be very time-consuming. Since the usefulness of such objects has been proven over the time, it is worth reformulating these trajectories in a way that fits in with the conventional framework of quantum mechanics, so that this useful tool can find its right place within the theoretical apparatus, without the need of additional postulates or even rhetorical reasoning.

In this chapter the focus is on the correct formulation of Bohmian trajectories. In Section 3.1 the status quo and scope of these trajectories is briefly recalled. In Section 3.2, on the other hand, it is shown that the continuity equation in quantum mechanics is the starting point to overcome all the rhetorical and philosophical problems regarding the Bohmian trajectories. Next, in Section 3.3 a clear and simple link to conventional quantum mechanics is found with the help of the Wigner function. The proposed approach to the Bohmian trajectories is illustrated in Section 3.4 by applying it to an ion trap, as example.

keywords

Bohmian mechanics, Bohmian trajectories, quantile motion.

3.1 Overview

3.1.1 *Conventional Bohmian trajectories*

Bohmian mechanics originated as a deterministic alternative to the (probabilistic) Copenhagen interpretation of quantum mechanics. The latter states that individual detections cannot be predicted, *e.g.*, due to uncontrollable interactions between the object and the measurement apparatus. Therefore, conventional quantum mechanics only determines the statistical outcome of a well-defined experiment on the microscopic scale [Bohr(1948)].

On the other hand, since its creation in 1952 the Bohmian school [Bohm(1952a), Bohm(1952b)] claims that the individual detections can actually be predicted and are related to a geometrical path in configuration space that they call “Bohmian trajectory”. As Bohm points out [Bohm(1952a)], it is then stated that the microscopic systems do follow those trajectories. Since the works of Bohm there is the hope that technical advances will enable the detection of those trajectories.

Besides the interpretative character of Bohmian mechanics, it is clear that Bohmian trajectories are fundamental elements of Bohm’s framework. Nevertheless, one gets the impression that within the Bohmian community there is no real consensus what a Bohmian trajectory is, not to mention a clear physical picture of its origin.

A quantum optical experiment by Alain Aspect [Aspect(1976)] showing a violation of Bell’s inequalities as well as more recent experiments with Stern–Gerlach interferometers [Englert(1992), Scully(1998)] indicate that the original idea of Bohm that his trajectories are indeed the paths that particle follow and provide an additional parameter to conventional quantum mechanics is not correct, as it is not in agreement with experimental results. Does this mean that the Bohmian theory has completely lost its foundation?

There is a meaningful alternative in the literature, the relationship between Bohmian trajectories and the cumulative probability function (CPF) used in statistics. In 1996, Oriols [Oriols(1996)] suggested the treatment of Bohmian trajec-

ries using the complementary CPF, $\int_x^\infty |\psi(x',t)|^2 dx'$, in order to study dwelling times in tunneling problems. The idea is strongly based on the noncrossing property of the Bohmian trajectories. Shortly after, in 1998, Brandt [Brandt(1998)] and more recently Coffey *et al.* [Coffey(2008)] pointed out that the dynamics defined via the above-mentioned integral expression matches the dynamics of the Bohmian trajectory, provided the continuity equation is fulfilled. However, in either case, a clear mathematical link between conventional quantum theory, Bohmian mechanics and the suggested definition of Bohmian trajectories is missing.

The question that has to be answered is therefore, what is actually a Bohmian trajectory if it is not a particle's trajectory and how can the answer be formulated mathematically consistent and in a clear physical picture. In the present work it is tried to rehabilitate the concept of Bohmian trajectories by removing all unnecessary metaphysical ballast. Instead, it is proven how these trajectories arise naturally from the conventional theory, so Bohm's approach is nothing but another alternative formulation for studying quantum systems. Further, it is shown how to define properly Bohmian trajectories in position and momentum representation without the need of any Bohmian postulate like quantum equilibrium hypothesis or guidance law [Holland(1995)].

3.1.2 Problems with the conventional definition of the Bohmian trajectories

The concept of Bohmian trajectories has its origin in the pilot wave theory of de Broglie [Solvay(1928)] in 1927 and was later adopted (independently of de Broglie's work) by Bohm [Bohm(1952a), Bohm(1952b)] in 1952. In Bohmian mechanics a system is not only described by its wave function that obeys the Schrödinger equation but in addition by its configuration, *i.e.*, the position coordinates of "quantum objects". These are considered as "particles" with well-defined positions. For historical reasons these additional properties are called "hidden variables", although in the Bohmian interpretation they should be actually the observables. The time-evolution of the (particle) positions is determined by an additional first order differential equation, the so-called guiding (or guidance) equation (see Eq. (2.1)). As we saw in Section 2.1.1, this equation is obtained when

one expresses the wave function¹ in polar form as shown in Eq. (2.3). In analogy to the classical Hamilton–Jacobi theory and in agreement with conventional quantum mechanics, the quantity,

$$v \doteq \frac{1}{m} \frac{\partial}{\partial x} S(x, t) \quad (3.1)$$

is interpreted as a “velocity”, actually the velocity that appears in the CE (2.5) for the density $\rho(x, t) = \psi^*(x, t)\psi(x, t)$, namely

$$\frac{\partial}{\partial t} \rho(x, t) + \frac{\partial}{\partial x} [\rho(x, t)v(x, t)] = 0. \quad (3.2)$$

What is now the meaning of this velocity? It cannot be $\frac{d}{dt}x$, as x is the independent variable of the Schrödinger equation, therefore $\frac{d}{dt}x = 0$. But it is also not the classical velocity, *i.e.*, the time-derivative of the classical trajectory $\frac{d}{dt}\langle x \rangle$ (where $\langle x \rangle$ denotes the mean value of position). This is quite obvious considering the Gaussian wave packet solutions of the time-dependent Schrödinger equation, what will be shown explicitly in Section 6. Therefore, it is assumed that the velocity on the lhs of Eq. (3.1) is the time-derivative of the Bohmian trajectory that we will write in the following as $q(t)$, changing (3.1) into

$$\frac{d}{dt}q(t) \doteq \frac{1}{m} \frac{\partial}{\partial x} S(x, t). \quad (3.3)$$

However, in Bohmian mechanics the equation of motion for the Bohmian trajectory is given, without further justification, as

$$\boxed{\frac{d}{dt}q(t) = \frac{1}{m} \frac{\partial}{\partial x} S(x, t) \Big|_{x=q(t)}}, \quad (3.4)$$

that means, just like a *deus ex machina* the independent variable x of the action S turns into the time-dependent Bohmian trajectory $q(t)$.

Despite this inconsistency in the definition of the Bohmian trajectories, the theory seems nevertheless to be able to reproduce the results of conventional quantum mechanics. In the following it will be shown under what conditions the replacement in (3.4) is justified and what the physical and mathematical consequences are.

¹ We restrict the discussion to one spatial dimension.

3.2 Proposed definition

3.2.1 Proposal of a correct definition of the Bohmian trajectories

To illustrate our idea how to obtain the guidance law in a correct consistent way, starting point is a little digression into thermodynamics.

Box 3.2.1 Maxwell relations

In thermodynamics it is always possible to construct a total differential of a function that represents a thermodynamic property of the system if Maxwell's relations are fulfilled. For a gas described by the variables volume V and entropy S (This symbol should not be confused with the one for the phase of the wave function, $S(x,t)$), the function $U(V,S)$ is the internal energy, the pressure P and the temperature T have to fulfill the Maxwell relations

$$\frac{\partial P}{\partial S} = -\frac{\partial T}{\partial V} \quad (3.5)$$

(where in each case the variable that is not the one of the partial derivative is kept constant) and the total differential is given by the expression

$$dU = -PdV + TdS. \quad (3.6)$$

This allows a parametrization of some processes; they can be “iso-energetic” for $U = \text{const}$, “isometric” for $V = \text{const}$ or “iso-entropic” for $S = \text{const}$. For instance, the Joule expansion of a gas is an iso-energetic process, *i.e.* $U = \text{const}$. Therefore, for this process $dU = 0$ is valid and one has to consider all the points in the (S,V) -space that fulfill this condition, *i.e.*,

$$0 = -P|_{U=\text{const}}dV|_{U=\text{const}} + T|_{U=\text{const}}dS|_{U=\text{const}}. \quad (3.7)$$

Considering not the whole (S,V) -space anymore, but only the subspace that fulfills the constraint $U = \text{const}$, one can introduce the following parametrization:

$$(\mathcal{S}, V)|_{U=\text{const}} \longrightarrow (\sigma, V) \quad (3.8)$$

with $\sigma = \sigma(V)$. It is important to mention that σ is no longer the independent variable \mathcal{S} , but a dependent variable in the subspace where U is constant. This parametrization allows to rewrite Eq. (3.7) in the form

$$0 = -PdV + Td\sigma(V), \quad (3.9)$$

or

$$Td\sigma(V) = PdV. \quad (3.10)$$

Since the temperature never reaches absolute zero, one can divide by T to obtain

$$d\sigma(V) = \frac{P}{T}dV, \quad (3.11)$$

or finally

$$\frac{d\sigma(V)}{dV} = \frac{P}{T}. \quad (3.12)$$

The specific form of the solutions of this equation depends on the equation of state of the system. For an ideal gas this is given by

$$PV = nRT \quad (3.13)$$

with R being the gas constant and n the mole number, turning Eq. (3.12) into

$$\frac{d\sigma(V)}{dV} = \frac{nR}{V}. \quad (3.14)$$

After integration one obtains the well-known result for the entropy change in the Joule free expansion of an ideal gas,

$$\sigma(V) = \sigma(V_0) + nR \ln \left(\frac{V}{V_0} \right), \quad (3.15)$$

i.e., logarithmic curves in the (S, V) -space parametrized by $\sigma = \sigma(V)$ for a given value of U . The key elements to obtain this family of curves are the Maxwell relations (3.5), the parametrization (3.8) in the considered space and the equation of state (3.13) of the system.

Following the same line of reasoning it will now be shown how to obtain the Bohmian trajectories in a consistent way. For this purpose one has to keep in mind that in quantum mechanics the probability density $\rho(x, t) = \psi^*(x, t)\psi(x, t)$ fulfills the CE (3.2) that is obtained from the imaginary part of the Schrödinger equation if the polar form of the wave function, $\psi(x, t) = \sqrt{\rho(x, t)} \exp\left[\frac{i}{\hbar}S(x, t)\right]$ is inserted. The CE, however, can also be written in the form

$$\boxed{\frac{\partial \rho(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[\rho(x, t) \frac{\partial S(x, t)}{m} \right]} \quad (3.16)$$

that reminds of the Maxwell relation (3.5) only P and S replaced by ρ and t as well as T and V by $\rho(x, t) \frac{1}{m} \frac{\partial S(x, t)}{\partial x}$ and x .

Therefore, using the same mathematical arguments, one can formulate a total differential for a function $B(x, t)$ that is called in the following “Bohm function” in the form²

$$\boxed{dB(x, t) = \left[-\rho(x, t) \frac{1}{m} \frac{\partial S(x, t)}{\partial x} \right] dt + \rho(x, t) dx.} \quad (3.17)$$

One should keep in mind that B is still a function of the independent variables x and t . In analogy to the thermodynamic example, now the case $B = \text{const}$ is interesting, leading with $dB = 0$ from (3.17) to

$$\begin{aligned} 0 = & -\rho(x, t) \Big|_{B=\text{const}} \frac{1}{m} \frac{\partial S(x, t)}{\partial x} \Big|_{B=\text{const}} dt \Big|_{B=\text{const}} \\ & + \rho(x, t) \Big|_{B=\text{const}} dx \Big|_{B=\text{const}}. \end{aligned} \quad (3.18)$$

² Compared with Eq. (3.6), the rhs of (3.17), is multiplied by minus one. This does not change the following results, as they are based on Eq. (3.9) where the lhs is equal to zero. The form in (3.17) is chosen to be consistent with the definition of the CPF. The opposite sign would lead to the complementary CPF that is used by Brandt *et al.* [Brandt(1998)] and simply defined via 1–CPF.

Now, one needs to find the parametrization of every point in the (x,t) -space that belongs to the geometric locus where B is constant. This locus will be called Bohmian trajectory in position representation,

$$\boxed{(x,t)|_{B=\text{const}} \longrightarrow (q,t),} \quad (3.19)$$

with $q = q(t)$, so that (3.18) turns into

$$0 = -\rho(q,t) \frac{1}{m} \frac{\partial}{\partial q} S(q,t) dt + \rho(q,t) dq \quad (3.20)$$

or

$$\rho(q,t) dq = \rho(q,t) \frac{1}{m} \frac{\partial}{\partial q} S(q,t) dt. \quad (3.21)$$

As $\rho(q,t)$ cancels on both sides, this can finally be written in the form

$$\frac{dq}{dt} = \frac{1}{m} \frac{\partial}{\partial q} S(q,t), \quad (3.22)$$

an expression that is identical with the guidance law (3.4), but without the unjustified *ad hoc* replacement $x \longrightarrow q(t)$. That means, the continuity equation (3.16) and the parametrization (3.19) are the true origin of the Bohmian trajectories, not a simple substitution, as commonly claimed. Therefore, the current assumption of Bohmian trajectories being paths of particles that can be observed is not correct.

It is straightforward to see that the Bohm function $B(x,t)$ in coordinate representation is identical with the CPF, *i.e.*,

$$\boxed{B(x,t) = \int_{-\infty}^x \rho(x',t) dx'} \quad (3.23)$$

with the partial derivatives

$$\frac{\partial}{\partial x} B = \rho(x,t) - \rho(-\infty,t) = \rho(x,t), \quad (3.24)$$

as ρ vanishes for $x = \pm\infty$, and

$$\begin{aligned}
\frac{\partial}{\partial t} B &= \int_{-\infty}^x \frac{\partial}{\partial t} \rho(x', t) dx' = \int_{-\infty}^x \frac{\partial}{\partial x'} \left(-\rho \frac{1}{m} \frac{\partial}{\partial x'} S \right) dx' \\
&= -\rho \frac{1}{m} \frac{\partial}{\partial x} S,
\end{aligned} \tag{3.25}$$

in agreement with Eq. (3.17).

After the parametrization, the limit of integration turns from x to $q(t)$ and thus, the Bohm function (3.23) is, apart from a change to the complementary integration interval merely for convenience, identical with the probability defined in Eq. (1) of [Brandt(1998)]. There, the integration limit $x_p(t)$ that corresponds to our $q(t)$ is called “quantile trajectory” with a corresponding “quantile velocity” $v_p(t) = \frac{d}{dt}x_p(t)$ that fulfills the guidance equation (3.4).

Concerning the physical interpretation of the Bohmian trajectory, one can therefore quote [Brandt(1998)], stating that “for the solution of this differential equation the initial condition $x(0) = x_0$ is needed as a hidden parameter. If we set Bohm’s initial position x_0 equal to the initial quantile position $x_p(0)$ the quantile trajectories are mathematically identical to Bohm’s particle trajectories. Conceptually, however, they are based on the probability interpretation of the conventional quantum mechanics.”

Taking into account our consistent derivation of the Bohmian trajectories and the corresponding guidance equation and the clear connection with the quantile position based on the conventional quantum mechanical probability interpretation, one comes to the conclusion, Bohmian mechanics does not turn quantum mechanics into a deterministic theory, but supplies an alternative formulation of this theory. This does not necessarily diminish its importance, as it might provide better tools to solve certain problems (like, *e.g.*, tunneling ones, see [Brandt(1998), Oriols(1996)]) than the established conventional formulations.

In the next Section it is tried to give a more illustrative picture of the meaning of Bohmian trajectories.

3.2.1.1 Meaning of the Bohmian trajectories

Two properties are essential for Bohmian trajectories, the non crossing rule that is based on the fact that the guidance equation is of first order and the relation between the Bohmian trajectories and the probability density $\rho(x, t)$, expressed in the quantum equilibrium hypothesis, stating that $\rho(x, t)$ describes both, the probability density and the density of Bohmian trajectories. That means that between two given Bohmian trajectories the same probability is embedded in that region

for all times. This also arises naturally from the fact that the Bohmian trajectories are just time-dependent parametrizations in the configuration space, when the Bohm function or the CPF (3.23) is constant. Therefore, contrary to common belief, Bohmian trajectories have nothing to do with physical entities, but with the borders that separate regions that enclose a fixed amount of probability.

The box diagram in Figure 3.1 (a) shall illustrate the situation. Let us assume each point in the long box represents the detection of a particle at a specific instant of time. The two smaller boxes above with the vertical borders q_1 , q_2 and q_3 represent areas that contain five points each, *i.e.*, the same number of detections, but the distance between q_1 and q_2 has not to be the same as between q_2 and q_3 . If we take another snapshot at a later time, the distribution of the points in the large box has changed, so to say the point density has changed. The same applies to the two small boxes, meaning that also the positions of the vertical lines q_1 , q_2 and q_3 has to change so that still five points are in each box. This can be represented for more snapshots at later times. At each snapshot the position of the q_i can change, so their position is a function of time, as indicated in Figure 3.1 (b). The Bohmian trajectories are then obtained by interpolation (see dashed lines). This also illustrates the relation between the (probability) density and the Bohmian trajectories. So it is not necessary to introduce another postulate, the quantum equilibrium hypothesis, since the Bohmian trajectories are just quantile trajectories for probabilities that are calculated with densities that fulfill the continuity equation.

Although by definition it is now impossible to measure Bohmian trajectories as path of a particle, this concept can still be useful. The importance of the Bohmian trajectories arises when one is interested in determining the probability that is distributed in configuration space. This happens to be crucial in tunneling problems, because in that case one is interested in knowing how much probability is transmitted into a given region of configuration space.

We would also like to emphasize that Bohmian mechanics in that sense is a complement to the Schrödinger picture. Both of them have different scopes. An aim of the Schrödinger picture is the calculation of mean values $\langle \hat{A} \rangle$ of an observable A , or higher moments $\langle \hat{A}^n \rangle$, $n = 2, 3, \dots$. For that purpose, the wave function $\psi(x, t)$ or the density $\rho(x, t)$ in the whole domain of definition is needed, as well as their time-evolution. The scope of Bohmian mechanics is rather the study of interval classes (percentile, quartile, median, etc.) with the help of the Bohm function $B(x, t) = \int_{-\infty}^x \rho(x', t) dx'$ through the analysis of the evolution of the limit of this interval, $q(t)$. The relation between Schrödinger's and Bohm's approach can be compared with the relation between statistical inference and descriptive statistics.

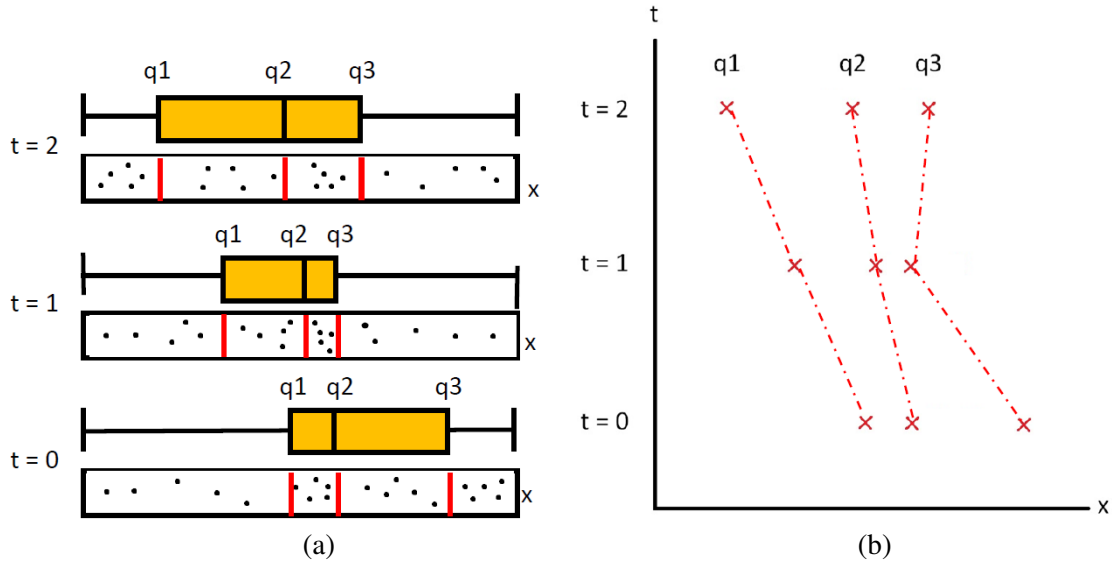


Fig. 3.1 Snapshots of position detections for different times and evolution of corresponding integration limits (=Bohmian trajectories) for three different instants of time. The probability for a detection between two neighboring q_i stays constant, only the limits change in time, *i.e.*, $q_i = q_i(t)$. Thus the density of points changes accordingly.

3.2.1.2 Conservation of probability via “thermodynamic” cycle

In Section 3.2.1 it has been shown that there exists a total differential dB ,

$$dB = \rho dx - j dt \quad (3.26)$$

with $j = \rho \frac{1}{m} \frac{\partial}{\partial x} S$.

This means that whenever an integration of B along a closed contour C is performed in the (x, t) -space, the result is zero,

$$\oint_C dB = 0. \quad (3.27)$$

Having this in mind, let us choose a simple rectangular-shaped contour as depicted in Figure 3.2 (a). The involved processes are characterized as follows:

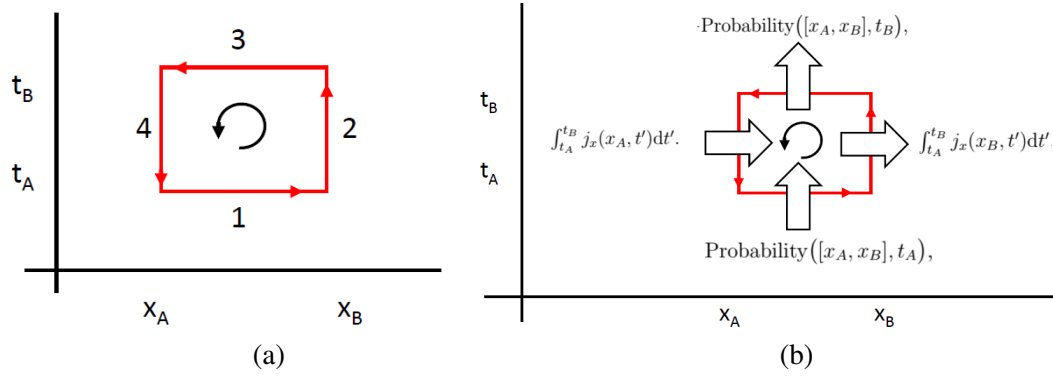


Fig. 3.2 (a) Contour integral within the (x, t) -space with two kinds of “processes”: 1 and 3 are iso-chronic ($t = \text{const}$), whereas 2 and 4 are iso-spatial ($x = \text{const}$). (b) Schematic representation of the effect of integrating along horizontal and vertical processes.

Process 1: $t = t_A = \text{const}$,
i.e., $dt = 0$ and $x_A \longrightarrow x_B$

Process 2: $x = x_B = \text{const}$,
i.e., $dx = 0$ and $t_A \longrightarrow t_B$

Process 3: $t = t_B = \text{const}$,
i.e., $dt = 0$ and $x_B \longrightarrow x_A$

Process 4: $x = x_A = \text{const}$,
i.e., $dx = 0$ and $t_B \longrightarrow t_A$.

Therefore, the integrals along the respective processes have the explicit form

$$\text{Process 1: } \int_1 dB = \int_{x_A}^{x_B} \rho(x', t_A) dx',$$

$$\text{Process 2: } \int_2 dB = - \int_{t_A}^{t_B} j(x_B, t') dt',$$

$$\text{Process 3: } \int_3 dB = - \int_{x_A}^{x_B} \rho(x', t_B) dx',$$

$$\text{Process 4: } \int_4 dB = \int_{t_A}^{t_B} j(x_A, t') dt'.$$

This can also be written as

$$\text{Process 1: } \int_1 dB = \text{Probability}([x_A, x_B], t_A),$$

$$\text{Process 2: } \int_2 dB = - \int_{t_A}^{t_B} j(x_B, t') dt',$$

$$\text{Process 3: } \int_3 dB = -\text{Probability}([x_A, x_B], t_B),$$

$$\text{Process 4: } \int_4 dB = \int_{t_A}^{t_B} j(x_A, t') dt'.$$

These expressions help to give a schematic representation of the line integrals in the (x, t) -space as shown in Figure 3.2 (b). The sign is determined by the orientation of the arrow: Inward arrows imply a plus sign, outward arrows a minus sign.

Going back to the closed contour integral

$$\oint dB = \int_1 dB + \int_2 dB + \int_3 dB + \int_4 dB = 0 \quad (3.28)$$

and inserting the contributions of the line integrals, after some rearrangement, this can be written as

$$\begin{aligned} & \text{Probability}([x_A, x_B], t_B) - \text{Probability}([x_A, x_B], t_A) \\ & + \int_{t_A}^{t_B} \left(j(x_B, t') - j(x_A, t') \right) dt' = 0. \end{aligned} \quad (3.29)$$

The difference of the probabilities at times t_A and t_B can also be expressed in the form

$$\begin{aligned} & \int_{t_A}^{t_B} \frac{\partial}{\partial t'} \text{Probability}([x_A, x_B], t') dt' \\ & + \int_{t_A}^{t_B} \left(j(x_B, t') - j(x_A, t') \right) dt' = 0. \end{aligned} \quad (3.30)$$

In a similar way, the differences of the probabilities and the currents at different positions (but the same time) can be expressed by integrations from x_A to x_B , finally leading to

$$\int_{t_A}^{t_B} \int_{x_A}^{x_B} \left(\frac{\partial}{\partial t'} \rho(x', t') + \frac{\partial}{\partial x'} j(x', t') \right) dx' dt' = 0, \quad (3.31)$$

i.e., the CE under the action of a double integration.

Considering the symmetry of the integration intervals it seems possible that contributions of two line integrals can cancel each other, so that the overall contour integral vanishes. But how is the situation if this symmetry is disturbed. What are then the contributions to the integration?

To answer this question, one has to recall that along a Bohmian trajectory B is constant, therefore, an integral of dB along a Bohmian trajectory vanishes, $\int_{\text{Bohmian trajectory}} dB = 0$. Let us therefore consider an integration along the cycle shown in Figure 3.3, *i.e.*, two horizontal lines of different lengths ($[x_A, x_B]$ and $[x_C, x_D]$) that connect two Bohmian trajectories at different times. As the contributions along the Bohmian trajectories vanish, the contour integral reduces to

$$\oint dB = \int_1 dB + 0 + \int_3 dB + 0 = 0, \quad (3.32)$$

or

$$\boxed{\text{Probability}([x_A, x_B], t_A) = \text{Probability}([x_C, x_D], t_B)}. \quad (3.33)$$

But this just reflects the typical characteristic of Bohmian trajectories: the probability between two given Bohmian trajectories is conserved in time.

However, in the conventional literature on Bohmian mechanics there is no mathematical proof of this property. Instead, the conventional “proof” is based on dialectic arguments: the non-crossing rule and the equivalence between $\rho(x, t)$ and the density of Bohmian trajectories (the latter one is actually only postulated). Our proof, in contrast, is a simple mathematical one that has no need to introduce postulates with the arbitrariness of their interpretation

3.2.2 Bohmian trajectories for general Gaussian wave packets

In order to give some specific examples for Bohmian trajectories and how they can be expressed in terms of mean values and uncertainties, cases are now con-

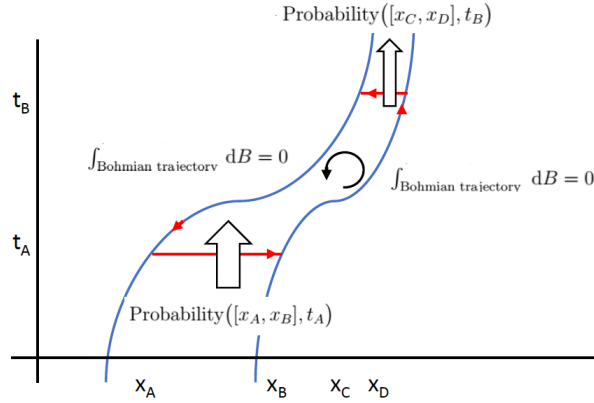


Fig. 3.3 When performing a “cycle” using two Bohmian trajectories (blue lines) as supports, there is a conservation of probability along the horizontal lines between those two Bohmian trajectories.

sidered where exact analytic expressions for the solutions of the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right\} \psi(x, t), \quad (3.34)$$

exist. This is fulfilled, as it is shown in Appendix A, for potentials that are at most quadratic in the position variable, particularly, the free motion, $V = 0$, and the harmonic oscillator, $V = \frac{m}{2} \omega_0^2 x^2$. In these cases solutions can be found having the form of Gaussian wave packets (A.1), characterized by their mean value and width, where both can be time-dependent.

Recall that the wave packets (A.1) can be written in the form

$$\psi(x, t) = N_x(t) \exp \left[\frac{i}{\hbar} \left(\frac{m}{2} \mathcal{C} \tilde{x}^2 + \langle p \rangle \tilde{x} + K(t) \right) \right] \quad (3.35)$$

with $\tilde{x} = x - \langle x \rangle = x - \eta(t)$, where the mean value $\langle x \rangle = \int_{-\infty}^{+\infty} dx \psi^* x \psi = \eta(t)$ corresponds to the classical trajectory and defines the maximum of the wave packet, $\langle p \rangle = m\dot{\eta}$ represents the classical momentum, $\mathcal{C}(t)$ in the coefficient of the quadratic term in the exponent is a complex function of time, related to the wave packet width. The (possibly time-dependent) normalization factor $N_x(t)$ and the purely time-dependent function $K(t)$ are not relevant for the following. The dynamical behavior of the involved parameters is summed up in Table A.1 of Appendix A. For the case of a harmonic oscillator in position space, the mean value η is ruled by the following Newtonian equation,

$$\dot{\eta} + \omega_0^2 \eta = 0. \quad (3.36)$$

Bear in mind that η describes the evolution of the maximum or mean value (the results for the free motion are obtained for $\omega_0 \rightarrow 0$). The complex quantity $\mathcal{C}(t)$ satisfies a complex quadratic nonlinear Riccati equation

$$\dot{\mathcal{C}} + \mathcal{C}^2 + \omega_0^2 = 0, \quad (3.37)$$

where \mathcal{C} determines the evolution of the width of the wave packet and thus of the position uncertainty. This can be seen from the fact that $\mathcal{C}_I = \frac{\hbar}{2m\langle\tilde{x}^2\rangle}$ where $\langle\tilde{x}^2\rangle = \langle x^2 \rangle - \langle x \rangle^2$ is the mean square deviation in position space and thus describes the position uncertainty. Introducing a new variable $\alpha(t)$ via $\mathcal{C}_I = \frac{1}{\alpha^2}$, real and imaginary parts of \mathcal{C} can be written as

$$\mathcal{C} = \mathcal{C}_R + i\mathcal{C}_I = \frac{\dot{\alpha}}{\alpha} + i\frac{1}{\alpha^2} \quad (3.38)$$

where $\alpha(t)$ is, via $\alpha = \sqrt{\frac{2m}{\hbar}\langle\tilde{x}^2\rangle}$, directly proportional to the wave packet width. For further details on the structural properties of the generalized coherent states see Appendix A.

The real part $\mathcal{C}_R(t)$ is important in the following, as it is part of the phase of the wave packet and thus enters the guidance law (3.22)

$$\frac{dq(t)}{dt} = \frac{1}{m} \frac{\partial}{\partial q} S(q, t) \quad (3.39)$$

in the form

$$\frac{dq(t)}{dt} = \mathcal{C}_R(q(t) - \eta(t)) + \frac{1}{m} \langle p \rangle(t). \quad (3.40)$$

As $\frac{1}{m} \langle p \rangle(t) = \dot{\eta}(t)$, in analogy to the definition of \tilde{x} , one can use $\tilde{q} = q - \eta$, instead of q , leading to

$$\frac{d\tilde{q}}{dt} = \mathcal{C}_R \tilde{q} = \frac{\dot{\alpha}}{\alpha} \tilde{q}, \quad (3.41)$$

what can be rewritten as

$$\frac{d}{dt} \ln \tilde{q} = \frac{d}{dt} \ln \alpha. \quad (3.42)$$

Integration from $t_0 = 0$ to time t finally leads to

$$\boxed{q(t) = \eta(t) + (q_0 - \eta_0) \frac{\alpha(t)}{\alpha_0}}. \quad (3.43)$$

Every Bohmian trajectory is determined by an initial point q_0 (in relation to the initial position η_0 of the classical trajectory) and the initial spreading α_0 of the Gaussian wave packet. As shown in Figure 3.3, the area between two Bohmian trajectories is important, as the probability is conserved within this interval. Therefore, one can define an interval $L = q_B - q_A$ with $q_A < q_B$ between two Bohmian trajectories q_A and q_B as

$$\boxed{L(t) = L_0 \frac{\alpha(t)}{\alpha_0}}. \quad (3.44)$$

That means the dynamics of this interval (broadening or narrowing) is determined by the evolution of $\alpha(t)$. In other words, one could say α determines how for a given probability the metric of the “probability-space time” is deformed.

It has been shown (see, *e.g.*, [Cruz(2015), Schuch(2018a)] and references therein) how $\alpha(t)$ can be determined, if two linear independent solutions η_1 and η_2 of the classical equation of motion (3.36) are known. Considering wave packets whose initial uncertainty product is minimal, *i.e.*, $\langle \tilde{x}^2 \rangle_0 \langle \tilde{p}^2 \rangle_0 = \frac{\hbar^2}{4}$, one can write $\alpha(t)$ in the form

$$\boxed{\alpha(t) = \sqrt{\frac{1}{(\alpha_0)^2} (\eta_1)^2 + (\alpha_0)^2 (\eta_2)^2}}. \quad (3.45)$$

It should be mentioned that due to the Gaussian shape of $\psi(x, t)$ and thus also of $\rho(x, t)$, the CPF $B(x, t)$ defined in (3.23) can always be expressed in terms of error functions.

Box 3.2.3

3.2.2.1 Bohmian trajectories in momentum representation

All the results obtained in the previous Sections can easily be taken over to the momentum representation. In [Bonilla(2020a)] it was shown that for a system of mass m under the influence of a general quadratic potential $U = a + bX + \frac{m}{2}\omega^2 X^2$ with X being the (complex) Bohmian position in momentum representation, the CE fulfilled in this case is of the same type as (3.16), namely

$$\frac{\partial \rho_p(p,t)}{\partial t} + \frac{\partial}{\partial p} \left[\rho_p(p,t) \left(-b - m\omega^2 \left(-\frac{\partial}{\partial p} S_p(p,t) \right) \right) \right] = 0. \quad (3.46)$$

As in Section 3.2.1, this implies the existence of a function, let us call it again Bohm function $B_p(p,t)$ in momentum representation, whose differential satisfies

$$dB_p = \rho_p(p,t) \left(b + m\omega^2 \left(-\frac{\partial}{\partial p} S_p(p,t) \right) \right) dt + \rho_p(p,t) dp. \quad (3.47)$$

Simple inspection shows that the Bohm function matches again the CPF criterium, but this time in momentum space,

$$B_p = \int_{-\infty}^p \rho_p(p',t) dp'. \quad (3.48)$$

Moreover, if we parametrize all the points where the Bohm function B_p is constant, we can define the guidance equation for the momentum space as well. So, after the parametrization

$$(p,t)|_{B_p=\text{const}} \longrightarrow (\pi,t), \quad (3.49)$$

with $\pi = \pi(t)$ follows the equation

$$\frac{d\pi}{dt} = -b - m\omega^2 \left(-\frac{\partial}{\partial p} S_p(\pi, t) \right). \quad (3.50)$$

The interpretations of Section 3.2.1.1 are valid correspondingly as well as the non-crossing property and its consequences, as discussed in Section 3.2.1.2. It is worth noticing that the expression (3.50) corresponds to the real part of Eq. (2.69).

3.2.2.2 Free motion

In the case of the free motion, $V = 0$, what is for our purpose also the same as $V = \text{const}$, as in both cases the force in (3.36) vanishes, two linear independent solutions of this equation are given by $\eta_1(t) = -t$, $\eta_2(t) = 1$. Inserted into (3.45) this yields

$$\alpha(t) = \alpha_0 \sqrt{\left(\frac{t}{\alpha_0^2} \right)^2 + 1}. \quad (3.51)$$

The explicit expression for the Bohmian trajectory (3.43) then takes the form

$$q(t) = \eta(t) + (q_0 - \eta_0) \sqrt{\left(\frac{t}{\alpha_0^2} \right)^2 + 1} \quad (3.52)$$

and

$$L(t) = L_0 \sqrt{\left(\frac{t}{\alpha_0^2} \right)^2 + 1}, \quad (3.53)$$

i.e., although $\frac{1}{\alpha_0}$ is cancelled by α_0 in front of the square root, $q(t)$ and $L(t)$ still depend on α_0 via the expression under the square root, as shown in Figures 3.4 (a) and (b), where $\sigma = \sqrt{\frac{\hbar}{2m}} \alpha_0$.

Expression (3.52) can be rewritten as an hyperbola in the probability-space-time,

$$\left(\frac{q(t) - \eta(t)}{q_0 - \eta_0} \right)^2 - \left(\frac{t}{\alpha_0^2} \right)^2 = 1. \quad (3.54)$$

Therefore, the further one goes away from the center of the Gaussian, the faster the hyperbolic trajectories get curved.

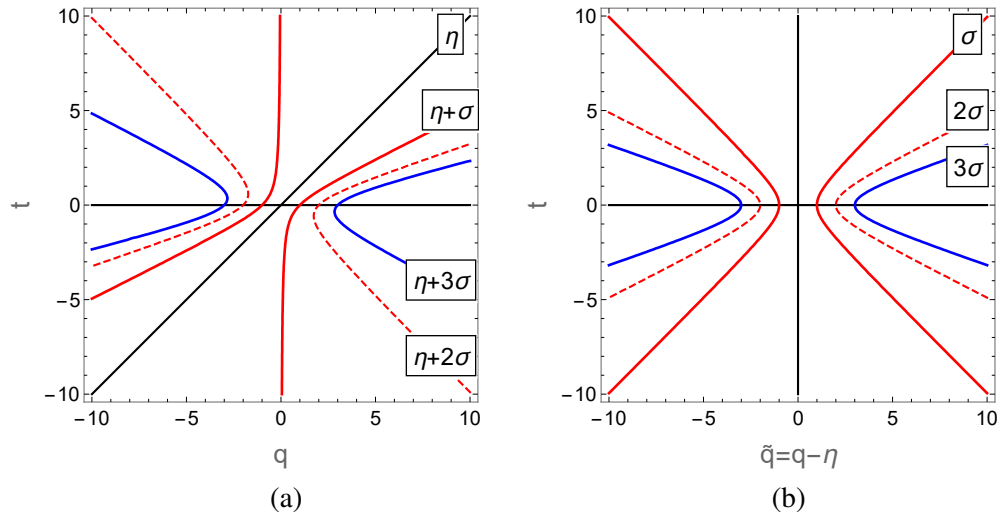


Fig. 3.4 (a) Bohmian trajectories for four different points of a general coherent state under the action of a constant potential. (b) The previous Bohmian trajectories, but now relative to the position mean value η . In every case $\frac{1}{\alpha_0^2} = 1$.

3.2.2.3 Harmonic oscillator

For the harmonic oscillator with potential $V = \frac{m}{2} \omega_0^2 x^2$, where the frequency ω_0 is constant, two linear independent solutions of Eq. (3.36) are $\eta_1(t) = -\frac{\sin \omega_0 t}{\omega_0}$ and $\eta_2(t) = \cos \omega_0 t$.

Inserting this into (3.45) leads to

$$\alpha(t) = \alpha_0 \sqrt{\left(\frac{\sin \omega_0 t}{\omega_0 \alpha_0^2} \right)^2 + \cos^2 \omega_0 t}. \quad (3.55)$$

In this case, the Bohmian trajectory $q(t)$ and $L(t)$ are given by

$$q(t) = \eta(t) + (q_0 - \eta_0) \sqrt{\left(\frac{\sin \omega_0 t}{\omega_0 \alpha_0^2}\right)^2 + \cos^2 \omega_0 t} \quad (3.56)$$

and

$$L(t) = L_0 \sqrt{\left(\frac{\sin \omega_0 t}{\omega_0 \alpha_0^2}\right)^2 + \cos^2 \omega_0 t}. \quad (3.57)$$

Eq. (3.57) determines how the metric in the probability-space-time is deformed for a harmonic oscillator. The Bohmian trajectory (3.56), as shown in Figure 3.5 (a) shows the superposition of two periodic evolutions, that of the classical trajectory $\eta(t)$ and that of the width $\alpha(t)$. Changing from $q(t)$ to the frame $\tilde{q} = q - \eta$ that moves with the classical trajectory $\eta(t)$, only the periodic motion of $\alpha(t)$ remains, as shown in Figure 3.5 (b). If the initial width of the Gaussian wave packet is that of the ground state of the harmonic oscillator, then $\frac{1}{\alpha_0^2} = \omega_0$ and the square root in (3.55) is equal to one, *i.e.*, there is no oscillation. That corresponds to the minimum uncertainty wave packet that Schrödinger himself found in 1926 [Schrödinger(1926e)]. In any other case, $\alpha(t)$ shows oscillations.

3.3 Connection between the Bohmian and the Wigner framework

In the decades that follow the construction of the conventional structure of quantum mechanics with the Copenhagen interpretation, there were different approaches to the microscopic systems that seek to propose a formulation as similar as possible to the concept of classical phase space. We can distinguish 3 main lines of thinking: the Wigner function, first introduced in 1932, was designed to give a formulation of quantum mechanics with a quasi probability distribution whose marginal distributions correspond to the position and momentum probability density functions. The term “quasi” accounts for its main conceptual drawback: the presence of negative values. Years later, Husimi proposed in 1940 an approach that was a smoothed version of the Wigner function with only positive values,

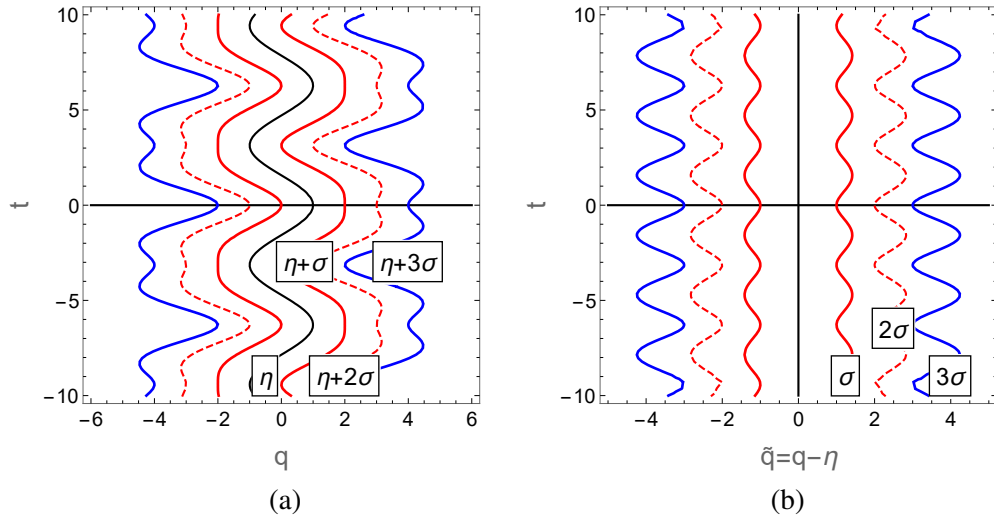


Fig. 3.5 (a) Bohmian trajectories for four different points of a general coherent state under the action of a harmonic oscillator. (b) The previous Bohmian trajectories, but now relative to the position mean value η . In every case $\frac{1}{\omega^2} \frac{1}{\alpha_0^2} - 1 = 1$, *i.e.*, $\omega_0 \neq \frac{1}{\alpha_0}$.

but the disadvantage is that it cannot provide correctly the probability density nor the density current. In 1952 though, Bohm claimed the possibility of a causal treatment of quantum mechanics through the use of trajectories that characterized individual detections. Its main critics are the lack of symmetry in position and momentum space (this was corrected by Bonilla and Schuch [Bonilla(2020a)]) and the disagreement with the Copenhagen interpretation.

Recently there has been a claim that the Bohmian framework is a better and more general scheme for the phase space formulation of quantum mechanics [Colomes(2015)]. Nevertheless, in this work it will be shown that Bohmian mechanics is nothing more than a projection of the Wigner formalism; therefore, Bohmian mechanics cannot be more general than the Wigner function in the first place. This misunderstanding is partly due to the misconception about the Bohmian trajectories themselves.

3.3.1 Bohmian mechanics as a projection of the Wigner function

An important feature of the Wigner function is that the marginal distributions match the probability density functions for the position and momentum representation, respectively, as it is recalled in what follows,

$$\int_{-\infty}^{\infty} W(x, p; t) dx = |\langle p | \psi(t) \rangle|^2 = \rho_p(p, t), \quad (3.58)$$

$$\int_{-\infty}^{\infty} W(x, p; t) dp = |\langle x | \psi(t) \rangle|^2 = \rho_x(x, t). \quad (3.59)$$

The corresponding cumulative probability functions (CPF) are of particular interest, because one obtains precisely the Bohm functions in the respective spaces,

$$\int_{-\infty}^p \int_{-\infty}^{\infty} W(x, p; t) dx dp = \int_{-\infty}^p \rho_p dp = B_p(p, t), \quad (3.60)$$

$$\int_{-\infty}^x \int_{-\infty}^{\infty} W(x, p; t) dp dx = \int_{-\infty}^x \rho_x dx = B_x(x, t). \quad (3.61)$$

Therefore, a Bohmian trajectory can be defined through the Wigner function. Indeed, a Bohmian trajectory is the set of positions $q = q(t)$ that share the same value for the Bohm function B_x , for all instants of time. Therefore, $q = q(t)$ is defined via

$$B_x(q, t) = \text{const}, \quad (3.62)$$

in the form

$$\int_{-\infty}^{q=q(t)} \int_{-\infty}^{\infty} W(x, p; t) dp dx = \text{const}. \quad (3.63)$$

A similar expression can be obtained for the momentum representation.

Now, this simple remark of the relationship between the Wigner and Bohm functions, allows us

- (1) to extend the concept of Bohmian trajectories to arbitrary representations. Indeed, it is only necessary to express the Wigner function in a couple of canonical variables (a, b) ; we then take the cumulative probability function of the marginal distribution of the Wigner function. Finally we set this expression to a

constant value, as it is indicated in what follows, for the Bohmian “trajectory”
 $a = a(t)$

$$\int_{-\infty}^{a=a(t)} \int_{-\infty}^{\infty} W(a', b; t) db da' = \text{const}; \quad (3.64)$$

- (2) to extend the Bohmian treatment to discrete level states, qubits, etc., since it is possible to assign to these cases a corresponding Wigner function.
- (3) Last but not least, this rehabilitates Bohmian mechanics as a projective feature of the Wigner formalism, leaving aside any interpretative or esoteric feature of Bohmian mechanics, *i.e.*, Bohmian mechanics does not need any additional postulates or interpretations with respect to conventional quantum mechanics.

It is also worth noticing that, contrary to the usual formulation (since 1952!), Bohmian mechanics and conventional quantum mechanics are not on the same level, because the former can be considered essentially as a projection of the Wigner function.

Nevertheless, this should not diminish the importance of Bohmian mechanics, but just clarifying its position in the theoretical corpus of quantum mechanics. Moreover, knowing the status of Bohmian mechanics helps to use this tool as a descriptive one for the probabilities in the representation-time space, *e.g.* (x, t) or (p, t) . Any further interpretation of the objects in this approach is meaningless.

3.3.2 Bohmian trajectories from the Wigner function

Now, let us repeat the dynamics of the Bohmian trajectories with respect to the Wigner function. For instance, it is known that the Bohmian trajectories $q = q(t)$ in position representation are governed by the following equation:

$$\frac{dq}{dt} = \frac{j_x}{\rho_x}, \quad (3.65)$$

where $\rho_x(x, t)$ and $j_x(x, t)$ are the probability density and probability density current in position space. For the momentum representation, the equation is analogous because, in both representations, the trajectories are parametrizations of a function that is build up from a CE.

One can rewrite the probability density current j_x by considering the Bohmian trajectories. By definition, Bohmian trajectories $q = q(t)$ are the locus where the Bohmian function $B(x, t)$ remains constant, namely

$$\int_{-\infty}^{q=q(t)} \rho_x(x, t) dx = \text{const.} \quad (3.66)$$

Differentiating with respect to the time t yields the following expression

$$0 = \frac{d}{dt} \int_{-\infty}^{q=q(t)} \rho_x(x, t) dx. \quad (3.67)$$

As one of the integration limits, $q(t)$, depends on time, one has to consider

$$0 = \rho_x(x, t) \frac{dq}{dt} + \int_{-\infty}^q \frac{\partial \rho_x}{\partial t} dx, \quad (3.68)$$

what, taking into account the relation (3.65) between the probability current and the Bohmian trajectories, provides

$$j_x = - \int_{-\infty}^q \frac{\partial \rho_x}{\partial t} dx. \quad (3.69)$$

Recall that the probability density function ρ_x in position space results from the integration of the Wigner function $W(x, p; t)$ over the complete momentum space, therefore,

$$j_x = - \int_{-\infty}^q \int_{-\infty}^{\infty} \frac{\partial W(x, p; t)}{\partial t} dp dx. \quad (3.70)$$

Bearing in mind that the time derivative of the Wigner function is given by $\frac{\partial W}{\partial t} = -\frac{p}{m} \frac{\partial W}{\partial x} + \frac{\partial U}{\partial x} \frac{\partial W}{\partial p}$, leads to

$$\begin{aligned}
j_x &= - \int_{-\infty}^q \int_{-\infty}^{\infty} \left(-\frac{p}{m} \frac{\partial W}{\partial x} + \frac{\partial U}{\partial x} \frac{\partial W}{\partial p} \right) dp dx \\
&= \int_{-\infty}^{\infty} \frac{p}{m} dp \int_{-\infty}^q \frac{\partial W}{\partial x} dx - \int_{-\infty}^q \frac{\partial U}{\partial x} dx \int_{-\infty}^{\infty} \frac{\partial W}{\partial p} dp.
\end{aligned} \tag{3.71}$$

Since, for the first integral, p is an independent variable, one can first evaluate $\int_{-\infty}^q \frac{\partial W}{\partial x} dx$. On the other hand, in the second integral, the potential U depends exclusively on the position; therefore, one can first evaluate $\int_{-\infty}^{\infty} \frac{\partial W}{\partial p} dp$. In other words, the previous equation takes the following form,

$$j_x = \int_{-\infty}^{\infty} \frac{p}{m} \left(W(q, p; t) - W(-\infty, p; t) \right) dp - \int_{-\infty}^q \frac{\partial U}{\partial x} \left(W(x, \infty; t) - W(x, -\infty; t) \right) dx. \tag{3.72}$$

Given that the Wigner function vanished at plus-minus infinity in the space (x, p) , the equation simplifies to

$$j_x = \int_{-\infty}^{\infty} \frac{p}{m} W(q, p; t) dp. \tag{3.73}$$

Note, that the Wigner function inside the integral is evaluated at q , *i.e.* a point belonging to the Bohmian trajectory; it is not anymore the independent variable x . With this expression, one can finally write down the dynamics of the Bohmian trajectory in terms of the Wigner function,

$$\frac{dq}{dt} = \frac{j_x}{\rho_x}, \tag{3.74}$$

as

$$\boxed{\frac{dq}{dt} = \frac{1}{m} \frac{\int_{-\infty}^{\infty} p W(q, p'; t) dp'}{\int_{-\infty}^{\infty} W(q, p''; t) dp''} = \frac{j_x}{\rho_x}}. \tag{3.75}$$

In the momentum representation, it is possible to obtain the dynamical equation for a corresponding Bohmian momentum $\pi = \pi(p, t)$ as

$$\boxed{\frac{d\pi}{dt} = \frac{\int_{-\infty}^{\infty} -\frac{\partial U}{\partial x} W(x', \pi; t) dx'}{\int_{-\infty}^{\infty} W(x'', \pi; t) dx''} = \frac{j_p}{\rho_p}}. \tag{3.76}$$

3.3.3 Application to coherent states

Let us illustrate how to recover the dynamical equation of the Bohmian trajectories from the Wigner function for the generalized coherent states. It is known that these states are characterized by the following Wigner function [Schuch(2018a)]

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{2}{\hbar^2} \left(\langle \tilde{p}^2 \rangle \tilde{x}^2 - \langle [\tilde{x}, \tilde{p}]_+ \rangle \tilde{x} \tilde{p} + \langle \tilde{x}^2 \rangle \tilde{p}^2 \right) \right], \quad (3.77)$$

where $\tilde{x} \doteq x - \langle x \rangle = x - \eta$ and $\tilde{p} \doteq p - \langle p \rangle$. Rewriting the previous equation in terms of uncertainties and correlation yields

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{2}{\hbar^2} \left(\sigma_p^2 \tilde{x}^2 - 2\sigma_{x,p} \tilde{x} \tilde{p} + \sigma_x^2 \tilde{p}^2 \right) \right] \quad (3.78)$$

or

$$\boxed{W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{4}{\hbar^2} \sigma_x^2 \sigma_p^2 \left(\frac{\tilde{x}^2}{2\sigma_x^2} - \frac{\sigma_{x,p}}{\sigma_x^2 \sigma_p^2} \tilde{x} \tilde{p} + \frac{\tilde{p}^2}{2\sigma_p^2} \right) \right]}. \quad (3.79)$$

This expression will be used in what follows to obtain the dynamical laws of the Bohmian trajectories for both the position and momentum space.

3.3.3.1 Position space

In this Section, Eq. (3.79) is handled in position space. For that purpose, the quadratic momentum term has to be isolated,

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{2}{\hbar^2} \sigma_x^2 \left(\frac{\sigma_p^2}{\sigma_x^2} \tilde{x}^2 - 2 \frac{\sigma_{x,p}}{\sigma_x^2} \tilde{x} \tilde{p} + \tilde{p}^2 \right) \right]. \quad (3.80)$$

Recall that the momentum uncertainty σ_p as well as the correlation $\sigma_{x,p}$ are related to the position uncertainty by a ratio (see Appendix A) so that the previous equation can be written in the following way,

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{2}{\hbar^2} \sigma_x^2 \left(m^2 |\mathcal{C}|^2 \tilde{x}^2 - 2m \mathcal{C}_R \tilde{x} \tilde{p} + \tilde{p}^2 \right) \right] \quad (3.81)$$

or

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{1}{m\hbar\mathcal{C}_I} \left(m^2 \mathcal{C}_I^2 \tilde{x}^2 + m^2 \mathcal{C}_R^2 \tilde{x}^2 - 2m \mathcal{C}_R \tilde{x} \tilde{p} + \tilde{p}^2 \right) \right]. \quad (3.82)$$

Besides, bearing in mind that $\mathcal{C}_I = \frac{\hbar}{2m} \frac{1}{\sigma_x^2} = \frac{1}{\alpha^2}$ allows us to write

$$W(x, p; t) = \frac{\sqrt{2\pi\sigma_x^2}}{\pi\hbar} \rho_x(x, t) \exp \left[-\frac{\alpha^2}{m\hbar} \left(p - (m\mathcal{C}_R \tilde{x} + \langle p \rangle) \right)^2 \right], \quad (3.83)$$

where $\rho_x = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp \left[-\frac{\tilde{x}^2}{2\sigma_x^2} \right]$ denotes the probability density in the position space. Now, we can identify the argument of the exponent in terms of the real part of the Bohmian momentum, P_R ,

$$W(x, p; t) = \frac{\sqrt{2\pi\sigma_x^2}}{\pi\hbar} \rho_x(x, t) \exp \left[-\frac{\alpha^2}{m\hbar} \left(p - P_R \right)^2 \right]. \quad (3.84)$$

Since this Wigner function is composed out of $\rho_x(x, t)$ and a Gaussian function with maximum at P_R in momentum space, calculating the mean value of momentum via integration in momentum space leads according to (3.75) to the probability current j_x in position space and thus to

$$\boxed{\frac{dq}{dt} = \frac{1}{m} P_R = \frac{j_x}{\rho_x}}. \quad (3.85)$$

This is precisely the dynamical equation for the Bohmian trajectory for the case of the generalized coherent states. In this way, it is shown how Bohmian mechanics is just a projective aspect of a more general formalism: the Wigner formalism.

3.3.3.2 Momentum space

In this Section, Eq. (3.79) is handled in momentum space. For that purpose, the quadratic position term has to be isolated,

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{2}{\hbar^2} \sigma_p^2 \left(\tilde{x}^2 - 2 \frac{\sigma_{x,p}}{\sigma_p^2} \tilde{x}\tilde{p} + \frac{\sigma_x^2}{\sigma_p^2} \tilde{p}^2 \right) \right]. \quad (3.86)$$

Recall again that the position uncertainty σ_x as well as the correlation $\sigma_{x,p}$ are related to the momentum uncertainty by a ratio (see Appendix A) so that the previous equation can be written in the following way,

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{2}{\hbar^2} \sigma_p^2 \left(\tilde{x}^2 - 2 \frac{\mathcal{U}_R}{m} \tilde{x}\tilde{p} + \frac{|\mathcal{U}|^2}{m^2} \tilde{p}^2 \right) \right]. \quad (3.87)$$

Bear in mind that the momentum uncertainty σ_p is expressed in terms of $\mathcal{U} = \frac{1}{\mathcal{C}}$ as $\sigma_p^2 = \frac{\hbar m}{2} \frac{1}{\mathcal{U}_I}$. This allows to rewrite Eq. (3.86) as,

$$W(x, p; t) = \frac{1}{\pi\hbar} \exp \left[-\frac{m}{\hbar} \frac{1}{\mathcal{U}_I} \left(\tilde{x}^2 - 2 \frac{\mathcal{U}_R}{m} \tilde{x}\tilde{p} + \frac{\mathcal{U}_R^2}{m^2} \tilde{p}^2 + \frac{\mathcal{U}_I^2}{m^2} \tilde{p}^2 \right) \right]. \quad (3.88)$$

Besides, bearing in mind that $\frac{\mathcal{U}_I}{m\hbar} = \frac{1}{2\sigma_p^2}$ allows to write

$$W(x, p; t) = \frac{\sqrt{2\pi\sigma_p^2}}{\pi\hbar} \rho_p(p, t) \exp \left[-\frac{m}{\hbar} \frac{1}{\mathcal{U}_I} \left(x - \left(\frac{\mathcal{U}_R}{m} \tilde{p} - \eta \right) \right)^2 \right]. \quad (3.89)$$

where $\rho_p = \sqrt{\frac{\mathcal{U}_I}{m\hbar\pi}} \exp \left[-\frac{\mathcal{U}_I}{m\hbar} \tilde{p}^2 \right] = \frac{1}{\sqrt{2\pi\sigma_p^2}} \exp \left[-\frac{\tilde{p}^2}{2\sigma_p^2} \right]$ denotes the probability density in the momentum space. Now, we can identify the argument of the exponent in terms of the real part of the Bohmian position X_R

$$W(x, p; t) = \frac{\sqrt{2\pi\sigma_p^2}}{\pi\hbar} \rho_p(p, t) \exp \left[-\frac{m}{\hbar} \frac{1}{\mathcal{U}_I} \left(x - X_R \right)^2 \right]. \quad (3.90)$$

Since this Wigner function is composed out of ρ_p and a Gaussian function with maximum at X_R , then Eq. (3.89) can be easily integrated and inserted into Eq. (3.76). It is then straightforward to write down for a general coherent state in the momentum space (do not loose sight of the fact that the generalized coherent states are solutions for a general potential $U = b\hat{X} + \frac{m\omega^2(t)}{2}\hat{X}^2$, with $\frac{\partial}{\partial \hat{X}} U = b + m\omega^2(t)\hat{X}$)

$$\boxed{\frac{d\pi}{dt} = b + m\omega^2(t)X_R = \frac{j_p}{\rho_p}.} \quad (3.91)$$

In this way, the dynamical law of the Bohmian trajectories in momentum space is obtained. Also, it is shown again that Bohmian mechanics is a projective aspect of the Wigner formalism.

3.4 Example: Ion trap

In the present Section, the results of Section 3.2 are illustrated through the example of an ion trap. That being said, let us remember the goal of an ion trap:

“The purpose of an atom or ion trap is to confine the motion of the atomic or ionic particles to a small region of space. The trapping of charged particles, which is understandably far easier than the confinement of neutral atoms, as the forces which can be exerted by electromagnetic fields on the latter are far smaller”[Rao(2001)].

In the next Box some applications that make the use of ion traps appealing are listed.

Box 3.4

Some applications of ion traps [Rao(2001)]

- (1) *Storage of charged particles in a very well controlled environment nearly free of unwanted perturbations enables the highly precise and accurate measurement of interaction constants, as the transit-time line broadening is nearly eliminated.*
- (2) *Extreme reduction of Doppler broadening can be achieved, due to the possibility of very effective cooling of the trapped ions. Several cooling techniques have been developed in order to reduce the kinetic energies, thereby*

minimising the first order as well as the second-order Doppler effects and localising the charged particles near the trap centre, thereby achieving very high resolution and accuracy in the spectroscopic measurements.

- (3) *The possibility of performing experiments on few ions or even a single ion reduces or eliminates the ion-ion Coulomb interactions and thus very rare species like anti-proton, positron, short-lived isotopes or exotic particles like C_{60} , can be investigated.*
- (4) *Ion traps are now routinely being used as a mass spectrometer. Highest mass resolving power and accuracy are obtained by Penning traps. Mass spectrometers based on Penning traps have been used for the accurate mass measurements of anti-protons, mass of light ions and, recently, measurements of mass of heavy ions.*

Let us consider a magnesium ion of mass $m = 4.03 \times 10^{-23} \text{ g}$, with an initial position uncertainty $\sigma_x = 1 \mu\text{m}$ and initial speed of $\dot{\eta}_0 = 1 \mu\text{m} \cdot \mu\text{s}^{-1}$, subjected to the action of an ion trap, whose influence on the x -axis is represented by a parametric oscillator $\frac{1}{2}m\omega^2(t)x^2$, with the frequency given by $\omega(t) = \frac{1}{at+b} \sim 1\text{MHz}$. Bear in mind from Section 2.3.2.1 that only generalized coherent states (2.75) are being considered. Therefore, in the x -direction the quantum state of the ion is described by $\langle x|\psi(t)\rangle = N(t) \exp\left[\frac{i}{\hbar}\left(\frac{m}{2}\mathcal{C}\tilde{x}^2 + \langle p\rangle\tilde{x} + f\right)\right]$, where the dynamics of the involved parameters is given by (see Appendix A):

$$\dot{\mathcal{C}} + \mathcal{C}^2 + \omega^2(t) = 0 \quad (3.92)$$

$$\frac{d}{dt}\langle p\rangle = -m\omega^2(t)\eta. \quad (3.93)$$

Bear in mind that the complex quantity \mathcal{C} is expressed as $\mathcal{C} = \frac{\dot{\alpha}}{\alpha} + i\frac{1}{\alpha^2}$, with $\alpha^2 \doteq \frac{2m}{\hbar}\sigma_x^2$. Since the behavior of the mean values is ruled by Newton's equation, it is straight forward to state $\eta = \frac{\langle p\rangle_0}{m\omega} \sin(\omega t)$, where we set the initial condition $\eta_0 = \langle x\rangle_0 = 0$ for our wave packet. The remaining dynamical parameters are determined through the associated Riccati equation,

$$\boxed{\dot{\mathcal{C}} + \mathcal{C}^2 + \frac{1}{(at+b)^2} = 0.} \quad (3.94)$$

The general solution will be determined with the help of a particular solution \mathcal{C}_p .

3.4.1 Particular solution

Given the form of the frequency $\omega(t) = \frac{1}{at+b}$, it is reasonable to propose the following particular solution,

$$\boxed{\mathcal{C}_p = \gamma \frac{1}{at+b}}, \quad (3.95)$$

where γ is a time-independent parameter to be found. Therefore the time derivative of the particular solution is given by

$$\dot{\mathcal{C}}_p = -a\gamma \frac{1}{(at+b)^2}. \quad (3.96)$$

Substitution into Riccati equation (3.94) and rearranging terms yields,

$$\left(\gamma^2 - a\gamma + 1\right) \frac{1}{(at+b)^2} = 0. \quad (3.97)$$

To obtain a non trivial solution, the parameter γ must satisfy the following relation,

$$\gamma^2 - a\gamma + 1 = 0, \quad (3.98)$$

leading to

$$\boxed{\gamma = \frac{a}{2} \pm \sqrt{\frac{a^2}{4} - 1}}. \quad (3.99)$$

That means that the parameter γ essentially depends on a . Therefore, from now on we will denote it as γ_a . Now, depending on the values that a may take, γ will have a different form. Let us consider the three possible cases:

$$\gamma_a = \frac{a}{2} \pm i\sqrt{1 - \frac{a^2}{4}}, \quad \text{for } 0 < a < 2 \quad (3.100)$$

$$\gamma_a = \frac{a}{2}, \quad \text{for } a = 2 \quad (3.101)$$

$$\gamma_a = \frac{a}{2} \pm \sqrt{\frac{a^2}{4} - 1}, \quad \text{for } 2 < a. \quad (3.102)$$

Hereafter, we will refer to (3.100), (3.101) and (3.102) as the underdamped, critically damped and overdamped cases, respectively.

3.4.2 General solution

As it is explained in Appendix B, the general solution \mathcal{C} of Riccati equation (3.94) is given by:

$$\mathcal{C} = \frac{1}{\mathcal{Y}} + \mathcal{C}_p(t; a), \quad (3.103)$$

where \mathcal{Y} is given by equation (B.3) of Appendix B:

$$\mathcal{Y} = \frac{\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt' + \exp \left[-2 \int^0 \mathcal{C}_p(t'; a) dt' \right] \mathcal{Y}_0}{\exp \left[-2 \int^t \mathcal{C}_p(t'; a) dt' \right]}. \quad (3.104)$$

Bearing in mind the expression (3.95) of the particular solution $\mathcal{C}_p(t; a)$ and the form (3.103) of the complex quantity \mathcal{C} , it is straightforward to relate the initial condition \mathcal{Y}_0 to the experimental parameters of spreading:

$$\mathcal{Y}_0 = \frac{1}{\mathcal{C}_0 - \frac{\gamma}{b}} = \frac{1}{\frac{\dot{\sigma}_{x,0}}{\sigma_{x,0}} - \frac{\gamma}{b} + i \frac{\hbar}{2m} \frac{1}{(\sigma_{x,0})^2}} \quad (3.105)$$

3.4.2.1 Case $a = 2$

For the case $a = 2$, the quantities involved in expression (3.104) are given by (see Appendix B):

$$\exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] = \frac{1}{2t' + b}, \quad (3.106)$$

$$\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt' = \frac{1}{2} \ln(2t + b) - \frac{1}{2} \ln(b). \quad (3.107)$$

Let us substitute the previous quantities into equation (3.101),

$$\mathcal{Y} = \frac{\frac{1}{2} \ln(2t + b) - \frac{1}{2} \ln(b) + \frac{1}{b} \mathcal{Y}_0}{\frac{1}{2t + b}}, \quad (3.108)$$

where $\mathcal{Y}_0 \in \mathbb{C}$.

Therefore the total solution of the Riccati equation is given by:

$$\begin{aligned} \mathcal{C} &= \frac{1}{\mathcal{Y}} + \frac{1}{2t + b} \\ &= \frac{1}{2t + b} + \frac{\ln(t + \frac{b}{2})}{(t + \frac{b}{2}) [1 + \ln^2(t + \frac{b}{2})]} + i \left(\frac{1}{(t + \frac{b}{2}) [1 + \ln^2(t + \frac{b}{2})]} \right), \end{aligned} \quad (3.109)$$

and the spreading in the position and momentum spaces are given by:

$$\sigma_x^2 = \frac{\hbar}{2m} \frac{1}{\mathcal{C}_I}, \quad (3.110)$$

$$\sigma_p^2 = m^2 |\mathcal{C}_I|^2 \sigma_x^2. \quad (3.111)$$

For this critical case $a = 2$, we depict the spreadings behavior in Figure 3.6 (a) and (b); we notice immediately that there is a divergent behavior in the position uncertainty σ_x after $t = 0.85 \mu s$.

Moreover, if we recall the proposed definition and interpretation of the Bohmian trajectories of Section 3.2.1.1, we can calculate the correspondent Bohmian trajectories for: $\eta \pm \sigma_x$, $\eta \pm 2\sigma_x$, $\eta \pm 3\sigma_x$. This choice is due to the fact that those are key points of a Gaussian distribution, as we can see in the following table:

Region	Area
$[\eta - \sigma_x; \eta + \sigma_x]$	68.3%
$[\eta - 2\sigma_x; \eta + 2\sigma_x]$	95.5%
$[\eta - 3\sigma_x; \eta + 3\sigma_x]$	99.7%

Table 3.1 Given a Gaussian distribution $\rho_x = \exp\left[-\frac{(x-\eta)^2}{2\sigma_x^2}\right]$, the area $\int \rho dx$ is computed for intervals of 1, 2 and 3 standard deviation σ_x away from the mean value η .

With Table 3.1 in mind, the Bohmian trajectories are depicted in Figure 3.6 (c). One can observe there how practically the whole wave packet is focused for a time $\Delta t = 0.85\mu s$, before starting a divergent spreading which tends to the free particle behavior. Bear in mind that the main goal of an ion trap is to maintain a wave packet within an initial region for a given time Δt . In this case, a parametric oscillator with $\omega(t) = \frac{1}{at+b}$ (hereafter b is set to $b = 1$) achieves that goal for a time $\Delta t < 2\mu s$. If the time intervals required to be greater than that, this parametric oscillator is not suitable for ion trapping.

3.4.2.2 Case $a \neq 2$

For the case when $a \neq 2$, the quantities involved in expression (3.104) are given by (see Appendix B):

$$\exp\left[-2\int^{t'} \mathcal{E}_p(t''; a) dt''\right] = \frac{1}{(at' + b)^{2\frac{\gamma}{a}}}, \quad (3.112)$$

$$\int_0^t \exp\left[-2\int^{t'} \mathcal{E}_p(t''; a) dt''\right] dt' = \frac{1}{a} \frac{1}{1-2\frac{\gamma}{a}} (at + b)^{-2\frac{\gamma}{a}+1} - \frac{1}{a} \frac{1}{1-2\frac{\gamma}{a}} b^{-2\frac{\gamma}{a}+1}. \quad (3.113)$$

Let us substitute the previous quantities into equation (3.104),

$$\mathcal{Y} = \frac{\frac{1}{a} \frac{1}{1-2\frac{\gamma}{a}} (at + b)^{-2\frac{\gamma}{a}+1} - \frac{1}{a} \frac{1}{1-2\frac{\gamma}{a}} b^{-2\frac{\gamma}{a}+1} + \frac{1}{b^{2\frac{\gamma}{a}}} \mathcal{Y}_0}{\frac{1}{(at+b)^{2\frac{\gamma}{a}}}}. \quad (3.114)$$

As in the previous Section, the total solution of the Riccati equation is given by:

$$\mathcal{E} = \frac{1}{\mathcal{D}} + \frac{\gamma}{2t+b}, \quad (3.115)$$

with γ having two possible values depending on the value of a relative to 2 (see equations (3.100) and (3.102)). Actually, for the overdamped case $a = 3 > 2$, as Figures 3.7 (a), (b) and (c) suggest, there is a more stable trapping until $\Delta t = 4\mu s$, before starting a divergent behavior which tends to the free particle behavior. Therefore, we notice that the overdamped regime for the considered potential is also not suitable for trapping.

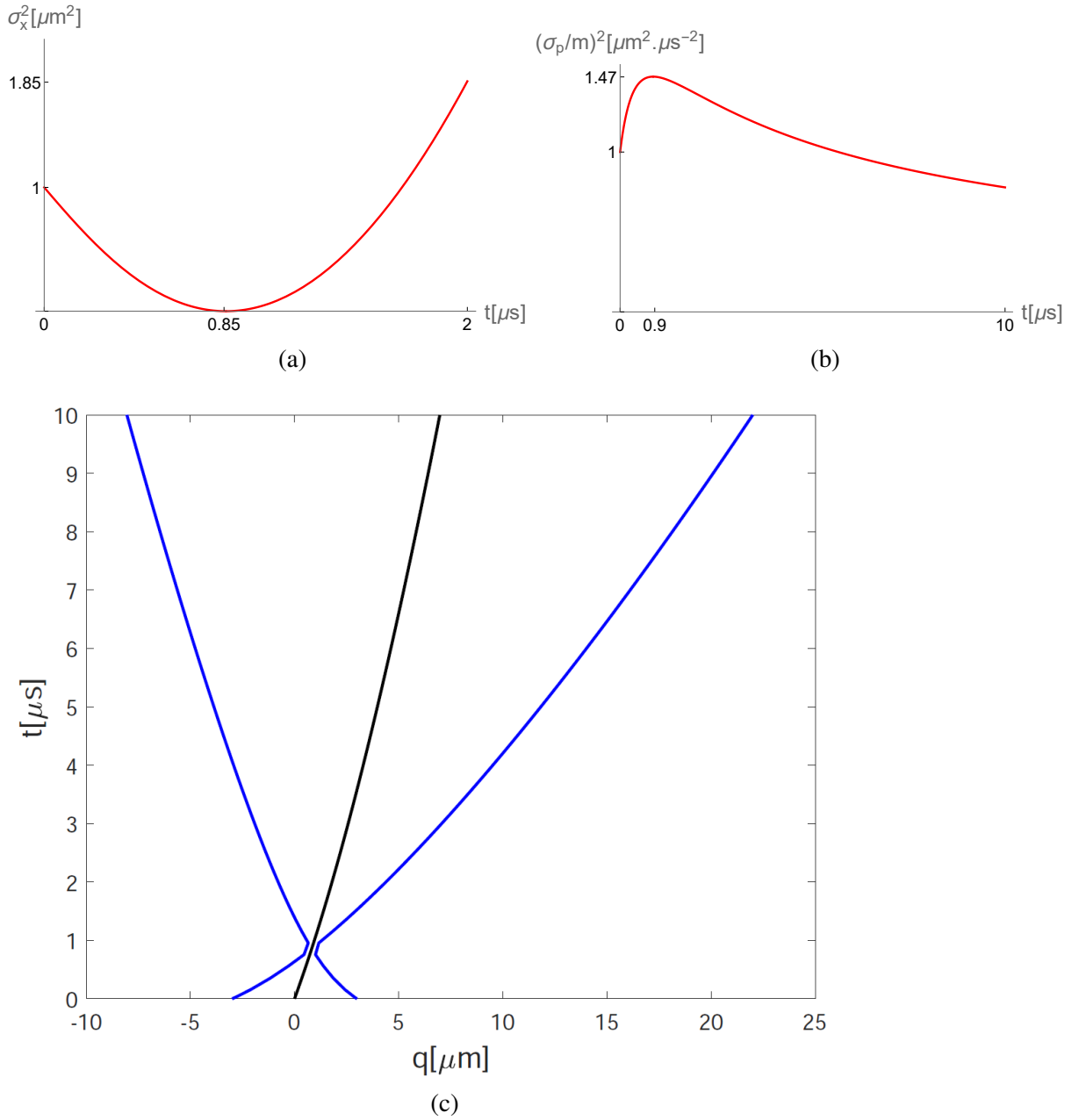


Fig. 3.6 Critical case $a = 2$ for a Mg-ion [Seidelin(2006)] under the action of a parametric oscillator whose frequency has 1MHz as order of magnitude (a) Position spreading for a general coherent state (b) momentum spreading for a general coherent state (c) Bohmian trajectories for the mean value (black line) and two other trajectories (blue lines) that are $3\sigma_x$ away from the maximum of the wavepacket. The previous Bohmian trajectories, in blue, contain 99.7% of the probability distribution according to Table 3.1 and the conservation equation (3.33). The initial conditions are given by $\eta_0 = 0$, $\dot{\eta}_0 = 1\mu\text{m} \cdot \mu\text{s}^{-1}$, $\sigma_{x,0} = 1\mu\text{m}$ and $\dot{\sigma}_x = 0$.

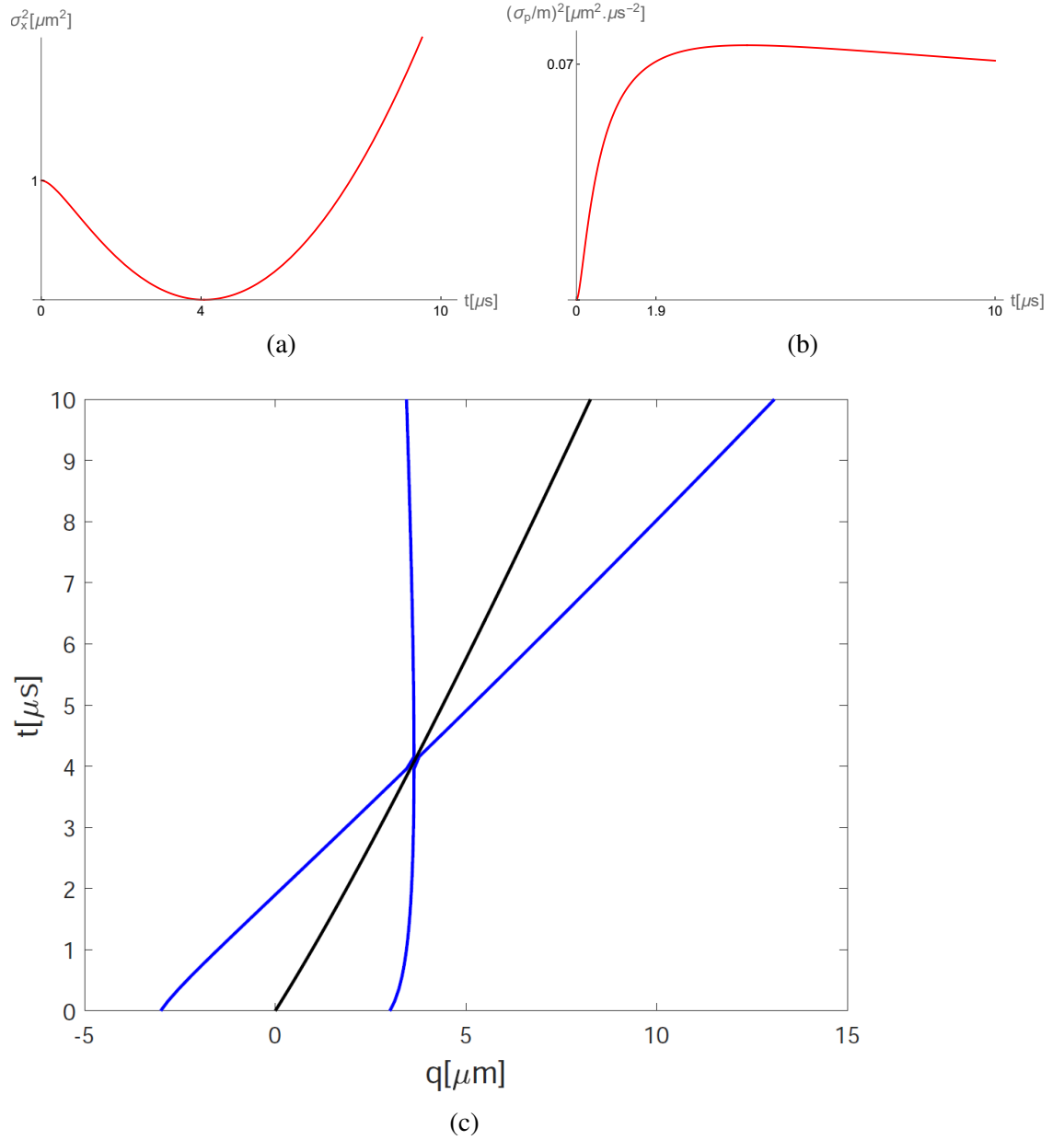


Fig. 3.7 Overdamped case $a = 3$ for a Mg-ion [Seidelin(2006)] under the action of a parametric oscillator whose frequency has 1MHz as order of magnitude (a) Position spreading for a general coherent state (b) momentum spreading for a general coherent state (c) Bohmian trajectories for the mean value (black line) and two other trajectories (blue lines) that are $3\sigma_x$ away from the maximum of the wavepacket. The previous Bohmian trajectories, in blue, contain 99.7% of the probability distribution according to Table 3.1 and the conservation equation (3.33). The initial conditions are given by $\eta_0 = 0$, $\dot{\eta}_0 = 1\mu\text{m} \cdot \mu\text{s}^{-1}$, $\sigma_{x,0} = 1\mu\text{m}$ and $\dot{\sigma}_x = 0$.

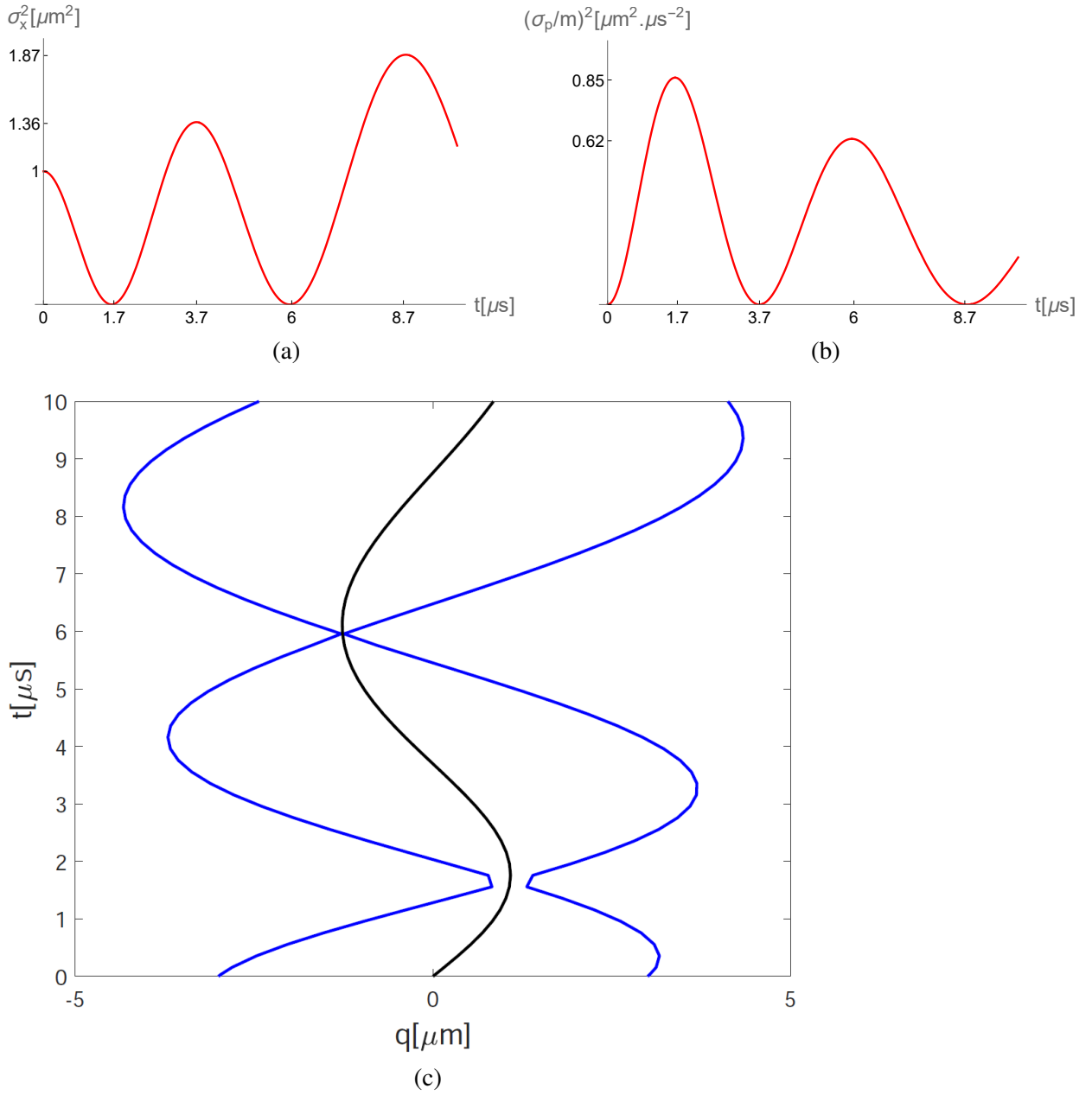


Fig. 3.8 Underdamped case $a = 0.1$ for a Mg-ion [Seidelin(2006)] under the action of a parametric oscillator whose frequency has 1MHz as order of magnitude (a) Position spreading for a general coherent state (b) momentum spreading for a general coherent state (c) Bohmian trajectories for the mean value (black line) and two other trajectories (blue lines) that are $3\sigma_x$ away from the maximum of the wavepacket. The previous Bohmian trajectories, in blue, contain 99.7% of the probability distribution according to Table 3.1 and the conservation equation (3.33). The initial conditions are given by $\eta_0 = 0$, $\dot{\eta}_0 = 1\mu\text{m} \cdot \mu\text{s}^{-1}$, $\sigma_{x,0} = 1\mu\text{m}$ and $\dot{\sigma}_x = 0$.

Regarding the underdamped case ($a < 2$), for $a = 0.1$, we see in Figures 3.8 (a) and (b) that the trapping stability is assured by a spreading that slowly increases periodically in time. The trapping function is assured to an interval of time $\Delta t = 10\mu s$, see Figure 3.8 (c).

This shows that the new interpretation of the Bohmian trajectories as “probability lanes” is useful to analyse the spatial spreading of probability. This occurs to be important in ion traps. Furthermore, it was shown that even a non-periodic frequency $\omega = \frac{1}{at+b}$ for a parametric oscillator can assure the trapping of a magnesium ion for at least intervals of times of the order of $10\mu s$ for the choice of parameter $a = 0.1$, *i.e.*, the underdamped regime.

3.5 Summary

■ In Section 3.1, it is recalled that the additional postulates are not necessary when defining and introducing the Bohmian trajectories. Especially the mathematical justification of the so called guidance law (3.4) is incoherent.

■ In Section 3.2, Bohmian trajectories are found without the need of additional postulates. They are the result of a specific parametrization of the respective continuity equations. This was shown for position and momentum representations

	Position representation	Momentum representation
Continuity equation	$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j_x}{\partial x} = 0$	$\frac{\partial \rho_p(p,t)}{\partial t} + \frac{\partial j_p}{\partial p} = 0$
Bohm function	$B_x = \int_{-\infty}^x \rho_x(x',t) dx'$	$B_p = \int_{-\infty}^p \rho_p(p',t) dp'$
Parametrization	$(x,t) _{B=\text{const}} \longrightarrow (q,t)$	$(p,t) _{B_p=\text{const}} \longrightarrow (\pi,t)$
Dynamical law	$\frac{dq}{dt} = \frac{j_x}{\rho_x}$	$\frac{d\pi}{dt} = \frac{j_p}{\rho_p}$

where $j_x = \rho_x(x,t) \frac{p_R}{m} = \rho_x(x,t) \frac{\partial_x S(x,t)}{m}$ and $j_p = \rho_p(p,t) (-b - m\omega^2 X_R) = \rho_p(p,t) (-b - m\omega^2 (-\frac{\partial}{\partial p} S_p(p,t)))$, with $\rho_x(x,t)$ and $\rho_p(p,t)$ representing the probability density in position and momentum space, respectively.

This was achieved by the use of a simple thermodynamic procedure involving Maxwell relations (see Box 3.2.1). Therefrom, after performing a contour integral in (x,t) -space, the non-crossing rule and the conservation of probability, so characteristic of Bohmian trajectories, was proven. This suggested naturally the interpretation of Bohmian trajectories not as possible paths, as it is commonly believed, but as borders of “probability lanes”. This idea was illustrated with the help of generalized coherent states.

■ In Section 3.3, a connection between conventional quantum mechanics and Bohmian mechanics was found. It was the Wigner formalism; the Bohmian framework is just a projected aspect of the Wigner function. This reinforced the idea of the proposed complex Bohmian quantities in Chapter 2, because they are projected effects of an observable on a continuous representation.

■ In Section 3.4, the new interpretation was used to analyse an ion trap characterized by a parametric oscillator of frequency $\frac{1}{at+b}$. After tuning the parameters of that parametric oscillator, the ion trapping time can decrease or increase. Contrary to usual frequencies in ion traps, this one is evidently non periodic and yet, it was proven, applying the new interpretation and handling of Bohmian trajectories, that it is useful for ion trapping when the intervals of interest are of the order of microseconds. Otherwise this potential can be discarded as candidate for trapping.

Chapter 4

Quantum hydrodynamics with complex quantities

Objective

In Chapter 2 a new formulation of Bohmian mechanics was introduced to clearly avoid any rhetorical and philosophical argumentation of quantum mechanics. In this sense, the projective structure of the action of the observables revealed to be the milestone of the Bohmian framework. On the other hand, Chapter 3 showed that the connection between conventional quantum mechanics and the Bohmian framework is the Wigner formalism. Bohmian mechanics is essentially a projective aspect of quantum mechanics. This does not diminish the importance of Bohmian mechanics. On the contrary, once the proper place of the theory is found, it allows to interpret the Bohmian trajectories in the correct way. They happen to be the borders of “probability lanes”. This is useful when approaching problems where the main interest is the spatial distribution of probability over the configuration space.

In Section 4.1, the status quo of the boundary conditions within Bohmian mechanics is mentioned. This is then extended in Sections 4.2 and 4.3 to the position and momentum representations, respectively, what can be achieved with the complex formulation of Bohmian mechanics.

keywords Hydrodynamic formulation, Bohmian mechanics, complex Bohmian quantities, momentum representation, transport equations, Eulerian equations.

4.1 Overview

Shortly after Schrödinger's first communication [Schrödinger(1926a)], Madelung published a formulation [Madelung(1927)] in terms of hydrodynamic equations using a polar form of the complex wave function resulting in two real equations instead of the one complex Schrödinger equation (SE). One of the equations is a CE for the (probability) density $\rho(x,t) = \psi^*(x,t)\psi(x,t)$ where $\psi(x,t)$ is the solution of the time-dependent SE and $\psi^*(x,t)$ its complex conjugate. The second equation is a mHJE, where the modification is an additional term depending on the density $\rho(x,t)$, thus introducing an (additional) coupling of Madelung's two equations.

This term is often called “quantum potential” or “Bohmian quantum potential”, as David Bohm used these two equations as basis for his formulation and interpretation of quantum mechanics [Bohm(1952a), Bohm(1952b)].

In this Chapter we will not discuss Bohm's attempt of a deterministic interpretation of quantum mechanics nor any ontological aspects, but essentially the formal similarities with hydrodynamics and extend the approach originally established by Madelung.

Further-reaching hydrodynamic aspects of quantum mechanics have been mentioned by other authors, *e.g.*, by Holland in [Holland(1995)]. In the context of quantum tunneling, Nassar [Nassar(1993)] tried to extend the similarities to include a kind of transport or Eulerian equations, adding equations of motion for a momentum density with an associated momentum flux density and an energy flux with energy flux density. The expressions for these equations are given explicitly, but there are no apparent structural relations or similarities amongst them recognizable.

In this study we want to show this missing structure using the complex quantities corresponding to physical quantities in the Bohmian formulation of quantum mechanics. Not only the equations of Nassar can be regained, but also in a form that is identical for the probability density (comparable to mass density in hydrodynamics), momentum and energy densities, but now for complex momentum and energy quantities.

An early criticism by Pauli [Pauli(1952)] and Heisenberg [Passon(2005)] against Bohm's approach was the asymmetric role of the canonical variables, *i.e.*, the description solely in terms of position and the absence of a description in terms of momentum, unlike in classical mechanics where the Hamiltonian formalism acts in phase space with position and momentum both being independent

variables, or in standard quantum mechanics that can equally well be formulated in position and momentum space.

In a Chapter 2 we have shown that the missing symmetry can be established just following the original approach of Bohm leading to a consistent momentum space version of this formalism.

This formulation will also be applied to the above mentioned transport equations in momentum space, leading to formally equivalent equations for position density (corresponding to momentum density in position space) and energy density in momentum space.

4.2 Transport equations in position representation

4.2.1 Dynamics of Bohmian quantities in position representation

Recall that, as we saw in Chapter 2, the formal basis of Bohmian mechanics is the already defined decomposition of the linear complex SE¹

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right\} \psi(x,t) \quad (4.1)$$

into two real equations that have similarity with hydrodynamic equations (see Eqs. (2.4-2.5)), namely the CE

$$\frac{\partial}{\partial t} \rho_x + \frac{\partial}{\partial x} \left[\rho_x \frac{\partial S_x}{\partial x} \right] = 0 \quad (4.2)$$

and a mHJE

$$\frac{\partial}{\partial t} S_x + \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V - \frac{\hbar^2}{2m} \frac{\frac{\partial^2 \sqrt{\rho_x}}{\partial x^2}}{\sqrt{\rho_x}} = 0 \quad (4.3)$$

by using the polar ansatz (2.3) for the wave function ψ , *i.e.*, in position representation $\psi(x,t) = \langle x | \psi(t) \rangle = \sqrt{\rho_x} \exp\left(\frac{i}{\hbar} S_x\right)$, where $\rho_x = \psi^* \psi$ and the subscript indicates the representation that is considered. This formulation was first introduced by Madelung [Madelung(1927)] in 1927 and 25 years later adopted by Bohm [Bohm(1952a), Bohm(1952b)] in his interpretation of quantum mechanics in terms of “hidden variables”. In the following we are not going into ontological

¹ Our discussion is restricted to the one-dimensional case.

interpretations of quantum mechanics, but stick to the formal structure that was established by Madelung and extend the similarities with hydrodynamics.

Now, we use the definition (2.9) introduced in Section 2.2.1, for Bohmian quantities F_{Bo} corresponding to an operator \widehat{F} (associated with an observable F),

$$F_{Bo}(x, t) = F(x, t) = \frac{\langle x | \widehat{F} | \psi \rangle}{\langle x | \psi \rangle} = F_R + iF_I. \quad (4.4)$$

Recall that Bohmian quantities $F(x, t)$ are in general (apart from purely multiplicative c-numbers) complex.

In position representation we consider again expressions (2.12-2.15) for the position operator $\widehat{X} = x$, momentum operator $\widehat{P} = \frac{\hbar}{i} \frac{\partial}{\partial x}$, Hamiltonian operator $\widehat{H}_x = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t)$ and the energy operator $\widehat{E} = i\hbar \frac{\partial}{\partial t}$. The corresponding Bohmian quantities are then

$$X = x \quad \text{real} \quad (4.5)$$

$$P = \frac{\partial}{\partial x} S_x - i \frac{\hbar}{2} \frac{\frac{\partial}{\partial x} \rho_x}{\rho_x} = \frac{\partial}{\partial x} S_x - i \frac{\hbar}{2} \frac{\partial}{\partial x} \ln \rho_x = P_R + iP_I \quad \text{complex} \quad (4.6)$$

$$H_x = T_x + V(x, t) = \frac{1}{2m} \left[(P)^2 + \frac{\hbar}{i} \frac{\partial}{\partial x} P \right] + V(x, t) \quad (4.7)$$

with

$$T_x = \frac{1}{2m} [P^2] = \frac{1}{2m} \left[(P_R^2 - P_I^2 + \hbar \frac{\partial}{\partial x} P_I) + i(2P_R P_I - \hbar \frac{\partial}{\partial x} P_R) \right] = T_R + iT_I \quad (4.8)$$

where

$$T_R = \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V_{qu,x} \quad (4.9)$$

and

$$V_{qu,x} = -\frac{1}{2m} \left[P_I^2 - \hbar \frac{\partial}{\partial x} P_I \right] = -\frac{\hbar^2}{8m} \left(\frac{\frac{\partial}{\partial x} \rho_x}{\rho_x} \right)^2 - \frac{\hbar^2}{4m} \frac{\partial}{\partial x} \left(\frac{\frac{\partial}{\partial x} \rho_x}{\rho_x} \right) = -\frac{\hbar^2}{2m} \frac{\frac{\partial^2}{\partial x^2} \sqrt{\rho_x}}{\sqrt{\rho_x}}. \quad (4.10)$$

The appearance of the “quantum potential” $V_{qu,x}$ distinguishes the mHJE (4.3) from the classical HJE for the action S_x .

Finally,

$$E = -\frac{\partial}{\partial t}S_x + i\frac{\hbar}{2}\frac{\frac{\partial}{\partial t}\rho_x}{\rho_x} = -\frac{\partial}{\partial t}S_x + i\frac{\hbar}{2}\frac{\partial}{\partial t}\ln\rho_x = E_R + iE_I \quad (4.11)$$

corresponds to the left hand side of the SE (4.1).

As shown in Section 2.2.1, combining E_I with T_I leads to the CE (4.2). In general, as also has been shown in [Bonilla(2020a)], it holds in any representation “ a ”, that:

$$H_R(a,t) = E_R(a,t) = -\frac{\partial}{\partial t}S_a, \quad (4.12)$$

$$H_I(a,t) = E_I(a,t) = \frac{\hbar}{2}\frac{\frac{\partial}{\partial t}\rho_a}{\rho_a}. \quad (4.13)$$

The dynamics of the Bohmian quantities can then be formulated using these relations.

The temporal change of the complex momentum can be expressed as

$$\begin{aligned} \frac{\partial}{\partial t}P &= \frac{\partial}{\partial t}\left[\frac{\partial}{\partial x}S_x - i\frac{\hbar}{2}\frac{\partial}{\partial x}\ln\rho_x\right] = \frac{\partial}{\partial x}\left[\frac{\partial}{\partial t}S_x - i\frac{\hbar}{2}\frac{\partial}{\partial t}\ln\rho_x\right] \\ &= -\frac{\partial}{\partial x}H_x(x,t). \end{aligned} \quad (4.14)$$

Finally, the time-derivative of the Bohmian Hamiltonian can be expressed using these relations as

$$\begin{aligned} \frac{\partial}{\partial t}H_x &= \frac{P}{m}\frac{\partial}{\partial t}P - i\frac{\hbar}{2m}\frac{\partial}{\partial x}\frac{\partial}{\partial t}P + \frac{\partial}{\partial t}V \\ &= -\frac{P}{m}\frac{\partial}{\partial x}H_x + i\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}H_x + \frac{\partial}{\partial t}V. \end{aligned} \quad (4.15)$$

Only if the potential V is explicitly time-dependent, *e.g.* for a parametric oscillator $V = \frac{m}{2}\omega(t)x^2$, the contribution $\frac{\partial}{\partial t}V$ does not vanish. But even for $\frac{\partial}{\partial t}V = 0$, the first two terms on the right hand side of equation (4.15) remain due to the nonlocality of the complex Bohmian Hamiltonian.

4.2.2 Bohmian transport equations in position representation

Considering first the dynamics of the Bohmian momentum density $\rho_x P \in \mathbb{C}$ by taking its time-derivative and using the CE (4.2) and Eq. (4.14) one obtains

$$\begin{aligned} \frac{\partial}{\partial t}(\rho_x P) &= P \frac{\partial}{\partial t} \rho_x + \rho_x \frac{\partial}{\partial t} P \\ &= -P \left[\frac{\partial}{\partial x} \left(\rho_x \frac{P_R}{m} \right) \right] - \rho_x \frac{\partial}{\partial x} H_x \end{aligned} \quad (4.16)$$

where

$$\frac{\partial}{\partial x} H_x = \frac{P}{m} \frac{\partial}{\partial x} P - i \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} P + \frac{\partial}{\partial x} V, \quad (4.17)$$

leading to

$$\frac{\partial}{\partial t}(\rho_x P) = -P \left[\frac{\partial}{\partial x} \left(\rho_x \frac{P_R}{m} \right) \right] - \rho_x \frac{P}{m} \frac{\partial}{\partial x} P + i \frac{\hbar}{2m} \rho_x \frac{\partial^2}{\partial x^2} P - \rho_x \frac{\partial}{\partial x} V. \quad (4.18)$$

In order to obtain the equation for the complex Bohmian quantity $\rho_x P$, the term $-iP \frac{\partial}{\partial x} \left(\rho_x \frac{P_I}{m} \right)$ has to be added and subtracted and the definition of P_I used, resulting in

$$\frac{\partial}{\partial t}(\rho_x P) = -\frac{\partial}{\partial x} \left[\left(\rho_x \frac{P_R}{m} \right) P \right] + i \frac{\hbar}{2m} \left[\rho_x \frac{\partial^2}{\partial x^2} P - P \frac{\partial^2}{\partial x^2} \rho_x \right] - \rho_x \frac{\partial}{\partial x} V. \quad (4.19)$$

Adding and subtracting $(\frac{\partial}{\partial x} \rho_x)(\frac{\partial}{\partial x} P)$ and using (2.59) this can be rewritten in a form where the time-derivative of the momentum density can be expressed essentially by the divergence of a flux, similar to the continuity equation, with $-\rho_x \frac{\partial}{\partial x} V$ as an external source-term,

$$\frac{\partial}{\partial t}(\rho_x P) + \frac{\partial}{\partial x} \left[\left(\rho_x \frac{\partial Q}{\partial t} \right) P + i \frac{\hbar}{2m} \left(P \frac{\partial}{\partial x} \rho_x - \rho_x \frac{\partial}{\partial x} P \right) \right] = -\rho_x \frac{\partial}{\partial x} V \quad (4.20)$$

where, according to the definition (2.59), $\frac{\partial Q}{\partial t} = \frac{P}{m}$.

Regarding next the Bohmian energy density $\rho_x H \in \mathbb{C}$, we follow the same scheme, *i.e.*, using the CE (4.2) and now equation (4.15),

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho_x H_x) &= H_x \frac{\partial}{\partial t} \rho_x + \rho_x \frac{\partial}{\partial t} H_x \\
&= -H_x \left[\frac{\partial}{\partial x} \left(\rho_x \frac{P_R}{m} \right) \right] - \rho_x \left(\frac{P}{m} \frac{\partial}{\partial x} H_x \right) + i \frac{\hbar}{2m} \rho_x \frac{\partial^2}{\partial x^2} H_x + \rho_x \frac{\partial}{\partial t} V.
\end{aligned} \tag{4.21}$$

Adding and subtracting this time $-iH_x \frac{\partial}{\partial x} \left(\rho_x \frac{P_I}{m} \right)$ and $\left(\frac{\partial}{\partial x} \rho_x \right) \left(\frac{\partial}{\partial x} H_x \right)$ and using again the definition of P_I and Eq. (2.61), this time leads to

$$\frac{\partial}{\partial t}(\rho_x H_x) + \frac{\partial}{\partial x} \left[\left(\rho_x \frac{\partial Q}{\partial t} \right) H_x + i \frac{\hbar}{2m} \left(H_x \frac{\partial}{\partial x} \rho_x - \rho_x \frac{\partial}{\partial x} H_x \right) \right] = \rho_x \frac{\partial}{\partial t} V. \tag{4.22}$$

Finally, the CE can be brought into the same form, starting from

$$\frac{\partial}{\partial t} \rho_x + \frac{\partial}{\partial x} \left(\rho_x \frac{P_R}{m} \right) = 0, \tag{4.23}$$

adding and subtracting $i \frac{\partial}{\partial x} \left(\rho_x \frac{P_I}{m} \right)$ and using the definition of P_I and Eq. (2.61)

$$\frac{\partial}{\partial t} \rho_x + \frac{\partial}{\partial x} \left[\rho_x \frac{\partial Q}{\partial t} + i \frac{\hbar}{2m} \frac{\partial}{\partial x} \rho_x \right] = 0, \tag{4.24}$$

what can be rewritten in a form like the one obtained for $\rho_x P$ and $\rho_x H_x$ by changing ρ_x into $\rho_x \cdot 1$, leading to

$$\frac{\partial}{\partial t}(\rho_x \cdot 1) + \frac{\partial}{\partial x} \left[\left(\rho_x \frac{\partial Q}{\partial t} \right) \cdot 1 + i \frac{\hbar}{2m} \left(1 \cdot \frac{\partial}{\partial x} \rho_x - \rho_x \frac{\partial}{\partial x} 1 \right) \right] = 0. \tag{4.25}$$

Therefore, all three cases (4.20), (4.22) and (4.25) can be summarized in the same (complex) form

$$\boxed{\frac{\partial}{\partial t}(\rho_x A) + \frac{\partial}{\partial x} \left[J_x A + i \frac{\hbar}{2m} \left(A \frac{\partial}{\partial x} \rho_x - \rho_x \frac{\partial}{\partial x} A \right) \right]} = f(x, t) \tag{4.26}$$

where $J_x \doteq \rho_x \frac{P}{m} = \rho_x \frac{\partial Q}{\partial t} = \rho_x \frac{\partial S_x}{\partial x} - i \frac{\hbar}{2m} \frac{\partial}{\partial x} \rho_x = J_{x,R} + i J_{x,I}$ and A can be 1, $P \in \mathbb{C}$ or $H_x \in \mathbb{C}$. The position dependent function $f(x, t)$ can also be written as a density

in the form $f(x) = \rho_x \frac{\partial}{\partial t} A_{cl}$ where A_{cl} is the classical quantity corresponding to the Bohmian quantity A , therefore $\frac{\partial}{\partial t} 1 = 0$, $\frac{\partial}{\partial t} P_{cl} = -\frac{\partial}{\partial x} V$ and $\frac{\partial}{\partial t} H_{cl} = \frac{\partial}{\partial t} V$.

The terms in the square bracket of equation (4.26) can still be simplified by going from a description in terms of only complex quantities (apart from $\rho_x \cdot 1$) to one where, like in the original CE (4.2), only the real part of the current density is used, *i.e.*, $J_{x,R} = \rho_x \frac{\partial S_x}{m}$ instead of $J_x = \rho_x \frac{P}{m}$. Equation (4.26) can then be reformulated as

$$\frac{\partial}{\partial t} (\rho_x A) + \frac{\partial}{\partial x} \left[J_{x,R} A - i \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A \right] = f(x, t). \quad (4.27)$$

In this form it is also easy to confirm the right hand side of equation (4.26), namely $f(x, t) = \rho_x \frac{\partial}{\partial t} A_{cl}$. Going from our local description in terms of densities to a global one by integrating equation (4.27) over the whole position space, *i.e.*,

$$\int_{-\infty}^{+\infty} dx \frac{\partial}{\partial t} (\rho_x A) + \int_{-\infty}^{+\infty} dx \frac{\partial}{\partial x} \left[\rho_x \left(\frac{\partial S_x}{m} \right) A - i \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A \right] = \int_{-\infty}^{+\infty} dx \rho_x \frac{\partial A_{cl}}{\partial t}. \quad (4.28)$$

The second integral on the left hand side yields just the values of the quantities in the square bracket at the boundaries, *i.e.*

$$\rho_x \left[\left(\frac{\partial S_x}{m} \right) \cdot A - i \frac{\hbar}{2m} \frac{\partial}{\partial x} A \right] \Big|_{-\infty}^{+\infty} = 0, \quad (4.29)$$

that vanish for square integrable wave functions, as ρ_x vanishes for $-\infty$ and $+\infty$.

In the other two integrals, integration and time-derivative can be interchanged, leading to

$$\frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dx \rho_x A = \frac{\partial}{\partial t} \langle A \rangle = \frac{\partial A_{cl}}{\partial t} \int_{-\infty}^{+\infty} dx \rho_x = \frac{\partial A_{cl}}{\partial t} \quad (4.30)$$

where the pointed brackets denote mean values or expectation values of the quantities within the brackets. Therefore, Eq. (4.30) is nothing but the Ehrenfest theorem [Ehrenfest(1927)] that states that on average, the classical equations of motion are valid

In the following, equation (4.27) is separated into real and imaginary parts, yielding

$$\frac{\partial}{\partial t}(\rho_x A_R) + \frac{\partial}{\partial x} \left[J_{x,R} A_R + \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A_I \right] = f(x,t), \quad (4.31)$$

$$\frac{\partial}{\partial t}(\rho_x A_I) + \frac{\partial}{\partial x} \left[J_{x,R} A_I - \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A_R \right] = 0. \quad (4.32)$$

For $A = 1 + i0$ it is straightforward to see that (4.32) is trivially fulfilled and (4.31) simply turns into the CE (4.2) or Eq. (4.23).

For $A = P = \frac{\partial}{\partial x} S_x - i \frac{\hbar}{2} \frac{\partial_x \rho_x}{\rho_x}$, the real part can be expressed as

$$\frac{\partial}{\partial t}(\rho_x \frac{\partial}{\partial x} S_x) + \frac{\partial}{\partial x} \left[\rho_x \frac{\partial_x S_x}{m} \left(\frac{\partial}{\partial x} S_x \right) - \frac{\hbar^2}{4m} \left(\frac{\partial^2}{\partial x^2} \rho_x - \frac{(\frac{\partial}{\partial x} \rho_x)^2}{\rho_x} \right) \right] = -\rho_x \frac{\partial}{\partial x} V, \quad (4.33)$$

or, using Nassar's notation [Nassar(1993)]:

$$\frac{\partial}{\partial t} (m J_{\text{Nassar}}) + \frac{\partial}{\partial x} [m P_{\text{Nassar}}] = -\rho_x \frac{\partial}{\partial x} V \quad (4.34)$$

where $J_{\text{Nassar}} = \rho_x v_{\text{Nassar}} = \rho_x \frac{\partial_x S_x}{m}$ is his momentum density and $P_{\text{Nassar}} = \rho_x \frac{(\frac{\partial_x S_x)^2}{m^2} - \frac{\hbar^2}{4m^2} \left(\frac{\partial^2}{\partial x^2} \rho_x - \frac{(\frac{\partial}{\partial x} \rho_x)^2}{\rho_x} \right)$ his momentum flux density (where in both cases his definition contains a factor $\frac{1}{m}$).

The imaginary part simply provides

$$\frac{\partial}{\partial x} \left\{ \frac{\partial}{\partial t} \rho_x + \frac{\partial}{\partial x} \left(\rho_x \frac{\partial_x S_x}{m} \right) \right\} = 0 \quad (4.35)$$

what essentially is the momentum operator applied to the CE,

$$\left(\frac{i}{\hbar} \right) \widehat{P}_{op} \{ \text{CE} \}. \quad (4.36)$$

Considering now $A = H_x = -\frac{\partial}{\partial t} S_x + i \frac{\hbar}{2} \frac{\partial_t \rho_x}{\rho_x}$, where (4.12) and (4.13) have been used, the real part yields

$$\frac{\partial}{\partial t} \left(-\rho_x \frac{\partial S_x}{\partial t} \right) + \frac{\partial}{\partial x} \left[\rho_x \frac{\partial_x S_x}{m} \left(-\frac{\partial}{\partial t} S_x \right) + \frac{\hbar^2}{4m} \rho_x \frac{\partial}{\partial x} \left(\frac{\partial_t \rho_x}{\rho_x} \right) \right] = \rho_x \frac{\partial}{\partial t} V, \quad (4.37)$$

what can again be expressed using Nassar's energy density $U_{\text{Nassar}} = \rho_x \left(\frac{m}{2} v_{\text{Nassar}}^2 + V + V_{qu,x} \right)$ and his energy density flux $Q_{\text{Nassar}} = v_{\text{Nassar}} U_{\text{Nassar}} + \frac{\hbar^2}{2m} \left(\sqrt{\rho_x} \frac{\partial^2 \sqrt{\rho_x}}{\partial x \partial t} - \left(\frac{\partial \sqrt{\rho_x}}{\partial x} \right) \left(\frac{\partial \sqrt{\rho_x}}{\partial t} \right) \right)$ in the form

$$\frac{\partial}{\partial t} U_{\text{Nassar}} + \frac{\partial}{\partial x} Q_{\text{Nassar}} = 0 \quad (4.38)$$

where $\frac{\partial}{\partial t} V = 0$ has been assumed (to be in agreement with [Nassar(1993)]).

The imaginary part now takes the form

$$\frac{\partial}{\partial t} \left\{ \frac{\partial}{\partial t} \rho_x + \frac{\partial}{\partial x} \left(\rho_x \frac{\partial S_x}{\partial x} \right) \right\} = 0 \quad (4.39)$$

what again can be expressed as the corresponding operator, in this case the energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$, applied on the CE,

$$-\frac{i}{\hbar} \hat{E} \{ CE \} = -\frac{i}{\hbar} \hat{H} \{ CE \}. \quad (4.40)$$

4.2.3 *Quantum transport equations and the associated Euler equations in position representation*

In classical mechanics a transport equation for a local density can be rewritten as an Euler equation in a co-moving frame [Greiner(1991)], provided the CE is fulfilled. To recall the procedure, a typical transport equation shall be considered,

$$\frac{\partial}{\partial t} (\rho A) + \frac{\partial}{\partial x} [(\rho v) A] = 0, \quad (4.41)$$

leading to

$$A \frac{\partial \rho}{\partial t} + \rho \frac{\partial A}{\partial t} + A \nabla \cdot (\rho v) + (\rho v) \cdot \nabla A = 0, \quad (4.42)$$

what, since the CE is fulfilled, can be written as an Euler equation in the form

$$\rho \frac{\partial A}{\partial t} + \rho v \cdot \nabla A = 0, \quad (4.43)$$

or for regions with $\rho \neq 0$, as

$$\frac{\partial A}{\partial t} + \mathbf{v} \cdot \nabla A = \frac{D}{Dt} A = 0, \quad (4.44)$$

where $\frac{D}{Dt}$ is the substantial time-derivative valid in a co-moving “coordinate” frame moving with velocity \mathbf{v} .

This procedure is now applied to the general Bohmian transport equation (4.27) in position representation,

$$\frac{\partial}{\partial t} (\rho_x A) + \frac{\partial}{\partial x} \left[J_{R,x} A - i \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A \right] = f(x,t),$$

leading to

$$\boxed{\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial t} \frac{\partial}{\partial x} A - i \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} A = \frac{f(x,t)}{\rho_x}}. \quad (4.45)$$

This is obviously a convection-diffusion equation or a Fokker–Planck-type equation in position space, also called Smoluchowski equation, for an incompressible medium with $\frac{\partial}{\partial x} \frac{\partial Q}{\partial t} = \frac{\partial P}{\partial x} = 0$ and a purely imaginary diffusion coefficient² $D_x = i \frac{\hbar}{2m}$. Expressing (4.45) in terms of real and imaginary parts leads to:

$$\boxed{\frac{\partial A_R}{\partial t} + \frac{P_R}{m} \frac{\partial}{\partial x} A_R - \frac{P_I}{m} \frac{\partial}{\partial x} A_I + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} A_I = \frac{f(x,t)}{\rho_x}}, \quad (4.46)$$

$$\boxed{\frac{\partial A_I}{\partial t} + \frac{P_R}{m} \frac{\partial}{\partial x} A_I + \frac{P_I}{m} \frac{\partial}{\partial x} A_R - \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} A_R = 0}. \quad (4.47)$$

For $A = P = P_R + iP_I$, *i.e.*, the complex Bohmian momentum, one obtains

$$\frac{\partial P_R}{\partial t} + \frac{P_R}{m} \frac{\partial}{\partial x} P_R - \frac{P_I}{m} \frac{\partial}{\partial x} P_I + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} P_I = -\frac{\partial}{\partial x} V, \quad (4.48)$$

$$\frac{\partial P_I}{\partial t} + \frac{P_R}{m} \frac{\partial}{\partial x} P_I + \frac{P_I}{m} \frac{\partial}{\partial x} P_R - \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} P_R = 0, \quad (4.49)$$

what can be rewritten as

² It should just be reminded that the time-dependent SE for the free motion, *i.e.*, $V = 0$, has exactly the form of a diffusion equation with this purely imaginary diffusion coefficient $D_x = i \frac{\hbar}{2m}$.

$$\frac{\partial P_R}{\partial t} + \frac{\partial}{\partial x} \left[\frac{P_R^2}{2m} - \frac{P_I^2}{2m} + \frac{\hbar}{2m} \frac{\partial}{\partial x} P_I + V \right] = 0, \quad (4.50)$$

$$\frac{\partial P_I}{\partial t} + \frac{\partial}{\partial x} \left[\frac{P_R P_I}{m} - \frac{\hbar}{2m} \frac{\partial}{\partial x} P_R \right] = 0. \quad (4.51)$$

In terms of real and imaginary parts of the Bohmian Hamiltonian, this yields

$$\frac{\partial P_R}{\partial t} + \frac{\partial}{\partial x} H_R = 0, \quad (4.52)$$

$$\frac{\partial P_I}{\partial t} + \frac{\partial}{\partial x} H_I = 0. \quad (4.53)$$

with $H_R = \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V + V_{qu,x}$, $H_I = \frac{i\hbar}{2} \frac{\partial}{\partial x} \ln \rho_x$ and $P_R = \frac{\partial}{\partial x} S_x$.
Exchanging temporal and spatial derivatives in (4.52) leads to

$$\frac{\partial}{\partial x} \left[\frac{\partial}{\partial t} S_x + \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V + V_{qu,x} \right] = 0 \quad (4.54)$$

what is just the momentum operator applied to the mHJE (4.3)

$$\frac{i}{\hbar} \hat{P} \{ \text{mHJE} \}. \quad (4.55)$$

On the other hand, applying $\frac{\partial}{\partial x}$ in Eq. (4.54) and replacing $\frac{\partial}{\partial x} S_x$ by P_R , this equation can be formulated as a Newtonian equation of motion with a substantial time-derivative of the (real) momentum and including the quantum potential $V_{qu,x}$,

$$\frac{\partial}{\partial t} P_R + \frac{P_R}{m} \frac{\partial}{\partial x} P_R + \frac{\partial}{\partial x} (V + V_{qu,x}) = 0, \quad (4.56)$$

or

$$\frac{D}{Dt} P_R = - \frac{\partial}{\partial x} (V + V_{qu,x}). \quad (4.57)$$

Equation (4.53) for the imaginary part provides

$$\frac{\partial}{\partial t} \left[- \frac{i\hbar}{2} \frac{\partial}{\partial x} \ln \rho_x \right] + \frac{\partial}{\partial x} \left[\frac{i\hbar}{2} \frac{\partial}{\partial t} \ln \rho_x \right] = 0 \quad (4.58)$$

what is obviously fulfilled, as spatial and temporal derivatives can be interchanged.

Considering the complex Bohmian Hamiltonian, Eqs. (4.46) and (4.47) turn into

$$\frac{\partial H_R}{\partial t} + \frac{P_R}{m} \frac{\partial}{\partial x} H_R - \frac{P_I}{m} \frac{\partial}{\partial x} H_I + \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} H_I = \frac{\partial}{\partial t} V, \quad (4.59)$$

$$\frac{\partial H_I}{\partial t} + \frac{P_R}{m} \frac{\partial}{\partial x} H_I + \frac{P_I}{m} \frac{\partial}{\partial x} H_R - \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} H_R = 0. \quad (4.60)$$

Bearing in mind the expression of the Bohmian Hamiltonian and the Bohmian momentum leads for the real part to

$$\frac{\partial}{\partial t} \left\{ \frac{\partial}{\partial t} S_x + \frac{P_R^2}{2m} - \frac{P_I^2}{2m} + \frac{\hbar}{2m} \frac{\partial}{\partial x} P_I + V \right\} = 0 \quad (4.61)$$

or

$$\frac{\partial}{\partial t} \left\{ \frac{\partial}{\partial t} S_x + \frac{1}{2m} \left(\frac{\partial}{\partial x} S_x \right)^2 + V_{qu,x} + V \right\} = 0 \quad (4.62)$$

what is, up to a constant factor, just the energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$ applied to the mHJE (4.3), *i.e.*,

$$-\frac{i}{\hbar} \hat{E} \{ \text{mHJE} \}. \quad (4.63)$$

For the imaginary part, one obtains

$$\frac{\partial}{\partial t} \left\{ \frac{\hbar}{2} \frac{\partial}{\partial t} \ln \rho_x - \frac{P_R P_I}{m} + \frac{\hbar}{2m} \frac{\partial}{\partial x} P_R \right\} = 0, \quad (4.64)$$

what, using the terms for E_I and H_I , can be written as

$$\frac{\partial}{\partial t} \{ E_I - H_I \} = 0, \quad (4.65)$$

being obviously correct according to Eq. (4.13).

4.3 Transport equations in momentum representation

4.3.1 Dynamics of Bohmian quantities in momentum representation

In analogy to Section 4.2.1, it is possible to formulate Bohmian mechanics in momentum representation.

Inserting again the polar form (2.3) of the wave function in momentum space, $\psi(p, t) = \langle p | \Psi \rangle = \sqrt{\rho_p} \exp(\frac{i}{\hbar} S_p)$, into the time-dependent SE allows again to “decouple” this complex equation into two real ones. The explicit form of these equations depends on the specific form of the potential V that itself depends on the position operator $\hat{X} = -\frac{\hbar}{i} \frac{\partial}{\partial p}$. To show the similarity and symmetry between the position and momentum representation, we restrict our discussion to potentials that are at most quadratic in the position variable in momentum space, as the kinetic energy in position space is quadratic in momentum. This will allow to show clearly the formal correspondence between the two formulations.

Therefore, hereafter the potential $V(\hat{X}_{op}) = a + b\hat{X}_{op} + \frac{m}{2}\omega^2\hat{X}_{op}^2 = a - b\frac{\hbar}{i}\frac{\partial}{\partial p} - \frac{m}{2}\omega^2\hbar^2\frac{\partial^2}{\partial p^2}$ is considered.

As we saw in Section 2.2.2.2 with Eqs. (2.33-2.34), the two hydrodynamic equations are then given by:

$$\frac{\partial}{\partial t} S_p + \frac{p^2}{2m} + V(-\frac{\partial}{\partial p} S_p) + V_{qu,p} = 0, \quad (4.66)$$

$$\frac{\partial}{\partial t} \rho_p + \frac{\partial}{\partial p} \left[\rho_p \left(-b - m\omega^2 \left(-\frac{\partial}{\partial p} S_p \right) \right) \right] = 0. \quad (4.67)$$

The additional term $V_{qu,p}$ in the mHJE (4.66) is a kind of “quantum potential” in momentum space due to its formal similarity with $V_{qu,x}$ in position representation, given in Eq. (4.10). The term $V_{qu,p}$ is also nonlocal and has the structure

$$V_{qu,p}(p, t) = -m\omega^2 \frac{\hbar^2}{4} \left[\frac{\frac{\partial^2}{\partial p^2} \rho_p}{\rho_p} - \frac{1}{2} \left(\frac{\frac{\partial \rho_p}{\partial p}}{\rho_p} \right)^2 \right] = -\frac{m}{2} \omega^2 \hbar^2 \frac{\frac{\partial^2}{\partial p^2} \sqrt{\rho_p}}{\sqrt{\rho_p}}. \quad (4.68)$$

Like in the position representation in Section 4.2.1, the Bohmian quantities F_{Bo} defined through (2.9) are employed. In addition, similar to the position repre-

sentation, we consider the position operator $\widehat{X}_p = -\frac{\hbar}{i} \frac{\partial}{\partial p}$ (which is now a differential operator), the momentum operator $\widehat{P} = p$ (which is now not a differential operator), the Hamiltonian operator $\widehat{H}_p = \frac{p^2}{2m} + a - b \frac{\hbar}{i} \frac{\partial}{\partial p} - \frac{m}{2} \omega^2 \hbar^2 \frac{\partial^2}{\partial p^2}$ and the energy operator $\widehat{E} = i\hbar \frac{\partial}{\partial t}$. The corresponding Bohmian quantities are, as we saw in Section 2.2.2.2 with Eqs. (2.22-2.25),

$$P = p \quad \text{real} \quad (4.69)$$

$$X = -\frac{\partial}{\partial p} S_p + i \frac{\hbar}{2} \frac{\frac{\partial}{\partial t} \rho_p}{\rho_p} = -\frac{\partial}{\partial p} S_p + i \frac{\hbar}{2} \frac{\partial}{\partial p} \ln \rho_p = X_R + iX_I \quad \text{complex} \quad (4.70)$$

$$H_p = \frac{p^2}{2m} + a + bX + \frac{m}{2} \omega^2 \left[(X)^2 - \frac{\hbar}{i} \frac{\partial}{\partial p} X \right] = \frac{p^2}{2m} + a + bX + \frac{m}{2} \omega^2 [X^2] = H_R + iH_I \quad (4.71)$$

with

$$\begin{aligned} H_R &= \frac{p^2}{2m} + a + bX_R + \frac{m}{2} \omega^2 X_R^2 - \frac{m}{2} \omega^2 \left[X_I^2 + \hbar \frac{\partial}{\partial p} X_I \right] \\ &= \frac{p^2}{2m} + a - b \frac{\partial}{\partial p} S_p + \frac{m}{2} \omega^2 \left(\frac{\partial}{\partial p} S_p \right)^2 + V_{qu,p} \end{aligned} \quad (4.72)$$

where the above defined ‘‘quantum potential’’ $V_{qu,p}$ can also be rewritten in terms of the imaginary part of the Bohmian position X_I as

$$V_{qu,p} = -\frac{m}{2} \omega^2 \left[X_I^2 + \hbar \frac{\partial}{\partial p} X_I \right] \quad (4.73)$$

and

$$H_I = bX_I + m\omega^2 X_R X_I + m\omega \frac{\hbar}{2} \frac{\partial}{\partial p} X_R. \quad (4.74)$$

Finally, the Bohmian energy corresponding to the left hand side of SE is given by

$$E = -\frac{\partial}{\partial t} S_p + i \frac{\hbar}{2} \frac{\frac{\partial}{\partial t} \rho_p}{\rho_p} = -\frac{\partial}{\partial t} S_p + i \frac{\hbar}{2} \frac{\partial}{\partial t} \ln \rho_p = E_R + iE_I. \quad (4.75)$$

As already mentioned in Section 4.2.1, in any representation, *i.e.*, also in momentum representation,

$$\mathbf{H}_R(p,t) = \mathbf{E}_R(p,t) = -\frac{\partial}{\partial t} S_p \quad (4.76)$$

$$\mathbf{H}_I(p,t) = \mathbf{E}_I(p,t) = \frac{\hbar}{2} \frac{\partial}{\partial t} \ln \rho_p = \frac{\hbar}{2} \frac{\partial}{\partial t} \ln \rho_p \quad (4.77)$$

is valid.

Using these relations, the dynamics of the Bohmian quantities in momentum space can be formulated.

For the temporal change of the Bohmian position one obtains

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{X} &= \frac{\partial}{\partial t} \left[-\frac{\partial}{\partial p} S_p + i \frac{\hbar}{2} \frac{\partial}{\partial p} \ln \rho_p \right] = \frac{\partial}{\partial p} \left[-\frac{\partial}{\partial t} S_p + i \frac{\hbar}{2} \frac{\partial}{\partial t} \ln \rho_p \right] \\ &= \frac{\partial}{\partial p} \mathbf{H}_p(p,t). \end{aligned} \quad (4.78)$$

With the variable $\Pi(p,t)$ (see Eq. (2.69)) defined previously in Chapter 2, the time-derivative of the Hamiltonian can finally be obtained via

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{H}_p &= (b + m\omega^2 \mathbf{X}) \frac{\partial}{\partial t} \mathbf{X} + i \frac{m}{2} \omega^2 \hbar \frac{\partial}{\partial p} \frac{\partial}{\partial t} \mathbf{X} \\ &= (b + m\omega^2 \mathbf{X}) \frac{\partial}{\partial p} \mathbf{H}_p + i \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} \mathbf{H}_p \\ &= -\frac{\partial \Pi}{\partial t} \frac{\partial}{\partial p} \mathbf{H}_p + i \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} \mathbf{H}_p. \end{aligned} \quad (4.79)$$

4.3.2 Bohmian transport equations in momentum representation

Following the same line of reasoning as in Section 4.2, the transport equations for the position density $\rho_p \mathbf{X}$, energy density $\rho_p \mathbf{H}_p$ and probability density ρ_p in momentum space can be derived using the CE (4.67) and the dynamical equations (4.78) and (4.79), thus leading to:

$$\frac{\partial}{\partial t}(\rho_p X) + \frac{\partial}{\partial p} \left[\left(\rho_p \frac{\partial \Pi}{\partial t} \right) X + i \frac{m}{2} \omega^2 \hbar \left(X \frac{\partial}{\partial p} \rho_p - \rho_p \frac{\partial}{\partial p} X \right) \right] = \rho_p \frac{P}{m} = \rho_p \frac{\partial}{\partial t} X_{cl}, \quad (4.80)$$

$$\frac{\partial}{\partial t}(\rho_p H_p) + \frac{\partial}{\partial p} \left[\left(\rho_p \frac{\partial \Pi}{\partial t} \right) H_p + i \frac{m}{2} \omega^2 \hbar \left(H_p \frac{\partial}{\partial p} \rho_p - \rho_p \frac{\partial}{\partial p} H_p \right) \right] = \rho_p \frac{\partial}{\partial t} V, \quad (4.81)$$

$$\frac{\partial}{\partial t}(\rho_p \cdot 1) + \frac{\partial}{\partial p} \left[\left(\rho_p \frac{\partial \Pi}{\partial t} \right) \cdot 1 + i \frac{m}{2} \omega^2 \hbar \left(1 \cdot \frac{\partial}{\partial p} \rho_p - \rho_p \frac{\partial}{\partial p} 1 \right) \right] = 0. \quad (4.82)$$

where $\frac{\partial \Pi}{\partial t}$ is given by (2.71), *i.e.*, $\frac{\partial \Pi}{\partial t} = -b - m\omega^2 X$.

These three equations can be summarized in the form

$$\boxed{\frac{\partial}{\partial t}(\rho_p A) + \frac{\partial}{\partial p} \left[J_p A + i \frac{m}{2} \omega^2 \hbar \left(A \frac{\partial}{\partial p} \rho_p - \rho_p \frac{\partial}{\partial p} A \right) \right]} = g(p, t), \quad (4.83)$$

where $J_p \doteq \rho_p \frac{\partial \Pi}{\partial t} = \rho_p (-b - m\omega^2 X_R) - i \frac{m}{2} \hbar \omega^2 \frac{\partial}{\partial p} \rho_p$ and A can be 1 , $X \in \mathbb{C}$ or $H_p \in \mathbb{C}$.

The momentum dependent function $g(p, t)$ can, similarly to the situation in position representation, be written as $g(p, t) = \rho_p \frac{\partial}{\partial t} A_{cl}$, where A_{cl} is the classical quantity corresponding to the Bohmian one, *i.e.* $\frac{\partial}{\partial t} 1 = 0$, $\frac{\partial}{\partial t} X_{cl} = \frac{p}{m}$ and $\frac{\partial}{\partial t} H_{cl} = \frac{\partial}{\partial t} V$.

Again, Eq. (4.83) containing only the complex quantities J_p and A (apart from $A = 1$) can be simplified using solely the real part of the current density J_p , *i.e.*, $J_{p,R} = \rho_p (-b - m\omega^2 X_R)$ like in CE (4.67), leading to

$$\frac{\partial}{\partial t}(\rho_p A) + \frac{\partial}{\partial p} \left[J_{p,R} A + i \frac{m}{2} \omega^2 \hbar \rho_p \frac{\partial}{\partial p} A \right] = g(p, t). \quad (4.84)$$

Integrating this equation over the whole momentum space confirms, again like in Section 4.2, Ehrenfest's theorem, now in momentum representation.

Separating equation (4.84) into real and imaginary parts leads to

$$\boxed{\frac{\partial}{\partial t}(\rho_p A_R) + \frac{\partial}{\partial p} \left[J_{p,R} A_R + \frac{m}{2} \omega^2 \hbar \rho_p \frac{\partial}{\partial p} A_I \right]} = g(p, t), \quad (4.85)$$

$$\boxed{\frac{\partial}{\partial t}(\rho_p A_I) + \frac{\partial}{\partial p} \left[J_{p,R} A_I - \frac{m}{2} \omega^2 \hbar \rho_p \frac{\partial}{\partial p} A_R \right]} = 0. \quad (4.86)$$

For $A = 1$, equation (4.86) trivially vanishes and equation (4.85) turns into the CE (4.67).

For $A = X = -\frac{\partial}{\partial p}S_p + i\frac{\hbar}{2}\frac{\partial}{\partial p}\frac{\rho_p}{\rho_p} = X_R + iX_I$, Eq. (4.85) for the real part yields

$$\begin{aligned} \frac{\partial}{\partial t} \left[\rho_p \left(-\frac{\partial}{\partial p} S_p \right) \right] + \frac{\partial}{\partial p} \left[\rho_p \left(-b - m\omega^2 \left(-\frac{\partial}{\partial p} S_p \right) \right) \left(-\frac{\partial}{\partial p} S_p \right) \right. \\ \left. - \frac{\hbar^2}{4} m\omega^2 \rho_p \left(\frac{\partial^2}{\partial p^2} \frac{\rho_p}{\rho_p} - \left(\frac{\partial}{\partial p} \frac{\rho_p}{\rho_p} \right)^2 \right) \right] = \rho_p \frac{p}{m}, \quad (4.87) \end{aligned}$$

what can be rewritten as:

$$\frac{\partial}{\partial t} [\rho_p X_R] + \frac{\partial}{\partial p} \left[\left(\rho_p \frac{\partial \Pi}{\partial t} \right) X_R - \frac{\hbar^2}{4} m\omega^2 \rho_p \frac{\partial}{\partial p} \left(\frac{\partial}{\partial p} \frac{\rho_p}{\rho_p} \right) \right] = \rho_p \frac{\partial}{\partial t} X_{cl}. \quad (4.88)$$

Changing the order of $\frac{\partial}{\partial t}$ and $\frac{\partial}{\partial p}$ in equation (4.86) shows easily that

$$\frac{\partial}{\partial p} \left\{ \frac{\partial}{\partial t} \rho_p + \frac{\partial}{\partial p} \left[\rho_p \left(-b - m\omega^2 X_R \right) \right] \right\} = 0 \quad (4.89)$$

is fulfilled, what is essentially the position operator applied to the CE in momentum space,

$$-\frac{i}{\hbar} \hat{X} \{ \text{CE} \}. \quad (4.90)$$

Considering finally $A = H_p = -\frac{\partial}{\partial t} S_p + i\frac{\hbar}{2}\frac{\partial}{\partial t}\frac{\rho_p}{\rho_p} = H_R + iH_I$, the real part leads via (4.85) to an equation formally similar to (4.88)

$$\frac{\partial}{\partial t} \left(\rho_p \left(-\frac{\partial S_p}{\partial t} \right) \right) + \frac{\partial}{\partial p} \left[\rho_p \frac{\partial \Pi}{\partial t} \left(-\frac{\partial S_p}{\partial t} \right) + \frac{\hbar^2}{4} m\omega^2 \rho_p \frac{\partial}{\partial p} \left(\frac{\partial}{\partial t} \frac{\rho_p}{\rho_p} \right) \right] = \rho_p \frac{\partial}{\partial t} V_{cl}, \quad (4.91)$$

Defining quantities similar to those used by Nassar in position space [Nassar(1993)], namely $U_{\text{Nassar},p} = \rho_p \left(\frac{p^2}{2m} + V + V_{qu,p} \right)$ and $Q_{\text{Nassar},p} = \frac{\partial \Pi_R}{\partial t} U_{\text{Nassar},p} + \frac{m}{2} \omega^2 \hbar^2 \left(\sqrt{\rho_p} \frac{\partial^2 \sqrt{\rho_p}}{\partial p \partial t} - \left(\frac{\partial \sqrt{\rho_p}}{\partial p} \right) \left(\frac{\partial \sqrt{\rho_p}}{\partial t} \right) \right)$, one can rewrite (4.91) (for $\frac{\partial V}{\partial t} = 0$) in a form similar to (4.38) in position space,

$$\frac{\partial}{\partial t} U_{\text{Nass,p}} + \frac{\partial}{\partial p} Q_{\text{Nass,p}} = 0. \quad (4.92)$$

Regarding the imaginary part H_I , Eq. (4.86) can be reduced to

$$\frac{\partial}{\partial t} \left\{ \frac{\partial}{\partial t} \rho_p + \frac{\partial}{\partial p} \left[\rho_p (-b - m\omega^2 X_R) \right] \right\} = 0, \quad (4.93)$$

what is now basically the energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$ applied to CE (4.67), *i.e.*,

$$-\frac{i}{\hbar} \hat{E} \{ CE \} = -\frac{i}{\hbar} \hat{H}_p \{ CE \}. \quad (4.94)$$

4.3.3 Quantum transport equations and the associated Euler equations in momentum representation

Similar to what has been shown for Eq. (4.27) in Section 4.2.3 for the position representation, will now be applied to the corresponding Eq. (4.84) in momentum space, *i.e.*,

$$\frac{\partial}{\partial t} (\rho_p A) + \frac{\partial}{\partial p} \left[J_{p,R} A + i \frac{m}{2} \omega^2 \hbar \rho_p \frac{\partial}{\partial p} A \right] = g(p, t),$$

leading with $J_{p,R} = \rho_p \frac{\partial \Pi_R}{\partial t}$ to

$$\boxed{\frac{\partial A}{\partial t} + \frac{\partial \Pi}{\partial t} \frac{\partial}{\partial p} A - i \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} A = \frac{g(p, t)}{\rho_p}}, \quad (4.95)$$

containing also a diffusion term with purely imaginary diffusion coefficient $D_p = i \frac{\hbar}{2} m \omega^2$.

Separated into real and imaginary parts this equation yields

$$\boxed{\frac{\partial A_R}{\partial t} + \frac{\partial \Pi_R}{\partial t} \frac{\partial}{\partial p} A_R - \frac{\partial \Pi_I}{\partial t} \frac{\partial}{\partial p} A_I + \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} A_I = \frac{g(p, t)}{\rho_p}}, \quad (4.96)$$

$$\boxed{\frac{\partial A_I}{\partial t} + \frac{\partial \Pi_R}{\partial t} \frac{\partial}{\partial p} A_I + \frac{\partial \Pi_I}{\partial t} \frac{\partial}{\partial p} A_R - \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} A_R = 0}. \quad (4.97)$$

In momentum space, first the complex Bohmian position shall be considered, leading to

$$\frac{\partial X_R}{\partial t} + \frac{\partial \Pi_R}{\partial t} \frac{\partial}{\partial p} X_R - \frac{\partial \Pi_I}{\partial t} \frac{\partial}{\partial p} X_I + \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} X_I = \frac{\partial x_{cl}}{\partial t} = \frac{p}{m} = \frac{\partial}{\partial p} \left(\frac{p^2}{2m} \right), \quad (4.98)$$

$$\frac{\partial X_I}{\partial t} + \frac{\partial \Pi_R}{\partial t} \frac{\partial}{\partial p} X_I + \frac{\partial \Pi_I}{\partial t} \frac{\partial}{\partial p} X_R - \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} X_R = 0. \quad (4.99)$$

Taking into account the time derivative (2.71) of Π and the expressions for H_p and $V_{qu,p}$ as given in (4.72)-(4.74) this can be rewritten as

$$\frac{\partial X_R}{\partial t} - \frac{\partial}{\partial p} \left[\frac{p^2}{2m} + V(X_R) + V_{qu,p} \right] = 0, \quad (4.100)$$

$$\frac{\partial X_I}{\partial t} - \frac{\partial}{\partial p} \left[bX_I + \frac{m}{2} \omega^2 \left(2X_R X_I + \hbar \frac{\partial}{\partial p} X_R \right) \right] = 0, \quad (4.101)$$

or, in terms of real and imaginary parts of the Bohmian Hamiltonian as

$$\frac{\partial X_R}{\partial t} - \frac{\partial}{\partial p} H_R = 0, \quad (4.102)$$

$$\frac{\partial X_I}{\partial t} - \frac{\partial}{\partial p} H_I = 0. \quad (4.103)$$

Changing the order of differentiation in $\frac{\partial X_R}{\partial t} = -\frac{\partial}{\partial t} \frac{\partial}{\partial p} S_p = -\frac{\partial}{\partial p} \frac{\partial}{\partial t} S_p$, Eq. (4.102) can be written as

$$-\frac{\partial}{\partial p} \left[\frac{\partial}{\partial t} S_p + \frac{p^2}{2m} + V(X_R) + V_{qu,p} \right] = 0 \quad (4.104)$$

what is nothing but applying the position operator in momentum space on the mHJE (4.66)

$$\frac{i}{\hbar} \widehat{X} \{ \text{mHJE} \}. \quad (4.105)$$

Using the definitions of X_I and H_I , Eq. (4.103) turns into

$$\frac{\partial}{\partial t} \left[\frac{i\hbar}{2} \frac{\partial}{\partial p} \ln \rho_p \right] - \frac{\partial}{\partial p} \left[\frac{i\hbar}{2} \frac{\partial}{\partial t} \ln \rho_p \right] = 0. \quad (4.106)$$

Inserting into (4.98) and (4.99) for A finally the Bohmian Hamiltonian, one obtains

$$\frac{\partial H_R}{\partial t} + \frac{\partial \Pi_R}{\partial t} \frac{\partial}{\partial p} H_R - \frac{\partial \Pi_I}{\partial t} \frac{\partial}{\partial p} H_I + \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} H_I = \frac{\partial V}{\partial t}, \quad (4.107)$$

$$\frac{\partial H_I}{\partial t} + \frac{\partial \Pi_R}{\partial t} \frac{\partial}{\partial p} H_I + \frac{\partial \Pi_I}{\partial t} \frac{\partial}{\partial p} H_R - \frac{m}{2} \omega^2 \hbar \frac{\partial^2}{\partial p^2} H_R = 0. \quad (4.108)$$

Using (4.12) and the definitions of $\frac{\partial \Pi}{\partial t}$ and H_p , Eq. (4.107) takes the form

$$-\frac{\partial}{\partial t} \left\{ \frac{\partial}{\partial t} S_p + \frac{p^2}{2m} + V(X_R) + V_{qu,p} \right\} = 0, \quad (4.109)$$

what is essentially the application of the energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$ on the mHJE (4.66),

$$\frac{i}{\hbar} \hat{E} \left\{ \text{mHJE} \right\}. \quad (4.110)$$

Taking into account Eqs. (4.12) and (4.13), the equation for the imaginary part can be expressed as

$$\frac{\partial}{\partial t} \left\{ H_I - \left[bX_I + m\omega^2 X_R X_I - \frac{m}{2} \omega^2 \frac{\partial}{\partial p} X_R \right] \right\} = 0 \quad (4.111)$$

where the terms in square brackets are according to (4.74) identical to H_I .

4.4 Summary

■ In Section 4.1, the lack of consistent hydrodynamical equations for position and momentum representation is summarized.

■ In Section 4.2, the complex hydrodynamical equations are found. Contrary to what is found in the current literature, they all share the same structure: a transport equation. Care must be taken not to make physical speculations regarding possible transport phenomena because the involved quantities are not real ones but complex ones.

For the case of position representation one obtains

$$\frac{\partial}{\partial t}(\rho_x A) + \frac{\partial}{\partial x} \left[J_x A + i \frac{\hbar}{2m} \left(A \frac{\partial}{\partial x} \rho_x - \rho_x \frac{\partial}{\partial x} A \right) \right] = f(x, t), \quad (4.26)$$

where $J_x \doteq \rho_x \frac{P}{m} = \rho_x \frac{\partial Q}{\partial t} = \rho_x \frac{\partial S_x}{\partial x} - i \frac{\hbar}{2m} \frac{\partial}{\partial x} \rho_x = J_{x,R} + i J_{x,I}$ and A can be 1, $P \in \mathbb{C}$ or $H_x \in \mathbb{C}$. The position dependent function $f(x, t)$ can also be written as a density in the form $f(x) = \rho_x \frac{\partial}{\partial t} A_{cl}$ where A_{cl} is the classical quantity corresponding to the Bohmian quantity A , therefore $\frac{\partial}{\partial t} 1 = 0$, $\frac{\partial}{\partial t} P_{cl} = -\frac{\partial}{\partial x} V$ and $\frac{\partial}{\partial t} H_{cl} = \frac{\partial}{\partial t} V$.

In the following, equation (4.27) was separated into real and imaginary parts, yielding

$$\frac{\partial}{\partial t}(\rho_x A_R) + \frac{\partial}{\partial x} \left[J_{x,R} A_R + \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A_I \right] = f(x, t), \quad (4.31)$$

$$\frac{\partial}{\partial t}(\rho_x A_I) + \frac{\partial}{\partial x} \left[J_{x,R} A_I - \frac{\hbar}{2m} \rho_x \frac{\partial}{\partial x} A_R \right] = 0. \quad (4.32)$$

For the case of the momentum representation one obtains

$$\frac{\partial}{\partial t}(\rho_p A) + \frac{\partial}{\partial p} \left[J_p A + i \frac{m}{2} \omega^2 \hbar \left(A \frac{\partial}{\partial p} \rho_p - \rho_p \frac{\partial}{\partial p} A \right) \right] = g(p, t), \quad (4.83)$$

where $J_p \doteq \rho_p \frac{\partial \Pi}{\partial t} = \rho_p (-b - m\omega^2 X_R) - i \frac{m}{2} \hbar \omega^2 \frac{\partial}{\partial p} \rho_p$ and A can be 1, $X \in \mathbb{C}$ or $H_p \in \mathbb{C}$.

The momentum dependent function $g(p, t)$ can, similarly to the situation in position representation, be written as $g(p, t) = \rho_p \frac{\partial}{\partial t} A_{cl}$, where A_{cl} is the classical quantity corresponding to the Bohmian one, *i.e.* $\frac{\partial}{\partial t} 1 = 0$, $\frac{\partial}{\partial t} X_{cl} = \frac{p}{m}$ and $\frac{\partial}{\partial t} H_{cl} = \frac{\partial}{\partial t} V$.

Separating equation (4.84) into real and imaginary parts leads to

$$\frac{\partial}{\partial t}(\rho_p A_R) + \frac{\partial}{\partial p} \left[J_{p,R} A_R + \frac{m}{2} \omega^2 \hbar \rho_p \frac{\partial}{\partial p} A_I \right] = g(p, t), \quad (4.85)$$

$$\frac{\partial}{\partial t}(\rho_p A_I) + \frac{\partial}{\partial p} \left[J_{p,R} A_I - \frac{m}{2} \omega^2 \hbar \rho_p \frac{\partial}{\partial p} A_R \right] = 0. \quad (4.86)$$

■ Like in hydrodynamics, it is possible to change the description from one that locally considers densities at a particular position (or momentum), corresponding to the Lagrangian point of view, to that of Euler, considering a co-moving frame, moving with the convection velocity of the system. This turns the transport equations for the densities into Euler equations that can be written as complex convection-diffusion equations with purely imaginary diffusion coefficient depending on \hbar .

Chapter 5

Conclusion

In 1952, Bohm challenged the Copenhagen interpretation through the suggestion of a deterministic interpretation in terms of “hidden variables” in the microscopic world [Bohm(1952a), Bohm(1952b)]. Paradoxically, Bohmian mechanics originally sought to become more general than its conventional counterpart [Bohm(1952a)], but in the process every analysis was performed solely in the position representation, a reason for the objections of Pauli [Pauli(1952)] and Heisenberg [Passon(2005)], mentioned in the beginning. Ever since, there have been numerous attempts at expressing Bohmian mechanics in the momentum representation in a causal form. It is important to bear in mind the relevant works of Epstein [Epstein(1953a), Epstein(1953b)] and Struyve [Struyve(2010)]. Although, to date, the previous works have been unable to write down explicitly a Hamilton–Jacobi and continuity equation for the momentum representation.

Three major problems can be found in Bohmian mechanics as it is currently formulated. First of all, there is no systematic treatment of other representations. Second, the Bohmian trajectories inadequately defined are inconsistently used. Third, the Bohmian hydrodynamic treatment seems to be composed of unrelated dynamical equations.

In this context, this thesis aims to take a mediating standpoint between Bohmian mechanics and conventional quantum mechanics, reformulate the former based on the latter and assign it its appropriate place in the quantum mechanical formalism, without additional postulates, interpretations or philosophical arguments. For this purpose, this work is based on three major pillars: a formulation that is independent of the chosen representation, a rational criticism of the Bohmian trajectory and, last but not least, the structure of the local transport equations that are assigned to the Bohmian trajectories.

Chapter 2 serves to reformulate Bohmian mechanics. Section 2.1 shows that the controversy over the formulation of Bohmian mechanics in momentum representation is still of interest; see Table 2.2 for the arguments related to the controversy. In Section 2.2, using the polar decomposition (2.6) of the wave function according to (2.9), complex Bohmian quantities such as position, momentum, kinetic and potential energies for the position (2.12-2.15) and momentum representation (2.22-2.25) are defined. The most remarkable property of these Bohmian quantities is that they are generally complex. One exception concerns the position and momentum, these are real quantities in their respective representations, but otherwise they are also complex. Furthermore, quadratic quantities such as kinetic and potential energies contain not only the squares of the real and imaginary parts of the corresponding complex quantities, but also an additional imaginary contribution that couples the original real and imaginary parts.

Advantages of using the Bohmian formulation in the momentum representation are illustrated using a linear potential for stationary states. Working in position space, the difficulty in solving a problem arises from the quadratic structure of the kinetic energy and the resulting quantum contribution in the modified Hamilton–Jacobi equation. Using, on the other hand, the Bohmian formulation in momentum space introduced in this work, the quantum contribution originates from the quadratic terms of the potential. For the linear potential, however, there is no quadratic contribution at all. This means that the complication due to the quantum contribution is absent in the momentum representation for the Bohmian framework.

In Section 2.3, it is stated that even if the modified Hamilton–Jacobi equation in Bohmian mechanics suggests a Hamiltonian structure, this is not the case due to the lack of canonically conjugated variables. Nevertheless, the complex dynamical equations are similar to the Newtonian counterparts, see for example (2.60-2.62) for the position and (2.70-2.72) for the momentum representation. Furthermore, these equations prove to be useful in finding constants of motion, such as the Ermakov invariant for time-dependent states like the generalized coherent states.

In Section 2.4 it turns out that the quantum potential, within the scheme of the formulation introduced in this work, is related to the quantum contribution to the position and momentum uncertainties, see (2.159-2.160) and (2.162-2.163). Indeed, the proposed formulation of Bohm’s approach allows the uncertainties to be separated into two types of contributions, one originating from the classical quantities, while the other arises from the so-called quantum potential. In this sense, the proposed formulation makes it clear that the quantum potential, even if the term suggests it, is not a potential, but a kinetic term that results from the uncer-

tainties associated with the classically conjugated variables. In addition, it is now possible to represent Heisenberg's uncertainty product in the form (2.164) since the position and momentum versions of Bohmian mechanics are now available. This is demonstrated using the example of the generalized coherent states.

Chapter 3 deals with a redefinition and reinterpretation of the Bohmian trajectories. For this purpose, Section 3.1 points out the inadequacy of the additional postulates in the definition and introduction of the Bohmian trajectories. In particular, the mathematical (and physical) justification of the guidance law (3.4) is inconsistent.

In Section 3.2, Bohmian trajectories are derived without additional postulates. This is the result of a specific parametrization of the respective continuity equations, in the case of the position space by (3.19) with the definition (3.23) of the associated Bohm function and in the momentum space (3.49) with the Bohm function (3.48).

This is achieved through the use of a simple thermodynamic procedure that involves Maxwell relations (see Box 3.2.1). Starting from this, after performing a contour integral in the $(x; t)$ -space, the non-crossing rule, characteristic of Bohmian trajectories, and the conservation of the probability are proven. Of course, this indicates that Bohmian trajectories should not be interpreted as (real) paths, as is generally assumed, but rather as the borders of probability lanes. This idea is illustrated using generalized coherent states. It is also suggested that this limits the applicability of Bohmian mechanics. This interpretation shows that the strength of the trajectories lies in the descriptive statistics, i.e., in the determination of percentile regions. This means that the use of trajectories is advisable for all those problems where one is interested in how the dection probability is distributed in a certain region, such as in tunneling or scattering problems. However, if the goal is to calculate mean values (or higher moments), Bohmian mechanics is rather cumbersome and the use of the conventional formalism is generally advisable.

In Section 3.3 a connection between conventional quantum mechanics and Bohmian mechanics is found through the Wigner formalism. The Bohmian framework can be viewed as a projected aspect of the Wigner function, see e.g. (3.75) and (3.76). This confirms the idea of complex Bohmian quantities introduced in Chapter 2, since they represent projections of observables onto continuous representations.

In Section 3.4 the new interpretation is used to analyze an ion trap, characterized by a parametric oscillator with the frequency $1/(at+b)$. In contrast to usual

frequencies for ion traps, this one is obviously aperiodic, but thanks to the new interpretation and the application of Bohmian trajectories it can be shown that such a trap would be useful for trapping a system for time intervals in the range of microseconds. If longer trapping times are required, this frequency is of course not adequate. At least the trapping times can be varied by changing the parameter of this oscillator (see Figures 3.6-3.8).

As a third aspect, a systematic treatment of the hydrodynamic viewpoint of Bohmian mechanics is presented in Chapter 4. Section 4.1 summarizes the lack of consistent hydrodynamical equations for position and momentum representation. The local Bohmian equations for momentum and energy do not have the structure of transport equations.

The complex hydrodynamical equations are obtained in Section 4.2. Contrary to what can be found in the current literature, they all have the same structure: they are transport equations. However, one must be careful with regard to speculations about possible transport phenomena, since the quantities involved are not real but complex (for the position representation see (4.26) and for the momentum representation (4.83)).

With all the above results, this thesis seeks to connect the loose ends of Bohmian mechanics, so that it can be viewed as a genuinely compatible and valuable part of the conventional quantum mechanical theory.

Appendix A

Time-dependent quantum systems and Riccati equation

In the time-independent case the SE possesses exact analytic solutions for the free motion ($V = 0$) and the constant potential ($V = V_0$), where both can be combined to form a step potential, a rectangular potential barrier, or a series of such barriers. In both cases ($V = 0$ and $V = V_0$), the solutions are given by plane waves that can be used to describe an incoming, a reflected and a transmitted part of the initial wave.

Also in the time-dependent case there are potentials that allow exact analytic solutions, this time in the form of Gaussian wave packets that exist for potentials that are at most quadratic in the position variable, *i.e.*, the free motion, a linear in-/decreasing potential and an oscillator potential $V = \frac{1}{2}m\omega^2x^2$. In the latter case an analytic form of the parameters determining the evolution of the wave packet can be given for a constant frequency $\omega = \omega_0$ (*i.e.*, the harmonic oscillator) and certain cases with time-dependent frequency, $\omega = \omega(t)$ (*i.e.*, the parametric oscillator; see, *e.g.*, [Schuch(2018b)]).

As already mentioned, the case of the harmonic oscillator wave packet was already considered by Schrödinger himself [Schrödinger(1926e)] shortly after he had published his first communications on wave mechanics. In the beginning, Schrödinger was very confident that similar stable wave packets could also be found, *e.g.*, for the Coulomb problem [Schrödinger(1926e)], but already the free motion wave packet with its spreading width showed that this was not possible and finally favoured the probabilistic interpretation of the wave function. In any case, it became clear that both parameters of the Gaussian function, the maximum and the width, are in general time-dependent.

Taking this also into account one can formulate a general Gaussian ansatz for the solution of the time-dependent SE (with at most quadratic Hamiltonian) in the form

$$\psi(x,t) = N_x(t) \exp \left[\frac{i}{\hbar} \left(\frac{m}{2} \mathcal{C} \tilde{x}^2 + \langle p \rangle \tilde{x} + K(t) \right) \right], \quad (\text{A.1})$$

where $\mathcal{C}(t)$ is a complex time-dependent quantity that is connected with the wave packet width via $\mathcal{C}_I = \frac{\hbar}{2m\langle \tilde{x}^2 \rangle}$ with $\langle \tilde{x}^2 \rangle(t) = \langle x^2 \rangle - \langle x \rangle^2 = \sigma_x^2$ being the mean square deviation in position space that is essentially the square of the width, $\tilde{x} = x - \langle x \rangle$ with $\langle x \rangle$ being the mean value of position, *i.e.*, the classical trajectory, indicating that the maximum of the Gaussian function is at the position of the corresponding classical particle. The quantities $N(t)$ and $K(t)$ are purely time-dependent and not relevant for the dynamics of the two essential parameters.

The equations of motion for these parameters can easily be obtained inserting ansatz (A.1) into the time-dependent SE

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right\} \psi(x,t). \quad (\text{A.2})$$

This leads to the Newtonian equation of motion for the maximum $\langle x \rangle(t) = \eta(t)$,

$$\ddot{\eta} + \omega^2(t)\eta = 0, \quad (\text{A.3})$$

(for the parametric oscillator with the special cases of the harmonic oscillator, $\omega = \omega_0$, and the free motion, $\omega = 0$) and the complex Riccati equation

$$\dot{\mathcal{C}} + \mathcal{C}^2 + \omega^2(t) = 0 \quad (\text{A.4})$$

for the parameter connected with the wave packet width via its imaginary part $\mathcal{C}_I(t)$.

Methods to solve this Riccati equation are well-known, but one gains further inside by rewriting this equation introducing a new variable $\alpha(t)$ that is defined via

$$\mathcal{C}(t) = \frac{\dot{\alpha}}{\alpha} + i \frac{1}{\alpha^2(t)} \quad (\text{A.5})$$

and is thus directly proportional to the wave packet width, as $\alpha(t) = \sqrt{\frac{2m}{\hbar} \langle \tilde{x}^2 \rangle} = \sqrt{\frac{2m}{\hbar}} \sigma_x$. Inserting (A.5) into (A.4) shows via the imaginary part of this equation that $\mathcal{C}_R(t) = \frac{\dot{\alpha}}{\alpha}$, *i.e.*, the relative change in time of the width. Therefore, for wave packets with time-dependent width the variable of the Riccati equation always

is complex. The case of the harmonic oscillator solution with constant width is the special case where the Riccati equation possesses a particular solution that is constant and only exists, if the initial width of the wave packet is that of the ground state wave function of the stationary case; in all other cases, also the width of the harmonic oscillator wave packet oscillates (for details, see *e.g.* [Schuch(2006), Schuch(2018a)]).

It is straightforward to show that position and momentum uncertainties can be expressed in terms of \mathcal{C}_R and \mathcal{C}_I , or, α and $\dot{\alpha}$ as

$$\sigma_x^2 = \frac{\hbar}{2m} \frac{1}{\mathcal{C}_I} = \frac{\hbar}{2m} \alpha^2 \quad (\text{A.6})$$

$$\sigma_p^2 = \frac{m\hbar}{2} \frac{\mathcal{C}_R^2 + \mathcal{C}_I^2}{\mathcal{C}_I} = \frac{m\hbar}{2} \left(\dot{\alpha}^2 + \frac{1}{\alpha^2} \right), \quad (\text{A.7})$$

hence the absolute square of \mathcal{C} attains the form

$$|\mathcal{C}|^2 = \mathcal{C}_R^2 + \mathcal{C}_I^2 = \frac{\dot{\alpha}^2 + \frac{1}{\alpha^2}}{\alpha^2} = \frac{1}{m^2} \frac{\sigma_p^2}{\sigma_x^2}. \quad (\text{A.8})$$

Inserting \mathcal{C}_I and \mathcal{C}_R in terms of $\alpha(t)$ into the real part of the Riccati equation (A.4) leads to

$$\ddot{\alpha} + \omega^2(t)\alpha = \frac{1}{\alpha^3}, \quad (\text{A.9})$$

the so-called Ermakov equation. Solving this equation directly provides the time-dependence of the wave packet width. Further, this formulation yields the advantage that the dynamics of this quantum property can be traced back to the dynamics of the classical system¹. It has been shown by Man'ko *et al.* [Malkin(1970), Dodonov(2003)] that, knowing two linear independent solutions η_1 and η_2 of the classical equation of motion (A.3), the solution of equation (A.9) can be written as

$$\alpha(t) = \sqrt{\frac{2m}{\hbar} \left(\sigma_{p,0}^2 \eta_1(t) + \sigma_{x,0}^2 \eta_2(t) \mp 2\sigma_{x0,p0} \eta_1 \eta_2 \right)} \quad (\text{A.10})$$

¹ There are other approaches to describe the dynamics of generalized coherent states like those based on the Dirac–Frenkel variational method [Dirac(1930), Frenkel(1934)]; but these are not applied here. As long as systems with exact analytical solutions are considered, they lead to the same result as our method.

with $\sigma_{x0}^2 = \langle (x - \langle x \rangle)^2 \rangle(t=0) = \langle x^2 \rangle(0) - \langle x \rangle^2(0)$, $\sigma_{p0}^2 = \langle (p - \langle p \rangle)^2 \rangle(t=0) = \langle p^2 \rangle(0) - \langle p \rangle^2(0)$ and $\sigma_{x0,p0} = \frac{1}{2} \langle [(x - \langle x \rangle)(p - \langle p \rangle)]_+ \rangle(t=0)$, where $\eta_1(t)$ is the classical trajectory and $[\ , \]_+$ the anticommutator (for further details, see also [Cruz(2015), Schuch(2018a)]). But also $\eta_2(t)$ is defined by the Riccati equation (A.4) up to a constant of integration. This is connected with the fact that any Riccati equation can be linearized using a logarithmic derivative. In this case

$$\mathcal{C}(t) = \frac{\dot{\lambda}}{\lambda} \quad (\text{A.11})$$

with $\lambda(t)$ being a complex variable fulfilling

$$\ddot{\lambda} + \omega^2(t)\lambda = 0, \quad (\text{A.12})$$

i.e., the classical equation of motion. It can be shown [Schuch(1992), Schuch(2006), Schuch(2018a)] that the imaginary part $z(t)$ of λ , when writing it in Cartesian coordinates as $\lambda = u + iz$, is, up to a constant factor, identical with the classical trajectory,

$$z = \frac{m}{\alpha_0 p_0} \eta(t). \quad (\text{A.13})$$

Furthermore, z and u are not independent of each other. This can be seen inserting definition (A.11) into the Riccati equation (A.4). From the imaginary part one obtains

$$\dot{z}u - \dot{u}z = 1, \quad (\text{A.14})$$

what allows to obtain $u(t)$ simply via integration, if $z(t)$ is known,

$$u = -z \int \frac{1}{z^2(t')} dt'. \quad (\text{A.15})$$

Therefore, $u(t)$ is (up to a constant factor) the second solution η_2 that is needed to obtain $\alpha(t)$ via (A.10).

Writing $\lambda(t)$ in polar coordinates as $\lambda = \alpha e^{i\varphi}$, it can be shown [Schuch(2018a), Schuch(2006)] that the amplitude α is identical with α defined in (A.5) and from the imaginary part of (A.4) one obtains the conservation law (A.14) now in the form

$$\dot{\varphi} = \frac{1}{\alpha^2}. \quad (\text{A.16})$$

From the polar form immediately follows

$$\lambda \lambda^* = \alpha^2 = u^2 + z^2, \quad (\text{A.17})$$

so knowing $z(t)$ and $u(t)$ also directly provides $\alpha(t)$.

The essence of this is that, up to initial conditions that have to be fixed, the complete dynamics of the quantum system can be obtained by solving the classical Newtonian equation of motion, because the connection between the different dynamical variables is provided via the complex Riccati equation (A.4). This might not be so spectacular in cases, where exact solutions of the Riccati or Ermakov equations are available, but, *e.g.*, for parametric oscillators without analytic solutions this might be advantageous. In this case, still numerical solutions of the linear Newtonian equation can be obtained which, when fed into the above-described algorithm, are able to supply the information about the corresponding quantum mechanical uncertainties, responsible for the wave packet spreading and thus scattering and tunneling properties. The algorithm is sketched again in Figure A.1.

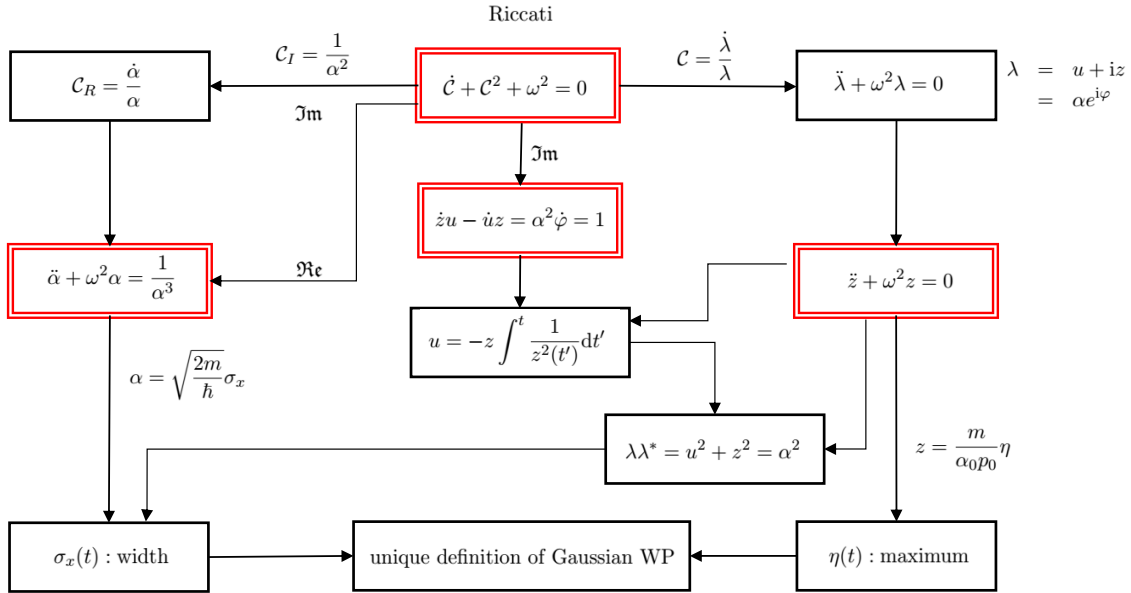


Fig. A.1 Schematic representation of the connection amongst the complex Riccati equation and the dynamics of the maximum and width of a Gaussian wave packet.

One further aspect of this combined Newton–Ermakov system (A.3) and (A.9) shall be mentioned that will not be exploited in this approach, but may open another aspect how to tackle time-dependent problems of the kind under investigation.

Already, in 1880 Ermakov [Ermakov(1880)] had shown that by eliminating the frequency ω from equations (A.3) and (A.9), a dynamical invariant can be obtained that is still a constant of motion, even when for $\omega = \omega(t)$ the corresponding Hamiltonian no longer has this property. This so-called Ermakov invariant has the form

$$I = \frac{1}{2} \left[(\dot{\eta}\alpha - \dot{\alpha}\eta)^2 + \left(\frac{\eta}{\alpha} \right)^2 \right] = \text{const.} \quad (\text{A.18})$$

It has been shown by Lewis [Lewis(1967)] in a quantum mechanical context, *i.e.*, replacing the momentum $m\dot{\eta}$ by the corresponding operator in position space, $\hat{p}_{op} = \frac{\hbar}{i} \frac{\partial}{\partial x}$, that one obtains a corresponding operator that has stationary solutions. It is possible to show that the problem of a time-dependent SE can be transformed to the solution of this stationary problem [Lewis(1969), Hartley(1982), Ray(1982)], what, in principle, should allow to apply methods from time-independent quantum mechanics to time-dependent problems, in our case scattering and tunneling.

Last, but not least it should also be mentioned that the operator corresponding to the Ermakov invariant can be factorized in a similar way as the Hamiltonian operator of the harmonic oscillator can be factorized in terms of creation and annihilation operators. The factorization of the invariant leads to generalized creation and annihilation operators [Castaños(2013)]

$$a^\dagger(t) = -i\sqrt{\frac{m}{2\hbar}} \alpha \left(\frac{1}{m} \hat{p}_{op} - \mathcal{C}^* x \right) \quad (\text{A.19})$$

$$a(t) = i\sqrt{\frac{m}{2\hbar}} \alpha \left(\frac{1}{m} \hat{p}_{op} - \mathcal{C} x \right) \quad (\text{A.20})$$

that depend on the complex Riccati variable $\mathcal{C}(t)$ and allow to obtain generalized coherent states with time-dependent width in the same way as the minimum uncertainty coherent states are obtained by the usual creation and annihilation operators. These are obtained for $\alpha = \alpha_0 = \text{constant}$, *i.e.*, $\mathcal{C}_R = \frac{\dot{\alpha}}{\alpha}$ vanishes and $\mathcal{C}_I = \frac{1}{\alpha^2}$ turns into $\mathcal{C}_I = \frac{1}{\alpha_0^2} = \omega_0$. The generalized coherent states

are again eigenstates of the (generalized) annihilation operator with corresponding complex eigenvalue. Whereas the Gaussian wave packet of the harmonic oscillator with constant width corresponds to the so-called frozen Gaussians (see Heller [Heller(1975), Heller(1981), Huber(1987)]), the generalized coherent states obtained using the general solutions of the complex Riccati equation could be called “thawed” Gaussian wave packets.

Now, these states can easily be treated in momentum space as well. After applying a Fourier transformation of (A.1), the projection of the generalized coherent states $|\psi\rangle$ onto the momentum representation $\{|p\rangle\}$ is given by

$$\langle p|\psi(t)\rangle = N_p(t) \exp \left[-\frac{i}{\hbar} \left(\frac{1}{2m} \mathcal{U} \tilde{p}^2 + \eta \tilde{p} + g(t) \right) \right], \quad (\text{A.21})$$

where $\tilde{p} = p - \langle p \rangle = p - m\dot{\eta}$ and the complex coefficient of \tilde{p}^2 is the inverse of the quantity $\mathcal{C}(t)$, fulfilling the Riccati equation (A.4), *i.e.*, $\mathcal{U} = \mathcal{C}^{-1}(t)$, the new symbol is used just for convenience. Also the dynamics of \mathcal{U} is ruled by a complex Riccati equation,

$$-\dot{\mathcal{U}} + \omega^2(t)\mathcal{U}^2 + 1 = 0 \quad (\text{A.22})$$

that turns into Eq. (A.4) if \mathcal{U} is replaced by \mathcal{C}^{-1} . Because of the dual properties relating the position $\{|x\rangle\}$ and momentum $\{|p\rangle\}$ representation, the wave functions (A.1) and (A.21) share common properties.

It is actually elucidating to express the general property of the generalized coherent states without recurring to the use of any representation. It is straightforward from (A.1) and (A.21) to notice that

$$\tilde{\mathbf{P}}|\psi(t)\rangle = m\mathcal{C}\tilde{\mathbf{X}}|\psi(t)\rangle, \quad (\text{A.23})$$

$$\tilde{\mathbf{X}}|\psi(t)\rangle = \frac{1}{m\mathcal{C}}\tilde{\mathbf{P}}|\psi(t)\rangle. \quad (\text{A.24})$$

After taking the adjoint of the previous expressions, one can compute the covariance $\sigma_{x,p}$ of position and momentum,

$$\sigma_{x,p} \doteq \frac{1}{2} \langle \psi(t) | (\tilde{\mathbf{X}}\tilde{\mathbf{P}} + \tilde{\mathbf{P}}\tilde{\mathbf{X}}) | \psi(t) \rangle, \quad (\text{A.25})$$

as

$$\sigma_{x,p} = \frac{1}{2} \left(\frac{\sigma_p^2}{m\mathcal{C}^*} + m\mathcal{C}^* \sigma_x^2 \right) = \frac{1}{2} \left(\frac{\mathcal{U}^*}{m} \sigma_p^2 + m\mathcal{C}^* \sigma_x^2 \right). \quad (\text{A.26})$$

Up to this point one can either work in position or momentum space. For the former, one needs to remember the correlation between the position and momentum uncertainties (A.8),

$$\sigma_{x,p} = \frac{1}{2} \left(m\mathcal{C} \sigma_x^2 + m\mathcal{C}^* \sigma_x^2 \right) = m\mathcal{C}_R \sigma_x^2. \quad (\text{A.27})$$

This directly allows to express the complex quantity \mathcal{C} with help of (A.6) as

$$\mathcal{C} = \frac{1}{m} \frac{\sigma_{x,p}}{\sigma_x^2} + i \left(\frac{\hbar}{2m} \right) \frac{1}{\sigma_x^2}. \quad (\text{A.28})$$

On the other hand, if the position uncertainty σ_x is expressed in terms of the momentum uncertainty σ_p according to (A.8) with $|\mathcal{C}|^2 = \frac{1}{|\mathcal{U}|^2}$, $\sigma_x^2 = \frac{|\mathcal{U}|^2}{m^2} \sigma_p^2$, Eq. (A.26) turns directly into

$$\sigma_{x,p} = \frac{\mathcal{U}_R}{m} \sigma_p^2. \quad (\text{A.29})$$

Bearing in mind (A.7), the complex quantity \mathcal{U} can be written in the form

$$\mathcal{U} = m \frac{\sigma_{x,p}}{\sigma_p^2} - i \left(\frac{m\hbar}{2} \right) \frac{1}{\sigma_p^2}. \quad (\text{A.30})$$

The relations given above provide the connections between the uncertainties and the variables fulfilling the complex Riccati equations in position and momentum space.

The dynamical parameters and corresponding equations for the generalized coherent states in position and momentum space are given in Table A.1.

	Position representation	Momentum representation
mean values	$\langle x \rangle = \eta$	$\langle p \rangle = m \frac{d}{dt} \eta$
dynamical laws	$m \frac{d^2}{dt^2} \eta = -m\omega^2(t)\eta$	$\frac{d}{dt} \langle p \rangle = -m\omega^2(t)\eta$
uncertainty variables	$\mathcal{C} = \frac{1}{m} \frac{\sigma_{x,p}}{\sigma_x^2} + i \left(\frac{\hbar}{2m} \right) \frac{1}{\sigma_x^2}$	$\mathcal{U} = m \frac{\sigma_{x,p}}{\sigma_p^2} - i \left(\frac{m\hbar}{2} \right) \frac{1}{\sigma_p^2}$
Riccati equations	$\dot{\mathcal{C}} + \mathcal{C}^2 + \omega^2(t) = 0$	$-\dot{\mathcal{U}} + \omega^2(t)\mathcal{U}^2 + 1 = 0$

Table A.1 Symmetric properties of the generalized coherent states for the position and momentum spaces regarding the mean values and uncertainties of the corresponding wave packets.

Appendix B

Riccati equation with a frequency $\omega(t) = \frac{1}{at+b}$

Let us consider the Riccati equation (A.4) for a frequency $\omega(t) = \frac{1}{at+b}$. As it will be seen later, this Riccati equation is parametrized by a . The general solution might be obtained by expressing $\mathcal{C} \in \mathbb{C}$ as a superposition of a particular solution \mathcal{C}_p and a function \mathcal{Y} (both functions depend on the time t and the specific value of the parameter a as well) to be determined,

$$\mathcal{C} = \mathcal{Y} + \mathcal{C}_p(t; a). \quad (\text{B.1})$$

Once this ansatz is used in the Riccati equation (A.4) and after some algebra, it yields the following Bernoulli equation,

$$\dot{\mathcal{Y}} - 2\mathcal{C}_p\mathcal{Y} = 1 \quad (\text{B.2})$$

where $\mathcal{Y} = \frac{1}{\mathcal{Y}}$. The method of integrating factor delivers the following solution,

$$\mathcal{Y} = \frac{\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt' + \exp \left[-2 \int_0^t \mathcal{C}_p(t'; a) dt' \right] \mathcal{Y}_0}{\exp \left[-2 \int^t \mathcal{C}_p(t'; a) dt' \right]}, \quad (\text{B.3})$$

where $\mathcal{Y}_0 \in \mathbb{C}$.

It should be noticed that the general solution depends on finding a particular solution of the Riccati equation \mathcal{C}_p . In the case of the frequency $\omega(t) = \frac{1}{at+b}$, it is easy to see that (3.95) constitutes a particular solution as long as the condition (3.99) is fulfilled. This in turn distinguishes three cases (3.100-3.102) depending on the values that a might take.

In what follows the detailed calculations regarding the integrals of (B.3) are presented depending on the different values of a .

B.1 Computation of the involved integrals for the case $a = 2$

Bear in mind that, for the case $a = 2$, a particular solution is given by $\mathcal{C}_p = \frac{1}{2t+b}$.

Integral $\exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right]$:

$$\exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] = \exp \left[-2 \int^{t'} \frac{1}{2t''+b} dt'' \right], \quad (\text{B.4})$$

$$= \exp \left(-\ln [2t' + b] \right) = \frac{1}{2t' + b}. \quad (\text{B.5})$$

Integral $\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt'$:

$$\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt' = \int_0^t \frac{1}{2t' + b} dt' \quad (\text{B.6})$$

$$= \frac{1}{2} \ln(2t' + b) \Big|_0^t = \frac{1}{2} \ln(2t + b) - \frac{1}{2} \ln(b) \quad (\text{B.7})$$

B.2 Computation of the involved integrals for the case $a \neq 2$

Bear in mind that, for the case $a \neq 2$, a particular solution is given by $\mathcal{C}_p = \frac{\gamma}{2t+b}$, where γ is in turn a parameter whose expression depends on the specific value of a (see for example Eqs. (3.100) and (3.102)).

Integral $\exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right]$:

$$\exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] = \exp \left[-2\gamma \int^{t'} \frac{1}{at''+b} dt'' \right], \quad (\text{B.8})$$

$$= \exp \left(-2\frac{\gamma}{a} \ln [at' + b] \right) = \frac{1}{(at' + b)^{\frac{2\gamma}{a}}}. \quad (\text{B.9})$$

Integral $\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt'$:

$$\int_0^t \exp \left[-2 \int^{t'} \mathcal{C}_p(t''; a) dt'' \right] dt' = \int_0^t (at' + b)^{-2\frac{\gamma}{a}} dt' \quad (\text{B.10})$$

$$= \frac{1}{a} \frac{1}{1 - 2\frac{\gamma}{a}} (at' + b)^{-2\frac{\gamma}{a} + 1} \Big|_0^t \quad (\text{B.11})$$

$$= \frac{1}{a} \frac{1}{1 - 2\frac{\gamma}{a}} (at + b)^{-2\frac{\gamma}{a} + 1} - \frac{1}{a} \frac{1}{1 - 2\frac{\gamma}{a}} b^{-2\frac{\gamma}{a} + 1} \quad (\text{B.12})$$

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