

## Shell-Model Treatment of Nuclear Reactions\*

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A method is developed for the calculation of resonant nuclear states which preserves as many features of the shell model as possible. It is an extension of the  $R$ -matrix theory. The necessary formulas are derived and a detailed description of the computational procedure is given. The method is valid up to the two-particle emission threshold. With the assumption of consecutive decay of the nucleus, the two-particle emission process can also be described. The treatment is antisymmetrized in all particles.

### I. INTRODUCTION

IN the present paper we develop a method which allows the shell-model techniques to be extended to include resonant continuum states. Bearing in mind the need for the eventual use of computing machines we aim to facilitate the actual computation of cross sections. The method is based on the  $R$ -matrix theory of Wigner *et al.*<sup>1-4</sup> In that theory the nuclear wave function is expanded in the internal region into a set of solutions of the Hamiltonian with an arbitrary boundary condition at the matching radius which separates the internal and the external regions. We utilize this arbitrariness and introduce the "natural" boundary conditions which are defined so as to provide the smoothest possible transition between the inside region and the outside region. As a consequence the computational difficulties of the  $R$ -matrix method are greatly reduced. Work to test the method in an actual calculation of resonant nuclear continuum states is in progress at this time.

The  $R$ -matrix theory seems to us to provide that approach to resonant states which is most closely related to the shell model, both in the picture it represents and in the techniques of computation. After all, the states in the internal region can be chosen to be nuclear Hartree-Fock states which are normalized to unity in the finite volume of the internal region. The usual shell-model techniques can then be applied to diagonalize the Hamiltonian and to obtain the "model" states and the energies of the system. The wave function here can be antisymmetrized without difficulty. Un-

fortunately, the usual  $R$ -matrix formulation has several drawbacks, viz., the model states and model eigen-energies of the system obtained this way have no particular physical significance. Further and more importantly, the expansion of the nuclear wave function into the model states does not converge uniformly at the matching radius, the radius which is chosen to separate the inside and the outside region. This is particularly unfortunate since all the important quantities, namely, the partial and the total widths and thus the cross sections, depend on the expansion of the wave function just at the matching radius. The number of terms needed to achieve a desired accuracy of the expansion therefore may be rather large. Finally, the conversion of the standing-wave inside solutions to the running- (incoming plane+scattered spherical)-wave outside solutions involves the inversion of a "matching" matrix, essentially the  $R$  matrix. This represents a formidable barrier which in general has to be overcome by numerical methods.

The method which we develop in the present paper consists in the specialization of the boundary condition to the "natural" boundary condition. This "natural" boundary condition is based on the observation that "in nature" the wave function of the scattered particle has to go smoothly through any point, including the matching boundary. We thus postulate that the logarithmic derivative of the inside wave function matches the logarithmic derivative of the outside wave function at the matching radius. As usual, the magnitude of the matching radius is determined by the "channel-orthogonality" requirement. We shall elaborate these points later.

With the natural boundary condition the  $R$ -matrix expansion  $R_{ee'} = \sum_{\lambda} \gamma_{\lambda e} \gamma_{\lambda e'} (E_{\lambda} - E)^{-1}$  reduces in the resonance exactly to one term, and also, the expansion of the wave function into the set of inside solutions converges uniformly at the matching radius. In this way the essential stumbling blocks for the practical application of the method are removed. Naturally, one

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<sup>1</sup> E. P. Wigner, Phys. Rev. **70**, 15 (1946).

<sup>2</sup> E. P. Wigner, Phys. Rev. **70**, 606 (1946).

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<sup>4</sup> E. Vogt, Rev. Mod. Phys. **34**, 723 (1962). More references are contained in this article.

has to pay for it somewhere. It turns out, however, that the price is not very high. It is one of the aims of the present paper to demonstrate this point.

As yet there does not exist a theory for three-body reactions.<sup>5</sup> We shall not attempt here to construct one. Strictly, the present method therefore is applicable only in the energy region below the two-particle threshold. Outgoing bound fragments, like a deuteron or an  $\alpha$  particle, naturally, can be treated. As long as the so-called simultaneous two-particle emission is unimportant and the two-particle decay can be described by two consecutive single-particle emission processes, one can use the method even above the two-particle threshold, as has been done before. However, we do not advocate this procedure. It represents just a stop-gap measure, pending the development of a genuine three-body theory.

Since the natural boundary conditions are different for the different resonances, one has to compute each state separately. This involves a repeated diagonalization of the Hamiltonian using a truncated set of the internal wave functions, which may contain ten to twenty states. In this respect our method is inferior to the usual  $R$ -matrix theory which uses one single boundary condition for all states. The gain thus lies in the replacement of the inversion of a large matrix, essentially the  $R$  matrix, by several diagonalizations of relatively small matrices. Furthermore, we can give an explicit and exact resonance formula and explicit expressions for the various partial widths. This is exceedingly difficult if not impossible if a large  $R$  matrix has to be inverted which itself is an expansion over many resonant terms.

The present method has certain similarities to the Kapur-Peierls procedure<sup>6</sup> in that the boundary conditions are energy-dependent. In contrast to that procedure our boundary conditions are real and the obtained states have an immediate physical meaning. The natural boundary conditions were first introduced by Siegert.<sup>7</sup> They were used by Peierls,<sup>8</sup> LeCouteur,<sup>9</sup> Humblet and Rosenfeld<sup>10-12</sup> in formal reaction theories and to some extent by Vogt<sup>4</sup> in the discussion of low-energy neutron scattering.

There still exists, however, one serious flaw in our work which we share with all shell-model treatments where a potential other than the harmonic oscillator potential is used. We have not treated the center-of-mass motion properly and we thus will encounter spurious-state problems. The only course we can offer at

this time is to check against the harmonic oscillator case where the spurious components can be identified. It is, however, clear that this is not a safe procedure. We have to leave this as an as yet unsolved problem.

Finally, we shall treat exclusively resonant states, i.e., the states into which the shell-model states develop as they pass the particle emission threshold. A formal criterion for a state to be resonant is for it to have decay modes which are independent of the mode of excitation. We assume this to be true in our case. The region in between the resonances merits special investigation.<sup>13-15</sup> It will be considered in a subsequent paper.

In Sec. II we define the natural boundary conditions and describe the iteration procedure needed to solve the problem by treating the scattering of a single particle on a potential well. In Sec. III we give the formal proof that the  $R$  function reduces to a single term at the resonance for the case of the natural boundary condition. In Sec. IV we formulate the theory for particle-hole states disregarding the residual interactions, and define precisely the channel orthogonality conditions. In Sec. V we formulate the  $R$ -matrix theory for the particle-hole description. In Sec. VI we add the residual interactions and in Sec. VII we finally develop formally the many-channel reaction theory. We conclude by describing in Sec. VIII certain difficulties which one encounters in applying the method, and we show how to deal with them. We give a resume in Sec. IX. The uniform convergence of the expansion of the wave function at the boundary is proven in an Appendix.

## II. THE NATURAL BOUNDARY CONDITION

We illustrate the essential points of the natural boundary condition by the simplest possible model, namely, the scattering of a neutral particle on a potential well. We first have to choose the matching radius  $a$ . We take it to be larger than the extent of the potential well. Then the wave functions in the outside region are given by the asymptotic form, namely, by the spherical Bessel and Neumann functions,  $j_l(kr)$  and  $n_l(kr)$ , multiplied by spherical harmonics. On the inside the wave functions are determined by the equation

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2}(E_\lambda - V) \right\} \varphi_\lambda = 0 \quad (1)$$

and the boundary condition

$$[r(d\varphi_\lambda/dr)]_{r=a} = [b\varphi_\lambda]_{r=a}, \quad (2)$$

with an arbitrary constant  $b$ .

<sup>5</sup> See, however, L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)].

<sup>6</sup> P. L. Kapur and R. E. Peierls, Proc. Roy. Soc. (London) **A166**, 277 (1938).

<sup>7</sup> A. F. J. Siegert, Phys. Rev. **56**, 750 (1939).

<sup>8</sup> R. E. Peierls, Proc. Roy. Soc. (London) **A253**, 16 (1959).

<sup>9</sup> K. J. LeCouteur, Proc. Roy. Soc. (London) **A256**, 115 (1960).

<sup>10</sup> J. Humblet, Mem. Soc. Roy. Sci. Liege **12**, No. 4 (1952).

<sup>11</sup> J. Humblet and L. Rosenfeld, Nucl. Phys. **26**, 529 (1961).

<sup>12</sup> L. Rosenfeld, Nucl. Phys. **26**, 594 (1961).

<sup>13</sup> This point was first brought to our attention by J. H. D. Jensen. We also acknowledge a fruitful discussion concerning this point with G. Suessmann.

<sup>14</sup> W. Brenig and R. Haag, Fortsch. Physik **7**, 183 (1959).

<sup>15</sup> G. Suessmann (to be published).

At a resonance the scattering phase shift is  $\delta_l = \pi/2$ . Then the outside wave function is a spherical Neumann function. We now want to achieve a smooth matching of the inside and outside wave functions. We thus want to take for  $b$  the value given by

$$b = \left[ \frac{r}{rn_l(kr)} \frac{d[rn_l(kr)]}{dr} \right]_{r=a}, \quad (3)$$

where  $k$  is determined by the resonance energy. However, we do not know the resonance energy as yet. The set of equations [(1), (2), and (3)] has the character of a self-consistency problem and must be used to determine this energy. We can solve for the resonance energy and simultaneously for the wave functions, by an iteration procedure. (i) We begin by guessing the resonance energy; we denote it by  $E^{(0)}$ . (ii) With this energy, and the corresponding momentum  $k^{(0)}$ , we compute  $b^{(0)}$  from (3). (iii) We now solve (1) with the boundary condition (2) putting  $b = b^{(0)}$ , obtaining the set of eigenvalues  $E_\lambda^{(1)}$ . In general, no value  $E_\lambda^{(1)}$  will coincide with our assumed energy  $E^{(0)}$ . We then take the eigenvalue, say  $E_\alpha^{(1)}$ , which lies closest to  $E^{(0)}$  and return to step (i) replacing  $E^{(0)}$  by the "once iterated energy"  $E_\alpha^{(1)}$ . This defines an iteration loop which can be repeated until the required accuracy has been reached. The boundary condition (2) with the value of  $b$ , say  $b_\alpha$ , obtained in this iterative procedure, i.e., for which (3) is fulfilled, we call the natural boundary condition for the state  $\varphi_\alpha$ . Its advantage over any other boundary condition lies in the fact that the wave function in the inside region is given by a single member of the set  $\varphi_\lambda$ , namely  $\varphi_\alpha$ , instead of by an infinite series involving all the functions  $\varphi_\lambda$ . In other words, here the state  $\varphi_\alpha$  has a definite physical meaning; it represents directly a scattering state. The price one has to pay is the necessity of going through a separate iteration procedure for each resonance.

To obtain solutions with the natural boundary conditions at other than resonance energies one has to go through the same iteration procedure, just using in (3), instead of  $n_l(kr)$ , a different function for the outside region, viz.,  $f = \sin \delta_l m_l(kr) - \cos \delta_l j_l(kr)$ .

### III. R-MATRIX THEORY FOR POTENTIAL SCATTERING

We now give the formal proof for the assertion that a single state  $u_\lambda$  represents the total wave function, i.e., that the  $R$  matrix at the energy corresponding to the natural boundary condition reduces to a single term. We therefore consider the usual expansion of the wave function at an arbitrary energy  $E$  in terms of the internal wave functions  $u_\lambda$  calculated with the natural boundary condition for the state  $\alpha$ , which corresponds to the energy  $E_\alpha$ .

Let  $U_E$  be the actual wave function for the scattering of a particle at energy  $E$  with the proper boundary

conditions at  $r=0$  and  $r=\infty$ . We now expand in the inside region

$$U_E = \sum_\lambda A_\lambda u_\lambda. \quad (4)$$

Returning to the reduced radial functions, already introduced in the previous section, we may write

$$\begin{aligned} \varphi_\lambda &= r(u_\lambda)_{\text{Rad}}, \\ \Phi_E &= r(U_E)_{\text{Rad}}, \end{aligned} \quad (5)$$

where  $(U)_{\text{Rad}}$  denotes the radial part of the wave function  $U$ , and the coefficients  $A_\lambda$  are given by the expression

$$A_\lambda = \int_0^a \varphi_\lambda \Phi_E dr. \quad (6)$$

Both  $\varphi_\lambda$  and  $\Phi_E$  satisfy Eq. (1), the latter with the replacement of  $E_\lambda$  by  $E$ . From (1) one obtains

$$\begin{aligned} \int_0^a \left( \varphi_\lambda \frac{d^2 \Phi_E}{dr^2} - \Phi_E \frac{d^2 \varphi_\lambda}{dr^2} \right) dr \\ + \frac{2M}{\hbar^2} (E - E_\lambda) \int_0^a \Phi_E \varphi_\lambda dr = 0. \end{aligned} \quad (7)$$

Integrating the first term by parts and substituting (6) in (7) yields

$$A_\lambda = \frac{\hbar^2}{2M} \frac{1}{E_\lambda - E} \left[ \varphi_\lambda \frac{d\Phi_E}{dr} - \Phi_E \frac{d\varphi_\lambda}{dr} \right]_{r=a}. \quad (8)$$

Rewriting (4) for the radial parts, and using (2) we have

$$\Phi_E = \frac{\hbar^2}{2M} \sum_\lambda \frac{1}{E_\lambda - E} \left[ \varphi_\lambda \left( r \frac{d\Phi_E}{dr} - b_\alpha \Phi_E \right) \right]_{r=a} \varphi_\lambda. \quad (9)$$

Introducing the  $R$  function [see Eq. (16), Ref. 4] by the defining equation

$$[\Phi_E]_{r=a} = R_E [r(d\Phi_E/dr) - b_\alpha \Phi_E]_{r=a} \quad (10)$$

we find, using (2), the relation

$$R_E = \sum_\lambda \gamma_\lambda^2 / (E_\lambda - E) \quad (11)$$

with

$$\gamma_\lambda^2 = (\hbar^2/2Ma) [\varphi_\lambda^2]_{r=a}. \quad (12)$$

One sees immediately from (9) that for  $E \rightarrow E_\alpha$  only the term  $\lambda = \alpha$  remains in the sum since then the brackets vanish like  $(E_\alpha - E)$ . Only in the term  $\lambda = \alpha$  is this cancelled by the energy denominator.

### IV. TREATMENT OF PARTICLE-HOLE STATES; RESIDUAL INTERACTIONS OMITTED

We now proceed to the next level of complication, namely, the case of independent particle-hole states. We consider a nucleus containing  $A$  particles,  $N$  of which are neutrons and  $Z$  of which are protons. The

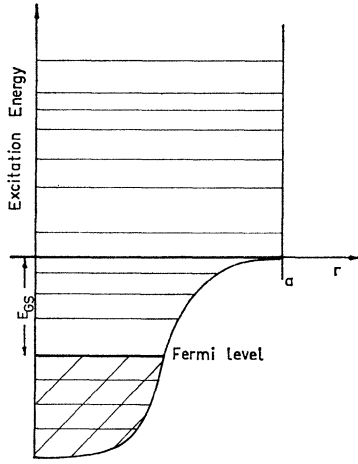


FIG. 1. Schematic picture of the single-particle level scheme of  $H^0$ .

single-particle states are given by

$$H^{(0)}u_\lambda = E^{(0)}u_\lambda \quad (13)$$

and we again impose the boundary condition (2) at a matching radius,  $a$  the constant  $b$  again being left unspecified for the time being.  $\lambda$  denotes all relevant quantum numbers, such as the total angular momentum and its  $Z$  projection, etc.

Some of the states  $u_\lambda$  are bound ( $E_\lambda^{(0)} < 0$ ); most of them are unbound ( $E_\lambda^{(0)} > 0$ ). Some of the bound single-particle states are completely filled up. Let us restrict ourselves to doubly closed shells and light nuclei where protons and neutrons fill the same shells. We call the last full shell the Fermi shell of the nucleus. Levels below the Fermi shell are filled in the ground state by definition. In excited states some of these levels are empty. We then speak of holes and call the hole wave functions

$$v_\lambda(E_\lambda) = T u_\lambda(E_\lambda); \quad E_\lambda \leq E_F, \quad (14)$$

where  $T$  is the time-reversal operator. Now it is easy to construct particle-hole wave functions  $\Phi^{(1)}$ ; two-particle-two-hole wave functions  $\Phi^{(2)}$ , etc., which are all eigenstates of  $H^{(0)}$ ; in general, we have for an  $n$ -particle- $n$ -hole wave function

$$\Phi_\Lambda^{(n)} = [u_{\lambda_1}, u_{\lambda_2}, \dots, u_{\lambda_n}; v_{\lambda_1'}, v_{\lambda_2'}, \dots, v_{\lambda_n'}]_\Lambda, \\ E = E_{\lambda_1} + E_{\lambda_2} + \dots + E_{\lambda_n} - E_{\lambda_1'} - E_{\lambda_2'} - \dots - E_{\lambda_n'}. \quad (15)$$

$E$  is the excitation energy of  $\Phi_\Lambda^{(n)}$  above the ground state;  $\Lambda$  stands for all quantum numbers necessary to specify the state; in particular it contains a quantum number specifying the different possible antisymmetrizations of this state; it is understood that (15) is completely antisymmetrized, e.g., it is a sum over different coupling schemes with the appropriate fractional-parentage coefficients.

The single-particle level scheme of  $H^{(0)}$  looks as shown in Fig. 1. The total level scheme of  $H^{(0)}$  is, however, much more complex since each particle state can

combine with several hole states and since, in addition to the one-particle-one-hole configurations, it furthermore includes the many-particle-many-hole configurations. In particular at higher excitation energy the level density will be much higher than the single-particle level density. A qualitative picture is shown in Fig. 2. Consider now the particle-hole state

$$\Phi_\alpha^{(1)} = [u_{\lambda_1}(E_1); v_{\lambda_1'}(E_1')]_\alpha. \quad (16)$$

We again define the boundary conditions by the equation

$$\left[ \frac{r}{u_\lambda} \frac{\partial u_\lambda}{\partial r} \right]_{r=a} = b_\alpha = \left[ \frac{r}{r n_i(kr)} \frac{\partial [r n_i(kr)]}{\partial r} \right]_{r=a}. \quad (17)$$

Now the conditions which govern the choice of the matching radius  $a$  can be explained. The function  $v$  in (24) describes a bound state. For  $r$  larger than the range of the potential in  $H^{(0)}$ , Eq. (13), it thus decays exponentially with increasing  $r$ . We now have to choose  $a$  so large that  $v$  at the radius  $a$  is sufficiently small so as to be negligible. One calls this neglect the "channel orthogonality assumption." On the other hand, one wants to keep the inside region, i.e., the matching radius  $a$ , as small as possible, because the density of the states  $u_\lambda$  increases with increasing  $a$ . Therefore, also, the size of the matrix which one will have to diagonalize when considering residual interactions becomes larger with increasing  $a$ . One thus has to make a compromise in the choice of the matching radius so that the size of the matrix is manageable while the channel orthogonality is not violated too badly. This requirement is actually not too costly to fulfill since the wave functions decay exponentially while the number of states increases only approximately linearly with increasing matching radius.

Up till now the particle and the hole energies have been defined by the one-body Hamiltonian (13). One may, however, follow present-day usage and consider the hole wave functions to represent the exact solutions of the  $A-1$  system. Then the different hole states represent the different excited states of the  $A-1$  system whose energies can be considered to be known, either by previous computation or by comparison with

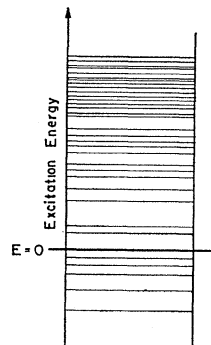


FIG. 2. Schematic picture of the many-particle-many-hole excitation spectrum. The higher the excitation energy, the larger is the level density.

experiment. The different particle-hole states thus represent different channels in which, at a given total energy of the  $A$  system, a nucleon scatters on the different energetically accessible excited states of the  $A-1$  system. Similar, commonly used excuses can be adduced to obtain the particle energies from the  $A+1$  system.

### V. R-MATRIX THEORY FOR PARTICLE-HOLE STATES

All developments of Sec. III can be immediately applied to this case by projecting out the particle wave functions. This is done by uncoupling (16), e.g., by multiplying with  $v_{\lambda_1}^*$  and integrating over the hole coordinates. We thus can continue by taking over everything up to Eq. (12).

We now shall give expressions for the cross section in the channel spin formalism.<sup>4</sup> Then we shall rewrite them in the  $j$ - $j$  coupling scheme which is the appropriate description for the particle-hole states. Writing

$$\Phi' \equiv [r(d\Phi/dr)]_{r=a}, \quad (18)$$

we find from (10) for the logarithmic derivative

$$[\Phi_E'/\Phi_E]_{r=a} = (1 + b_\alpha R_E)/R_E. \quad (19)$$

On the other hand at  $r=a$ , already the asymptotic form applies:

$$[\Phi_E]_{r=a} = I_{E'l} - U_{E'l} O_{E'l} \quad (20)$$

with

$$\begin{aligned} I_{E'l} &= -i(\pi kr/2)^{1/2} H_{l+1/2}^{(2)}(kr) \sim e^{-i(kr-l\pi/2)}, \\ O_{E'l} &= i(\pi kr/2)^{1/2} H_{l+1/2}^{(1)}(kr) \sim e^{i(kr-l\pi/2)}. \end{aligned} \quad (21)$$

Inserting (20) in (19) we find

$$\begin{aligned} U &= (O + bRO - RO')^{-1} (I + bRI - RI') \\ &= (I/O) [(1 - RL^*) / (1 - RL)], \end{aligned} \quad (22)$$

where

$$\begin{aligned} L &= (O'/O) - b \equiv S + iP, \\ O' &= [r(dO/dr)]_{r=a}. \end{aligned} \quad (23)$$

The scattering cross section is now given by

$$\sigma_{\alpha\alpha} = \pi \lambda_\alpha^2 \sum_I G_\alpha^I \sum_{l_s} \{1 - 2 \operatorname{Re} U_{\alpha s l, \alpha s l}^I + \sum_{l' s'} |U_{\alpha s' l', \alpha s l}^I|^2\}, \quad (24)$$

where we have supplemented the index  $\alpha$  with  $s$  and  $l$  which denote the channel spin and relative angular momentum, respectively. In the present case  $l=l_p$ , the particle orbital angular momentum. The statistical factor is given by

$$G_\alpha^I = \frac{2I+1}{(2s_p+1)(2J_\alpha+1)}, \quad (25)$$

where  $s_p = \frac{1}{2}$  is the spin of the particle and  $J_\alpha$  is the angular momentum of the  $A-1$  system. In the present case it is just the hole angular momentum  $j_h$  (see Fig. 3).  $I$  and  $M$  are the quantum numbers of the total angular momentum of the  $A$  system.

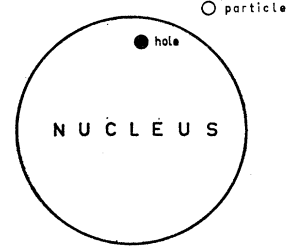


FIG. 3. The hole characterizes the target nucleus. The total angular momentum of the hole is that of the target nucleus. This coupled with the intrinsic spin of the particle ( $\frac{1}{2}$ ) gives the channel spin.

In (24) the matrix elements  $U_{\alpha s' l', \alpha s l}^{IM}$  of the scattering matrix are understood to be taken between channel spin-wave functions

$$\tilde{\Psi}_{\alpha s l_p}^{IM} = (\varphi_\alpha / r_p) \sum (s m_s l_p m_p | IM) \chi_{s m_s} Y_{l_p m_p}, \quad (26)$$

$$\chi_{s m_s} = \sum (j_h m_h s_p \sigma_p | s m_s) v_{j_h m_h} \zeta_{\sigma_p}, \quad (27)$$

$\zeta_{\sigma_p}$  is the spin function of the particle

The wave functions (26) are particle-hole wave functions in a different than the usual coupling scheme. We can denote the channel spin coupling scheme by

$$[[\mathbf{j}_h \times \mathbf{s}_p]^{[s]} \times \mathbf{I}_p]^{[I]}, \quad (28)$$

while the usual particle-hole coupling scheme is the  $j$ - $j$  coupling

$$[\mathbf{j}_h \times [\mathbf{I}_p \times \mathbf{s}_p]^{[j_p]}]^{[I]}. \quad (29)$$

Let us denote the wave functions of the  $j$ - $j$ -coupling scheme (29) by

$$\begin{aligned} \Psi_{\alpha j_p j_h}^{IM} &= (\varphi_\alpha / r_p) \sum (j_h m_h j_p m_p | IM) v_{j_h m_h} \tilde{u}_{j_p m_p} \\ &\equiv \varphi_\alpha \tilde{\Psi}_{\alpha j_p j_h}^{IM}. \end{aligned} \quad (30)$$

Here  $\tilde{u}_{j_p m_p}$  is the angular part of the particle wave function. The connection between the wave functions (26) and (30) is then given by the recoupling formula

$$\tilde{\Psi}_{\alpha s l_p}^{IM} = \sum_{j_p} K_{j_p s}^{(l_p)} \Psi_{\alpha j_p j_h}^{IM}, \quad (31)$$

where

$$\begin{aligned} K_{j_p s}^{(l_p)} &= (-)^{j_p + j_h + I} ((2s+1)(2j_p+1))^{1/2} \\ &\quad \times \begin{Bmatrix} l_p & s_p & j_p \\ j_h & I & s \end{Bmatrix}. \end{aligned} \quad (31a)$$

We obtain therefore for the  $U$ -matrix element

$$U_{\alpha' s' l', \alpha s l}^{IM} = \sum_{j_p j_p'} K_{j_p' s'}^{(l_p')} K_{j_p s}^{(l_p)} U_{\alpha j_p' j_h, \alpha j_p j_h}^{IM}. \quad (32)$$

Inserting this into (24) yields

$$\begin{aligned} \sigma_{\alpha\alpha} &= \pi \lambda_\alpha^2 \sum_I G_\alpha^I \sum_{l_p s} \{1 - 2 \operatorname{Re} \sum_{j_p' j_p} K_{j_p' s'}^{(l_p')} K_{j_p s}^{(l_p)} \\ &\quad \times U_{\alpha j_p' j_h, \alpha j_p j_h}^{IM} \\ &\quad + \sum_{l' s'} |\sum_{j_p j_p'} K_{j_p' s'}^{(l_p')} K_{j_p s}^{(l_p)} U_{\alpha j_p' j_h, \alpha j_p j_h}^{IM}|^2\}. \end{aligned} \quad (33)$$

By use of the orthogonality relations

$$\sum_l K_{f l} K_{g l} = \delta_{f g}, \quad \sum_l K_{l f} K_{l g} = \delta_{f g}, \quad (34)$$

we find for the second term in the braces of (24) or (33)

$$\sum_s K_{j_p' s}^{(l_p')} K_{j_p s}^{(l_p)} = \delta_{j_p j_p'} \quad (35)$$

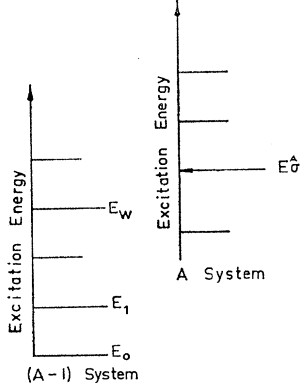


FIG. 4. The energy levels of the  $(A-1)$  system are shown qualitatively together with the continuum of the  $A$  system. The latter is represented by a set of discrete compound levels. If the considered compound level  $E_{\alpha}^A$  of the system drops below the level  $E_W$  of the  $(A-1)$  system, this level drops out as a possible channel for the decay of the  $A$  system.

and for the third term in the braces of (33)

$$\sum_{ss'} \sum_{j_p j_p'} \sum_{\tilde{j}_p \tilde{j}_p'} K_{j_p' s' (l_p')} K_{\tilde{j}_p' s' (l_p')} K_{j_p s (l_p)} K_{\tilde{j}_p s (l_p)} \times U_{\alpha j_p' j_h, \alpha \tilde{j}_p j_h}^{IM} U_{\alpha \tilde{j}_p' j_h, \alpha j_p j_h}^{IM*} = \sum_{j_p j_p'} |U_{\alpha j_p' j_h, \alpha j_p j_h}^{IM}|^2. \quad (36)$$

Therefore we have finally for the elastic scattering cross section in the particle-hole formalism

$$\sigma_{\alpha\alpha} = \pi \lambda_{\alpha}^2 \sum_I G_{\alpha}^I \sum_{l_p j_p} \{1 - 2 \operatorname{Re} U_{\alpha j_p j_h, \alpha j_p j_h}^{IM} + \sum_{l_p' j_p'} |U_{\alpha j_p' j_h, \alpha j_p j_h}^{IM}|^2\}. \quad (37)$$

At the energy  $E_{\alpha}$  the  $R$  number is given solely by (see the discussion at the end of Sec. III)

$$R_{\alpha} = \gamma_{\alpha}^2 / (E_{\alpha} - E). \quad (38)$$

By means of (22) and (23) the  $U$  matrix reduces to

$$U_{\alpha} = \begin{pmatrix} I \\ -O \end{pmatrix} \frac{E - E_{\alpha} - \gamma_{\alpha}^2 (S - iP)}{E - E_{\alpha} - \gamma_{\alpha}^2 (S + iP)}. \quad (39)$$

For the elastic scattering section we need  $1 - U_{\alpha}$  which is

$$1 - U_{\alpha} = \frac{(O+I)i\Gamma_{\alpha}/2}{O(E - \bar{E}_{\alpha} - i\Gamma_{\alpha}/2)} + \frac{(O-I)(E - \bar{E}_{\alpha})}{O(E - \bar{E}_{\alpha} - i\Gamma_{\alpha}/2)}, \quad (40)$$

where

$$\Gamma_{\alpha}/2 = \gamma_{\alpha}^2 P. \quad (41)$$

Here  $P$  is the penetrability<sup>4</sup> and

$$\bar{E}_{\alpha} = E_{\alpha} + \gamma_{\alpha}^2 S. \quad (42)$$

The second term vanishes if the hard-sphere phase shift  $\varphi$ , defined by  $(I/O)_{\alpha} = e^{2i\varphi}$ , vanishes.

The scattering cross section is proportional to  $|1 - U_{\alpha}|^2$ . From our previous considerations concerning the natural boundary conditions it is clear that the cross section should have a resonance at  $E = E_{\alpha}$ . This is not formally obvious from (40). The first term has a resonance at  $E = \bar{E}_{\alpha}$  while the second term does not have a resonance at all and vanishes at  $E = \bar{E}_{\alpha}$ . We are now going to show that by (40) *de facto* a resonance is described which lies at the unshifted energy  $E = E_{\alpha}$ . To this end we consider the case where the matching radius  $a$  has been chosen so large that the outside wave

functions can be replaced by their asymptotic form. The scattering wave function for neutrons has the form

$$A_i [\cos \delta_l j_l(kr) - \sin \delta_l m_l(kr)]$$

which in the case  $\delta_l = \pi/2$  becomes asymptotically

$$-A_l m_l(kr) \rightarrow -[(2l+1)i^l/2ikr] \times [e^{i(kr-l\pi/2)} + e^{-i(kr-l\pi/2)}] = [(2l+1)i^l/2ikr][I_l + O_l]. \quad (43)$$

The quantity  $L$  is given by

$$L = \left[ \frac{r}{O} \frac{dO}{dr} - \frac{r}{rn_l} \frac{d(rn_l)}{dr} \right]_{r=a} = -ka^2 \left[ i - \frac{\sin(ka - \frac{1}{2}l\pi)}{\cos(ka - \frac{1}{2}l\pi)} \right] \equiv S + iP, \quad (44)$$

Thus

$$P = -ka^2, \quad S = ka^2 \tan(ka - \frac{1}{2}l\pi). \quad (45)$$

From (40) we find for the cross section

$$\sigma(E) \propto |1 - U_{\alpha}|^2 \equiv V(E) = \frac{|i(\Gamma_{\alpha}/2)(O+I) + (O-I)(E - \bar{E}_{\alpha})|^2}{|O|^2[(E - \bar{E}_{\alpha})^2 + (\Gamma_{\alpha}^2/4)]}. \quad (46)$$

It is straightforward to compute the extrema of the function  $V(E)$  from

$$\partial V(E)/\partial E = 0.$$

We find for the energies where the extrema occur

$$E_{\text{Res}} = E_{\alpha} + \gamma_{\alpha}^2 \left[ S - P \frac{\operatorname{Re}(IO^*) \pm |IO^*|}{\operatorname{Im}(IO^*)} \right]. \quad (47)$$

Inserting the values for  $S$  and  $P$  from (45) and the asymptotic expressions for  $I$  and  $O$  from (21) we find that indeed

$$E_{\text{Res}} = E_{\alpha}. \quad (48)$$

The shift  $\bar{E}_{\alpha} - E_{\alpha}$  which occurs in the resonating part of (40) is cancelled by the nonresonating part of the amplitude, the hard-sphere contribution.

## VI. TREATMENT OF PARTICLE-HOLE STATES; RESIDUAL INTERACTIONS INCLUDED

In the previous sections we have progressed up to the scattering of particles in several disconnected channels. We now shall introduce the residual interactions which will both couple the different channels, thus allowing inelastic processes, and shift the resonance energies. We therefore have to generalize our procedure for the determination of the natural boundary conditions in that we have to include the necessary diagonalizations. We again begin by leaving the boundary conditions open for the time being. We write the wave

function (30), splitting off explicitly the radial functions  $\varphi_c$  and summing over the different channels

$$\Psi = \sum_c \psi_c \varphi_c. \quad (49)$$

The necessary expansion coefficients have been absorbed in the  $\varphi_c$ . The most general wave function is

$$\Psi = \sum_c C_c (\mathcal{G}_c - \sum_{c'} U_{cc'} \mathcal{O}_{c'}) \quad (50)$$

and the reduced radial wave function in the channel  $c$  is then

$$\varphi_c(r_{pc}) = (C_c I_c - \sum_{c'} C_{c'} U_{cc'} O_{c'}) v_c^{-1/2}. \quad (51)$$

We have used the notation

$$\begin{aligned} \mathcal{G}_c &= I_{\alpha_j p l_p} \tilde{\psi}_{\alpha_j p h}^{I M}, \\ \mathcal{O}_c &= O_{\alpha_j p l_p} \tilde{\psi}_{\alpha_j p h}^{I M}, \end{aligned} \quad (52)$$

where  $I$  and  $\tilde{\psi}$  are given by (21) and (30). We now introduce quantities analogous to  $(rd\varphi/dr)_{r=a}$  of Eq. (2),

$$\Delta_c \equiv \left[ r \frac{\partial \varphi_c}{\partial r} \right]_{r=a} = a v_c^{-1/2} \left[ C_c \frac{dI_c}{dr} - \sum_{c'} U_{cc'} \frac{dO_{c'}}{dr} \right]_{r=a}. \quad (53)$$

Here  $v_c$  is the relative velocity in the channel  $c$ . We introduce now again an internal set of eigenfunctions which satisfy the Schrödinger equation and a boundary condition

$$\begin{aligned} H X_\lambda &= E_\lambda X_\lambda, \\ H &= H_0 + H'. \end{aligned} \quad (54)$$

The states  $X_\lambda$  are superpositions of various  $p$ - $h$  channels. The radial wave functions  $\varphi_{\lambda c}$  involved in the states  $X_\lambda$  shall fulfill the boundary condition

$$\Delta_{\lambda c} = B_c [\varphi_{\lambda c}]_{r=a} \quad (55)$$

or

$$\left[ \frac{r}{\varphi_{\lambda c}} \frac{d\varphi_{\lambda c}}{dr} \right]_{r=a} = B_c = \left[ \frac{r}{r n_l(k_c r)} \frac{d[r n_l(k_c r)]}{dr} \right]_{r=a}. \quad (55')$$

The energies in the different channels, and thus the wave numbers  $k_c$ , are connected because of the assumed previous knowledge of the spectrum of the  $A-1$  system (see Fig. 4). Only a finite number of channels can participate at a given energy. In the different channels therefore the constants  $B_c$  have different, albeit related, values.

With this boundary condition we again require that the various  $p$ - $h$  states contained in  $X_\lambda$  should have phase shifts of  $\pi/2$  for particles in all channels at the energy  $E$  of the  $A$  system. This postulate implies the assumption of a resonating character for the reaction, as emphasized in the introduction. In the general case no fixed relation exists between the phase shifts in the different channels.

The iteration procedure discussed earlier in Sec. II must here be modified in a rather obvious manner. We describe now the complete procedure. (1) One chooses

an energy  $E_\alpha^{(0)}$  for the  $A$  system. (2) One then determines from the level scheme of the  $A-1$  system the particle energies in the different channels and obtains according to (55) the set  $B_c^{(0)}$ . (3) With these boundary conditions one computes for each channel separately a complete set of particle states. (4) One constructs the wave functions  $\Psi_\nu$ , Eq. (49) for the desired state of the  $A$  system by diagonalization of the Hamiltonian. (5) One searches for the eigenvalue closest to the assumed value  $E_\alpha^{(0)}$ , and calls it  $E_\alpha^{(1)}$ . This closes the iteration loop. After reaching the desired accuracy one has a wave function which consists of a well-determined mixture of states in the different channels. Thus now the channels are coupled and reactions, e.g., inelastic scattering, are contained in the description of the system.

To obtain the different excited states of the system one has to go through a separate iteration procedure for each state. This way one can find the spectrum of the resonant states in the  $A$  system. We call these compound states

$$\tilde{\chi}_{\alpha\nu}, \quad \nu = 1, 2, 3, \dots \quad (56)$$

The index  $\nu$  merely denotes the sequence of the resonances of the  $A$  system.  $\alpha$  characterizes all other quantum numbers. We emphasize that the different inside wave functions  $\tilde{\chi}_{\alpha\nu}$  obey different boundary conditions and therefore are not orthogonal. However, the nuclear wave functions defined in the whole space, obtained by joining the outside region to the inside region and matching the outside wave functions to  $\tilde{\chi}_{\alpha\nu}$  at the boundary, are indeed orthogonal. This is the correct behavior of a wave function belonging to the continuum.

In the diagonalization of the Hamiltonian which one has to carry out when going through the iteration procedure a complete set of eigenstates is generated in addition to the state  $\tilde{\chi}_{\alpha\nu}$ . The other states are, however, not needed and do not even have to be calculated.

In the present formulation the closed channels do not present any problems whatsoever. When going through the iteration one may find that, for example, the energy of a state gets lower in consecutive iteration steps. Once the energy passes the threshold of the lowest energy channel (the channel associated with the highest excited state of the  $A-1$  system) in the next iteration step that channel automatically drops out (see Fig. 4).

## VII. MANY-CHANNEL R-MATRIX REACTION THEORY FOR PARTICLE-HOLE STATES

The functions  $\chi_\lambda^{(\alpha\nu)}$  are normalized according to

$$\int \chi_\lambda^{(\alpha\nu)} \chi_{\lambda'}^{(\alpha\nu)} d\tau = \delta_{\lambda\lambda'}, \quad (57)$$

$$H \chi_\lambda^{(\alpha\nu)} = E_\lambda^{(\alpha\nu)} \chi_\lambda^{(\alpha\nu)}. \quad (58)$$

The total wave function  $\Psi$  in (40) is a solution of the

same Hamiltonian, i.e.,

$$H\Psi = E\Psi. \quad (59)$$

Only the boundary conditions are different; namely, they are fixed at infinity. We expand  $\Psi$  in the interior region (all  $r_c < a$ )

$$\Psi = \sum_{\lambda} A_{\lambda} \chi_{\lambda}^{(\alpha\nu)}, \quad (60)$$

with

$$A_{\lambda} = \int_{\tau} \chi_{\lambda}^{(\alpha\nu)*} \Psi d\tau. \quad (61)$$

In order to evaluate (61) we deduce from (58) and (59) the relation

$$\begin{aligned} \int_{\tau} d\tau \left( \sum_i \chi_{\lambda}^{(\alpha\nu)*} \frac{\hbar^2}{2m} \nabla_i^2 \Psi - \Psi \frac{\hbar^2}{2m} \nabla_i^2 \chi_{\lambda}^{(\alpha\nu)*} \right) \\ = (E_{\lambda}^{(\alpha\nu)} - E) \int_{\tau} \chi_{\lambda}^{(\alpha\nu)*} \Psi d\tau. \end{aligned}$$

Using Green's theorem, we get in the usual way

$$\begin{aligned} (E_{\lambda}^{(\alpha\nu)} - E) \int_{\tau} \chi_{\lambda}^{(\alpha\nu)*} \Psi d\tau \\ = \sum_c \int_{S_c} \frac{\hbar^2}{2M_c} \left( \chi_{\lambda}^{(\alpha\nu)*} \frac{\partial \Psi}{\partial r_c} - \Psi \frac{\partial \chi_{\lambda}^{(\alpha\nu)*}}{\partial r_c} \right) dS. \quad (62) \end{aligned}$$

We now equate the form (49) and (60) for the wave function at the surface

$$[\chi_{\lambda}^{(\alpha\nu)}]_{r=a} = \sum_c [\psi_c \varphi_{\lambda c}^{(\alpha\nu)}]_{r=a} \quad (63)$$

so that

$$\begin{aligned} (E_{\lambda}^{(\alpha\nu)} - E) \int_{\tau} \chi_{\lambda}^{(\alpha\nu)*} \Psi d\tau \\ = \sum_c \frac{\hbar^2}{2M_c} \left[ \varphi_{\lambda c}^{(\alpha\nu)*} \frac{d\varphi_c}{dr_c} - \varphi_c \frac{d\varphi_{\lambda c}^{(\alpha\nu)*}}{dr_c} \right]_{r=a} \\ = \sum_c \frac{\hbar^2}{2M_c a} [\varphi_{\lambda c}^{(\alpha\nu)*} \Delta_c - \varphi_c \Delta_{\lambda c}^{(\alpha\nu)*}]_{r=a}. \quad (64) \end{aligned}$$

Therefore, according to (61),

$$\begin{aligned} A_{\lambda} = \sum_c \frac{\hbar^2}{2M_c a} \frac{1}{E_{\lambda}^{(\alpha\nu)} - E} \\ \times [\varphi_{\lambda c}^{(\alpha\nu)*} \Delta_c - \varphi_c \Delta_{\lambda c}^{(\alpha\nu)*} \varphi_{\lambda c}^{(\alpha\nu)*}(a)]_{r=a} \\ = \sum_c \frac{\hbar^2}{2M_c a} \frac{\varphi_{\lambda c}^{(\alpha\nu)*}}{E^{(\alpha\nu)} - E} [\Delta_c - B_c^{(\alpha\nu)} \varphi_c]_{r=a}. \quad (65) \end{aligned}$$

Inserting this result into (60), we obtain

$$\begin{aligned} \Psi(E) = \sum_c [\Delta_c - B_c^{(\alpha\nu)} \varphi_c]_{r=a} \frac{\hbar^2}{2M_c a} \\ \times \sum_{\lambda} \frac{\varphi_{\lambda c}^{(\alpha\nu)*}}{E_{\lambda}^{(\alpha\nu)} - E} \chi_{\lambda}^{(\alpha\nu)} \quad (66) \end{aligned}$$

and for the radial function

$$\begin{aligned} \varphi_c(E_1 r_c) = \sum_{c'} [\Delta_{c'} - B_{c'}^{(\alpha\nu)} \varphi_{c'}]_{r=a} \frac{\hbar^2}{2M_{c'} a} \\ \times \sum_{\lambda} \frac{\varphi_{\lambda c'}^{(\alpha\nu)*}(a) \varphi_{\lambda c}^{(\alpha\nu)}(r_c)}{E_{\lambda}^{(\alpha\nu)} - E}. \quad (67) \end{aligned}$$

The  $R$  matrix is then defined as

$$\begin{aligned} [\varphi_c(E_1 a)] (M_c a)^{-1/2} \\ = \sum_{c'} R_{cc'}^{(\alpha\nu)}(E_1 E_{\lambda}) \\ \times [\Delta_{c'}(E) - B_{c'}^{(\alpha\nu)}(E) \varphi_{c'}(E_1 a)] (M_{c'} a)^{-1/2}. \quad (68) \end{aligned}$$

From the comparison of (63) and (67) it follows that

$$\begin{aligned} R_{cc'}^{(\alpha\nu)}(E_1 E_{\lambda}) = \sum_{\lambda} \frac{\gamma_{\lambda c}^{(\alpha\nu)} \gamma_{\lambda c'}^{(\alpha\nu)}}{E_{\lambda}^{(\alpha\nu)} - E}, \\ \gamma_{\lambda c}^{(\alpha\nu)} = (\hbar^2 / 2M_c a)^{1/2} \varphi_{\lambda c}^{(\alpha\nu)}(a). \quad (69) \end{aligned}$$

From (68) we can deduce an important result: At the energy  $E_{\lambda=1}^{(\alpha\nu)}$  the state  $\tilde{\chi}_{\alpha\nu}$ , Eq. (56) is identical with  $\chi_{\lambda=1}^{(\alpha\nu)}$  of the complete set (57); as a matter of fact the iteration procedure described above was chosen in order to achieve this result. If  $E \rightarrow E_{\lambda=1}^{(\alpha\nu)}$  then in (68) the quantity

$$[\Delta_{c'}(E) - B_{c'}^{(\alpha\nu)}(E_{\lambda=1}^{(\alpha\nu)}) \varphi_{c'}(E_1 a)] \propto (E - E_{\lambda=1}^{(\alpha\nu)}) \quad (70)$$

because of the boundary condition (55). In other words: Since the reduced radial function

$$\begin{aligned} \varphi_c(E_1 a) \rightarrow [r m_i(kr)]_{r=a} \\ k^2 \rightarrow (2M_c / \hbar^2) E_{\lambda=1}^{(\alpha\nu)} \quad (71) \end{aligned}$$

the quantities in (70) vanish for  $E \rightarrow E_{\lambda=1}^{(\alpha\nu)}$  at least linearly. This means that in the  $R$ -matrix sum (69) only one single term, namely,

$$\begin{aligned} R_{cc'}(E = E_{\lambda=1}^{(\alpha\nu)}) \\ = \gamma_{\lambda=1, c}^{(\alpha\nu)} \gamma_{\lambda=1, c'}^{(\alpha\nu)} / E_{\lambda=1}^{(\alpha\nu)} - E \quad (72) \end{aligned}$$

contributes in the vicinity of  $E = E_{\lambda=1}^{(\alpha\nu)}$ . The contributions of all the other terms in (69) vanish *exactly* for  $E = E_{\lambda=1}^{(\alpha\nu)}$ .

Therefore, it is relatively easy to compute the  $R$  matrix for the resonance states  $\tilde{\chi}_{\alpha\nu}$  in (56). Depending on the number,  $N$ , of channels, e.g.,  $p\hbar$  configurations which are contained in  $\tilde{\chi}_{\alpha\nu}$ , one obtains for the  $R$  matrix an  $N$  by  $N$  matrix.

The  $U$  matrix can be evaluated from the  $R$  matrix by

$$\begin{aligned} U = (ka)^{1/2} O^{-1} [1 - RL_0]^{-1} [1 - RL_0^*] I (ka)^{-1/2}, \\ L_0 = L - B; \quad L_0^* = L^* - B, \quad (73) \end{aligned}$$

where

$$\begin{aligned} I_{cc'} &= I \delta_{cc'}, \\ L_{cc'} &= a(O_c' / O_c) \delta_{cc'}, \\ L_{cc'}^* &= a(I_c' / I_c) \delta_{cc'}, \\ B_{cc'} &= B_c \delta_{cc'}. \quad (74) \end{aligned}$$



This form of the collision matrix was originally obtained by Wigner and Eisenbud.<sup>3</sup> It involves the inversion of the matching matrix  $[1-R(L-B)]$ . A new form of the  $U$  matrix has been introduced by Thomas.<sup>16</sup> It can be obtained as follows:

We define a new matrix  $A_{\lambda\lambda'}$  by

$$([1-RL_0]^{-1}[1-RL_0^*])_{cc'} = \delta_{cc'} + 2iP_{c'}\gamma_{\lambda c}\gamma_{\lambda c'}A_{\lambda\lambda}. \quad (75)$$

In contrast to Ref. 4 we do not have to write a sum over  $\lambda$  and  $\lambda'$  on the right-hand side since in our case the left-hand side contains only a single  $\lambda$ . Multiplication of both sides in (75) with  $(1-RL_0)$  from the left yields

$$\begin{aligned} \delta_{cc'} - [\gamma_{\lambda c}\gamma_{\lambda c'}/(E_\lambda - E)]L_{0c'}^* \\ = \delta_{cc'} - [\gamma_{\lambda c}\gamma_{\lambda c'}/(E_\lambda - E)]L_{0c'} + 2iP_{c'}\gamma_{\lambda c}\gamma_{\lambda c'}A_{\lambda\lambda} \\ - \sum_{c''} [\gamma_{\lambda c}\gamma_{\lambda c''}/(E_\lambda - E)]L_{0c''} 2iP_{c''}\gamma_{\lambda c}\gamma_{\lambda c'}A_{\lambda\lambda}. \end{aligned} \quad (76)$$

This can be written as

$$[2iP_{c'}\gamma_{\lambda c}\gamma_{\lambda c'}/(E_\lambda - E)] \times [\delta_{\lambda\lambda'} - (E_\lambda - E)A_{\lambda\lambda} + \xi_{\lambda\lambda}A_{\lambda\lambda}] = 0, \quad (77)$$

with

$$\begin{aligned} \xi_{\lambda\lambda} &= \sum_{c''} \gamma_{\lambda c}\gamma_{\lambda c''}L_{0c''} \\ &\equiv -\Delta_{\lambda\lambda} + \frac{1}{2}i\Gamma_{\lambda\lambda}. \end{aligned} \quad (78)$$

It follows

$$(A^{-1})_{\lambda\lambda'} = [(E_\lambda - E) + \Delta_{\lambda\lambda} - \frac{1}{2}i\Gamma_{\lambda\lambda}]\delta_{\lambda\lambda'}. \quad (79)$$

In general, this matrix has to be inverted. In our problem, however, as a result of the natural boundary condition, this matrix becomes diagonal at the resonances  $E = E_{\lambda=1}^{(\alpha\nu)}$  according to (72). The inversion is therefore simply the inversion of numbers. We now compute explicitly the matrix elements of the  $U$  matrix (73) at the resonance energy, generalizing to charged particles. Then, following Ref. 4,

$$I_c = O_c^* = (G_c - iF_c)e^{i\omega_c}, \quad (80)$$

where  $G_c$  and  $F_c$  are the irregular and regular Coulomb functions, respectively, and  $\omega_c$  is the Coulomb phase shift

$$\omega_c \equiv \sum_{n=1}^{l_c} \arctan \frac{\eta_c}{n}, \quad \eta_c = \frac{Z_1 Z_2 e^2}{\hbar v_c}. \quad (81)$$

$F_c$  and  $G_c$  are normalized according to

$$r_c(dF_c/dr_c)G_c - r_c(dG_c/dr_c)F_c = k_c r_c. \quad (82)$$

From

$$L_{0c} = (r_c/O_c)(dO_c/dr_c) - B_c \equiv S_c + iP_c, \quad (83)$$

we obtain

$$\begin{aligned} P_c &= \left[ \frac{k_c r_c}{F_c^2 + G_c^2} \right]_{r_c=a}; \\ S_c &= -B_c + \left[ \frac{r_c}{F_c^2 + G_c^2} \left( F_c \frac{dF_c}{dr_c} + G_c \frac{dG_c}{dr_c} \right) \right]_{r_c=a}. \end{aligned} \quad (84)$$

<sup>16</sup> R. G. Thomas, Phys. Rev. 92, 224 (1955).

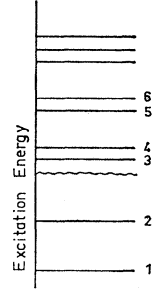


FIG. 5. Hartree-Fock single-particle energies calculated with some arbitrary boundary condition.

With these formulas we obtain

$$\begin{aligned} (k_c r_c)^{1/2} O_c^{-1} I_{c'} (k_{c'} r_{c'})^{-1/2} \\ = e^{i(\omega_c + \omega_{c'})} (k_c r_c / k_{c'} r_{c'})^{1/2} [(G_{c'} - iF_{c'}) / (G_c + iF_c)] \\ = e^{i(\Omega_c + \Omega_{c'})} P_c^{1/2} P_{c'}^{-1/2}, \end{aligned} \quad (85)$$

where

$$\Omega_c \equiv \omega_c - \arctan(F_c/G_c).$$

Inserting this into (73) we obtain

$$\begin{aligned} U_{cc'} &= e^{i(\Omega_c + \Omega_{c'})} \\ &\times \left[ \delta_{cc'} + i \frac{\Gamma_{\lambda=1,c}^{1/2} \Gamma_{\lambda=1,c'}^{1/2}}{E - E_{\lambda=1}^{(\alpha\nu)} + \Delta_{\lambda=1,\lambda=1} - \frac{1}{2}i\Gamma_{\lambda=1,\lambda=1}} \right], \end{aligned} \quad (86)$$

where

$$\Gamma_{\lambda c}^{1/2} = (2P_c)^{1/2} \gamma_{\lambda c}^{(\alpha\nu)}$$

has the same sign as the reduced width amplitude  $\gamma_{\lambda c}^{(\alpha\nu)}$ .

For uncharged particles the same result holds except that  $F_c$  and  $G_c$  then are spherical Bessel functions.<sup>17</sup>

### VIII. DETAILS CONCERNING THE CONSTRUCTION OF THE INSIDE WAVE FUNCTION

We describe now in detail the treatment of some particular problems which arise in the construction of a complete set of linearly independent orthonormal states for the inside wave function. As will be seen, it is easy to obtain a complete set. The difficulties are associated with the elimination of the redundant states. Although it is not necessary to eliminate them for practical computations—the Hamiltonian matrix in that case just has a number of zero eigenvalues equal to the number of supernumerary states—it still is advantageous to do so.

We begin with the simplest case, namely, that of a single open channel. The structure of the level scheme is shown in Figs. 5 and 6. The wavy line represents the beginning of the continuum. The bound states (1 through 5) are independent of the boundary condition since the wave function is sufficiently small at the matching radius  $a$ . The states with positive energy (6 and up) depend explicitly on the boundary conditions. We consider that the  $(A-1)$  problem has been solved.

<sup>17</sup> A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1958).

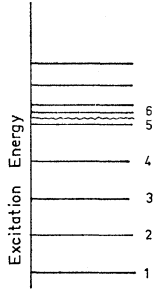


FIG. 6. Energy spectrum of the  $A-1$  system after diagonalization with the set of single particle functions of Fig. 5.

We now turn to the  $A$  system, and we consider an excitation energy such that only one channel is open, namely, the ground-state transition (see Fig. 7). To know the threshold energy one has to have calculated the binding energy of the  $A$  system. This can be done by usual shell-model methods and we consider that this has been done too.

We now write the wave function of the  $A$  system assuming that only a single angular momentum is available in the open channel. Asymptotically it has simply the form

$$\Psi = \psi_1 \varphi_1. \quad (87)$$

For our present purpose it is better to change from the channel wave function to a more explicit form. To that end we introduce the wave function for the  $A-1$  system, denoting it by  $\omega_\lambda$ . Then (87) becomes

$$\Psi = \omega_1 u_1. \quad (88)$$

In the inside region we need a complete set of states. This is supplied, for example, by the expansion

$$\Psi_i = \sum_{\lambda, \nu} a_{\lambda, \nu} \omega_\lambda u_\nu, \quad (89)$$

where the summations over  $\lambda$  and  $\nu$  are to be performed independently covering the complete sets of solutions of the  $A-1$  system and the single particle. The set  $(\lambda, \nu)$  is however not linearly independent. We now proceed to eliminate this drawback. We expand the wave function  $\omega_\lambda$  into Hartree-Fock states, and, more precisely, into particle-hole states. Then (89) becomes simply

$$\Psi_i = \sum a_{\alpha\beta\cdots\mu\lambda; \nu} u_\alpha u_\beta \cdots v_\mu v_\lambda u_\nu. \quad (90)$$

It is now sufficient to eliminate all partitions  $(\alpha\beta\cdots\nu)$  which correspond to permutations between the channel particle  $u_\nu$  and the core particle  $u_\alpha$ . This can be performed very easily in practice when one builds up the set of states for the  $A-1$  system systematically starting with hole states, and continuing with particle-two hole states, two-particle-three-hole states, etc. No problem is now encountered in the antisymmetrization of the state.

At this point only the boundary condition for the state  $\nu$  has been determined by the "naturalness" criterion. For the states with other angular momenta the boundary conditions can be still chosen at will.

This freedom can be used to advantage in the case of several channels, to which we now proceed.

We thus consider the case when at the energy  $E_1$  (Fig. 7) particles with, say, two different angular momenta contribute to the decay. Such a situation obtains, for example, in the giant resonance of  $O^{16}$ , where  $1\bar{p}_{1/2}2s_{1/2}$  and  $1\bar{p}_{1/2}1d_{3/2}$  both participate in the ground-state transitions. The asymptotic form of the wave function then is

$$\Psi = \psi_1 \varphi_1 + \psi_2 \varphi_2 = a_1 \omega_1 u_1 + a_2 \omega_2 u_2. \quad (91)$$

Here, the particle functions  $u_1$  and  $u_2$  are calculated with different boundary conditions according to their different angular momenta. We indicate this by adding a superscript. In the inside again we expand into a complete set and obtain

$$\Psi_i = \sum_{\lambda, \nu} a_{1\lambda, \nu} \omega_\lambda^{(1)} u_\nu^{(1)} + \sum_{\lambda, \nu} a_{2\lambda, \nu} \omega_\lambda^{(2)} u_\nu^{(2)}. \quad (92)$$

We have also indicated the boundary conditions at the wave functions  $\omega^{(n)}$  since the unbound states depend on the boundary conditions. It is, namely, very desirable to use the boundary conditions of  $u_\nu$  in those components  $u_\alpha$  of the product  $\omega_\lambda u_\nu$  which have the same angular momentum as  $u_\nu$  since otherwise the antisymmetrization is very difficult to perform. Again, in the first sum only the boundary conditions for the states with the quantum numbers of  $u_1$  are determined; similarly in the second sum they are fixed only for the states with the quantum numbers of  $u_2$ . One therefore can assign to the states of the first sum with the quantum numbers of  $u_2$  the boundary conditions valid for the second sum and vice versa. Then there is no difference left between the boundary conditions in the two sums and one can combine them formally into one sum, again watching out for possible repeats of states as in the above described case of one open channel. In practice, again the procedure is straightforward when constructing the states in a systematic manner.

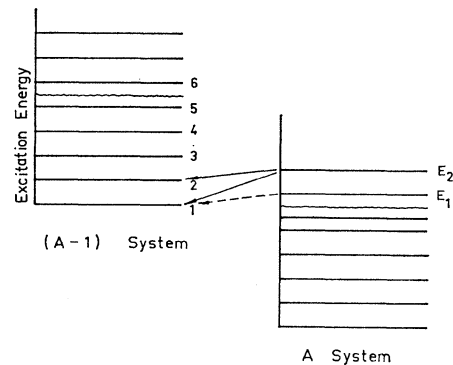


FIG. 7. Energy diagram for the  $A$  and  $A-1$  systems. At the excitation energy  $E_1$  only the ground state of the  $A-1$  system can be reached. However, several channels corresponding to different angular momenta of the outgoing particle can be involved. At the energy  $E_2$  both the ground and the first excited state can be reached, each possibly involving several channels.

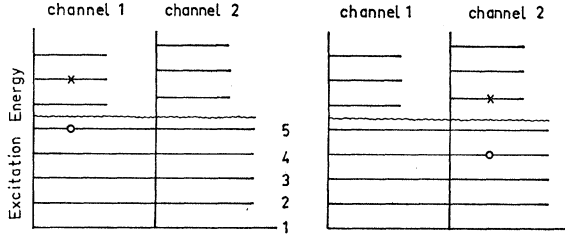


FIG. 8. The left figure shows the particle and the hole representing the ground-state transition in the asymptotic wave function. The right picture shows the same for the excited-state transition. Each picture has two sets of unbound levels corresponding to the two different natural boundary conditions of the two channels. The bound levels do not depend on the boundary condition.

We now proceed to the case where the energy allows transitions into both the ground state and the first excited state of the  $A-1$  system, i.e., to  $E_2$  of Fig. 7. It now may happen that particles with the same angular momentum can be emitted in both channels. This case must be discussed in detail. We again consider the case of two channels only, i.e., we assume that only one and the same angular momentum is involved in both transitions. The asymptotic form of the wave function then is again (91). It is schematically depicted in Fig. 8.

Now we have to construct a complete set of linearly independent states for the purpose of diagonalization of the Hamiltonian. A state of such a set is given by the expression

$$\psi = a_1 \omega_1 u_1^{(1)} + \sum_{\lambda'} a_{\lambda'} \omega_{\lambda'} u_{\nu}^{(1)} + a_2 \omega_2 u_2^{(2)} + \sum_{\lambda''} b_{\lambda''} \omega_{\lambda''} u_{\nu}^{(2)}. \quad (93)$$

This state is constructed as follows. First one adds all product terms containing the excited states of the  $A-1$  system  $\omega_{\lambda}^{(1)}$ , and the particle states  $u_{\nu}^{(1)}$ , both computed with the boundary condition of channel 1. The term with  $\lambda = \nu = 1$  is left out since it appears already explicitly in the asymptotic form. In constructing the sum one leaves out all superfluous states as discussed in the single-channel case. This is indicated by the prime at the summation sign. Now one turns to channel 2. First we consider those states  $\omega_{\lambda}$  which belong to the bound spectrum of the  $A$  system. Since they are independent of the boundary condition, and since both the sets  $u_{\nu}^{(1)}$  and  $u_{\nu}^{(2)}$  form a complete set of states we leave out all terms in the sum which contain a function  $\omega_{\lambda}$  which has already appeared in the first sum. This will eliminate most of the states; in particular all unbound states will be eliminated this way. The double prime at the summation symbol indicates the selection procedure. The remaining states thus form a complete orthonormal set which can be easily antisymmetrized.

Now the diagonalization and iteration procedure can be carried out.

To obtain the needed radial functions one just projects from (92) with  $\omega_n$  or, with the appropriate  $\psi_c$ , Eq. (49), which may be obtained from (30) by dropping the factor  $(\varphi_{\alpha}/r_{\alpha})$ . This then completes the detailed description of the method.

## IX. RESUME

In this paper we have described a method for the computation of resonant states which is both conceptually transparent and, we believe, easily applicable in practice. Being interested in collective states we have specialized our treatment to the particle-hole language. We have derived the necessary formulas and we have discussed in detail the difficulties which one will encounter in applying the method. The method is applicable in the energy region below the two-particle emission threshold. One may exceed that limit in certain cases, i.e., where the two-body decay is unimportant, or where the two-body decay goes mainly through two consecutive one-body decays, the intermediate state being well represented by a resonant state. In our treatment the total wave function is antisymmetric. We have not attempted to treat the nonresonating states, the center-of-mass motion, and the genuine three-body decays.

## APPENDIX

We prove here for completeness the uniform convergence at the boundary of the expansion of the wave function into the set of inside wave functions. We have

$$\Psi = \sum_{\lambda} a_{\lambda} \varphi_{\lambda}, \quad (A1)$$

where the  $\varphi_{\lambda}$  obey the boundary condition

$$\left[ r \frac{d\varphi_{\lambda}}{dr} \right]_{r=a} = b [\varphi_{\lambda}]_{r=a}, \quad (A2)$$

with constant  $b$ , and  $\Psi$  obeys the same boundary condition. Multiplying both sides of (A1) by  $b/a$  we obtain:

$$(b/a)\Psi = (b/a) \sum_{\lambda} a_{\lambda} \varphi_{\lambda} = \sum_{\lambda} a_{\lambda} (b/a) \varphi_{\lambda} = \sum_{\lambda} a_{\lambda} [d\varphi_{\lambda}/dr]_{r=a}. \quad (A3)$$

Multiplication by a constant and summation can always be exchanged. Since the left-hand side of (A3) equals  $[d\Psi/dr]_{r=a}$  one sees that in this case a formal differentiation inside the sum leads to a correct result in that the series of derivatives converges if the series of the functions converges.