

Scattering Resonances and the R Function*

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The relationship between scattering resonances and R -function states is explored by investigation of the separate properties of the "hard-sphere" and " R -function" portions of the phase shift. The R -function states are found to be good models for bound states and for some resonances below potential barriers, but they have no direct relation to scattering resonances above barriers. An R -function proof and explication are given for Levinson's theorem, according to which the number of scattering resonances is in general finite and small even though the spectrum of R -function states is infinite. Implications of the lack of high-energy resonances for the many-body problem are mentioned.

The purpose of this paper is to discuss the relationship between R -matrix states and scattering resonances in single-channel potential scattering and to note the implications of these results for the case of many channels.

The fact that R -matrix states do not bear a one-to-one relation to the scattering resonances was brought out very early by Wigner and Eisenbud's demonstration¹ that an infinite spectrum of discrete R -matrix states could be constructed which corresponds to no scattering at all and, hence, to no resonances. Nevertheless, in most R -matrix calculations, the number of resonances calculated equals the number of R -matrix states included in the calculation and, indeed, the infinite discrete spectrum of R -matrix states has often served as a model for resonance spectra. For example, the resonance density² up to quite high energies in the compound system has commonly been calculated as if resonances resulted from the distribution of nucleons among the states of an infinite discrete spectrum of single-particle states such as R -matrix states. Other properties, such as resonance widths, are frequently estimated by arguments which consider the compound-nucleus resonances as bound R -matrix-like states whose decays are treated by perturbation theory.

In addition, the R -matrix theory provides a powerful tool for resonance reaction calculations employing shell-model wave functions for the construction of R -matrix states.³ In principle, such an R -matrix shell-model spectrum can be arbitrarily large. In practice, the number of R -matrix states used is limited according to the nature of the phenomena under investigation and the size of the computational problem that can be handled. However, the number of resonances computed is usually equal to the number of R -matrix states included in the calculation.

Other recent calculations of resonance reactions⁴ employ only the finite spectrum of single-particle states in a finite shell-model potential well to construct a strictly finite number of compound-nucleus resonances. Since such theories work with incomplete sets of basis states (only one nucleon at a time can be in the continuum) it is of interest to discover, using the complete R -matrix theory, whether the actual number of resonances is finite or whether resonance densities continue to increase at high energies.

In the single-channel case it is well known that for a finite well-behaved single-particle potential of finite range each scattering phase shift approaches a constant value at high energies. This implies the absence of resonances at sufficiently high energies. Let us see how this lack of resonances arises from the infinite sequence of R -function states.

We consider scattering by a potential $V(r)$ that is zero beyond a certain radius r_0 . In R -matrix theory the phase shift δ for any partial wave is the sum of a "hard-sphere phase shift" δ_H and an " R -function phase shift" δ_R :

$$\delta = \delta_H + \delta_R, \quad (1)$$

where δ_R is given in terms of the R function R , the penetrability P , and the shift function S by

$$\delta_R = \tan^{-1}[PR/(1-SR)]. \quad (2)$$

This separation of the phase shift is accomplished by separating coordinate space into an "interior" with $r \leq a$ and an "exterior" with $r > a$ at a channel radius a which can be freely chosen so long as $a \geq r_0$. All the quantities defined depend on angular momentum and energy. Most of them also depend on the choice of a and on the choice of a real boundary-condition value B . For example $(S+B+iP)$ is given by the logarithmic derivative of an outgoing

wave evaluated at $r=a$, and $e^{2i\delta_H}$ is given by the ratio of the value of an incoming to that of an outgoing wave at $r=a$. The R function itself is defined by saying that $R^{-1}+B$ equals the logarithmic derivative of the radial part of the actual scattering wave function at $r=a$.

These relationships are such that S and R depend on the choice of both a and B , while P , δ_R , and δ_H depend only upon a . The dynamical details of the potential enter only through the R function R .

The R function so defined is an increasing function of E with an infinite sequence of poles at the energies $E=E_n$, where the logarithmic derivative of the scattering wave function at $r=a$ equals B . These energies E_n comprise a complete spectrum of solutions of the Schrödinger equation in the "interior" subject to the boundary condition B on the logarithmic derivative of the radial wave function at $r=a$. The states associated with that discrete spectrum are the R -function states.

Associated with the spectrum E_n is an infinite discrete spectrum \bar{E}_n of "R-function resonances" at the poles of $PR/(1-SR)$, where δ_R passes through $(n-\frac{1}{2})\pi$ for every positive integer n . Since S is a finite continuous function of the energy, the values of \bar{E}_n alternate with those of E_n . We want to compare this spectrum \bar{E}_n with the spectrum \mathcal{E}_n of bound states of the potential V and its scattering resonances which are defined as occurring whenever δ passes through $(n-\frac{1}{2})\pi$ for every positive integer n .

We consider first the case of s-wave scattering of an uncharged particle of mass M by a spherically symmetric potential V . In that case $S=-B$, and we may choose $B=S=0$, so that $\bar{E}_n=E_n$ corresponds to a pole of PR . We also have for s waves

$$P = -\delta_H = ka, \quad (3)$$

where $k=(2ME/\hbar^2)^{1/2}$ is the wave number of the particle.

We first note that for zero potential, $V=0$, there is no scattering and $\delta^{(V=0)}=0$. Hence from Eqs. (1) and (3)

$$\delta_R^{(V=0)} = -\delta_H = ka \quad (4)$$

and from Eq. (2)

$$R^{(V=0)} = (ka)^{-1} \tan(ka). \quad (5)$$

Consequently the R -function spectrum for zero potential is given by¹

$$E_n^{(V=0)} = (n-\frac{1}{2})^2 (\pi\hbar)^2 / 2Ma^2 = E_n^H. \quad (6)$$

This is identical to the spectrum E_n^H of the hard-sphere resonances where δ_H passes through $(n-\frac{1}{2})\pi$. The only difference between $\delta_R^{(V=0)}$ and δ_H is that the former ascends through $(n-\frac{1}{2})\pi$ at $E=E_n^H=E_n^{(V=0)}$, while the latter descends. The consequent cancel-

lation of δ_R and δ_H leads to no resonances in δ and indeed to no scattering, as required.

We can now extend this result to the case of high-energy scattering with finite V by applying first-order perturbation theory to the eigenstates of the zero-potential R function

$$\begin{aligned} E_n &= E_n^{(V=0)} + \Delta_n, \\ \Delta_n &= \frac{2}{a} \int_0^a dr V(r) \sin^2(k_n^H r) \\ &\rightarrow \frac{1}{a} \int_0^a dr V(r), \quad \text{as } n \rightarrow \infty, \end{aligned} \quad (7)$$

where k_n^H is the wave number at $E=E_n^{(V=0)}=E_n^H$.

Adopting the convention that at $E=0$, $\delta = \delta_R = \delta_H = 0$, we find that

$$\delta_R(E=E_n) = (n-\frac{1}{2}-N)\pi, \quad (8)$$

where N is the number of negative-energy R -function states of the potential V . On the other hand, from Eqs. (3) and (7) we have that to first order in Δ_n/E_n^H

$$\delta_H(E=E_n) = -(n-\frac{1}{2})\pi - (Ma/k_n^R \hbar^2) \Delta_n, \quad (9)$$

and hence

$$\begin{aligned} \delta(E=E_n) &= -(Ma/k_n^R \hbar^2) \Delta_n - N\pi \\ &\rightarrow -\frac{M}{k_n^R \hbar^2} \int_0^a dr V(r) - N\pi, \end{aligned} \quad (10)$$

which will be recognized as the first Born approximation for wave number $k_n^R = k(E=E_n)$. Assuming that the Born approximation is valid not only at $E=E_n$ but at all sufficiently high energies, we see that δ approaches the value $-N\pi$, and does not contain any high-energy resonances. The reason for this is seen in the fact that at high energies the R -function resonances are "cancelled" by the hard-sphere resonances. Except for the weakly energy-dependent Born term, δ_H decreases at the same rate as δ_R increases. Thus while both δ_R and δ_H continue to pass through $(n-\frac{1}{2})\pi$ at high energies, their sum does not. Moreover, even though in the high-energy limit both δ_H and δ_R depend strongly on the choice of channel radius a , their sum δ does not, provided that $V=0$ for $r>a$.

The result of Eq. (10) is equivalent to Levinson's theorem, which states that between zero and infinite energy the phase shift must descend through $N\pi$, where the number N of negative-energy R -function states equals the number of bound states of the potential V . This is so because on the one hand an R -function state with zero derivative at $r=a$ must have a lower energy than the corresponding bound state. On the other hand, if a zero-boundary-condition R -function state falls at zero energy its wave function is identical to the corre-

sponding “zero-energy” bound state. Consequently, the bound-state spectrum lies above the negative-energy R -function spectrum, but the difference goes to zero at zero energy.

An easy way to illustrate the behavior of δ , δ_H , and δ_R is to consider a square well of depth $-V$ and radius a , equal to the R -function channel radius. The R function follows directly from Eqs. (3) and (5) and the fact that R depends only on the boundary condition and the Hamiltonian in the interior:

$$R = (k'a)^{-1} \tan k'a, \tag{11}$$

where

$$k' = [2M(E + V)/\hbar^2]^{1/2},$$

and therefore

$$\tan \delta_H = -\tan(ka) \tag{12}$$

and

$$\tan \delta_R = (k/k') \tan(k'a). \tag{13}$$

For large values of k , Eq. (13) yields

$$\delta_R \cong -N\pi + k'a + d, \tag{14}$$

where

$$|d| \leq (1/2ka) |ka - k'a|. \tag{15}$$

For $2ka \gg 1$, the R -function phase shift becomes

$$\begin{aligned} \delta^R &\cong -N\pi + k'a \\ &\cong -N\pi + ka + MVa/\hbar k, \end{aligned} \tag{16}$$

whose second line is again the Born phase shift. The values of δ_R , $-\delta_H$, and δ are plotted for all energies in Fig. 1 for the case of a square-well potential of depth $V = 3.15\pi^2\hbar^2/2Ma^2$. The curves labeled $\delta_R(a)$ and $\delta_H(a)$ are computed according to Eqs. (12) and (13). For large values of k , δ_R approaches a line parallel to $-\delta_H = ak$ and a distance 2π below ak . As a result, δ approaches -2π for large k when its zero-energy value is chosen to be zero. This limit is in accordance with Levinson's theorem because the above potential has just two bound states at the energies indicated in Fig. 1:

$$\begin{aligned} \mathcal{E}_1 &= -2.43 \hbar^2/2Ma^2 \\ \mathcal{E}_2 &= -0.50 \hbar^2/2Ma^2 \end{aligned} \quad \text{bound states.}$$

Since the value of δ has a range of 2π and δ is a monotone function of k , there are just two resonances, as indicated by the heavy arrows at the energies where δ passes through $-\pi/2$ and $-3\pi/2$:

$$\begin{aligned} \mathcal{E}_3 &= +0.22 \hbar^2/2Ma^2 \\ \mathcal{E}_4 &= +7.80 \hbar^2/2Ma^2 \end{aligned} \quad \text{resonances.}$$

Corresponding to these two poles of the collision function there are two peaks in the cross section as shown in the top part of Fig. 1. Resonances of this type have been called “echoes” by McVoy because δ descends rather than ascends where they occur.⁵ We note that the “width” of the resonance depends only upon the slope with which δ passes through $(n - \frac{1}{2})\pi$ and not on whether δ is ascending or descending. Thus in this case, δ passes steeply down through $-\pi/2$ producing a fairly narrow “echo” resonance at $ak \approx 0.5$. On the other hand, δ descends at a shallow angle through $-3\pi/2$, resulting in a broad “echo” resonance at $ak = 2.8$.

In contrast to these two bound states and two resonances, there are infinitely many R -function states at the energies E_n^R indicated by light arrows in Fig. 1. Two of these states occur at the negative energies E_1^R and E_2^R corresponding to the two bound states \mathcal{E}_1 and \mathcal{E}_2 . On the other hand the infinite sequence E_n^H of hard-sphere resonances has only positive energies. Thus, while at zero ener-

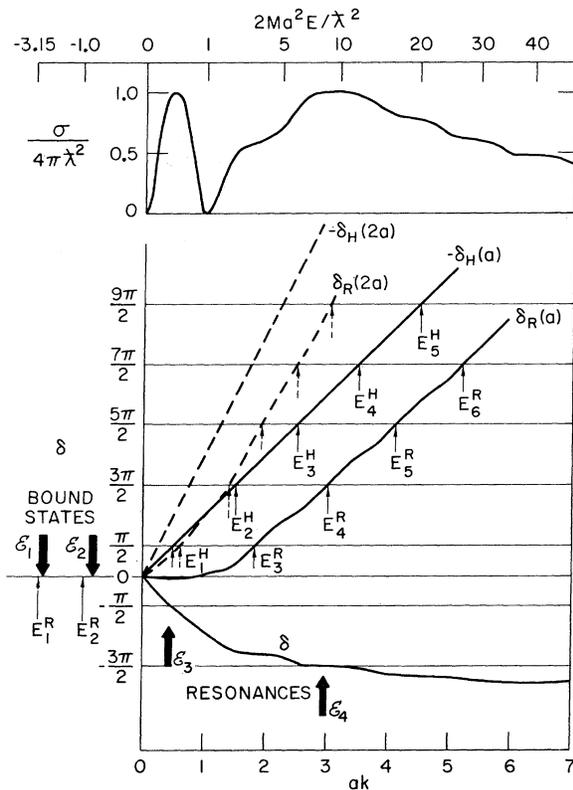


FIG. 1. Phase shift $\delta = \delta_R + \delta_H$ and cross section σ as a function of momentum k or energy E for an s -wave neutron of mass M scattered by a square-well potential of radius a and depth $V = 3.15\pi^2\hbar^2/Ma^2$. The bound states are at energies \mathcal{E}_1 and \mathcal{E}_2 , the scattering resonances at \mathcal{E}_3 and \mathcal{E}_4 . The R -function states for matching radius a have energies E_n^R and the hard sphere scattering resonances occur at E_n^H .

gy the E_n^H start out two levels behind the E_n^R , they must eventually catch up, because according to Eqs. (6) and (7) $E_n^H - E_n^R$ for large n . The resulting shift of 2π between δ_R and δ_H accounts for the two resonances \mathcal{E}_3 and \mathcal{E}_4 and for Levinson's theorem.

The equation for bound-state momenta in a square well is well known to be

$$R^{-1} = (k'a) \cot(k'a) = -|k|a, \quad (\text{bound state}). \quad (17a)$$

Using Eqs. (12) and (13) to calculate the poles of $\tan\delta$ as given by Eq. (1), we obtain a similar equation for the positive-energy resonances of a square-well potential

$$R^{-1} = (k'a) \cot(k'a) = -(ka) \tan(ka), \quad (\text{resonance}). \quad (17b)$$

The solutions of Eq. (17a) have been studied exhaustively by Nussenzveig⁶ to obtain the poles of the scattering function $e^{2i\delta}$. However, as we see, the high-energy poles do not lead to scattering resonances. Their effect on the scattering amplitude is largely cancelled by the influence of the hard-sphere factor's essential singularity at infinity. General expressions for the asymptotic distribution of poles have been given by Humblet and Regge.⁷

Note added in proof: It is important to distinguish between the "resonances" \mathcal{E}_n , which are the subject of this paper, and the poles of the scattering function which are discussed in Refs. 6, 7.

Changing only the boundary condition does not change either δ_R or δ_H and hence also does not change δ . Different boundary conditions change R and S so that $PR/(1 - SR)$ in Eq. (3) remains the same as PR for the zero boundary condition.

Changing the R -function matching radius does change both δ_R and δ_H , but in such a way that their sum δ is unaffected. This is illustrated by the curves $\delta_R(2a)$, $\delta_H(2a)$ in Fig. 1 which were computed for the same potential but with the matching radius at twice the potential radius a . Even though δ and therefore the cross section is the same as before, the new R -matrix states indicated by the dashed arrows at the bottom of Fig. 1 are more closely spaced than those of $\delta_R(a)$. At high energies these more densely spaced R -function states are compensated by a correspondingly denser set of hard-sphere resonances.

One interesting feature of the square-well phase shift and cross section in Fig. 1 is that they display structure that is correlated with the positions of the R -function states for a matching radius at the hard-sphere radius a . This structure does not correlate, however, with R -function states obtained with other matching radii, such as $2a$. This is due to the sharp edge of the square-well potential, which causes strong reflections of the scat-

tered wave at the same energies where total reflections at $r=a$ would produce the R -function states.

When the edges are not sharp, as in a diffuse Woods-Saxon potential, these size fluctuations disappear. For example, s -wave phases of δ_R , δ_H , and δ were obtained by numerical integration for the Woods-Saxon potential:

$$U(r) = V_0 \rho(r) + V_{so} \left(\frac{\hbar}{\mu c} \right)^2 \vec{I} \cdot \vec{s} \frac{1}{r} \frac{d\rho}{dr}, \quad (18a)$$

where

$$\rho(r) = (1 + e^{-(r-R)/a})^{-1} \quad (18b)$$

and

$$\begin{aligned} a &= 0.94 \text{ fm}, & R &= 3.58 \text{ fm}, \\ V_0 &= 42.4 \text{ MeV}, & \text{and } V_{so} &= 9.6 \text{ MeV}. \end{aligned} \quad (18c)$$

The values of the phases are shown in Fig. 2. Though no size fluctuations are evident, all other

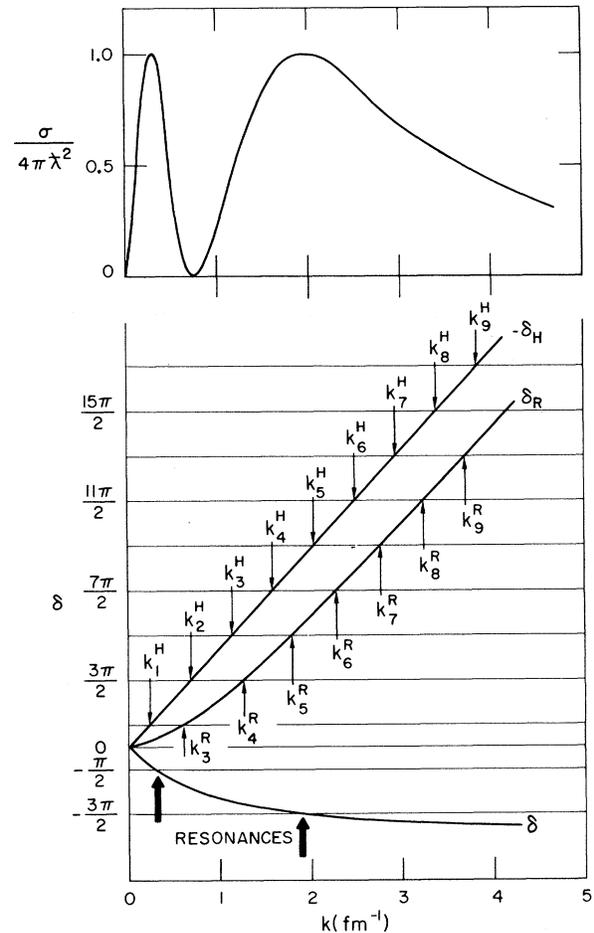


FIG. 2. Phase shifts $\delta = \delta_R + \delta_H$ and cross section σ for the scattering of s -wave neutrons by the Woods-Saxon potential of Eq. (18).

features discussed in connection with the square-well case remain the same.

Next we turn to the relation between R -function states and resonances in the presence of a potential barrier. As an example, the phase shift $\delta = \delta_R + \delta_H$ and cross sections for $d_{3/2}$ -wave neutron scattering by the Woods-Saxon potential (18) are shown in Fig. 3. There appears a sharp "resonance" where δ abruptly rises through $\pi/2$ and a wide resonance "echo" where δ slowly descends through $\pi/2$. The potential does not have a bound state of this particular partial wave, so that $\delta \rightarrow 0$ at large k , as seen in Fig. 3. The arrows indicate the positions of k_n^H and k_n^R for $a = 7$ fm.

In this case, where a potential barrier is present, the behavior of δ_R , δ_H , and δ differs from the s -wave-neutron case in two important ways. At low energies δ_H is very small because the repulsive centrifugal barrier keeps the neutrons away from the potential well. Therefore at low energies we have $\delta \approx \delta_R$. In our example the first R -matrix state lies in this low-energy region and therefore corresponds closely to the location of the first scattering resonance. Moreover, because of the centrifugal barrier, the d -wave penetrability P is also very small at the first resonance. It follows from Eq. (2) that δ_R rises through $\pi/2$ very steeply, almost like a step-function, rather than almost linearly with ka , as in the s -wave case. The same behavior is shared by δ , resulting in the very nar-

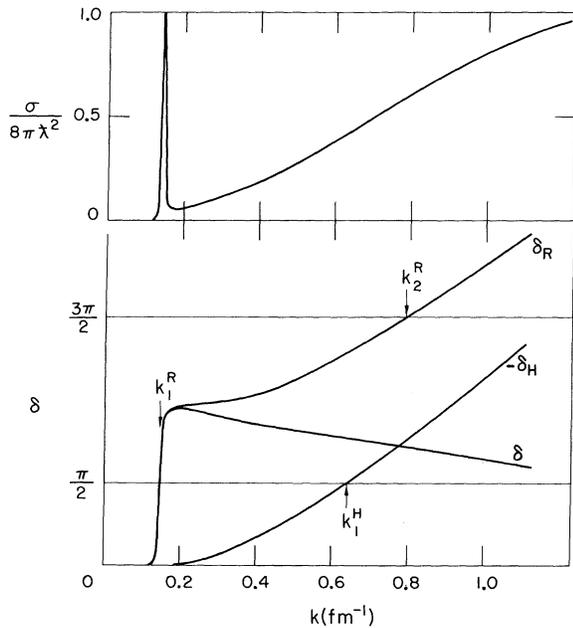


FIG. 3. Phase shifts $\delta = \delta_R + \delta_H$ and cross section σ for the scattering of $d_{3/2}$ -wave neutrons by the potential of Eq. (18).

row first resonance. Such narrow resonances below potential barriers are therefore closely associated with the corresponding R -function state and may be thought of as quasistationary states.

The close association of a sharp resonance below the barrier with an R -function state is quite insensitive to a change in boundary conditions or channel radius provided the channel radius is small enough so that at the resonance both δ_H and P remain small. In the case of the $d_{3/2}$ resonance shown in Fig. 3 the first R -function state remains close to the first resonance for channel radius up to 30 fm.

Above the centrifugal barrier the qualitative relationship between R -function states and resonances is again the same as for s -wave neutrons. In the example of Fig. 3, there is a second very broad (echo) resonance at $k = 1.5$ fm $^{-1}$, where δ descends through $\pi/2$ on its way to zero as required by Levinson's theorem. Again there is an infinite spectrum of R -function states, causing a steady rise in δ_R which is cancelled by an equal rise in $-\delta_H$.

We see that there are two kinds of R -function states which have direct physical meanings. By choice of a boundary value $B = -1$, the R -function states with negative energies are related one to one to the bound states of the potential. Furthermore, the wave function of such an R -function state is very similar to that of the corresponding bound state, as was pointed out by Mahaux and Weidenmüller.⁸ Such an R -function state is therefore a good representation of the bound state. Another type of R -function state is one associated with the sharp resonance below the peak of a potential barrier. Here again the wave function of the R -function state is very similar to the internal wave function at the sharp scattering resonance. The R -function state is therefore interpreted as the quasistationary state giving rise to the resonance.

Other resonances, particularly those occurring at higher energies are diffraction phenomena that are not associated with well-defined states in the interior and are therefore also not associated with particular R -function states. Such diffraction phenomena have been called echoes by McVoy,⁵ and they arise in R -function theory from the difference in the rates of increase of the R -function and hard-sphere phase shifts. These diffraction echoes are also limited, as we have seen, to the number specified by Levinson's theorem. Thus the infinite sequence of high-energy R -function states does not generate an infinite sequence of resonances. We may conclude therefore that also in the many-body case the number of resonances is effectively confined to those generated by single-particle bound

or quasibound states, and that therefore the resonance level density does not keep increasing exponentially at higher energies.⁹ Similarly, there is

therefore no reason to expect that cross-section fluctuations due to resonance terms in the S matrix continue to very high energies.

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R-Matrix Shell-Model Calculations of Scattering and Reaction Cross Sections*

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The Wigner-Eisenbud R -matrix theory is applied to the calculation of neutron total and inelastic scattering cross sections for a system consisting of two neutrons interacting with an inert ^{16}O core through a spherically symmetric Woods-Saxon potential and interacting with each other through a δ -function force. The calculational method employed has the advantages that it includes the effects of shell-model configurations in which both neutrons are unbound, that it presents no obstacles to inelastic or reaction calculations, that it permits antisymmetrization of the compound space wave functions, and that it requires only one shell-model diagonalization for the computation of cross sections up to 5-MeV neutron energy. Use of antisymmetrized wave functions is shown to reduce substantially the number of compound-nucleus resonances and to reduce the magnitude of the inelastic cross section. By the correct calculation of the distant resonance contribution to the R matrix, it is shown that the calculated cross sections are independent of the choice of channel radii. The application of the method to more complex systems with larger numbers of neutrons as well as protons and holes and also with direct coupling between channels is discussed. A selection rule encountered in the calculations suggests a possible J^π dependence of the absorptive part of the optical-model potential.

I. INTRODUCTION

The nuclear shell model is the basic theoretical tool for the description of atomic nuclei and has been used to calculate the properties of nuclear bound states. More recently, there has been considerable interest in the application of the shell model to the calculation of nuclear continuum states.¹ This paper deals with the analysis of the R -matrix method for the application of the shell model to nuclear cross-section calculations.

A bound-state shell-model calculation proceeds by the following five steps:

(1) A single-particle potential U is chosen. Most simply this is a spherically symmetric harmonic-oscillator plus spin-orbit potential.

(2) The single-nucleon spectrum of U is calculated by solving the single-particle Schrödinger equation

$$[K + U]\phi_{nljm} = E_{nlj}^{\text{SP}}\phi_{nljm}, \quad (1)$$

where K is the kinetic-energy operator, and ϕ_{nljm} is the single-nucleon state with principal quantum numbers n , orbital and total angular momentum quantum numbers l , j , and z -component m .² The energy of the single-particle state ϕ_{nljm} is denoted by E_{nlj}^{SP} . The ϕ_{nljm} are orthonormal.

(3) A set of N -nucleon independent-particle states or configurations $|pJM\rangle$ is formed as the antisymmetrized product of N single-particle states, cou-