

Stabilization Method of Calculating Resonance Energies: Model Problem*

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(Received 6 October 1969)

We have applied the stabilization method of calculating resonance energies to the elastic scattering from a one-dimensional model potential containing a barrier. For sufficiently large basis sets, the stabilization method yields good approximations to the inner part of the exact scattering wave functions at energies equal to the eigenvalues of the truncated matrix of the Hamiltonian in *both* the resonant and nonresonant energy regions. We have calculated good approximations to the exact phase shifts from the square-integrable wave functions produced by the stabilization method. We have derived a simple model to explain the behavior of the eigenvalues as a function of the size of the basis. The degree of stability of the eigenvalues approximating the resonance energy is proportional to the width of the resonance. Both the energy and the width of the resonance can be calculated from the change in the stable eigenvalue as the size of the basis increases.

I. INTRODUCTION

The resonant scattering of electrons from atoms and molecules has attracted considerable attention from both experimentalists and theoreticians. The recent literature has been critically reviewed by Burke¹ and by Taylor.² The resonant scattering process is well understood qualitatively, and elegant mathematical formulations have been developed independently by Feshbach³ and by Fano.⁴ Qualitatively, resonant scattering involves the formation of a metastable, quasiscrete state, which, because of its nonstationary character, decays after a short time into one of the open channels. The scattering cross section is a rapidly varying function of the incident energy in the resonant region and can be characterized by the Breit-Wigner expression containing two parameters: the resonance energy E_r and the width Γ . The resonance energy can be interpreted as the energy of the metastable state, whereas the width is related to its lifetime through the uncertainty relationship $\tau = \hbar/\Gamma$. From the practical point of view, one needs to know only the energy and the width of a resonance to calculate, from the Breit-Wigner expression, its contribution to the cross section.

In recent years, a number of methods have been proposed to calculate the energies and widths of resonances. In the close-coupling approximation¹ used by Burke and co-workers, the scattering wave function is expanded in a truncated set of product functions. Each of the product functions consists of the wave function of a target state mul-

tiplied by a function representing the scattered electron. The latter function is a continuum function satisfying the appropriate boundary conditions in the asymptotic region for an open channel. The phase shifts, as a function of energy, are extracted from the approximate open-channel functions, and then fitted to a Breit-Wigner formula to yield indirectly the energy and the width of the resonance.

In the truncated orthogonalization procedure of Holøien and Midtdal,⁵ the truncated diagonalization method of Lipsky and Russek,⁶ and the stabilization method of Eliezer *et al.*,⁷ one takes a conceptually different approach in that one attempts to calculate the energy of a resonance directly. These methods, which are closely related but differ in their emphasis, are based on the fact that the inner part of the scattering function, at an energy in the resonant region, very much looks like the wave function of a bound state. The amplitude of the scattering wavefunction in the asymptotic region is much smaller (depending on the magnitude of Γ) than the amplitude of its inner part. In these methods, therefore, the wave function is expanded in a set of discrete exponentially decaying functions, and then the Hamiltonian is diagonalized to yield the approximate resonance energies directly. The width of the resonances cannot be directly extracted from such bound approximations to the scattering functions. However, Miller⁸ has suggested that the width be calculated as an off-diagonal matrix element of H between the bound-function and a zeroth-order continuum function at the resonance energy.

Recently, Perkins⁹ introduced a variational bound method to calculate the energies of autoionizing states in two-electron systems. He showed that in Holóien's procedure appropriately chosen roots are true upper bounds to the eigenvalues of QHQ introduced by Feshbach.²

Although the stabilization method has produced accurate resonance energies for real systems such as $e^- + H_2$,⁷ a number of fundamental questions remain unanswered. For example, what is the basic reason for stability, i. e., why do certain eigenvalues of the truncated Hamiltonian matrix remain essentially unchanged as the size of the basis set varies? One intuitively feels that with the proper choice of basis set one is expanding the bound-state-like inner part of the scattering function ($Q\psi$ in the language of the projection operator formalism),³ and, of course, the expansion of the wave function of a bound state in terms of square-integrable basis functions converges. But, one would still like to know whether the stable eigenvalues will eventually diverge as the size of the basis set further increases; after all, the expansion of a continuum function in terms of square-integrable functions certainly diverges. In other words, what difficulties, if any, arise from the use of incorrect boundary conditions? In a similar problem, the Stark effect,¹⁰ it is well known that the perturbation expansion for the energy of the metastable (autoionizing or resonant) level embedded in the continuum is only an asymptotic series and eventually diverges even for small field strengths. Unfortunately, this conclusion cannot be directly applied to a scattering problem because in the Stark effect the potential goes to $-\infty$ instead of zero at large distances from the origin. One would like to know also the significance, if any, of the nonstable eigenvalues and the corresponding eigenfunctions. Can these functions be approximations to scattering functions representing potential scattering at energies far from the resonance energy? Finally, are there convenient ways of extracting the width from the square-integrable approximations to the scattering functions in order to complete the description of resonances?

In order to attempt to answer some of these questions, we have studied the elastic scattering exhibiting resonance phenomenon from a simple one-dimensional model potential. We have compared the exact scattering solutions to those obtained by the stabilization method. In addition, we have carefully analyzed the behavior of the eigenvalues of the truncated Hamiltonian matrix as a function of the size of the basis set. Our results show that with adequate basis sets the stabilization method yields good approximations, apart from a normalization constant, to the exact scattering wave functions at energies in the resonant *as well as* the nonresonant regions. We have calculated good approximations

to the exact phase shifts, including both the resonant and potential scattering contributions, from square-integrable wave functions through the use of an amplitude independent integral formula. This result, of course, implies that one can obtain both the energy and the *width* of resonances from square-integrable wave functions. The eigenvalues obtained in the stabilization method clearly demonstrate stability at energies near the resonance energy. We have developed a simple model to study the criteria that determine the eigenvalues for any expansion length and to demonstrate that the degree of stability is related to the width of the resonance and the region of space spanned by the basis set.

In Sec. II, we briefly describe the model potential and the procedure of the stabilization method. In Sec. III, we present the results of our numerical calculations including the approximate phase shifts extracted from square-integrable approximations to the scattering functions. Finally, in Sec. IV, we analyze the stabilization method in terms of a simple model.

II. MODEL POTENTIAL AND METHODS OF SOLUTION

We have chosen to study a one-dimensional potential with a barrier, which is continuous in the range $-\infty \leq x \leq \infty$, and which immediately suggests a natural basis of square-integrable functions to be used in the stabilization method. The model potential is given by

$$V(x) = \frac{1}{2} x^2, \quad x \leq 0 \quad (1a)$$

$$V(x) = \frac{1}{2} x^2 e^{-\lambda x^2}, \quad x \geq 0 \quad (1b)$$

with $\lambda > 0$. Both $V(x)$ and its first derivative are continuous at $x = 0$. The potential, which is shown in Fig. 1 for $\lambda = 0.225$, has the desirable feature that $V(x) \rightarrow 0$ as $x \rightarrow \infty$. Since, as $\lambda \rightarrow 0$, $V(x)$ approaches the harmonic oscillator potential, we have chosen the eigenfunctions of the harmonic oscillator

$$\psi_n(x) = (2^n n! \pi^{1/2})^{-1/2} H_n(x) \exp(-\frac{1}{2} x^2), \quad n = 0, 1, \dots \quad (2)$$

as our basis functions. In Eq. (2), $H_n(x)$ denotes the n th Hermite polynomial. The parameter λ determines the width and the height of the potential barrier ($V_{\max} \approx 1/5.4 \lambda$). Increasing λ decreases the size of the barrier and therefore increases the width of the resonances. Of course, for $\lambda = 0$, $V(x)$ has an infinite barrier and only bound states (with zero width) exist. We have studied both narrow and broad resonances by varying λ between 0.1 and 0.26.

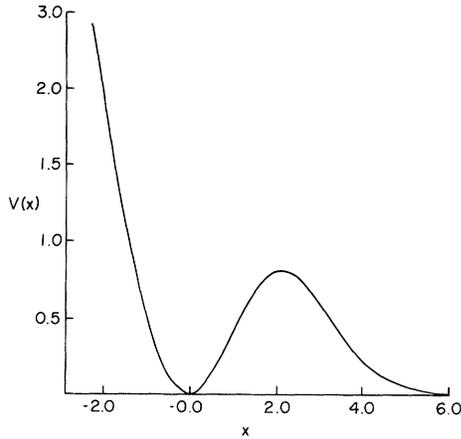


FIG. 1. Model potential $V(x)$ for $\lambda=0.255$ [see Eq. (1)].

The scattering problem is defined by the differential equation

$$\frac{d^2\Psi_E(x)}{dx^2} + [k^2 - 2V(x)]\Psi_E(x) = 0, \quad (3)$$

and the boundary conditions on $\Psi_E(x)$. The potential $V(x)$ is given in Eq. (1), and the energy E is equal to $\frac{1}{2}k^2$. In order to obtain the exact scattering wave function as a function of E , we have numerically integrated Eq. (3) subject to the boundary conditions:

$$\Psi_E(x) \rightarrow 0, \quad x \rightarrow -\infty, \quad (4a)$$

$$\text{and } \Psi_E(x) \rightarrow \sin(kx + \eta), \quad x \rightarrow \infty, \quad (4b)$$

where the phase shift η is a function of E . For a scattering process in which only isolated resonances occur, the phase shift, at energies near a resonance energy, is assumed to have the form

$$\eta(E) = \eta_{\text{pot}}(E) + \tan^{-1}\left(\frac{\Gamma/2}{E - E_\gamma}\right), \quad (5)$$

where E_γ and Γ are the energy and the width of the resonance, respectively. The contribution of the potential scattering to the phase shift $\eta_{\text{pot}}(E)$ is assumed to be a slowly varying function of E near E_γ , and is usually fitted to a polynomial in E . Once we have calculated the exact $\eta(E)$ from the numerical solutions to Eq. (3), we fitted $\eta(E)$ to the form given in Eq. (5) to obtain the exact resonance parameters E_γ and Γ , as well as $\eta_{\text{pot}}(E)$.

The procedure used in the stabilization method has been discussed in detail elsewhere.² Here, we discuss only those features, which are essen-

tial for the present analysis. For a given $V(x)$, we compute the matrix of the exact Hamiltonian $H(x)$ in a finite basis set consisting of the first N functions given in Eq. (2). For a given N , the matrix elements of H^N are given by

$$H_{nm}^N = \langle \psi_n(x), H(x)\psi_m(x) \rangle, \quad (6a)$$

with

$$\delta_{nm} = \langle \psi_n(x), \psi_m(x) \rangle, \quad n, m = 1, \dots, N. \quad (6b)$$

In the present work we have used up to 50 functions. We diagonalize the matrix H^N to yield a set of N eigenenergies ϵ_i^N , and the corresponding eigenfunctions $\Phi_i^N(x)$:

$$\epsilon_i^N \delta_{ij} = \langle \Phi_i^N(x), H(x)\Phi_j^N(x) \rangle. \quad (7)$$

The eigenfunctions are linear combinations of the first N functions in Eq. (2):

$$\Phi_i^N(x) = \sum_{n=1}^N C_{in} \psi_n(x), \quad \text{each } i. \quad (8)$$

Like the basis functions $\psi_n(x)$, the eigenfunctions are square integrable and can be normalized such that

$$\delta_{ij} = \langle \Phi_i^N(x), \Phi_j^N(x) \rangle. \quad (9)$$

We repeat the procedure for increasing values of N , changing N by unity if necessary, and carefully observing the behavior of ϵ_i^N and $\Phi_i^N(x)$ as a function of N .

III. RESULTS

In Sec. IIIA, we discuss the qualitative features of the numerical results and give a precise interpretation to the eigenvalues and eigenfunctions produced in the stabilization method. In Sec. IIIB, we present a simple method for the calculation of scattering information (e.g., the phase shift) from the square-integrable eigenfunctions.

A. Interpretation of the Eigenfunctions

For a given expansion length N the stabilization method yields a set of N eigenvalues and the corresponding eigenfunctions [see Eqs. (7)–(9)]. In the case of a Hamiltonian containing a potential with a barrier, such as our model potential, we find that certain of the eigenenergies change very little compared to the other eigenvalues as N changes over a relatively large range, e.g., $\Delta N \sim 20$. Furthermore, the “stable” eigenenergy is very close to the exact resonance energy E_γ . Table I illus-

TABLE I. "Stable" eigenenergy and the expansion coefficients as a function of N . $\lambda = 0.19$, $E_\gamma = 0.453536$, $\Gamma = 0.002805$.

N	j	ϵ_j^N	C_{jn}^N						
			$n: 1$	2	3	10	15	20	30
15	1	0.452846	0.9827	0.1046	0.0845	0.0280	0.0063
20	1	0.449656	0.9527	0.1112	0.0945	0.0776	0.0575	0.0132	...
25	2	0.456984	0.9738	0.0906	0.0670	-0.0383	-0.0611	-0.0444	...
30	2	0.454416	0.9845	0.0998	0.0782	0.0026	-0.0201	-0.0257	-0.0040
35	2	0.453508	0.9830	0.1026	0.0818	0.0172	-0.0052	-0.0186	-0.0133
40	2	0.452659	0.9784	0.1048	0.0849	0.0309	0.0088	-0.0119	-0.0221
45	2	0.451045	0.9597	0.1078	0.0897	0.0560	0.0350	0.0010	-0.0382

trates the behavior of a "stable" eigenenergy ϵ_j^N for $\lambda = 0.19$. At this point, we must emphasize that the "stable" eigenenergy is not necessarily the lowest eigenvalue of the matrix H^N . Indeed, at certain values of N , the "stable" eigenenergy becomes the next higher eigenvalue, that is, as N increases, a "nonstable" eigenvalue sometimes passes by the "stable" eigenenergy from above. This feature, which is indicated by the increase of j from 1 to 2 in Table I, and its significance will be discussed in detail in Sec. IV. The behavior of the eigenfunction Φ_j^N as a function of N is described by the expansion coefficients C_{jn}^N . Table I shows some of the C_{jn}^N belonging to the "stable" eigenenergy. An inspection of Table I shows, as expected, that the eigenfunction Φ_j^N corresponding to a "stable" eigenenergy also changes relatively little with N .

The behavior of the "stable" eigenenergies, as a function of N , is similar to the behavior of the approximate eigenvalues in the truncated diagonalization of a Hamiltonian with true bound states. In the case of such a Hamiltonian, as the expansion length increases, the j th approximate eigenvalue converges to the j th eigenvalue of the Hamiltonian from above. This convergence is a consequence of the Hylleraas-Undheim theorem.¹¹ The apparent convergence of the "stable" eigenenergy to a value near the exact resonance energy E_γ suggests that the "stable" eigenenergy and the corresponding eigenfunction are associated in some way with the resonant state. A qualitative inspection of the eigenfunctions produced by the diagonalization procedure supports this suggestion. Table I shows that the Φ_j^N associated with the "stable" eigenenergy ϵ_j^N has significant contributions from only the basis functions with small n , i. e., only those basis functions that have large amplitudes inside the potential barrier near $x=0$. As a result, Φ_j^N itself has a large amplitude inside the barrier, a behavior also exhibited by the exact scattering wave function at energies near E_γ . In contrast, the eigenfunctions associated with the other eigenvalues have significant contributions from basis

functions that have large amplitudes outside the potential barrier. Therefore, the Φ_j^N corresponding to "nonstable" eigenvalues apparently are not associated with the resonant state.

The behavior of the "stable" eigenenergies and eigenfunctions as a function of λ provides additional qualitative evidence. We already noted that as λ increases the size of the potential barrier decreases, and the resonance becomes broader and broader. We find that for larger λ the "stable" eigenenergy changes more significantly as the expansion length increases, i. e., it becomes less "stable." Also, the basis functions with large n and large amplitude outside the barrier contribute more and more to the expansion of Φ_j^N associated with the "stable" eigenenergy. Accordingly, as λ increases, the amplitude of Φ_j^N outside the barrier increases relative to the amplitude near $x=0$. The resonant scattering wave function again exhibits a similar behavior. It is well known that as the width of a resonance increases (λ increases) the ratio of outer to inner amplitudes of the exact wave function near E_γ increases indicating a greater probability of decay through the barrier. All of these qualitative arguments indicate that the "stable" eigenenergy ϵ_j^N and the corresponding square-integrable eigenfunction Φ_j^N are associated with the metastable resonant state.

In order to give a more precise interpretation of ϵ_j^N and Φ_j^N , we made a detailed study of the wave functions produced by the diagonalization procedure. We evaluated the Φ_j^N as a function of x and compared them with the exact scattering wave functions at various energies.

First, we compare the eigenfunction belonging to a "stable" ϵ_j^N with the exact scattering function Ψ_E at $E = E_\gamma$ and at $E = \epsilon_j^N$. The difference between Ψ_{E_γ} and Ψ_ϵ depends on the difference $\Delta E = E_\gamma - \epsilon_j^N$, which is clearly a function of both N and λ . It is important to realize that Ψ_{E_γ} and Ψ_ϵ can differ significantly even for a relatively small ΔE , because the phase shift is a rapidly varying function of E near E_γ [see Eq. (5) and the discussion of Fig. 2]. Figure 2 compares the Φ_j^N associated

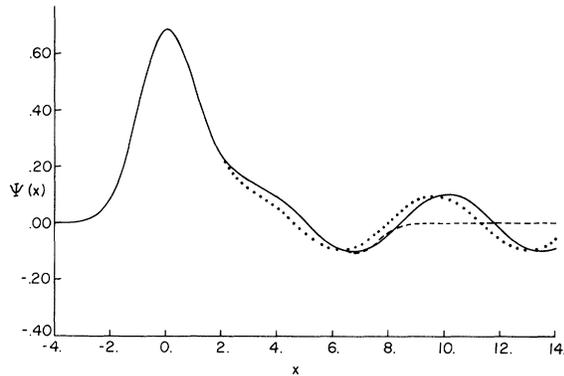


FIG. 2. Comparison of the exact and approximate wave functions in the resonant region for $\lambda=0.255$. (dashed line) Φ_j^N with $N=35$, $j=2$, and $\epsilon_j^N=0.439463$; (dotted line) Ψ_E for $E=E_\gamma=0.441333$; (solid line) Ψ_E for $E=\epsilon_j^N$.

with a “stable” eigenenergy to the exact scattering wave functions for $\lambda=0.225$. Each scattering wave function is arbitrarily normalized so that its amplitude corresponds to the amplitude of Φ_j^N at the first maximum or minimum. The selected ϵ_j^N for $N=35$ differs from the exact E_γ by 0.00187 a. u. As a result, the phase shifts of Ψ_{E_γ} and Ψ_ϵ differ by 0.39. Figure 2 clearly shows that, apart from the arbitrary normalization factor, the Φ_j^N associated with the “stable” ϵ_j^N accurately reproduces Ψ_ϵ out to $x=9$. At that point Φ_j^N quickly drops to zero, as it must, because it is a linear combination of exponentially decaying basis functions [see Eq. (8)]. The eigenfunction Φ_j^N differs significantly from Ψ_{E_γ} , however, even for $x<9$. Our results conclusively show that for the range of λ considered and for reasonable expansion lengths ($N\geq 20$) the square-integrable eigenfunction Φ_j^N associated with a “stable” eigenenergy ϵ_j^N is a good approximation, apart from a normalization factor, to the inner part of the exact scattering wave function at $E=\epsilon_j^N$. For small λ , where ϵ_j^N is very close to the exact resonance energy E_γ , Φ_j^N also approximates the inner part of the exact wave function at $E=E_\gamma$. Furthermore, when the basis set is large enough so that it spans the range of x beyond the range of $V(x)$, the square-integrable function Φ_j^N properly describes even the asymptotic part of the scattering wave function at $E=\epsilon_j^N$. Of course, for any expansion length, there is a value of x at which Φ_j^N quickly decays to zero, and therefore Φ_j^N is never a true scattering wave function. Figure 3 compares Φ_j^N to Ψ_ϵ for $\lambda=0.225$ and $N=50$, the largest expansion length used in the present work. In the range of $7<x\leq 10$, the exact wave function Ψ_ϵ almost completely settled down to its asymptotic form but it is still closely approximated by Φ_j^N .

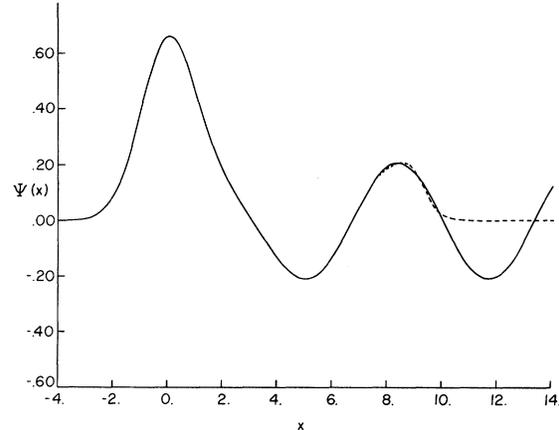


FIG. 3. Comparison of the exact and approximate wave functions in the resonant region for $\lambda=0.225$. (dashed line) Φ_j^N with $N=50$, $j=3$, and $\epsilon_j^N=0.450892$; (solid line) Ψ_E for $E=\epsilon_j$.

At $x\approx 10$, however, $\Phi_j^N(x)$ rapidly decreases to zero.

Encouraged by the results obtained for the “stable” eigenvalues, we next compare the Φ_i^N belonging to “nonstable” eigenvalues ϵ_i^N (which are far from the resonance energy E_γ) with the exact scattering functions at $E=\epsilon_i^N$. Figure 4 shows representative results for $\lambda=0.225$. Again, the scattering wave function is arbitrarily normalized so that its amplitude agrees with that of the eigenfunction Φ_i^N at the first maximum or minimum. The graph clearly indicates that the Φ_i^N belonging to “nonstable” eigenvalues ϵ_i^N as given by the diagonalization procedure, closely approximate,

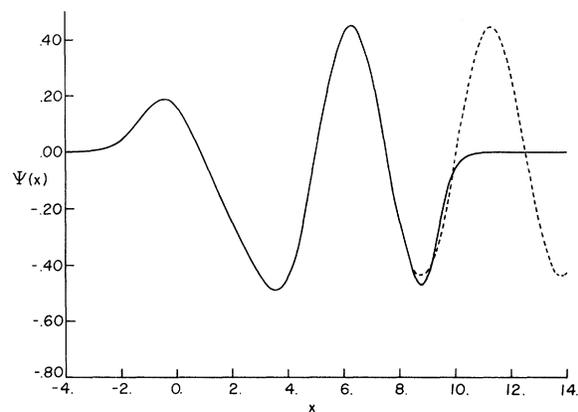


FIG. 4. Comparison of the exact and approximate wave functions in the nonresonant region for $\lambda=0.225$. (solid line) Φ_j^N with $N=50$, $j=4$, and $\epsilon_j^N=0.788675$; (dashed line) Ψ_E for $E=\epsilon_j^N$.

apart from a normalization constant, the inner part of the exact scattering functions Ψ_E at $E = \epsilon_l^N$, even though these Ψ_E represent nonresonant scattering.¹² This is a somewhat surprising result because the functions Φ_l^N are linear combinations of exponentially decaying basis functions, i. e., functions which exhibit incorrect behavior asymptotically.

Originally, the use of square-integrable functions to approximate the inner part of resonant scattering functions was justified by the argument that at energies near E_γ the amplitude of Ψ_E inside the potential barrier is much larger than that in the asymptotic region.² Therefore, if one neglects the relatively small (dependent on the width Γ) amplitude of Ψ_{E_γ} outside the range of $V(x)$, the function Ψ_{E_γ} looks like the wave function of a true bound state. But now we can make the much stronger statement that provided the basis of square-integrable functions spans the physically interesting region of x [defined by the range of $V(x)$], the stabilization or truncated diagonalization procedure yields good approximations, apart from a normalization factor, to the exact scattering functions at energies equal to the eigenvalues, *both in the resonant and nonresonant regions*,

In order to judge the adequacy of a given basis set, one must use intuition and all the physical information available about the problem. In this regard, a calculation of scattering states is no different from a variational calculation of true bound states. We note, however, that the expansion lengths required to produce a good approximation of the inner part of the scattering wave function near E_γ are usually smaller than those required for the wave functions at energies far from E_γ . This is simply a consequence of the fact that, apart from a relatively small asymptotic tail, the exact Ψ_E

near the resonance energy is much more localized in space than the potential scattering wave functions at energies far from E_γ . For example, a comparison of Figs. 3 and 4 shows that for $\lambda = 0.225$ a basis set spanning the range $-4 \leq x \leq 4$ is required to reproduce the most important inner part of the resonant wave function. On the other hand, a basis set that spans at least the range $-4 \leq x \leq 8$ is needed to approximate the nonresonant scattering wave function (at $E = 0.7887$) out to the third node.

B. Evaluation of Phase Shifts from the Eigenfunctions

In Sec. IIIA, we showed that for sufficiently large basis sets, the diagonalization procedure yields good approximations to the exact scattering functions even outside the range of the potential. In view of this fact, we conclude that the square-integrable eigenfunction must contain the desired scattering information, such as the phase shift. The problem therefore becomes how to extract the phase shift from the exponentially decaying eigenfunctions. Immediately, two possible difficulties are apparent. The eigenfunctions are not properly normalized for a scattering problem and have incorrect asymptotic behavior for large enough x . Of course, in a one-dimensional problem, we can always determine the phase shift from the logarithmic derivative of the approximate wave function at a value of x beyond the range of the potential but before the point where the function decays to zero. However, we are looking for a more general method that can be possibly applied to many-dimensional many-particle problems.

One possible procedure is to use the stationary expression for $\tan\eta$ originally developed by Schwinger¹³:

$$\tan\eta = \frac{[\int_0^\infty \Psi(x)V(x)\sin kx dx]^2}{\int_0^\infty \Psi(x)V(x)\Psi(x)dx - \int_0^\infty \int_0^\infty \Psi(x)V(x)G(x,x')V(x')\Psi(x')dx dx'} \quad (10)$$

where $G(x, x')$ is the free-particle Green's function

$$G(x, x') = \frac{1}{k} \sin kx' \cos kx, \quad x' < x \quad (11a)$$

$$G(x, x') = \frac{1}{k} \sin kx \cos kx', \quad x < x' \quad (11b)$$

The expression in (10) has the advantage that $\tan\eta$ is independent of the amplitude of the trial function $\Psi(x)$. It is also independent of the asymptotic behavior of $\Psi(x)$ since the boundary condition is incorporated into $G(x, x')$. However, it is difficult to use Eq. (10) in an actual calculation because of

the complexities involved in the evaluation of the double integral over the Green's function. An alternative expression, incorporating the above mentioned advantages, is desirable.

It can be easily shown that for an exact scattering wave function satisfying the equation

$$[E - H(x)] \Psi_E(x) = \left(\frac{1}{2} k^2 + \frac{1}{2} \frac{d^2}{dx^2} - V(x) \right) \Psi_E(x) = 0 \quad (12)$$

$\tan\eta$ can be calculated from the expression¹⁴

$$\tan\eta = - \frac{\int_0^\infty \Psi_E^* [E - H(x)] f(x) \sin kx dx}{\int_0^\infty \Psi_E^* [E - H(x)] f(x) \cos kx dx} . \quad (13)$$

The function $f(x)$ must satisfy the conditions:

$$f(x) \rightarrow 1, \quad x \rightarrow \infty \quad (14a)$$

$$f(0) = 0, \quad (14b)$$

$$\text{and } \left. \frac{df}{dx} \right|_{x=0} = 0, \quad (14c)$$

but it is otherwise arbitrary. For example, we have used the function $f(x) = 1 - \exp(-\lambda x^2)$, $\lambda > 0$ in our calculations. The purpose of introducing this function is explained below. The expression in (13) has the two desired features. The value of $\tan\eta$ is independent of the amplitude of $\Psi(x)$. Also, no particular asymptotic behavior of $\Psi(x)$ is required because the kinetic energy operator does not act on $\Psi(x)$.¹⁵ However, the value of $\tan\eta$ obtained from (13) is stationary only under certain conditions (see the discussion below). We have approximated the exact phase shifts at energies equal to the eigenvalues ϵ_j^N , by substituting the square-integrable eigenfunctions $\Phi_j^N(x)$ for $\Psi_E(x)$ in Eq. (13).

Before presenting our results, we wish to comment on the relationship of Eq. (13) to the variational method recently proposed by Harris.¹⁶ In his method, the exact scattering function $\Psi_E(x)$ is approximated by

$$\Psi_t(x) = \sum_{i=1}^N \alpha_i \Phi_i(x) + S(x) + \tan\eta C(x), \quad (15)$$

where the $\Phi_i(x)$ are eigenfunctions of H in an N -dimensional truncated basis set. The functions $S(x)$ and $C(x)$ are zero at the origin and behave like $\sin kx$ and $\cos kx$, respectively, at large x . The approximate phase shifts at $E = \epsilon_j$, the eigenvalues, are given by

$$\tan\eta = - \frac{\int_0^\infty \Phi_j^*(x) [\epsilon_j - H(x)] S(x) dx}{\int_0^\infty \Phi_j^*(x) [\epsilon_j - H(x)] C(x) dx} . \quad (16)$$

Recently, Nesbet has shown¹⁷ that Eq. (16) yields the same phase shifts at the eigenvalues ϵ_j as the Hulthén variational method¹⁸ would with a trial function of the form given in Eq. (15). Since our procedure, described in the previous paragraph, reduces Eq. (13) to Eq. (16), it is operationally identical to the Harris method and yields approximations to $\tan\eta$, which are stationary with respect to first-order corrections in the trial function. However, our interpretation is conceptually different,

in that we find for large enough basis sets the eigenfunction Φ_j by itself is a good approximation to Ψ_{ϵ_j} even beyond the range of the potential. Therefore, the explicit inclusion of the other eigenfunctions $\Phi_i (i \neq j)$ and the asymptotic functions $S(x)$ and $C(x)$ is not necessary. In fact, a careful examination of the Hulthén method shows that at $E = \epsilon_j$, the coefficient α_j of the function $\Phi_j(x)$ is infinite, i.e., the best approximation to Ψ_{ϵ_j} in the framework of the Hulthén variational principle is just the square-integrable eigenfunction $\Phi_j(x)$.

In our calculations, we included the function $f(x) = 1 - \exp(-\lambda x^2)$ in Eq. (13) to ensure the equivalence of $\tan\eta$ as given by Eq. (13) to that given by the Hulthén method for a problem defined over the range of $-\infty \leq x \leq \infty$.

Tables II and III compare the exact phase shifts to those obtained from the square-integrable eigenfunctions through the use of Eq. (13) for $\lambda = 0.15$ and $\lambda = 0.225$, respectively. The column labeled N gives the size of the basis set which yielded the particular eigenvalue and the approximate phase shift at that energy. The agreement between exact and approximate phase shifts is excellent in both the resonant and the nonresonant energy regions. We obtained the approximate resonance energies and widths by fitting the approximate phase shifts to the form given in Eq. (5). Table IV compares the exact and approximate resonance parameters for several values of λ . As expected, excellent agreement is obtained for both narrow and broad resonances. It is interesting to note that the difference between the exact and approximate resonance energies increases as the width of the resonance

TABLE II. Comparison of exact and approximate phase shifts: $\lambda = 0.15$, $E_r = 0.466105$, $\Gamma = 0.0003210$.^a

E	Exact η	Approximate η	N
0.1986012	0.25441	0.25448	45
0.2432740	-0.01298	-0.01301	40
0.3067471	-0.33681	-0.33661	35
0.4659006	-0.29226	-0.29216	50
0.4660346	0.19811	0.19845	45
0.4661222	0.71752	0.71749	40
0.4662023	1.15593	1.15614	36
0.4662291	1.26965	1.26985	35
0.4662616	1.38428	1.38455	34
0.4663029	1.50066	1.50062	33
0.4663590	1.61860	1.61896	32
0.4664427	1.73842	1.73924	31
0.4665855	1.85945	1.86032	30
0.4668974	1.98113	1.98177	29
0.5614866	1.90252	1.90244	50
0.6479890	1.69428	1.69448	45
0.7570471	1.48282	1.48295	40

^aAll quantities are in a.u. unless stated otherwise.

TABLE III. Comparison of exact and approximate phase shifts: $\lambda=0.225$, $E_\gamma=0.441333$, $\Gamma=0.008996$.^a

E	Exact η	Approximate η	N
0.1829543	1.16758	1.16719	35
0.3903266	0.52853	0.52853	50
0.4242980	0.61987	0.61968	45
0.4356381	1.00578	1.00573	40
0.4388743	1.40092	1.40078	36
0.4394626	1.50580	1.50623	35
0.4400106	1.61273	1.61291	34
0.4405336	1.72162	1.72117	33
0.4410453	1.83248	1.83225	32
0.4415584	1.94521	1.94572	31
0.4426438	2.17635	2.17595	29
0.4508920	3.00670	3.00662	50
0.4737665	3.26400	3.26393	45
0.5338320	3.25045	3.25056	40
0.6209181	3.16135	3.16143	35
0.7886753	3.07880	3.07890	50

^aReference a, Table II.

increases. Presumably, this is a consequence of the fact that for broader resonances potential scattering is relatively more important. As we have already noted at the end of Sec. III A, it is more difficult to obtain good approximations to the scattering function off resonance because larger basis sets are required to span the physically important region of x .

IV. MODEL FOR BEHAVIOR OF EIGENVALUES IN STABILIZATION PROCEDURE

The results presented in Sec. III A reinforce the qualitative idea previously used to justify the sta-

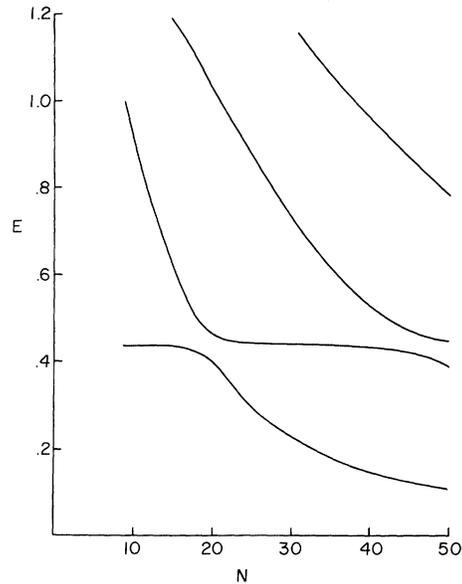


FIG. 5. Behavior of the four lowest eigenvalues as a function of the expansion length N for $\lambda=0.225$.

bilization method as an efficient way of approximating the resonance energy E_γ . Figure 2 clearly shows that at energies near E_γ the amplitude of the exact scattering wave function inside the range of the potential is much larger than its amplitude in the asymptotic region. However, so far we have not discussed in detail the behavior of the eigenvalues ϵ_j^N as a function of N .

Figure 5 shows the behavior of the few lowest ϵ_j^N as a function of N for $\lambda=0.225$.¹⁹ The "stable" behavior of the eigenvalues at energies near E_γ is very clear. Accepting for the moment the as-

TABLE IV. Comparison of the exact and approximate resonance parameters. The values in column 3 were determined from the approximate phaseshifts given by Eq. (13). The values in column 4 were determined by fitting the calculated $\Delta\epsilon/\Delta N$ to Eq. (31) [see Sec. IV].

λ		Exact	Approximate	Model
0.125	E_γ	0.472940	0.472940	0.472940
	Γ	0.3607×10^{-4}	0.3604×10^{-4}	0.3595×10^{-4}
0.15	E_γ	0.466105	0.466106	0.466106
	Γ	0.3210×10^{-3}	0.3225×10^{-3}	0.3176×10^{-3}
0.19	E_γ	0.453536	0.453540	0.453534
	Γ	0.002805	0.002820	0.002776
0.225	E_γ	0.441333	0.441326	0.441347
	Γ	0.008996	0.009032	0.008945
0.26	E_γ	0.429033	0.428985	0.429056
	Γ	0.01976	0.01979	0.01978

sumption that the stable ϵ_j^N approximates E_γ , it is obvious that we can easily estimate E_γ with good accuracy from such graphs. In order to show that the "stable" ϵ_j^N indeed approximates E_γ we now show that when one of the eigenvalues is near E_γ , its slope, $\Delta\epsilon_j^N/\Delta N$ is very small compared to the slopes of the other "nonstable" ϵ_i^N . Indeed, when $\epsilon_i^N = E_\gamma \Delta\epsilon_j^N/\Delta N$ (treated as a continuous function of N) is proportional to the exact width of the resonance to a very good approximation. Before proceeding with the argument, one should remember that the Hylleraas-Undheim theorem requires that $\Delta\epsilon_i^N/\Delta N \leq 0$ for each i .¹¹ This behavior is clearly seen in Fig. 5. Now let us consider the discrete energy spectrum obtained by solving $H\psi = E\psi$ in the region $-L \leq x \leq L$ subject to the condition $\psi(L) = \psi(-L) = 0$. Since the true spectrum of H in $-\infty < x < \infty$ is continuous for $E > 0$, we assume that for a very large L , the discrete spectrum is densely packed for $E \geq 0$. Indeed, one can always find a finite L so that the m lowest eigenvalues are below E_γ regardless how large m is. As the basis set becomes complete for $-L \leq x \leq L$, L finite, each ϵ_j^N approaches the corresponding exact discrete eigenvalue (of the box problem) from above. Therefore, if we treat N as a continuous variable, each ϵ_j^N must "cross" the line $E = E_\gamma$ for some value of N . More precisely, for some integer value of N there is an eigenvalue near E_γ .

To proceed, we must find the conditions which determine the ϵ_i^N for a given expansion length N . In a problem involving true bound states, the discrete eigenvalues are determined by the boundary condition $\Phi_i(x) \rightarrow 0$ as $x \rightarrow \infty$. In a scattering problem, different boundary conditions apply and a continuous energy spectrum results. However, in the stabilization method, we diagonalize the Hamiltonian in a truncated set of exponentially decaying functions. Therefore, presumably the eigenvalues are determined by the condition that $\Phi_i(x) \approx 0$ at some value of x yet unknown. If the basis functions $\psi_m(x)$ are properly ordered so that each $\psi_m(x)$ decays to zero at approximately x_m , which is an increasing function of m , then the eigenfunction $\Phi_j^N(x)$, which is a linear combination of $\psi_1 \dots \psi_N$ [see Eq. (8)] must certainly be zero for $x \geq x_N$. Thus, we have

$$\Phi_i^N(x_N) \approx 0, \quad i = 1, \dots, N. \quad (17)$$

The discussion of the eigenfunctions presented in Sec. IIIA shows that indeed the basis set $\psi_1 \dots \psi_N$ spans the region $x \leq x_N$, but not beyond.²⁰ Equation (17) can be taken as the boundary condition that determines the ϵ_i^N for a given N . Of course, this procedure is equivalent to placing an infinite potential (wall) at $x = x_N$, and then solving $(H - E)\Psi = 0$ within this wall.

If the point x_N is beyond the range of the potential, all the solutions of $(H - E)\Psi = 0$ must behave like

$$\Phi_j(x) \sim \sin[k_j x + \eta(k_j)] \quad (18)$$

for x near x_N . The eigenvalue ϵ_j^N equals $1/2k_j^2$. The boundary condition in Eq. (17) requires that

$$k_j x_N + \eta(k_j) = j\pi, \quad j = 1, \dots, N. \quad (19)$$

If the potential under consideration has a finite number of bound states for $E < 0$, then the lowest allowed value of j in Eq. (19) is $N_B + 1$, where N_B is the number of bound states. This implies that for $N > N_B$, the N_B lowest eigenvalues obtained in the diagonalization would approximate the N_B true discrete eigenvalues of H .

In order to obtain a result which is independent of the particular basis set used, we first consider the behavior of ϵ_j^N as a function of the boundary at x_N . We can differentiate Eq. (19) with respect to x_N provided we know the functional form of the phase shift η . For a problem exhibiting an isolated resonance, we can assume that η has the form given in Eq. (5). Differentiating Eq. (19) we obtain

$$\frac{\partial \epsilon_j^N}{\partial x_N} = -2\epsilon_j^N \left(x_N + \frac{2\Gamma k_j}{4(E_\gamma - \epsilon_j^N)^2 + \Gamma^2} \right)^{-1}, \quad (20)$$

where we have assumed that $\partial\eta_{\text{pot}}/\partial E = 0$. This is a good approximation provided we use Eq. (20) in a narrow energy region where $\eta_{\text{pot}}(E)$ is a slowly varying function of E . Equation (20) is the desired result because it relates the behavior of ϵ_j^N as a function of x_N (and N) to the resonance parameters. Also, it demonstrates the "stability" of an eigenvalue at energies very near E_γ .

Let us assume that for a given x_N one of the eigenvalues ϵ_i^N equals E_γ . We obtain

$$\frac{\partial \epsilon_i^N}{\partial x_N} = -2E_\gamma / (x_N + 2k_\gamma / \Gamma), \quad (21)$$

where $1/2k_\gamma^2 = E_\gamma$. In addition, let us assume that Γ is small enough so that no other eigenvalue is near E_γ within Γ and

$$x_N > \frac{\Gamma k_j}{2(E_\gamma - \epsilon_j^N)^2}, \quad j \neq i. \quad (22)$$

Using Eq. (22), we get

$$\frac{\partial \epsilon_j^N}{\partial x_N} \approx -\frac{2\epsilon_j^N}{x_N}, \quad j \neq i. \quad (23)$$

But if Γ is small enough so that

$$x_N \ll 2k_r/\Gamma, \quad (24)$$

Eqs. (21) and (23) reduce to

$$\frac{\partial \epsilon_i^N}{\partial x_N} \approx -\frac{1}{2} k_r \Gamma \quad (25)$$

and

$$\frac{\partial \epsilon_i^N}{\partial x_N} \left(\frac{\partial \epsilon_j^N}{\partial x_N} \right)^{-1} \approx \frac{E_r}{\epsilon_j} \frac{x_N \Gamma}{2k_r}, \quad j \neq i. \quad (26)$$

Equation (24) implies that

$$\frac{\partial \epsilon_i^N}{\partial x_N} \left(\frac{\partial \epsilon_j^N}{\partial x_N} \right)^{-1} \ll 1, \quad j \neq i. \quad (27)$$

We now have the result that, provided the assumption in Eq. (24) is valid, the slope of the "stable" eigenvalue ϵ_i^N is much smaller than those of the other eigenvalues. In addition, Eqs. (25) and (26) imply that the narrower is the resonance the more pronounced is the "stability."

Now let us examine the assumption in Eq. (24) in more detail. Since we originally assumed that the point x_N was beyond the range of the potential, say x_v , we can rewrite Eq. (24) in the form

$$x_v \ll \frac{2k_r}{\Gamma}. \quad (28)$$

The above restriction is certainly not too severe in the case of electron scattering off neutral atoms or molecules. For example, in the case of the well-known 19.3-eV resonance of He^- with an estimated width of 0.006 eV in the elastic channel¹ one has the requirement that $x_v \ll 10^4$ a.u. In the case of a broader low-lying resonance, say with $E_r \sim 2.7$ eV and $\Gamma \sim 0.3$ eV, Eq. (28) requires that $x_v \ll 90$ a.u. Because of the asymptotic form assumed in Eq. (18), the present analysis does not directly apply to scattering from the long-range Coulomb potential. However, if one repeats the analysis using an asymptotic form appropriate for Coulomb functions one again reaches the conclusion that "stability" of some eigenvalues will occur for narrow enough resonances. In this case, the width must satisfy Eq. (28), where now x_v denotes the range of the non-Coulomb (short-range) part of $V(x)$. This conclusion is in agreement with previous computational studies of the systems $e + \text{He}^{+6}$ and $e + \text{H}_2^{+}$,^{21, 22} in which "stabilization" of certain

eigenvalues was indeed observed.

Equations (21) and (23) also describe the behavior of the eigenvalues for very large expansion lengths. For large enough N , we have

$$x_N \gg 2k_r/\Gamma, \quad (29)$$

even in the case of very narrow resonances. Under this condition the slope of every eigenvalue is described by Eq. (23); i.e., there is no longer a unique so-called "stable" root. As N and x_N increase, no divergence results, but one is no longer able to select a particular ϵ_j^N for special consideration. This result agrees with the previous prediction that as N increases the density of eigenvalues becomes so large that one loses track of the particular ϵ_j^N that was "stable" for smaller N .²

The analysis also illustrates why the selection of an appropriate basis set for a given problem is so important:

(a) In deriving the expression for the slope of the eigenvalues, Eq. (20), we had to assume that the basis set spans the range of the potential.

(b) "Stability" occurs when there is an eigenvalue near E_r . This condition can occur only when the basis set is adequate to describe the inner part of the resonant scattering function, because it is this part which determines the value of E_r .

(c) If initially one chooses an inadequate basis set, one needs to add many other functions to obtain an ϵ_j^N near E_r . In such a case, the condition in Eq. (24) may not be satisfied by the time "stability" of an ϵ_j^N results. Once the inequality $x_N \ll 2k_r/\Gamma$ does not hold, no unique eigenvalue exists.

If one knows the explicit dependence of x_N on the expansion length N , one can use Eq. (20) to extract the resonance parameters E_r and Γ from the computed slopes of the "stable" eigenvalue. For the harmonic oscillator functions, we obtain (in a.u.)

$$x_N = 2N - 1. \quad (30)$$

Using Eq. (30) and assuming that N is a continuous variable, we can transform Eq. (20) into

$$\frac{\Delta \epsilon_j^N}{\Delta N} = -2\epsilon_j^N \times \left(2N - 1 + \frac{2\Gamma k_j (2N - 1)^{1/2}}{4(E_r - \epsilon_j^N)^2 + \Gamma^2} \right)^{-1}. \quad (31)$$

Table IV shows the resonance parameters obtained by fitting the computed slopes of the "stable" eigenvalues to Eq. (31). The good agreement obtained

between the exact and approximate values of both E_γ and Γ gives us confidence in our model as a valid explanation of the behavior of the eigenvalues as a function of N . The slightly increasing discrepancy between the exact and approximate resonance energies for increasing λ is probably due to the assumption $\partial\eta_{\text{pot}}/\partial E=0$. For broader resonances, ϵ_j^N is less "stable" so that one needs to use Eq. (20) over a larger energy range, over which η_{pot} may not be constant. For added computational accuracy, one could introduce $\partial\eta_{\text{pot}}/\partial E$ into Eq. (20) as an additional parameter, but this is not our purpose here.

Finally, we wish to comment on an interesting and perhaps puzzling feature of Fig. 5 illustrating the behavior of ϵ_j^N as a function of N . At certain values of N there are avoided crossings of two neighboring eigenvalues. Holøien and Middtdal⁵ found a similar behavior when they plotted the eigenroots obtained in the truncated orthogonalization method as a function of the variable screening parameter in the basis functions. The peculiar behavior of ϵ_j^N at certain values of N is a consequence of the Hylleraas-Undheim theorem¹¹ and Eq. (26). Let us consider an isolated "stable" eigenvalue ϵ_j^N . Since the next higher eigenvalue, denoted by ϵ_{j+1}^N , decreases much more rapidly with N than the "stable" ϵ_j^N [see Eq. (26)], $\epsilon_{j+1}^N - \epsilon_j^N$ must decrease until the two eigenvalues are nearly degenerate. As ϵ_j^N is pushed away from E_γ by ϵ_{j+1}^N approaching from above, it becomes less "stable." On the other hand, ϵ_{j+1}^N is approaching E_γ and thus becomes "stable." The behavior of the corresponding eigenfunction provides additional insight into the nature of the crossing region. The eigenfunction Φ_{j+1} belonging to the "stable" ϵ_{j+1} right of the crossing is almost identical to the Φ_j belonging to the "stable" ϵ_j left of the avoided crossing, except the former has one additional node. Therefore, the unstable region represented by the "avoided crossing" is associated with the addition of a new node to the eigenfunction that approximates the resonant scattering function. As N and x_N increase a new node is introduced for each half wavelength. In a problem for which the boundary condition in Eq. (18) is applicable, the wavelength is approximately $2\pi/k_\gamma$ and is independent of $x_N(N)$. As a result, the avoided crossings do not come closer as x_N increases and do not lead to any difficulty for large expansion lengths.

Our major conclusions are as follows: When the

exact Hamiltonian is diagonalized in a large enough basis of exponentially decaying functions, the resulting eigenfunctions closely approximate, apart from an arbitrary normalization factor, the inner part of the exact scattering functions at energies equal to the corresponding eigenvalues in both the resonant and nonresonant energy regions. However, in general, larger basis sets are required to obtain a good representation of the scattering wave functions at energies far from E_γ . Using appropriate amplitude independent formulas one can extract scattering information from the exponentially decaying approximations to the scattering wave function. We have analyzed a model which explains the behavior of the eigenvalues as a function of the expansion length. The analysis shows that for adequate basis sets the slope of an eigenvalue at E_γ is proportional to the width and is much smaller, in magnitude, than the slopes of the other eigenvalues. This phenomenon is called "stability," and it occurs provided $x_v < x_N \ll 2k_\gamma/\Gamma$, where x_N defines the range spanned by the basis set and x_v is the range of the potential. In the case of very-large basis sets, for which the above condition does not hold, the diagonalization no longer yields a unique stable eigenvalue. For increasing expansion lengths, the stabilization procedure becomes useless as the consequence of the incorrect boundary condition employed in the scattering problem.

We are presently investigating the extension of our method to many-dimensional problems in which both shape resonances and compound state resonances occur in the elastic as well as the inelastic channels. The results of this study will be reported in the future.

ACKNOWLEDGMENTS

We wish to thank Professor B. A. Lippmann and Professor S. R. Berry for helpful suggestions. One of us (AUH) also wishes to thank Dr. M. Fels for many useful conversations. This research was supported in part by the National Science Foundation Grant No. GP-7861, and in part by the National Aeronautics and Space Administration Grant No. NGL 05-007-003. We have also benefited from the use of facilities provided by the Campus Computing Network of the University of California at Los Angeles.

* Part of work reported at the Sixth International Conference on the Physics of Electronic and Atomic Collisions, 1969.

† Postdoctoral Fellow supported by the Air Force Office of Scientific Research during 1967-68 at the Uni-

versity of Southern California.

‡ Contribution No. 2460.

§ Alfred P. Sloan Foundation Fellow.

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Interpretation of Interference Structure in Elastic Scattering Using the Semiclassical Action*†

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(Received 29 October 1969)

We show how to interpret the Ford-Wheeler semiclassical expression for the scattering amplitude as an integral, over both positive and negative impact parameters, of a quantity depending on the action. This formulation clarifies the relationship between the action and the phase of the semiclassical expression for the scattering amplitude. Using this formulation, we show that interference processes in both one- and two-channel elastic scattering are analogous to those occurring in the two-slit diffraction of light.

I. INTRODUCTION

In quantum-mechanical treatments of scattering, the impact parameter cannot be known because of the uncertainty principle (the transverse momentum before the collision is fixed by the incident angle and momentum). If the de Broglie wavelength

$$\lambda = \hbar/p = \hbar(2mE)^{-1/2} \quad (1)$$

is much smaller than the scale of variation of the potential, however, the impact parameter b becomes physically significant. One can imagine that each portion of the incident wave can be followed through the collision; its deflection being determined only by the impact parameter b (and the reduced potential).

This idea forms the basis of this paper. In Sec. II, we show how the semiclassical scattering amplitude may be expressed as an integral over all impact parameters, and in Sec. III, we show the close relationship between the action and the phase of various contributions to the scattering amplitude. In Sec. IV, we give a simple interpretation of interference phenomena in single-channel (one-potential) scattering, which is extended to two-channel interference phenomena (e.g., resonant exchange) in Sec. V.

II. SCATTERING AMPLITUDE INTEGRAL

Ford and Wheeler¹ have shown that a considerable mathematical simplification in the usual partial-wave treatment of scattering results when the de Broglie wavelength is smaller than the scale of