# Calculation of Energies and Widths of Compound-State Resonances in Elastic Scattering: Stabilization Method

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In a previous paper, the stabilization method of calculating resonance parameters was applied to a one-dimensional model problem of potential scattering. The method is here extended to compound-state resonances in elastic scattering, and its application to a model problem for a target with two bound states is examined. The resonance parameters are calculated by two methods which use information obtained in the diagonalization of the exact Hamiltonian in appropriately chosen sets of square-integrable basis functions: One is presented for the first time here; the other is similar to the procedure used in the potential-scattering problem. In addition to the stabilization method, we have applied to the model problem some other techniques, which have been previously proposed for the calculation of resonance parameters. The availability of the exact solutions enables us to make some preliminary assessments of the reliability and the difficulty that might be expected from these approximation methods.

## I. INTRODUCTION

Methods for calculating resonance parameters may be divided into two categories.[1] In one, the experimentalist's approach is followed: The entire scattering problem is solved, in some approximation, for many energies, and the resonance energy and width are extracted from the energy-dependent cross section. The method of close coupling falls into this category.[1] In the other, $E_r$ and $\Gamma$ are calculated directly from approximations to the exact resonance wave function. One example is the stabilization method[2,3] which we propose to study here.

In a previous paper,[3] the stabilization method was applied to scattering from a one-dimensional model potential whose barrier gave rise to so-called single-particle resonances. The understanding of the method was enhanced by the possibility of comparison with the exact results. Often the resonances of interest, such as those in $e$-H or $e$-$He^+$ scattering, are examples of "compound" resonances, i.e., resonances which are associated with excited states of the target.[1,2] In this paper, we shall extend the stabilization method to elastic scattering from a target and study its application to a model problem which simulates the scattering from a target, and in which compound resonances occur.

The stabilization method for finding resonance parameters may be briefly summarized: After the choice of an appropriate basis of square-integrable functions, the complete Hamiltonian $H$ is diagonalized in successively larger bases. For sufficiently large basis sets, the presence of a "stable" root indicates a resonance, and the degree of stability of that root is a measure of the width.

In the course of studying the model problem of potential scattering in I, it was learned that the $N$ eigenvectors resulting from the diagonalization of $H$ in an $N$-dimensional basis were approximations to the exact wave functions at energies given by the corresponding roots. The eigenvectors represented those exact solutions which have a node approximately where the (square-integrable) eigenvectors exponentially go to zero. By examining the "wall" at which the last added basis function goes to zero, the slope of the stable root as a function of the basis size could be related to the resonance energy and width. The resulting values for $E_r$ and $\Gamma$ obtained from this application of the stabilization method compared favorably with the exact results.

When extended to scattering from a target, the stabilization method is complicated by the presence of the target states. The simplest kind of basis, where exchange does not enter, might consist of product functions $u_m(\vec{r})\varphi_t(\vec{r}_0)$ where $\varphi_t$ represent the target states and $\{u_m\}$ is the basis for the scatterer. In I, all of the basis elements contributed in the scattering region; in elastic scattering from the ground state $\varphi_1$ of the target, basis functions of the type $u_m\varphi_1$ contribute in the scattering region, whereas all others contribute only in the inner region. This may be seen by an analogy with close coupling,[1] where the complete (no-exchange) wave function may be written

$$\Psi_E = \sum_{t=1}^{\infty} \varphi_t(\vec{r}_0) F_t(\vec{r}) \ . \tag{1.1}$$

For elastic scattering, only $F_1(\vec{r})$ is nonzero in the asymptotic region. We write the $j$th eigenvector associated with the eigenvalue $\epsilon_j$ that results from the diagonalization procedure as

$$\Phi_j = \sum_{t=1}^{T} \varphi_t(\vec{r}_0)\left( \sum_{m=1}^{M_t} u_m(\vec{r})\, c_{m1}^{(j)} \right) \ . \tag{1.2}$$

In this expression, the $t=1$ term $\sum_{m=1}^{M_1} u_m(\vec{r})\, c_{m1}^{(j)}$

will represent the scattering function $F_1(\vec{r})$. When the eigenvector associated with the resonance state has been identified, information from the scattering part of the eigenvector, i.e., the $t=1$ term of Eq. (1.2), will yield the resonance parameters. In the following, we refer to basis functions of the form $\varphi_t(\vec{r}_0)u_m(\vec{r})$ as "type-$t$" functions, $t=1, 2, \ldots T$.

The extension of the stabilization method to compound resonances is discussed in Sec. II A. Two methods for calculating $E_r$ and $\Gamma$ (and, in some cases, the potential phase shift $\delta_p$) are developed in Sec. II B. The first is a new method which expresses the change in energy due to the addition of a type-1 basis function in terms of the resonance parameters; the second is an elaboration of the method used in I.

We shall apply the stabilization method to compound resonances occurring in the elastic scattering from a fictitious target which has two states. In Sec. III, we discuss this model problem and its exact solution in detail, and present the results of the stabilization methods. In Sec. IV, we apply some additional approximation methods for finding resonance parameters to the model problem. These methods, in general, make use of Feshbach's projection-operator formalism,[4] and range in complexity from complete neglect of the continuum of $QHQ$[5] to inclusion of all continuum states by a perturbation approach. In addition, we study two methods recently proposed, the "adiabatic" approximation of Muckerman[6] and the "Golden-rule-like formula" of Miller.[7] We conclude the paper with a few remarks concerning the comparative virtues of the methods considered.

## II. STABILIZATION METHOD

### A. Qualitative Remarks

For scattering from a target with internal states at energies $E_i$, $i=1, 2, \ldots$, the exact (no-exchange) scattering wave function is given by Eq. (1.1). In Eq. (1.1) $\vec{r}_0$ represents the coordinates of the target particles, $\vec{r}$ is the coordinate of the scatterer, and $E$ is the total energy. In the case of elastic scattering from the ground state of the target ($E_1 < E < E_2$), $\varphi_1(\vec{r}_0)$ is the exact ground-state wave function. The other functions $\varphi_t(\vec{r}_0)$, $t \geq 2$, may represent either the true excited states[1] or pseudostates[8] chosen to improve the convergence of the expansion in Eq. (1.1). In the stabilization method for specific energies the channel functions $F_t(\vec{r})$, including the continuum function $F_1$, are expanded in terms of a set of square-integrable basis function $u_m(\vec{r})$, $m=1, 2, \ldots$. Thus, the scattering wave function $\Psi_E$ is approximated by the expression in Eq. (1.2). The specific energies $\epsilon_j$ and the expansion coefficients $c_{mt}^{(j)}$ are just the eigenvalues and the corresponding eigenvectors obtained from the diagonalization of the complete Hamiltonian in the basis $\{\varphi_t(\vec{r}_0)u_m(\vec{r})\}$ $t=1, \ldots T$, $m=1, \ldots M_t$.

Next, we come to the major assumptions of the stabilization method. Let us assume that the basis set is sufficiently large to span the range of the potentials involved in the problem. Then the expansion of the closed-channel functions $F_t$, $t \geq 2$, in terms of $\{u_m\}$ converges because for $t \geq 2$ the functions $F_t$ themselves are exponentially decaying in the asymptotic region. The expansion of the continuum function $F_1$, however, cannot converge in the strict mathematical sense. Nevertheless, based on the results of I, we assume that the expansion of $F_1$ in terms of the square-integrable basis functions determines the specific energies $\epsilon_j$ and contains the scattering information. For a given basis set $\{u_m\} m=1, \ldots M$, those eigenenergies $\epsilon_j$ (between $E_1$ and $E_2$ for elastic scattering) are produced by the diagonalization for which the open-channel function $F_1(\vec{r})$ has a node at the point where the amplitude of the basis function $u_M(\vec{r})$ becomes negligible, say $r_M$. The point $r_M$ is not uniquely defined, but in most cases one can reasonably assume that it equals the outer classical turning point of $u_M(\vec{r})$. This is the definition we adopt for the discussion that follows. (Here we take the basis set to be so ordered that $r_m > r_{m-1}$ for all $m$.) Correspondingly, the expansion

$$S_1(\vec{r}) = \sum_{m=1}^{M} u_m(\vec{r}) c_{m1}^{(j)} \tag{2.1}$$

is a good approximation, apart from an arbitrary normalization constant, to the function $F_1$ out to $r_M$. The numerical results presented in Sec. III show that these assumptions are essentially correct

Next, we briefly discuss the "stabilization" property of certain eigenvalues obtained in the diagonalization. Let us assume that for a given basis set (large enough such that $r_M$ is greater than the range of the potentials) one of the eigenenergies, say $\epsilon_j$, is close to the resonance energy $E_r$. Then, based on the results of I, we predict that $\epsilon_j$ will be stable with respect to the addition of basis functions $\varphi_t u_{M+1}$, regardless of the value of $t$. For $t \geq 2$, $\epsilon_j$ will not change significantly as $\varphi_t u_{M+1}$ is added to the basis because, if $r_M$ is greater than the range of the potentials, then the expansion of $F_t$ in terms of $\{u_M\} m=1, \ldots M$ has already converged. The fact that $\epsilon_j$ will decrease only slightly (depending on the magnitude of the width $\Gamma$) with the addition of $\varphi_1 u_{M+1}$ to the basis can be shown using arguments exactly analogous to those given in Sec. IV of I, with the open-channel function $F_1(\vec{r})$ substituted for the scattering function $\Psi(x)$ of I. Qualitatively, it is known that, for energies near $E_r$, $\Psi_E$ has a much smaller amplitude in the asymptotic region than in the inner region. We can argue that, since $r_M$ is greater than the range of the potential, $\varphi_1 u_{M+1}$

contributes only to the asymptotic part of $\Psi_E$ which has relatively small amplitude. As a result, $u_{M+1}$ enters the expansion of $F_1$ with a small coefficient, and the eigenenergy $\epsilon_j$ is only slightly affected. Again, the numerical results presented in Sec. III show that these arguments are essentially correct.

In addition to the stabilization property of an eigenvalue near $E_r$, the behavior of the expansion coefficients in the associated eigenvector $\Phi_j$ also indicates that a root near $E_r$ represents the resonance state. In the sense that a resonance state is a "quasibound" state, and thus $\Phi_j$ is larger in the inner region than in the asymptotic region, we expect for a resonance associated with the $t$th target state that $c_{mt}^{(j)}$ (for one or more $m$ values) in Eq. (1.2) will be large for the $u_m$ which contribute most in the inner region. In particular, large $c_{m1}^{(j)}$ will indicate single-particle resonances while large $c_{mt}^{(j)}$ for $t \neq 1$ will indicate compound resonances. Hence, we can apply the stabilization method equally well to both types of resonances.

The Hylleraas-Undheim theorem ensures[9] that, with the addition of basis functions, all roots decrease, i.e., $\epsilon_i^{(N+1)} < \epsilon_i^{(N)}$ for all $i$, where $N$ is the total number of basis functions ($N = \sum_{t=1}^{T} M_t$). Since for elastic scattering $F_1$ contains the scattering information, the variation of the resonance root $\epsilon_j$ with the addition of $\varphi_1 u_m$ basis functions enables us to determine the resonance energy $E_r$ and, to a good approximation, the width $\Gamma$.

### B. Calculation of Resonance Parameters

Since the eigenvector associated with the stable root is a good approximation in the inner region (save, for an over-all normalization factor) to the exact resonance eigenfunction, and since it is known how to extract resonance parameters from the exact eigenfunction, one might hope to develop a normalization-independent formalism in which the resonance parameters can be extracted from the eingenvector produced by stabilization. This is accomplished by considering the change in the $j$th root in going from an $N$- to $(N+1)$-dimensional basis, i.e., $\Delta\epsilon^{(N+1)} \equiv \epsilon_j^{(N+1)} - \epsilon_j^{(N)}$. Taking $\{\psi_i\}$ as the basis [e.g., $\psi_i = \varphi_t(\vec{r}_0) u_m(\vec{r})$], let $\Phi_j$ be the $j$th eigenvector from the diagonalization of $H$ using $N$ basis functions, and let $\chi_j$ be the corresponding eigenvector from $N+1$ functions. Then it can easily be shown—and will be so done in Appendix A—that for the $j$th root we have

$$\Delta\epsilon^{(N+1)} = \frac{\langle \Phi_j H \psi_{N+1} \rangle \langle \psi_{N+1} \chi_j \rangle}{\langle \Phi_j \chi_j \rangle} . \tag{2.2}$$

In order to introduce resonance parameters, we make the assumption that $\chi_j$, apart from the normalization, is a good approximation to the *inner part* of the exact wave function $\Psi_E^+$ at $E = \epsilon_j^{(N+1)}$. Guided by the Feshbach formalism of projection operators, we define $Q = |\chi_j\rangle\langle\chi_j|$, and construct $Q\Psi_\epsilon^+$ which for $\epsilon_j^{(N+1)}$ near $E_r$ gives a relationship between $\chi_j$ and $\Psi_\epsilon^+$,

$$|\Psi_\epsilon^+\rangle = e^{i\alpha}(\Gamma/2\pi)^{1/2}(\epsilon_j^{(N+1)} - E_r + \tfrac{1}{2} i\Gamma)^{-1} |\chi_j\rangle . \tag{2.3}$$

(Here, we write $\epsilon$ for $\epsilon_j^{(N+1)}$ in all relevant subscripts.) It should be emphasized that Eq. (2.3) is valid only in the inner region where $\chi_j$ is significantly different from zero. For $l = 0$ scattering, $\alpha$ is the so-called potential phase shift $\delta_p$. Details of the derivation and the generalization to $l \neq 0$ scattering are given in Appendix B. Thus, we can write for $E = \epsilon_j^{(N+1)}$ near $E_r$,

$$\langle \psi_{N+1} \chi_j \rangle = \langle \psi_{N+1} \Psi_\epsilon^+ \rangle (\epsilon_j^{(N+1)} - E_r + \tfrac{1}{2} i\Gamma) e^{-i\delta_p} (\Gamma/2\pi)^{-1/2} \quad \text{for } l = 0 . \tag{2.4}$$

If the $N+1$ dimensional basis $\{\psi_i\}$ spans into the asymptotic region and the last-added basis function $\psi_{N+1}$ contributes only in the asymptotic region, then in the integral $\langle \psi_{N+1} \Psi_\epsilon^+ \rangle$, $\Psi_\epsilon^+$ may be replaced by its asymptotic form

$$(k\pi)^{-1/2} r^{-1} Y_{00}(\hat{r}) e^{i\delta} \sin(kr + \delta) \varphi_1(\vec{r}_0) ,$$

where $k^2 = \epsilon_j^{(N+1)} - E_1$.[10] We see here the justification for our previous statement that resonance information is obtained from the addition of type-1 functions to the basis set, for otherwise in this approximation $\langle \psi_{N+1} \Psi_\epsilon^+ \rangle = 0$. If one writes

$$\psi_{N+1} = [u_{M+1}(r)/r] Y_{00}(\hat{r}) \varphi_1(\vec{r}_0) ,$$

where $N = M + \sum_{t=2}^{T} M_t$, then after some simple algebra one may express $\Delta\epsilon^{(N+1)}$ in terms of the three resonance parameters $E_r$, $\Gamma$, and $\delta_p$:

$$\Delta\epsilon^{(N+1)} = \frac{\langle \Phi_j H \psi_{N+1} \rangle}{\langle \Phi_j \chi_j \rangle} (\tfrac{1}{2} k\Gamma)^{-1/2} [(\epsilon_j^{(N+1)} - E_r)(S_{M+1} \cos\delta_p + C_{M+1} \sin\delta_p) + \tfrac{1}{2}\Gamma(S_{M+1} \sin\delta_p - C_{M+1} \cos\delta_p)], \tag{2.5}$$

where

$$S_{M+1} = \int_0^\infty dr \sin kr\, u_{M+1}(r) ,$$

$$C_{M+1} = \int_0^\infty dr \cos kr\, u_{M+1}(r) .$$

By use of the eigenvectors for several stable roots, the values of $\Delta\epsilon^{(N+1)}$ are fitted against the function in (2.5) to produce approximate values for $E_r$, $\Gamma$, and $\delta_p$. The reader is reminded that this method can be expected to give good results only when $\chi_j$ is a good approximation to the exact resonance

eigenfunction in the inner region (we shall see better what is meant by this during the calculation), and when $\psi_{N+1}$ does contribute only in the asymptotic region.

The second method expresses $d\epsilon_j^{(N)}/dM$ as a function of $E_r$ and $\Gamma$. Its derivation is essentially the same as the derivation of Eq. (31) in I, so our discussion here will be brief. If we assume that the point $r_M$ at which the $M$th function $u_M$ becomes negligible coincides with a node in the exact eigenfunction for $k_j^2 = \epsilon_j^{(N)} - E_1$, then the boundary condition[11]

$$k_j r_M + \delta(\epsilon_j^N) = n\pi \tag{2.6}$$

($n$ is some integer) together with the Breit-Wigner form for the phase shift

$$\delta(E) = \delta_p(E) + \tan^{-1}\frac{\frac{1}{2}\Gamma}{E_r - E} \tag{2.7}$$

yields an expression for $d\epsilon_j^{(N)}/dr_M$ in terms of $E_r$ and $\Gamma$[12]:

$$\frac{d\epsilon_j^{(N)}}{dr_M} = -2\epsilon\left(r_M + \frac{4\Gamma k_j}{4(E_r-\epsilon)^2+\Gamma^2}\right)^{-1} . \tag{2.8}$$

As before, $N = M + \sum_{t=2}^{T} M_t$; and we have simply written $\epsilon$ for $\epsilon_j^{(N)}$ in the right-hand side of the last equation. Here the potential phase shift is assumed constant over the energy range considered; if we wish to relax this restriction, the expression in Eq. (2.8) becomes altered by adding $d\delta p/dE$ to $2\Gamma/[4(E_r-\epsilon)^2+\Gamma^2]$, the latter being $d\delta_{res}/dE$. The criteria for the validity of this expression are discussed in I, and may be summarized in the statement:

$$\text{range of potential} < r_M \ll 4k_j/\Gamma .$$

In order to convert Eq. (2.8) into an expression for $d\epsilon_j^{(N)}/dM$, one must know the relationship between $r_M$ and $M$ for a given basis set $\{u_m\}$. The explicit expression for $d\epsilon_j^{(N)}/dM$ applicable to the harmonic-oscillator basis set, which we use in the treatment of the model problem in Sec. III, is presented in Appendix C. After calculating the slope $d\epsilon_j^{(N)}/dM$ of the stable roots resulting from the diagonalization of $H$, approximations to $E_r$ and $\Gamma$ (and, if desired, $d\delta p/dE$) are calculated by fitting the slopes of $\epsilon_j^{(N)}$ with the function in Eq. (C1).

In Sec. III, after discussing the model problem and its exact solution, we shall use the two methods described here to find approximate values of the resonance parameters.

## III. MODEL PROBLEM

The model problem to be examined consists of a target with two bound states and an incoming particle with insufficient energy to excite the target out of its ground state. The target states $\varphi_1(y)$ and $\varphi_2(y)$ are eigenstates of $H_0$, with eigenenergies, respectively, $E_1$ and $E_2$. For this fictitious problem in which there exist no additional eigenstates of $H_0$, the eigenfunction of the complete $H$ at some energy $E$ may be written

$$\times\Psi(x,y) = F_1(x)\varphi_1(y) + F_2(x)\varphi_2(y) . \tag{3.1}$$

The equation $(E-H)\Psi = 0$ may be equivalently written as two coupled equations,

$$\left(E - E_1 + \frac{d^2}{dx^2} - V_{11}(x)\right)F_1(x) = V_{12}(x)F_2(x) , \tag{3.2a}$$

$$\left(E - E_2 + \frac{d^2}{dx^2} - V_{22}(x)\right)F_2(x) = V_{21}(x)F_1(x) , \tag{3.2b}$$

where

$$V_{ij}(x) = \int dy\, \varphi_i(y)\, \mathcal{V}(x,y)\, \varphi_j(y)$$

$$\text{for } H = H_0 - \frac{d^2}{dx^2} + \mathcal{V}(x,y) .$$

We consider the region $x \geq 0$ and solutions for which $F_1(0) = F_2(0) = 0$. The potentials $V_{ij}(x)$ are taken to be square wells:

$$\begin{aligned} V_{ii}(x) &= \lambda_i && \text{for } x \leq a , \\ V_{21}(x) &= V_{21}(x) = \eta && \text{for } x \leq a , \\ V_{ij}(x) &= 0 && \text{for } x > a , \quad i,j = 1,2. \end{aligned} \tag{3.3}$$

In addition, the energy $E$ satisfies $E_1 < E < E_2$. By taking $V_{22}(x)$ to be sufficiently deep to hold a bound state, resonances associated with the second target state occur.

These equations call to mind the radial equations for $l = 0$ resulting from truncation of the close-coupling expansion in Eq. (1.1) after the first two terms. Thus, we may hope that observations made concerning the various approximation methods for this specific model might be applicable to more realistic situations.

The exact solution of the model problem is easily found. Briefly, by eliminating $F_2(x)$ from Eqs. (3.2) for $x \leq a$ we obtain a fourth-order equation for $F_1(x)$ whose solution is of the form

$$F_1(x) = a_1 \sin(\beta_- x) + a_2 \sin(\beta_+ x) .$$

Here $\beta_\pm$ depend explicitly on the parameters of the problem: $E_1$, $E_2$, $\lambda_1$, $\lambda_2$, $\eta$, and $a$. The function $F_2$ is immediately determined from $F_1$ by Eq. (3.2b). By connecting $F_1$ and $F_2$ and their first derivatives at $x = a$ to the asymptotic solutions

$$F_1 = e^{-ik_1 x} + \alpha_1 e^{ik_1 x} ,$$

$$F_2 = \alpha_2 e^{ik_2 x}$$

(where $k_i^2 = E - E_i$ for $i = 1, 2$) and their derivatives, the four unknowns $a_1$, $a_2$, $\alpha_1$, and $\alpha_2$ are determined. This, of course, is valid for all $E$. For $E_1 < E < E_2$ when only elastic scattering is energetically allowed, $F_2$ is a square-integrable function (i.e., $ik_2 \equiv -\varkappa_2$

is real). From the conservation relation $|\alpha_1|^2 = 1$ the phase shift $\delta$ is given by

$$\tan\delta = -\,\mathrm{Im}\alpha_1 (1 - \mathrm{Re}\alpha_1)^{-1} \quad .$$

Our procedure was to choose a set of parameters ($E_i$, $\lambda_i$, $\eta$, and $a$) and calculate the phase shift $\delta$ for a range of $E$ values sufficient to exhibit resonance behavior. We fitted the resulting values of $\delta(E)$ against the Breit-Wigner form in Eq. (2.7), where $\delta_p$ was taken to be a second-degree polynomial in $E$, and thus computed the resonance parameters $E_r$, $\Gamma$, and $\delta_p$ at $E = E_r$.

To obtain resonances of varying widths, we repeated this procedure for several values of the coupling $\eta$, holding the other parameters fixed. In particular, we chose the following parameters for the problem: $\lambda_1 = 5$, $\lambda_2 = -16$ (which has a bound state at $E_b = -9.8765$), $E_1 = 0$, and $E_2 = 100$ for wells of width $a = 1$. The values of coupling considered were $\eta = 1.0$, 10, and 20. It may be noted that equivalent results are obtained for a well of width $a \neq 1$, if the energy and potential parameters are reduced by a factor $a^2$.

To be free from all approximations (even that introduced by the fitting of $\delta$ with the Breit-Wigner form), the $T$ matrix, as defined in $F_1 \sim \sin k_1 x - Te^{ik_1 x}$, was calculated in the complex-energy plane. One can define the position of the pole as $E_r - \frac{1}{2}i\Gamma$ in absolute terms, without reference to the potential or resonant part of $T$. The pole position calculated for $\eta = 10$ agreed to better than 0.1% with the result found from the Breit-Wigner fit. We thus refer to the resonance parameters obtained from the Breit-Wigner fit of the exact phase shifts as the "correct results"—these results are presented in the first column of Table I, for the three couplings considered. To facilitate comparison among the various approximation methods studied throughout the paper, representative results of each method will be included in Table I along with the exact results.

With the correct results available for comparison, we are now ready to apply the stabilization method to the model problem. For our basis we choose functions of the form $\varphi_i(y) u_m(x)$ $(i = 1, 2)$, where the functions $u_m(x)$ are the odd (i.e., zero at $x = 0$) harmonic-oscillator functions, normalized on an interval $[0, \infty]$. In terms of the Hermite polynomials $h_m(\alpha x)$, we have

$$u_m(x) = \left(\frac{\alpha}{2^{(2m-2)}(2m-1)!\sqrt{\pi}}\right)^{1/2} h_{2m-1}(\alpha x)\, e^{(-1/2)\alpha^2 x^2} \,,$$

where $\alpha^2 = \frac{1}{2}\omega$. It is useful to write the matrix representation of $H$ in four blocks

$$(H) = \begin{pmatrix} H11 & H12 \\ H21 & H22 \end{pmatrix} \quad ,$$

where

$$(HIJ)_{mn} = \int_0^\infty u_m(x) \left( -\frac{d^2}{dx^2}\,\delta_{IJ} + V_{IJ}(x) \right) u_n(x)\, dx \quad .$$

Here, of course, $V_{IJ}(x)$ are the square wells given in Eq. (3.3). These matrix elements are easily evaluated with the aid of recursion relations for $u_m$. The dimensionality of $HII$ is $M_I \times M_I$, so that complete $H$ is $N \times N$ where $N = M_1 + M_2$.

Before proceeding, we seek a frequency $\omega$ for which a reasonable number (say, 20 to 40) of functions $u_m$ spans the entire range of the potential. Diagonalizing $H22$ (i.e., a square well of depth $\lambda_2$) in a basis of $M_2$ functions, we obtained the best results with $\omega = 30$: The lowest root gave the bound-state energy to five places of accuracy, whereas the corresponding eigenvector represented the exact eigenfunction to better than four figures. Hence, for the diagonalization of complete $H$, we used basis functions with $\omega = 30$.

TABLE I. Comparison of the exact and approximate resonance parameters. Columns $A$ and $B$: stabilization method with Eqs. (2.5) and (2.8), respectively. Column $C$: Feshbach's method neglecting the continuum of $QHQ$. Column $D$: Feshbach's method with $P\Phi_0^{(3)}$ [Eq. (4.8)]. Column $E$: Muckerman's adiabatic method. Column $F$: Miller's method.

| $\eta$ | | Exact results | Approximate results $A$ | $B$ | $C$[a] | $D$ | $E$[b] | $F$ |
|---|---|---|---|---|---|---|---|---|
| | $E_r$ | 90.1346 | 90.1347 | 90.1347 | 90.1346 | ••• | 90.1346 | ••• |
| 1.0 | $\Gamma$ | 0.001472 | 0.001484 | 0.001591 | 0.001470 | 0.001473 | 0.001473 | 0.001494 |
| | $\delta_p$ | −0.2718 | −0.3012 | ••• | −0.2727 | −0.2718 | −0.2719 | ••• |
| | $E_r$ | 91.2161 | 91.2161 | 91.2155 | 91.2185 | ••• | 91.2151 | ••• |
| 10.0 | $\Gamma$ | 0.1720 | 0.1711 | 0.1666 | 0.1537 | 0.1737 | 0.1713 | 0.1747 |
| | $\delta_p$ | −0.1854 | −0.1802 | ••• | −0.2694 | −0.1832 | −0.2001 | ••• |
| | $E_r$ | 94.3836 | 94.3869 | 94.3818 | 94.3875 | ••• | 94.3592 | ••• |
| 20.0 | $\Gamma$ | 0.7912 | 0.7869 | 0.7883 | 0.6633 | 0.8063 | 0.8185 | 0.7721 |
| | $\delta_p$ | 0.0507 | 0.0775 | ••• | −0.2600 | 0.1336 | −0.0113 | ••• |

[a]Unshifted energy: $W_r = 90.1235$ for each $\eta$.

[b]Unshifted energy: $W_r = 90.1350$ for $\eta = 1$, $W_r = 91.2483$ for $\eta = 10$, and $W_r = 94.3444$ for $\eta = 20$.

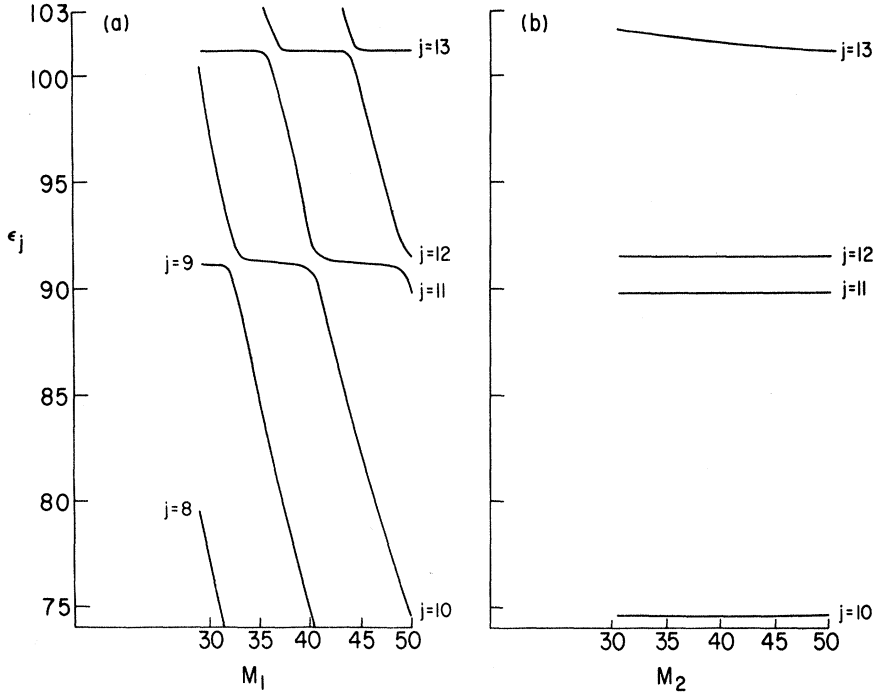


FIG. 1. Variation of the eigenvalues $\epsilon_j^{(N)}$ with basis-set size $N=M_1+M_2$ for $\eta=10$. (a) $M_1$ is varied for $M_2=50$; (b) $M_2$ is varied for $M_1=50$.

Let us proceed with the diagonalization. We shall discuss only the case of intermediate coupling, i.e., $\eta=10$, in detail. However, we comment in advance that the behavior discussed in the following is typical of the three couplings considered. From the criteria for stability already discussed, we are looking for a root below excitation threshold $E_2$ which is stable with respect to a variation of $M_1$($M_2$ constant) and a variation of $M_2$($M_1$ constant). Figures 1(a) and 1(b) show some of the roots plotted as a function of basis size: In Fig. 1(a), the size of the $H11$ matrix (i.e., $M_1$) varies, whereas in Fig. 1(b) $M_2$ varies. It is evident that several roots are stable under variation of $M_1$ or $M_2$; but only one below $E_2$—the 11th in this case—is stable under the addition of both types of functions. It is this root that we call the stable root, from which the resonance parameters will be calculated.

In Paper I, the "crossing of roots," wherein the $j$th root takes on the character of the $(j-1)$ root as $N$ increases, was attributed to a change in $x_N$ by a half-wavelength for $k^2=\epsilon_j^{(N)}$. For the elastic scattering problem, this behavior of the roots appears uncomplicated by the presence of more than one type of basis functions. For example, in Fig. 1(a), when the 11th root is the stable root for $41 \lesssim M_1 \lesssim 49$, spanning an additional half-wavelength is accomplished by adding eight or nine basis functions—just the number added before the 12th root becomes the stable root at $M_1=50$.

Figure 1(b) shows that when type-2 functions are added, all roots below the inelastic threshold, i.e., for $\epsilon_j < E_2 = 100$, are extremely stable. In fact, changing $M_2$ from 30 to 50 (for $M_1=50$) caused $\epsilon_{12}$ (the stable root) to change by less than 0.0002%. In addition, Fig. 2 shows that the sum $S_2 = \sum_{m=1}^{M_2} u_m(x) c_{m2}^{(j)}$ is a very good approximation to the exact function $F_2(x)$. Although, the root $\epsilon_j$ considered here is near $E_r$, the function $F_2$, due to its bounded nature, was equally well approximated for *all* roots below $E_2$. These results show that the expansion of $F_2$ in terms of $\{u_m\}$ has indeed converged for $M_2 \geq 30$.

How well does the sum $S_1$ given in Eq. (2.1) represent the scattering function $F_1$ for $E < E_2$? Guided

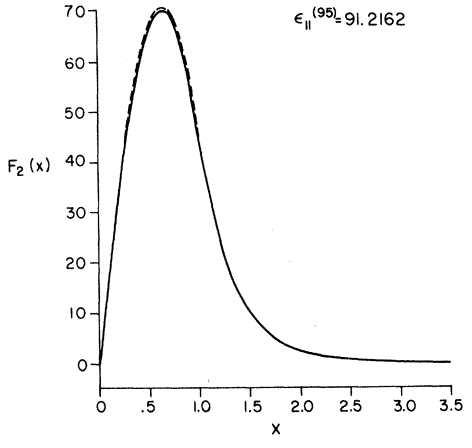


FIG. 2. Comparison of approximate and exact closed-channel functions for $E$ near $E_r$, $\eta=10$: (dashed line) $S_2$ in $\Phi_j^{(N)}$ and (solid line) $F_2$ in $\Psi_E$ calculated at $E=\epsilon_j^{(N)}$, for $j=11$ and $N=M_1+M_2$ with $M_1=45$ and $M_2=50$.

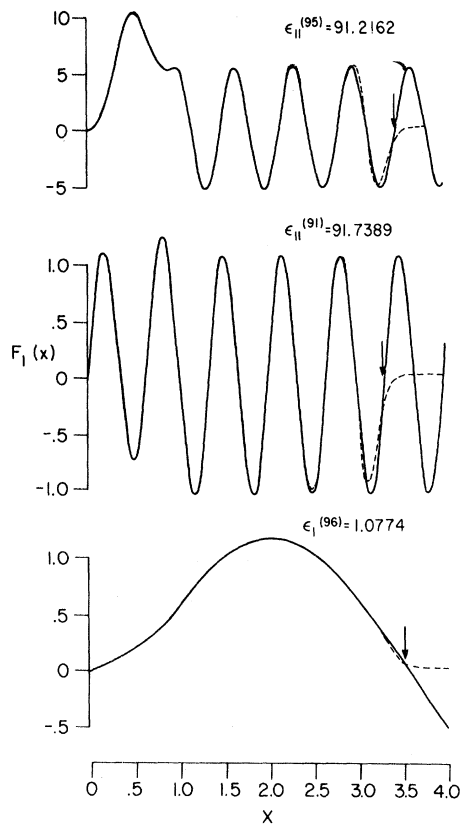


FIG. 3. Comparison of the approximate function $S_1$ (dashed line) with the exact open-channel function $F_1$ (solid line) at $E=\epsilon_j^{(N)}$ ($\eta=10$, $M_2=50$) for $\epsilon_j^{(N)}$ nearest $E_r$, i.e., $j=11$ and $N=95$; for another $\epsilon_j^{(N)}$ in the stable region, i.e., $j=11$ and $N=91$; and for the lowest eigenvalue $\epsilon_1^{(N)}$ with $N=96$. Arrows indicate the appropriate values of $x_M$ given by Eq. (3.4) for $M=M_1$.

by the behavior observed for the wave function in I, we expect a good approximation to $F_1$ in a region $x<x_M$, where $x_M$ is the point at which $S_1(x)$ becomes negligible and, in addition, coincides with a node of $F_1(x)$ in the asymptotic region. For the harmonic-oscillator basis $x_M$ is taken to be the classical turning point for the last function $u_M(x)$ in the basis, so that $M=M_1$ and

$$x_M^2=(8M-2)/\omega\,. \tag{3.4}$$

In Fig. 3, $F_1$ and the approximation $S_1$ are plotted for $\epsilon_j$ near resonance, slightly off resonance, and for an energy far from $E_r$. On each graph, the position of the appropriate $x_M$ is indicated. Off resonance, $F_1$ resembles the wave function of the well $V_{11}(x)$, while near $E_r$, $F_1$ loses nodes in the inner region, where it takes on the character of a quasibound state.[13] It appears that the expansion in terms of $\{u_m\}$ well approximates the (structured) inner region of $F_1$ at *all* energies, and, in addition, the "wall theory" of I concerning the coincidence of $x_M$ with a node in $F_1$ is equally valid for the elastic scattering from a target.

As in I, $\Phi_j$ approximates the inner part of $\Psi_E$ only within a normalization factor; hence the functions $S_i(x)$ were multiplied by a constant in Figs. 2 and 3. In all cases, of course, $S_1$ and $S_2$ were renormalized by the same factor, otherwise $\Phi_j$ would not approximate $\Psi_E$. For energies near $E_r$, the ratio of the maxima of $F_2$ and $F_1$ (or $S_2$ and $S_1$) was large (a value of 7 for the root nearest $E_r$), while off resonance the ratio was small (a value of 0.04 for $\epsilon_1$). In addition, for the stable roots, the coefficients of the first few type-2 functions are large, i.e., $c_{m2} > c_{m1}$ for small $m$, indicating that the resonance is associated with the excited state $\varphi_2$ of the target.

Now that we have found the stable root $\epsilon_j^{(N)}$ for several values of $N$, and demonstrated that the corresponding eigenvectors $\Phi_j^{(N)}$ are good approximations to $\Psi_E$ at $E=\epsilon_j$, we are ready to use the methods described in Sec. II to calculate the resonance parameters. The expression in Eq. (2.5) requires the use of $\Delta\epsilon^{(N+1)}=\epsilon_j^{(N+1)}-\epsilon_j^{(N)}$, along with $\Phi_j^{(N+1)}$ and $\Phi_j^{(N)}$ for several values of $N$. For the expression in Eq. (C1), the derivative $d\epsilon_j^{(N)}/dM$ is computed numerically from $\epsilon_j^{(n)}$ for $n=N$ and $N\pm1$. Clearly, any number of the available stable roots may be used to find a fit for these functions of $E_r$ and $\Gamma$; we have carried out the fitting procedure, for both these methods, using several different sets of points.

In Table II we present the values of $E_r$, $\Gamma$, and $\delta_p$ obtained from using fits of $\Delta\epsilon^{(N+1)}$ given in Eq. (2.5), or approximation $A$. For each coupling, three results for $E_r$, $\Gamma$, and $\delta_p$ are shown. The first column, under each $\eta$ indicates how close one can get to the exact results by a judicious (and perhaps fortuitous) choice of points. The second and third columns show how decreasing or increasing, respectively, the number of points causes the results to vary. It is apparent that the dependence on the number of points used in the fits increases for larger coupling; this increase in ambiguity is especially pronounced for $E_r$. Since in deriving Eqs. (2.3) and (2.5) we assumed that the eigenvalue $\epsilon_j$ was near $E_r$, the roots and corresponding eigenvectors used in the fit must lie in the stable region. We observed in the calculation that as we introduced roots from the edge of the stable region (i.e., near the crossing of roots), where $\epsilon_j$ is far from $E_r$ and where $\Phi_j$ does not well represent the exact $\Psi$ at $E_r$, the fit became worse. On the other hand, too few points gave insufficient information about the curvature of $\epsilon_j$ to allow determination of an accurate width. In general, best results were obtained for a number of points somewhere between the two extremes: for $\eta=10$ the set of stable roots between $M_1=41$ and $M_1=47$ [Fig. 1(a)] fits this description

TABLE II. Dependence of the approximate resonance parameters on the number of points used in the fitting of Eq. (2.5) with approximation $A$ and Eq. (2.8) with approximation $B$.

| Method | Number of points[a]: | $\eta=1$ 7 | $\eta=1$ 5 | $\eta=1$ 9 | $\eta=10$ 7 | $\eta=10$ 5 | $\eta=10$ 9 | $\eta=20$ 8 | $\eta=20$ 6 | $\eta=20$ 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| $A$ | $E_r$ | 90.1347 | 90.1347 | 90.1347 | 91.2161 | 91.2182 | 91.2183 | 94.3869 | 94.3547 | 94.4236 |
| | $\Gamma$ | 0.001484 | 0.001371 | 0.001459 | 0.1711 | 0.1599 | 0.1730 | 0.7869 | 0.8346 | 0.8059 |
| | $\delta_p$ | −0.3012 | −0.2138 | −0.2543 | −0.1802 | −0.1783 | −0.1603 | 0.0775 | 0.0020 | 0.1506 |
| $B$ | $E_r$ | 90.1347 | 90.1347 | 90.1347 | 91.2149 | 91.2155 | 91.2162 | 94.3749 | 94.3818 | 94.3771 |
| | $\Gamma$ | 0.001262 | 0.001591 | 0.001200 | 0.1658 | 0.1666 | 0.1656 | 0.8221 | 0.7883 | 0.8172 |

[a]The number of points listed refers to the number $\epsilon_j$ values used in approximation $A$, and to the number of $(d\epsilon_j/dM)$ values in approximation $B$.

and gave the results shown in column $A$ of Table I.

The resonance parameters calculated with the second method, or approximation $B$, are also presented in Table II. The three sets of results $(E_r, \Gamma)$ for each coupling show the variation observed from the use of different sets of points. In the use of Eq. (2.8), $d\delta p/dE$ was included as a third parameter, since for the problem at hand we found that its inclusion, in general, gave values of $E_r$ and $\Gamma$ which were less dependent on the number of points used in the fit. However, the resulting $d\delta p/dE$ was neither independent of the number of points nor a good approximation to the known value. Using this method, we obtained the best results, shown in column $B$ of Table I, with a relatively small number of points: five or six for the harmonic-oscillator basis with a frequency of $\omega = 30$.

For the three values of $\eta$ investigated, the first method gives the somewhat better results. The fact that we have obtained reasonable results from $A$ is encouraging, since its use requires only information readily available from the stabilization procedure. In contrast, approximation $B$ demands a knowledge of the functional dependence of the "wall" $x_M$ on the basis size, which for some bases will not be available. In their requirement of a fitting procedure, both methods suffer from a certain ambiguity of the results. But if it turns out that the range of values obtained from a reasonable set of roots is more accurate than a unique result from another approximation method, then the ambiguity may well be a price worth paying.

Up until now, we have discussed only those roots which are below the excitation threshold. For $E > E_2$, the function $F_2$ as well as $F_1$ is nonzero in the asymptotic region. For scattering in which two channels are open, there exist two linearly independent regular solutions of which some linear combination yields the desired boundary conditions. By analogy with roots below threshold, we postulate that the eigenvector $\Phi_j^{(N)}$ produced by the diagonalization represents *some* eigensolution of $H$ at energy $\epsilon_j^{(N)} > E_2$. In particular, the root $\epsilon_j^{(N)}$ and the corresponding solution $\Phi_j^{(N)}$ which appear are determined by the two requirements that $S_1$ go to zero at a node in $F_1$ *and* $S_2$ go to zero at a node in $F_2$. (This was verified numerically by finding the particular solution which some $\Phi_j^{(N)}$ represented.) A more detailed discussion will be deferred to a future paper on inelastic scattering.

## IV. ADDITIONAL APPROXIMATIONS

Feshbach's method of projection operators[4] for finding resonance parameters is easily formulated for the two-dimensional model. Writing $H$ in the matrix representation of target states, i.e.,

$$H = \begin{pmatrix} E_1 - \frac{d^2}{dx^2} + V_{11}(x) & V_{12}(x) \\ V_{12}(x) & E_2 - \frac{d^2}{dx^2} + V_{22}(x) \end{pmatrix}, \tag{4.1}$$

we may choose

$$P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad Q = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Thus solving

$$(W_i - QHQ)\,\xi_i = 0, \tag{4.2}$$

for $\xi_i$ bounded, becomes equivalent to finding the bound states of the attractive well $V_{22}(x)$ at energies $W_i - E_2$. Assuming only one bound state $\xi_r$, the width and resonance energy require the solution of

$$(E - PH'P)\,P\Phi_0 = 0. \tag{4.3}$$

Here $PH'P = PHP + PH_0P$ with

$$H_0 = \int dW_s\, HQ\xi_s\rangle (E - W_s)^{-1} \langle \xi_s QH\,.$$

The functions $\xi_s$ are the continuum solutions of Eq. (4.2) at energy $W_s$, and $P\Phi_0$ is the solution of Eq. (4.3) at $E_r$ which takes on the asymptotic behavior

$$P\Phi_0 \sim (k\pi)^{-1/2} e^{i\delta_p} \sin(kx + \delta_p). \tag{4.4}$$

If $G(x, x')$ is the standing-wave Green's function for Eq. (4.3) at $E = E_r$, then the width and resonance energy are given by

$$\Gamma = 2\pi \left| \langle \xi_r V_{12} P\Phi_0 \rangle \right|^2, \tag{4.5a}$$

$$E_r = W_r + \Delta_r, \tag{4.5b}$$

and

$$\Delta_r = \langle \xi_r V_{12} G(x, x') V_{12} \xi_r \rangle, \tag{4.5c}$$

where

$$PHQ = QHP = V_{12}.$$

Since the exact solution of Eq. (4.3) is very difficult even for the simple problem at hand, one is led naturally to performing various approximations on the so-called optical potential $PH'P$, which connects $\xi_r$ to the continuum of the attractive well, via $V_{12}$. We do this now for the model problem.

The first, and simplest, approximation we can make is to neglect completely the continuum of $V_{22}$, giving the solution $P\Phi_0^{(0)}$ of $(E - PHP)P\Phi_0^{(0)} = 0$; we call this approximation $C$. For the model problem, $P\Phi_0^{(0)}$ is the scattering solution of $V_{11}$ at $E_r$. Taking

$$G_0 = \frac{\mathcal{P}}{E - PHP},$$

we may write

$$G_0(x, x') = -(1/k)\, v_1(x_<) v_2(x_>), \tag{4.6}$$

where $x_<$ ($x_>$) is the lesser (greater) of the two quantities $x$ and $x'$, and $v_i$ are solutions of $(E - PHP)v_i = 0$. Specifically, $v_i$ is the regular solution at the origin with asymptotic behavior $\sin(kx + \delta_0)$ while $v_2$ is the irregular solution which connects asymptotically to $\cos(kx + \delta_0)$. Because of the simple nature of the solutions of the square well, $\Delta_r$ and $\Gamma$ can be expressed in closed form. The resulting values of $E_r$, $\Gamma$, and $\delta_p$ (i.e., $\delta_0$) are shown in column $C$ of Table I.

Higher-order approximations to $\Gamma$ may be made by calculating a better solution $P\Phi_0$ of Eq. (4.3). We do this by treating $PH_0P$ as a perturbation, so that $P\Phi_0$ becomes a solution of the integral equation

$$P\Phi_0 = P\Phi_0^{(0)} + G_0 PH_0 P\Phi_0 . \tag{4.7}$$

By iteration we get

$$P\Phi_0^{(n)}(x) = P\Phi_0^{(0)}(x) + \int dW_s (E - W_s)^{-1} \int dx'\, G_0(x, x') V_{12} \xi_s(x') \int dx''\, \xi_s(x'') V_{12} P\Phi_0^{(n-1)}(x''), \tag{4.8}$$

where the continuum solutions $\xi_s$ of $V_{22}$ are normalized to give $\sin(k_s x + \delta_s)\,(\pi k_s)^{-1/2}$ for $x > a$. Using Eq. (4.6) for $G_0(x, x')$, we numerically integrated over $x''$ and $W_s$ in Eq. (4.8) to obtain $P\Phi_0$ and $\Gamma$ in successive approximations (i.e., $P\Phi_0^{(1)}$ from $P\Phi_0^{(0)}$, etc.). In Table III we show the improved values of $\Gamma$, and those of $\delta_p$, as approximated by the phase shift of $P\Phi_0^{(n)}$ for $n = 1, 2, 3$. It is apparent that for $\eta = 1$ and 10 the first iteration compensates for most of the contribution from the continuum of $V_{22}$. For comparison with the other methods we include the results obtained from the third iteration in column $D$ of Table I.

Is it feasible to carry out a similar iterative procedure for $\Delta_r$? Since in theory $P\Phi_0$ may be calculated to arbitrary accuracy, one might wonder whether the full $G$ in $\Delta_r$ could be constructed from two homogeneous solutions of Eq. (4.3), similar in form to $G_0$ in Eq. (4.6). The resulting (numerical) Green's function would yield $\Delta_r$ to arbitrary accuracy. Unfortunately, the nonlocality of $PH'P$ prohibits such a product construction of $G$. In fact, it appears that one is left with the unwieldy task of expressing $G$ in terms of a complete set of solutions of Eq. (4.3); a task far too costly even for the simple problem at hand. In view of the result that approximation $C$, which neglects the continuum of $V_{22}$, yields a far better shift than width, at least for this model problem, it is fortunate that by improving $P\Phi_0$, $\Gamma$ is the quantity which benefits.

TABLE III. Convergence of the iterative procedure used in approximation $D$ to obtain improved values of $\Gamma$ and $\delta_p$ in Feshbach's formalism.

| | $\eta = 1$ | | $\eta = 10$ | | $\eta = 20$ | |
|---|---|---|---|---|---|---|
| $n$ | $\Gamma$ | $\delta_p$ | $\Gamma$ | $\delta_p$ | $\Gamma$ | $\delta_p$ |
| 1 | 0.001 473 | −0.2718 | 0.1775 | −0.1381 | 1.0902 | −1.0357 |
| 2 | 0.001 473 | −0.2718 | 0.1736 | −0.1850 | 0.7778 | 0.4335 |
| 3 | 0.001 473 | −0.2718 | 0.1737 | −0.1832 | 0.8063 | 0.1336 |

In a recent paper,[6] Muckerman applied the so-called adiabatic method for calculating the width to the problem of scattering by a rigid rotor. Since his results were encouraging, we have applied the technique, or approximation $E$, to our model problem. Essentially this method differs from the Feshbach approach described in approximation $C$ in that it uses a basis, given by $\chi_i = C_{i1}\varphi_1 + C_{i2}\varphi_2$, in which the Hamiltonian minus the kinetic-energy term is diagonal, rather than the basis $\varphi_i$ in which the kinetic energy is diagonal. This approach gives two coupled equations, like Eqs. (3.2), where $V_{11}$ and $V_{22}$ are replaced by new square wells $\mathcal{S}_1(x)$ and $\mathcal{S}_2(x)$, and the equations are now coupled by the kinetic-energy operator. If $R_1(x)$ is the scattering solution for the potential $\mathcal{S}_1(x)$ at energy $E_r$ and if $R_2(x)$ is the bound-state solution of $\mathcal{S}_2(x)$ at energy $W_r$, then the expressions for the width and shift resemble those used in approximation $C$. For our model problem

$$\Gamma = (2/k)\eta_{eff}^2 \left| \int_0^a R_1(x) R_2(x)\, dx \right|^2 \qquad (4.9a)$$

and

$$\Delta_r \equiv E_r - W_r = \eta_{eff}^2 \int_0^a dx\, R_2(x) \int_0^a dx'\, G_0(x, x') R_2(x') + \mathrm{ST}\,, \qquad (4.9b)$$

where $\eta_{eff}$ is a constant equal to $(\mathcal{E}_2 - \mathcal{E}_1)C_{12}/C_{11}$ for $x < a$. Here $G_0(x, x')$ is the Green's function for the potential $\mathcal{E}_1(x)$, and ST is the surface term resulting from an integration by parts. The resulting values of $E_r$, $\Gamma$, and $\delta_p$ [where $\delta_p$ is taken as the phase shift of $R_1(x)$], which are presented in column $E$ of Table I, give a marked improvement over the results of approximation $C$. In both approximation $C$ and $E$ the continuum of the attractive well was neglected; however, in the adiabatic approximation the continuum is coupled to $P\Phi_0$ only through the kinetic energy—apparently a weaker coupling than the potential $V_{12}(x)$. In addition, this method assumes that the kinetic energy commutes with $(C_{12}/C_{11})$, an assumption which is rigorously, rather than approximately, valid between zero and $a$ for the square-well problem. Therefore, although one might expect to see improved results from working in the adiabatic basis, the extremely good accuracy of the results may indeed be an artifact of the model problem.

As the final method, or approximation $F$, we shall discuss a calculation of the width proposed by Miller.[7] Using as a guide Feshbach's formula [Eq. (4.5a)], Miller calculates the width from

$$\Gamma = (2/k) \left| \int_0^\infty f(x) \sin(kx + \delta_0)(H - E)\Phi_r\, dx \right|^2 , \qquad (4.10)$$

where $\Phi_r$ is a good (bound) approximation to the exact wave function at $E_r$ in the nonasymptotic region and $\delta_0$ is the exact potential phase shift. If $\Phi_r$ is such a function, then $(H - E)\Phi_r$ is approximately zero in the inner region and the only contribution to the integral in Eq. (4.5a) is from the region in which $P\Phi_0$ has the asymptotic behavior in (4.4)—thus the *raison d'être* of Eq. (4.10). [The operator $(H - E)$ instead of $H$ appears in order to orthogonalize $\Phi_r$ and $P\Phi_0$.] The function $f(x)$ in Eq. (4.10) did not appear in Miller's original expression[7] for $\Gamma$, in which case a surface term results for $\delta_0 \neq 0$. Recently, Miller has suggested[14] the use of some function $f(x)$ for which $f(0) = 0$ and $f \to 1$ as $x \to \infty$, so that $P\Phi_0$ is approximated by a function which is zero at $x = 0$. For the model problem, we have calculated $\Gamma$ using

(i) $f(x) = 1$ for all $x$

and

(ii) $f(x) = 1 - e^{-\lambda x^2/2}$.

In particular, $\lambda = 5$ was chosen so that $f \to 1$ at a value of $x$ not too close to zero but less than $x_M$.

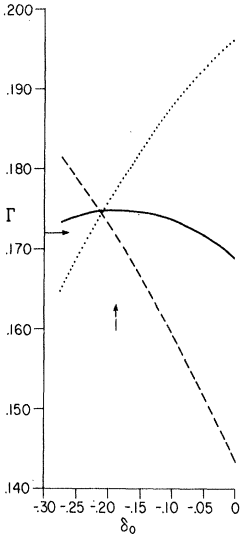


FIG. 4. Dependence of $\Gamma$ on $\delta_0$, in method (ii) of Miller, for three eigenvalues near $E_r$ ($\eta = 10$ and $M_2 = 50$): $\epsilon_{11}^{(95)} = 91.2162$ (solid line); $\epsilon_{11}^{(94)} = 91.2485$ (dotted line); $\epsilon_{11}^{(96)} = 91.1840$ (dashed line). Arrows indicate the exact values of $\Gamma$ and $\delta_p$.

From the application of the stabilization procedure, we have available eigenvectors which satisfy Miller's requirement for $\Phi_r$. Taking the eigenvector associated with the root closest to the resonance energy found by the stabilization method, we have computed $\Gamma$ for various "guesses" of $\delta_0$. Specifically, for each coupling, we have tried $\delta_0 = 0$, $\delta_0 = -0.27$ (approximately the phase shift due to scattering from $V_{11}$), and the correct value of $\delta_p$. The results from both methods (i) and (ii), presented in Table IV, show the sensitivity of $\Gamma$ to the choice of $\delta_0$. For method (ii), the best results are obtained from the correct value of $\delta_p$ and they become more reliable as the coupling is decreased; neither of these trends appear for method (i). In addition it turns out that $\Gamma$ is sensitive to the choice of stable eigenvector used. In Fig. 4 we show the values of $\Gamma$ as a function of $\delta_0$, computed by method (ii) (for $\eta = 10$) from three eigenvectors associated with the roots nearest $E_r$. Each of the $\Phi_j$ is a good approximation to $\Psi_E$ at $E = E_r$ and thus satisfies Miller's criterion. It is evident that the dependence of $\Gamma$ on the choice of the stable eigenvector used disappears in the neighborhood of $\delta_0 = \delta_p$. We have found the same behavior for all values of $\eta$. These results suggest that if in a

TABLE IV. Dependence of the calculated widths on the assumed values of the potential phase shift $\delta_0$ in methods (i) and (ii) of Miller.

| $\delta_0$ | $\eta = 1.0$ | | $\eta = 10$ | | $\eta = 20$ | |
|---|---|---|---|---|---|---|
| | (i) | (ii) | (i) | (ii) | (i) | (ii) |
| exact[a] | 0.001372 | 0.001494 | 0.1722 | 0.1747 | 0.7226 | 0.7721 |
| 0.0 | 0.001304 | 0.001326 | 0.1635 | 0.1689 | 0.7409 | 0.7734 |
| −0.27 | 0.001372 | 0.001494 | 0.1724 | 0.1734 | 0.7727 | 0.7152 |

[a]The values of the exact $\delta_p$ for each $\eta$ are given in Table I.

problem the correct $\delta_p$ is not known, Miller's formula should be computed for a number of stable roots (if available) and then $\delta_0$ should be varied until all the roots yield essentially the same $\Gamma$. The validity of this procedure for the calculation of $\Gamma$ and $\delta_p$ will be examined in a future paper.[15] For comparison with the other approximations, we list the widths calculated with method (ii) for $\delta_0 = \delta_p$ in column *F* of Table I.

## V. CONCLUSIONS

We have completed the discussion of all results presented in Table I. What, if any, conclusions are we able to draw concerning the comparative validity of the approximation methods tried? For small coupling, for which a small width is expected, a Feshbach calculation which neglects the continuum of *QHQ* (i.e., the potential giving rise to the resonance) gives satisfactory resonance parameters. On the other hand, as the coupling increases, additional work is necessary to obtain accurate values of $E_r$ and $\Gamma$. The adiabatic method (approximation *E*), when feasible, seems (from Muckerman's work and the work here) to give better results than other approximation methods which involve the same amount of effort (e.g., approximation *C* here). The two methods described in Sec. II, which use information from the stabilization procedure, give reliable values for $E_r$. For the problem considered here, approximation *A*, involving explicit use of the square-integrable eigenvectors, gives more accurate widths; obviously, we are not in a position to generalize this conclusion to more complicated systems.

We conclude with final remarks about the stabilization procedure. The observations made in I for single-particle resonances in potential scattering are found to be valid for compound-state resonances occurring in elastic scattering as well. In particular, when the exact $H$ is diagonalized in a large enough set of square-integrable basis functions, those eigenenergies below excitation threshold appear for which the exact open-channel function has a node at the "wall" defined by the basis set. Furthermore, the square-integrable eigenfunctions are good approximations, apart from a normalization factor, to the inner parts of the exact scattering wave function at energies equal to the corresponding eigenvalues in both the resonant and nonresonant energy regions. Roots occurring near the exact resonance energy are stable; the corresponding eigenfunctions represent the quasibound or resonance state. Since for sufficiently large basis sets the addition of type-1 (open-channel) basis functions affects only the asymptotic region, we were able to derive expressions relating the resonance parameters, $E_r$ and $\Gamma$, to the variation in the stable root with increasing basis sets. The coincidence of a node in the exact open-channel function with the wall defined by the basis set will hopefully enable us to extend the formalism to resonances occurring in inelastic scattering.

## ACKNOWLEDGMENTS

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## APPENDIX A

In order to derive Eq. (2.2), let $\{\Phi_i\}$ and $\{\epsilon_i\}$ be the $N$ eigenvectors and eigenvalues resulting from the diagonalization of $H$ in the orthonormal basis set $\{\psi_i\}\, i = 1, \cdots N$, and let $\{\chi_i\}$ and $\{W_i\}$ be the corresponding quantities from the diagonalization in the set $\{\psi_i\} i = 1, \cdots N+1$. If we define the projection operator

$$Q_M = \sum_{i=1}^{M} |\psi_i\rangle\langle\psi_i|$$

for any $M$, then $Q_N$ is equivalent to $\sum_{i=1}^{N} |\Phi_i\rangle\langle\Phi_i|$ and

$$Q_{N+1} = Q_N + |\psi_{N+1}\rangle\langle\psi_{N+1}| \ . \tag{A1}$$

The eigenvectors $\chi_i$ satisfy

$$(W_i - Q_{N+1} H Q_{N+1})\chi_i = 0 \ . \tag{A2}$$

By taking the scalar product of $\Phi_j$ with Eq. (A2) and then using Eq. (A1) with the relationships $\langle\Phi_i H \Phi_j\rangle = \delta_{ij}\epsilon_i$, and $\langle\Phi_i \Phi_j\rangle = \delta_{ij}$, $i, j \leq N$, we obtain

$$W_i\langle\Phi_j \chi_i\rangle - \epsilon_j\langle\Phi_j \chi_i\rangle - \langle\Phi_j H\psi_{N+1}\rangle\langle\psi_{N+1}\chi_i\rangle = 0 \ . \tag{A3}$$

If we define $\Delta\epsilon^{(N+1)} \equiv W_j - \epsilon_j$, then the rearranging of Eq. (A3) for $i = j$ yields Eq. (2.2).

## APPENDIX B

In the usual Feshbach formalism, if we define $Q = |\chi_r\rangle\langle\chi_r|$ and $P = 1 - Q$, then the solution of

$$(E - H)\Psi_E^+ = 0$$

gives

$$Q\Psi_E^+ = \frac{|\chi_r\rangle\langle\chi_r QHP\Phi_E^+\rangle}{E - W_r - \Delta_r + \frac{1}{2}i\Gamma} \ .$$

As usual,

$$\Gamma = 2\pi\left|\langle\chi_r QHP\Phi_E^+\rangle\right|^2$$

and

$$\Delta_r = \left\langle\chi_r QHP \frac{\mathcal{P}}{E - PHP} PHQ\chi_r\right\rangle ,$$

where $P\Phi_E^+$ is the solution of

$$(E - PHP)\,P\Phi_E^+ = 0 \ .$$

For elastic scattering from a spherically symmetrical potential, we expand

$$\Psi_E^+ = (\pi k)^{-1/2} r^{-1} \sum_l R_l(r)\, Y_{l0}(\hat{r}) \ , \tag{B1}$$

where

$$R_l(r) \xrightarrow[r\to\infty]{} i^l e^{i\delta_l} \sin(kr + \delta_l - \tfrac{1}{2} l\pi) \ . \tag{B2}$$

For a resonance with angular momentum $L$ we take

$$\begin{aligned} \langle \vec{r} \,|\, \chi_r \rangle &= r^{-1} \chi(r)\, Y_{L0}(\hat{r}) \ , \\ \langle \vec{r} \,|\, \psi_{N+1} \rangle &= r^{-1} \psi_{N+1}(r)\, Y_{L0}(\hat{r}) \ . \end{aligned} \tag{B3}$$

If we assume that $\psi_{N+1}$ contributes only in the asymptotic region, then using Eqs. (2.3), (B1), (B2), and (B3) we obtain

$$\langle \psi_{N+1} \chi_r \rangle = (2/k\Gamma_L)^{1/2} (E - E_r + \tfrac{1}{2} i\Gamma_L)\, i^L e^{i(\delta_L - \alpha_L)} I_L \ . \tag{B4}$$

Here

$$I_L = \int_0^r dr \, \sin(kr + \delta_L - \tfrac{1}{2} L\pi)\, \psi_{N+1}(r),$$

and $\alpha_L$ is the phase of $\langle \chi_r QHP\Phi_E^+ \rangle$. Again evoking the Breit-Wigner expression in Eq. (2.7), we take $\delta_L = \delta_p^L + \delta_r^L$, where

$$\tan\delta_r^L = \tfrac{1}{2}\Gamma_L/(E_r - E) \ ,$$

so that

$$E - E_r + \tfrac{1}{2} i\Gamma_L = -e^{i(\delta_p^L - \delta_L)} \left[ (E - E_r)^2 + (\tfrac{1}{2}\Gamma_L)^2 \right]^{1/2} . \tag{B5}$$

To ensure reality of $\langle \psi_{N+1} \chi_r \rangle$, we take $\alpha_L = \delta_p^L$ for $L$ even and $\alpha_L = \delta_p^L - \tfrac{1}{2}\pi$ for $L$ odd. Then substituting Eq. (B5) together with the definitions

$$S_N = \int_0^\infty dr \, \sin kr \, \psi_N(r) \ , \qquad C_N = \int_0^\infty dr \, \cos kr \, \psi_N(r)$$

into the expression in (B4), we obtain, for $L$ even,

$$\langle \psi_{N+1} \chi_r \rangle = (2/k\Gamma_L)^{1/2} \left[ (E - E_r)(S_{N+1} \cos\delta_p^L + C_{N+1} \sin\delta_p^L) + \tfrac{1}{2}\Gamma_L (S_{N+1} \sin\delta_p^L - C_{N+1} \cos\delta_p^L) \right]$$

and, for $L$ odd,

$$\langle \psi_{N+1} \chi_r \rangle = (2/k\Gamma_L)^{1/2} \left[ (E - E_r)(C_{N+1} \cos\delta_p^L - S_{N+1} \sin\delta_p^L) + \tfrac{1}{2}\Gamma_L (C_{N+1} \sin\delta_p^L + S_{N+1} \cos\delta_p^L) \right] .$$

A remark should be made concerning the sign of $\chi_r$. The eigenvectors produced from a diagonalization of $H$ are unique only within a sign. It is evident from Eq. (2.2) that $\Delta\epsilon^{(N+1)}$ is independent of the sign of $\chi_r$ or $\Phi_r$; this must also be true for Eq. (2.5). In theory, the proportionality factor between $\chi_r$ and $Q\Psi_E^+$, whose sign is affected by the choice of $\alpha_L$, determines the over-all sign of the eigenvectors to be used in Eq. (2.5). For the model problem, consistency between Eqs. (2.2) and (2.5) was maintained by choosing the signs of $\chi_r$ and $\Phi_r$ such that $\langle \Phi_r \chi_r \rangle > 0$.

## APPENDIX C

For an harmonic oscillator of mass $\mu$ centered around $x = a_0$, the relationship between the classical turning point $x_m$ and $m$ for the $m$th harmonic-oscillator function is given by

$$\tfrac{1}{2}\mu\omega^2 (x_m - a_0)^2 = (m - \tfrac{1}{2})\hbar\omega \ .$$

In this case, an expression for $d\epsilon_j/dm$ is obtained from Eq. (2.8)

$$\frac{d\epsilon_j}{dm} = -2\epsilon_j \Bigg/ \left[ a_0 \left( \frac{\mu\omega(2m-1)}{\hbar} \right)^{1/2} + (2m-1) + \frac{2\Gamma}{4(E_r - \epsilon_j)^2 + \Gamma^2} \left[ 2\epsilon_j \hbar\omega (2m-1) \right]^{1/2} \right] . \tag{C1}$$

Here the criterion of validity is generalized to

$$\text{range of potential} < x_m \ll \frac{2\hbar}{\Gamma} \left( \frac{2E_r}{\mu} \right)^{1/2} .$$

In the model problem, where $M$ odd harmonic-oscillator functions comprised the basis, the number $m$ in Eq. (C1) is replaced by $2M$.

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[10]Throughout the calculation Rydberg units are used, and the mass of the scatterer is taken to be the mass of the electron, i.e., $\mu = \frac{1}{2}$.

[11]This, of course, is valid for $l = 0$ only; for $l \neq 0$ the formalism may be generalized by taking $j_l(k_j r_M + \delta_l) = 0$.

[12]This expression differs from Eq. (20) in I, because here we use Rydberg instead of atomic units.

[13]In the diagonalization of $H$ for a potential-scattering problem, the orthogonality of the eigenvectors is accomplished by each possessing a different number of nodes. Here the disappearance of nodes described can occur

because

$$\langle \Phi_i \Phi_j \rangle = \langle S_1^{(i)} S_1^{(j)} \rangle + \langle S_2^{(i)} S_2^{(j)} \rangle = 0, \quad i \neq j$$

may hold even when $S_1^{(i)}$ and $S_1^{(j)}$ have the same number of nodes.

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