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Calculation of Energies and Widths of Resonances in Inelastic Scattering: Stabilization Method*

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In previous work, the stabilization method of calculating resonance parameters was applied to potential scattering and to elastic scattering from a target. The method is here extended to compound-state resonances in inelastic scattering and its application to a model problem for a target with three bound states is examined. The eigenfunctions associated with eigenvalues ϵ_j obtained from the diagonalization of the exact Hamiltonian in appropriately chosen sets of square-integrable basis functions are good approximations, in the inner region, to particular linear combinations of the degenerate exact scattering solutions at $E=\epsilon_j$ (above inelastic threshold). The partial widths are calculated from a Fermi's-"Golden-Rule"-like formula involving the matrix elements of the exact Hamiltonian between the square-integrable eigenfunctions representing the resonance state and potential-scattering solutions at the same energy. The slowly varying (as a function of E) potential-scattering S matrix, knowledge of which is required in the calculation of the decay widths, is determined using the criterion that several good approximations to the resonance state yield exactly the same widths. For the exactly soluble model problem studied here, the resonance parameters obtained with the stabilization method compare well with the exact values, especially for narrow resonances. The theoretical limitations of the method are discussed.

I. INTRODUCTION

For collision processes which involve the formation and decay of a quasidiscrete resonance state, the energy dependence of the cross section can be expressed in terms of a few physically meaningful parameters, such as the resonance energy E_r, the width Γ (or the decay lifetime $\hbar/\Gamma$), and the slowly varying potential-scattering S matrix. In recent years, several methods[1,2] have been proposed for the direct calculation of these parameters from approximations to the exact resonance wave function, without recourse to solution of the complete energy-dependent cross section. One example is the stabilization method[3–5] which, until now, has been applied only to resonances occurring in elastic scattering. Since many processes of interest involve excitation of the target, we investigate here the extension of the method to inelastic scattering.

In Paper I,[3] the stabilization method was applied to scattering from a one-dimensional model potential whose barrier gave rise to so-called single-particle resonances. Later in II,[4] we extended the method to elastic scattering from a target and studied its application to a model problem in which compound resonances occurred. In III,[5] we proposed a new method for the calculation of all the resonance parameters including the potential-scattering or background phase shift. This method utilizes approximate resonance wave functions obtained from the stabilization procedure, together with a Fermi's-"Golden-Rule"-like formula originally proposed by Miller.[6] In this paper, we shall extend the stabilization method to inelastic scattering and study its application to a model problem in which compound resonances decay into two open channels. Also, we shall generalize the method proposed in III for the calculation of the resonance parameters, so that, in principle, the stabilization method may be applied to problems with an arbitrary number of open channels.

In order to establish the framework for the discussion that follows, we summarize briefly the stabilization method as applied to elastic scattering.[4,5] For scattering from a target, the complete (no-exchange) wave function may be written in the form

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

where $\vec{r}_0$ represents the coordinates of the target particles, $\vec{r}$ is the coordinate of the scatterer, and E is the total energy. The functions ϕ_t represent the target states. For elastic scattering, only F_1 is nonzero in the asymptotic region. After choosing an appropriate basis of square-integrable functions $\{u_m(\vec{r})\}$, one expands the channel functions F_t, $t=1, \ldots, T$ (including the continuum function F_1) in terms of the $\{u_m\}$ for specific energies ϵ_j. The resulting approximate wave function has the form

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

The specific energies ϵ_j and the expansion coefficients $c_{mt}^{(j)}$ are determined by diagonalizing the complete Hamiltonian in the basis set $\{\phi_t(\vec{r}_0)u_m(\vec{r})\}$, $m=1, \ldots, M_t$, $t=1, \ldots, T$. To search for a resonance, one diagonalizes the Hamiltonian in successively larger basis sets. The presence of a "stable" root, i.e., one which does not change significantly as the size of the basis increases, indicates a resonance. The eigenfunction corresponding to a stable eigenvalue ϵ_j is a good approximation to the inner part of the exact resonance function, and can be used to calculate the resonance parameters.[5]

The extension of the stabilization method to inelastic scattering is complicated by several factors. At a total energy E, for which N channels are open, the equation $(E-H)\Psi_E = 0$ has N linearly independent solutions. Based on the results obtained for elastic scattering, we may anticipate that Φ_j, obtained in the diagonalization of H, is a good approximation to the inner part of an exact solution at energy ϵ_j. But the important question is *which* particular exact solution? In the case of elastic scattering, those eigenvalues ϵ_j are obtained for a given basis set, say, $\{\phi_t(\vec{r}_0)u_m(\vec{r})\}$, $m=1, \ldots, M_t$, $t=1, \ldots, T$, for which the *only* open-channel function F_1 has a node approximately at the point where the amplitudes of the functions $\{u_m\}$, $m=1, \ldots, M_1$, become negligible. In other words, the ϵ_j are determined by the channel radius or "wall" defined by the one-particle basis set $\{u_m\}$, $m=1, \cdots, M_1$. In the case of inelastic scattering, however, there are N open-channel functions and, correspondingly, N-channel radii defined by the one-particle basis sets $\{u_m,\ m=1, \cdots, M_t\}$, $t=1, \cdots, N$. Since the sizes of the basis sets M_t can be varied independently, the N independent-channel radii appear to overdetermine the eigenvalue ϵ_j. As we shall see, these problems have a common resolution. For sufficiently large basis sets, the square-integrable Φ_j approximates a particular solution which is a linear combination of the N exact linearly independent solutions with, for example, outgoing boundary conditions. The $N-1$ linear coefficients (Nth being determined by the over-all normalization) and the eigenvalue ϵ_j are uniquely determined by the N-channel radii.

The calculation of the resonance parameters in the inelastic case is complicated by the fact that even for one partial wave there are N partial widths and $N(N+1)/2$ background parameters (e.g., the elements of the potential-scattering S matrix). We have been able to derive a practical procedure for the calculation of the resonance parameters by working within the eigenphase representation of the potential-scattering S matrix. The formalism is relatively simple in this representation because a given partial width depends on only one of the background eigenphases.

The extension of the stabilization method to inelastic scattering is discussed qualitatively in Sec. II. The method for calculating the resonance parameters is formulated in Sec. III. To show the utility of the method, we apply it to compound resonances occurring in an exactly soluble model problem which simulates the inelastic scattering of a projectile from a fictitious target with three states. In Sec. IV we discuss the model problem and its exact solution, and present the results of the stabilization method.

II. QUALITATIVE DISCUSSION OF STABILIZATION METHOD

We consider the scattering of a projectile from a target with internal states at energies E_t, $t=1, 2, \ldots$. In the case of scattering at a total energy E, where $E_N < E < E_{N+1}$, the exact (no-exchange) scattering wave functions with outgoing boundary condition can be written in the form[1]

$$\Psi_{E\alpha}^{+} = \sum_{t=1}^{\infty} \phi_t(\vec{r}_0)\, F_{t\alpha}^{+}(\vec{r}), \quad \alpha = 1, \ldots, N. \tag{2.1}$$

Here, α labels the N linearly independent solutions of $(E-H)\,\Psi = 0$ that result in the case of N open channels. The functions $\phi_t(\vec{r}_0)$, $t=1, \ldots, N$, must be the exact wave functions of the N lowest internal states of the target, whereas $\phi_t(\vec{r}_0)$, $t>N$, may represent either true excited states or pseudostates[7] chosen to improve the convergence of the expansion in Eq. (2.1).

Now consider a particular solution of $(E-H)\Psi = 0$:

$$\Psi_{E\beta} = \sum_{\alpha=1}^{N} d_\alpha \Psi_{E\alpha}^{+} \ . \tag{2.2}$$

By defining a set of particular channel functions $G_t(\vec{r})$:

$$G_t(\vec{r}) = \sum_{\alpha=1}^{N} d_\alpha F_{t\alpha}^{+}(\vec{r}) \ , \tag{2.3}$$

we can rewrite Eq. (2.2) in the form

$$\Psi_{E\beta} = \sum_{t=1}^{\infty} \phi_t(\vec{r}_0) G_t(\vec{r}). \tag{2.4}$$

In the stabilization method, for specific energies

the channel functions $G_t(\vec{r})$, including the continuum functions G_1, G_2, ..., G_N, are expanded in terms of an appropriate set of square-integrable functions $u_m(\vec{r})$ $m=1, \ldots$. Thus, the scattering wave function $\Psi_{E\beta}$ is approximated by the expression in Eq. (1.2). The specific energies ϵ_j and the expansion coefficients $c_{mt}^{(j)}$, $j=1, \ldots, M_0$, are just the eigenvalues and the corresponding eigenvectors obtained from the diagonalization of the complete Hamiltonian in the basis $\{\phi_t(\vec{r}_0)u_m(\vec{r})\}$ $m=1, \ldots, M_t$, $t=1, \ldots, T$ (where $M_0=\sum_{t=1}^{T} M_t$). Here we emphasize that because the approximate wave function contains open-channel components [terms $t=1, \ldots, N$ in Eq. (1.2)], the stabilization method differs significantly from previous methods[8] in which the approximate resonance functions are obtained by projecting out the open-channel components.

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 G_t, $t>N$, in terms of $\{u_m\}$ converges because for $t>N$ the G_t themselves are exponentially decaying in the asymptotic region. The expansion of the open-channel functions G_t, $t\leq N$, however, cannot converge in the strict mathematical sense. Nevertheless, based on the results obtained in I and II, we shall assume that the expansion of G_t, $t\leq N$, in terms of the square-integrable basis functions, determines the specific energies ϵ_j and contains the scattering information. In order to discuss this assumption in more detail, we need to consider the point r_m, at which the amplitude of the basis function $u_m(\vec{r})$ becomes negligible. The point r_m is not uniquely defined, but in most cases one can reasonably assume that it equals the outer classical turning point associated with u_m. This is the definition we adopt for the following discussion. If the basis $\{u_m(\vec{r})\}$ is so ordered that $r_m>r_{m-1}$ for all m, then the amplitude of any function expanded in terms of $\{u_m\}$, $m=1, \ldots, M$, must become negligible for $r\geq r_M$. This result was utilized in the case of elastic scattering[3] to find a relationship between r_M and the eigenvalues ϵ_j obtained in the diagonalization. In particular, for a given basis $\{u_m\}$, $m=1, \ldots, M$, those ϵ_j (between E_1 and E_2) are obtained, for which the only open-channel function has a node at r_M. In the case of inelastic scattering, however, one cannot find a particular ϵ_j for which, simultaneously, $F_{1\alpha}^{+}(\vec{r})$ has a node at r_{M_1}, $F_{2\alpha}^{+}(\vec{r})$ has a node at r_{M_2}, etc., for any α. Fortunately, there are N linearly independent solutions, so that one can construct a particular solution with channel functions G_t [see Eqs. (2.3) and (2.4)] which, for selected energies ϵ_j, have nodes at r_{M_t}, $t\leq N$, respectively. Correspondingly, the expansion

$$Z_t(\vec{r})=\sum_{m=1}^{M_t} u_m(\vec{r})\, c_{mt}^{(j)} \tag{2.5}$$

is a good approximation (apart from a t-independent but otherwise arbitrary normalization constant) to the function $G_t(\vec{r})$ out to r_{M_t}, and decays exponentially to zero for $r>r_{M_t}$. The numerical results presented in Sec. IV show that these assumptions are essentially correct.

The linear coefficients $\{d_\alpha\}$ are determined by the set of homogeneous equations

$$G_t(\vec{r}_{M_t})=\sum_{\alpha=1}^{N} d_\alpha F_{t\alpha}^{+}(\vec{r}_{M_t})=0, \quad t=1, \ldots, N. \tag{2.6}$$

In order to obtain a nontrivial solution for $\{d_\alpha\}$, one must require that

$$\det \mathcal{F}(E)=0 \ , \tag{2.7}$$

where $\mathcal{F}$ is the $N\times N$ matrix with elements $F_{t\alpha}^{+}(\vec{r}_{M_t})$. (Here, we explicitly denote the energy dependence of $\mathcal{F}$, because the channel functions $F_{t\alpha}^{+}$ are, of course, energy dependent.) The eigenvalues ϵ_j that result from the diagonalization of H in a particular basis set are given by the roots of Eq. (2.7). For each ϵ_j there is a corresponding set of coefficients $\{d_\alpha(\epsilon_j)\}$.

From Eqs. (2.6) and (2.7) it is clear that as the basis set is enlarged (i.e., the corresponding M_t increase), different sets of eigenvalues $\{\epsilon_j\}$ result. More specifically, the Hylleraas-Undheim theorem[9] predicts that all the eigenvalues must decrease as the number $M_0=\sum_{t=1}^{T} M_t$ increases. It is the different behavior of eigenvalues near and far from the exact resonance energy E_r that allows the identification of a resonance.

In the case of elastic scattering,[3,4] we found that, as the Hamiltonian is diagonalized in successively larger bases, the presence of a stable eigenvalue (i.e., one which changes only slightly as the basis is increased) indicates the existence of a resonance. Now we must consider the stabilization property of eigenvalues representing resonances at energies above inelastic threshold. The Hylleraas-Undheim theorem[9] ensures that for some basis set there will be an eigenvalue, say ϵ_j, close to E_r.[10] Let us assume that this basis is large enough so that each r_{M_t} ($t=1, \ldots, T$) is greater than the range of the potentials in the problem. Then, based on the results of Papers I and II, we predict that ϵ_j will be stable with respect to addition of basis function $\phi_t u_{M_t+1}$, regardless of the value of t. For $t>N$, ϵ_j will not change significantly as $\phi_t u_{M_t+1}$ is added to the basis, because, if r_{M_t} is greater than the range of potentials, then the expansion of the closed-channel functions G_t in terms of $\{u_M\}$, $m=1, \ldots, M_t$, has already converged. For $t\leq N$, ϵ_j will decrease only slightly (depending on the magnitude of the width) with the addition of $\phi_t u_{M_t+1}$ to the basis;

this behavior can be argued as follows. It is known that for energies near E_r, $\Psi_{E\beta}$ has a much smaller amplitude in the asymptotic region than in the inner region. If r_{M_t} is greater than the range of potentials, then $\phi_t u_{M_t+1}$, $t \leq N$, contributes only to the asymptotic part of $\Psi_{E\beta}$ which has a relatively small amplitude. As a result, u_{M_t+1} enters the expansion of G_t (an open-channel function) with a small coefficient, and the eigenvalue is only slightly affected. Again, the numerical results presented in Sec. IV show that these arguments are essentially correct.

Here we wish to emphasize that in searching for a stable eigenvalue representing a physical resonance, it is very important to test the stability of ϵ_j with respect to *all* types of basis functions which may contribute to the open-channel part of $\Psi_{E\beta}$. If this is not done, one can be misled by an *apparently* stable root to conclude that a physical resonance exists. For example, it is conceivable that for a problem in which no physical resonances occur, a particular open-channel function (or functions), say G_v, has a much smaller asymptotic amplitude than G_t, $t \neq v$, $t \leq N$. In this case, ϵ_j will be relatively stable with respect to the addition of $\phi_v u_{M_v+1}$, but it will decrease significantly when $\phi_t u_{M_t+1}$, $t \neq v$, is added to the basis. Fortunately, only for physical resonances, i.e., at E_r, will the asymptotic amplitudes of *all* the open-channel functions be smaller than the inner part of $\Psi_{E\beta}$. Thus, only those eigenvalues ϵ_j which represent physical resonances will be stable with respect to the addition of all $\phi_t u_m (t = 1, \ldots, T)$ to the basis.

In addition to the stabilization property of an eigenvalue near E_r, the magnitudes of the expansion coefficients in the associated eigenvector Φ_j also indicate that a stable root represents the resonance state. In the sense that a resonance state is a "quasibound" state, and thus Φ_j is larger in the inner region than in the asymptotic region, we expect, for a resonance associated with the tth 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 $c_{mt}^{(j)}$ for $\epsilon_j > E_t$ will indicate single-particle resonances while large $c_{mt}^{(j)}$ for $\epsilon_j < E_t$ will indicate closed-channel, or compound, resonances. Hence, we can apply the stabilization method equally well to both types of resonances.

III. CALCULATION OF RESONANCE PARAMETERS

As the eigenfunction Φ associated with a stable root ϵ is a good approximation, apart from an overall normalization constant, to the inner part of a particular exact solution $\Psi_{E\beta}$ at $E = \epsilon$, Φ satisfies the criterion for its use in the computation of the decay widths.[5,6] In this section, we utilize the analysis of the method developed previously for elastic scattering[5] to derive explicit formulas for the resonance energy and partial widths which are applicable to inelastic processes.

Guided by the Feshbach formalism[11] of projection operators, we define $Q = |\Phi\rangle\langle\Phi|$ and $P = 1 - Q$, and construct $Q\Psi^+_{E\alpha}$:

$$|Q\Psi^+_{E\alpha}\rangle = |\Phi\rangle\langle\Phi HP\tilde{\psi}^+_{E\alpha}\rangle(\epsilon - E_r + i\Gamma/2)^{-1} \ . \quad (3.1)$$

The lth partial wave of the potential scattering solution $P\tilde{\psi}^+_{E\alpha}$, which satisfies $(E - PHP)P\tilde{\psi}^+_{E\alpha} = 0$, has the asymptotic form[12]

$$(\mu/2\hbar^2\pi)^{1/2}\, i^{l+1} \sum_{t=1}^{N} \phi_t(\vec{r}_0)\left[\delta_{t\alpha} k_\alpha^{-1/2} e^{-ik_\alpha r} + (-)^{l+1} k_t^{-1/2} \mathcal{S}^p_{t\alpha} e^{ik_t r}\right] , \quad (3.2)$$

where $E = E_t + \hbar^2 k_t^2/2\mu$, $t = 1, \ldots, N$. $P\tilde{\psi}^+_{E\alpha}$ and $\mathcal{S}^p$ are slowly varying functions of E and represent the background or nonresonant part of the scattering. The total width Γ is a sum over open channels:

$$\Gamma = 2\pi \sum_{\alpha=1}^{N} |\langle\Phi HP\tilde{\psi}^+_{E\alpha}\rangle|^2 \equiv \sum_{\alpha=1}^{N} \tilde{\Gamma}_\alpha \ , \quad (3.3)$$

where $\hbar/\tilde{\Gamma}_\alpha$ is the lifetime for the decay of the resonance into the αth physical channel.

In order to express the proportionality constant between Φ and $Q\Psi^+_{E\alpha}$ in terms of the resonance parameters, it is convenient to work with the functions $P\psi^+_{E\gamma}$ in the eigenphase representation of $\mathcal{S}^p$. The relationship between the two representations is

$$P\psi^+_{E\gamma} = \sum_{\alpha=1}^{N} P\tilde{\psi}^+_{E\alpha} \mathfrak{U}_{\alpha\gamma} \ , \quad (3.4)$$

where the real orthogonal matrix $\mathfrak{U}$ diagonalizes $\mathcal{S}^p$ to give the background eigenphases $\{\Delta_\gamma\}$:

$$\mathfrak{U}^\dagger \mathcal{S}^p \mathfrak{U} = e^{2i\Delta} \ . \quad (3.5)$$

In Eq. (3.5), $e^{2i\Delta}$ represents the diagonal matrix with nonzero elements $e^{2i\Delta_\gamma}$. The lth partial wave of $P\psi^+_{E\gamma}$ has the asymptotic form

$$(2\mu/\hbar^2\pi)^{1/2}\, e^{i\Delta_\gamma} \sum_{t=1}^{N} \phi_t(\vec{r}_0) k_t^{-1/2}\, \mathfrak{U}_{t\gamma} \sin(k_t r - l\pi/2 + \Delta_\gamma) \ . \quad (3.6)$$

Without loss of generality, one may define a set of partial widths $\{\Gamma_\gamma\}$ according to

$$\Gamma_\gamma = 2\pi |\langle\Phi HP\psi^+_{E\gamma}\rangle|^2 \ , \quad (3.7)$$

where $\langle\Phi HP\psi^+_{E\gamma}\rangle$ is the amplitude for the decay of the resonance into the γth eigenchannel of $\mathcal{S}^p$. Of course, the total width is invariant under the transformation $\mathfrak{U}$ and is a simple sum of partial widths, $\Gamma = \sum_\gamma \Gamma_\gamma$. In Eq. (3.6) all the factors except $e^{i\Delta_\gamma}$ are real, so one may write[13]

$$\langle\Phi HP\psi^+_{E\gamma}\rangle = (2\pi)^{-1/2} e^{i\Delta_\gamma} \Gamma_\gamma^{1/2} \ . \quad (3.8)$$

Substituting Eqs. (3.4) and (3.8) into (3.1), one

finally obtains

$$|Q\Psi^{+}_{E\alpha}\rangle = |\Phi\rangle(2\pi)^{-1/2}(E-E_r+i\Gamma/2)^{-1}\sum_{\gamma=1}^{N}\mathfrak{U}_{\alpha\gamma}e^{i\Delta_\gamma}\Gamma_\gamma^{1/2}\ . \tag{3.9}$$

Next we assume that the normalization constant relating Φ and $\Psi_{E\beta}$ can be deduced from the proportionality constant given in Eq. (3.9). Using the definition of $\Psi_{E\beta}$ in terms of $\Psi^{+}_{E\alpha}$ [Eq. (2.2)], together with Eq. (3.9), we obtain, for $E=\epsilon$,

$$|\Psi_{\epsilon\beta}\rangle = |\Phi\rangle(2\pi)^{-1/2}(\epsilon-E_r+i\Gamma/2)^{-1} \times\sum_{\gamma=1}^{N}\sum_{\alpha=1}^{N}d_\alpha(\epsilon)\mathfrak{U}_{\alpha\gamma}e^{i\Delta_\gamma}\Gamma_\gamma^{1/2}\ . \tag{3.10}$$

It should be emphasized that Eq. (3.10), in contrast to (3.9), is valid only in the inner region where the square-integrable function Φ is significantly different from zero.

If the exact solutions $\Psi^{+}_{E\alpha}$ are defined according to the usual outgoing boundary conditions, then the lth partial wave of $\Psi_{E\beta}$ has the asymptotic form, for $E=\epsilon$,

$$(\mu/2\hbar^2\pi)^{1/2}i^{l+1}\textstyle\sum_\alpha d_\alpha(\epsilon)\sum_t\phi_t(\vec{r}_0)[\delta_{t\alpha}k_\alpha^{-1/2}e^{-ik_\alpha r} + (-)^{l+1}k_t^{-1/2}\mathcal{S}_{t\alpha}e^{ik_t r}]. \tag{3.11}$$

(Henceforth, all sums run from 1 to N, unless specifically noted otherwise.) In terms of the resonance parameters, the elements of the full energy-dependent S matrix are given by[14]

$$\mathcal{S}_{t\alpha}=\textstyle\sum_\omega\sum_\gamma\mathfrak{U}_{t\omega}e^{i\Delta_\omega}[\delta_{\omega\gamma}-i(\Gamma_\gamma\Gamma_\omega)^{1/2} \times(E-E_r+i\Gamma/2)^{-1}]\mathfrak{U}_{\alpha\gamma}e^{i\Delta_\gamma}\ . \tag{3.12}$$

While considering practical methods for the computation of decay widths, Miller suggested[6] that if Φ is a good approximation to the inner part of the exact solution of $(E-H)\Psi=0$, then the matrix element in Eq. (3.8) has no contribution from the inner region. As a result, in evaluating $\langle\Phi HP\psi^{+}_{E\gamma}\rangle$ one may replace $P\psi^{+}_{E\gamma}$ by a function χ_E, which has exactly the same asymptotic form as $P\psi^{+}_{E\gamma}$, but whose inner part is arbitrary. This procedure simplifies the computation of the widths, because, provided the assumption about Φ is correct, one needs to know only the asymptotic behavior of $P\psi^{+}_{E\gamma}$, i.e., the elements of $\mathcal{S}^p$ or $e^{i\Delta}$ and $\mathfrak{U}$, but not its functional form for all r. Unfortunately, in most cases one does not know *a priori* the potential-scattering parameters; so in order to compute Γ_γ one must either solve $(E-PHP)P\psi^{+}_{E\gamma}=0$, a bleak prospect, or estimate $\mathcal{S}^p$. Even the second alternative seems to be impractical, because, as we have found for the case of elastic scattering,[5] the computed width appears to depend strongly on the assumed value of the potential-scattering phase shift δ_p. Fortunately, in the elastic case we were able to use this dependence of the computed width on δ_p to good advantage by recognizing that, in general, two slightly different but equally good resonance functions Φ give exactly the same width only if the assumed value of δ_p is close to the exact value. Thus, if at least two good Φ are available, say from the stabilization procedure, then one can determine both Γ and δ_p by requiring that the two Φ give exactly the same Γ.

We now show that an exactly analogous behavior of the computed widths holds for resonances above inelastic threshold, and suggest a procedure for the calculation of all the resonance parameters. We propose to calculate the partial widths from Eq. (3.8) by replacing $P\psi^{+}_{E}$ by a function χ_E whose lth partial wave has the asymptotic form

$$(2\mu/\hbar^2\pi)^{1/2}\textstyle\sum_t\phi_t(\vec{r}_0)k_t^{-1/2}\mathcal{V}_t e^{i\tau}\sin(k_t r-l\pi/2+\tau)\ , \tag{3.13}$$

but is otherwise arbitrary. The variables τ and $\mathcal{V}$ represent the "trial" values for a given Δ and the corresponding column of $\mathfrak{U}$, respectively. Writing the computed *partial* widths as $\Gamma(\epsilon,\tau,\mathcal{V})$ to show their dependence on Φ, ϵ, and the "trial" background parameters, we have, from Eq. (3.8),

$$\Gamma(\epsilon,\tau,\mathcal{V})^{1/2}=e^{-i\tau}\langle\Phi(H-\epsilon)\chi_\epsilon\rangle(2\pi)^{1/2}\ . \tag{3.14}$$

In Eq. (3.14) the operator $H-\epsilon$ instead of H appears in order to remove the restrictions that χ_ϵ be orthogonal to Φ. If R is the point at which the square-integrable function Φ becomes negligible, then the matrix element in Eq. (3.14) has no contribution from $r>R$. Assuming that Φ is proportional to $\Psi_{\epsilon\beta}$ for $r<R$, we may substitute Eq. (3.10) into (3.14) to obtain

$$\Gamma(\epsilon,\tau,\mathcal{V})^{1/2}=2\pi e^{-i\tau}(\epsilon-E_r-i\Gamma/2) \times[\textstyle\sum_\gamma\sum_\alpha d_\alpha^*(\epsilon)\mathfrak{U}_{\alpha\gamma}e^{-i\Delta_\gamma}\Gamma_\gamma^{1/2}]^{-1}\langle\Psi_{\epsilon\beta}(H-\epsilon)\chi_\epsilon\rangle\ . \tag{3.15}$$

If the point R is beyond the range of interactions, then the matrix element in Eq. (3.15) can be evaluated using the asymptotic forms of $\Psi_{\epsilon\beta}$ and χ_ϵ given by Eqs. (3.11) and (3.13), respectively. The derivation, whose details are given in Appendix A, yields the following expression for the computed partial widths:

$$\Gamma(\epsilon,\tau,\mathcal{V})^{1/2}=\textstyle\sum_\omega L_\omega e^{i(\tau-\Delta_\omega)}\Gamma_\omega^{1/2}+2D(\epsilon-E_r-i\Gamma/2) \times\sum_\omega L_\omega[\sum_\alpha d_\alpha^*(\epsilon)\mathfrak{U}_{\alpha\omega}]e^{-i\Delta_\omega}\sin(\tau-\Delta_\omega)\ , \tag{3.16}$$

where

$$L_\omega=\textstyle\sum_t\mathcal{V}_t\mathfrak{U}_{t\omega}$$

and

$$D=[\textstyle\sum_\omega\sum_\alpha d_\alpha^*(\epsilon)\mathfrak{U}_{\alpha\omega}e^{-i\Delta_\omega}\Gamma_\omega^{1/2}]^{-1}\ .$$

Before discussing the implications of Eq. (3.16), we

emphasize that the validity of the results depends on the assumption embodied in Eq. (3.10).

Equation (3.16), which is the generalization of Eq. (10) of Paper III to inelastic scattering, shows the dependence of the computed widths on the resonance function Φ through $d_\alpha^*(\epsilon)$ and ϵ, the eigenvalue associated with Φ. In addition, as expected from the results obtained for elastic scattering, $\Gamma(\epsilon,\tau,\mathcal{U})$ becomes independent of ϵ and Φ, and reduces to the exact partial widths when the "trial" background parameters become equal to the corresponding exact parameters. Specifically, if $\mathcal{U}_t = \mathfrak{U}_{t\gamma}$, $t=1, \ldots, N$, then $L_\omega = \delta_{\gamma\omega}$ because $\mathfrak{U}$ is a real orthogonal matrix, and Eq. (3.16) reduces to

$$\Gamma(\epsilon,\tau,\bar{\mathfrak{U}}_\gamma)^{1/2} = e^{i(\tau-\Delta_\gamma)}\,\Gamma_\gamma^{1/2} + 2D(\epsilon - E_r - i\Gamma/2)e^{-i\Delta_\gamma} \times \sin(\tau-\Delta_\gamma)\textstyle\sum_\alpha d_\alpha^*(\epsilon)\,\mathfrak{U}_{\alpha\gamma} \ . \quad (3.17)$$

(Here $\bar{\mathfrak{U}}_\gamma$ denotes the γth column of the matrix $\mathfrak{U}_{\gamma\cdot}$.) If, in addition, $\tau = \Delta_\gamma$, then Eq. (3.17) becomes

$$\Gamma(\epsilon,\Delta_\gamma,\bar{\mathfrak{U}}_\gamma)^{1/2} = \Gamma_\gamma^{1/2} \ . \quad (3.18)$$

To summarize, all resonance functions Φ that satisfy Eq. (3.10) give the exact partial widths via Eq. (3.14) provided the function χ_ϵ has exactly the same asymptotic behavior as $P\psi_{\epsilon\gamma}^+$; or, equivalently, if the background parameters associated with χ_ϵ are equal to the corresponding exact parameters in $P\psi_{\epsilon\gamma}^+$.

Based on the results contained in Eq. (3.16), we suggest the following practical procedure for the computation of *all* the resonance parameters from several good resonance functions Φ, which are obtained from the diagonalization of H in successively larger basis sets.

(a) By requiring that several different Φ give exactly the same partial width Γ_γ computed from Eq. (3.14) for $\tau = \Delta_\gamma$ and $\mathcal{U}_t = \mathfrak{U}_{t\gamma}$, $t=1, \ldots, N$, one can determine approximations to the background eigenphases Δ_γ and the matrix $\mathfrak{U}$.

(b) Once the potential-scattering parameters, and thus $\mathcal{S}^p$, are known, one can calculate Γ_γ from Eq. (3.14).

(c) After Δ_γ, $\mathfrak{U}$, and Γ_γ are known, approximations to E_r may be found from an expression equivalent to Eq. (3.16) for each Φ.

To see how the first step of the above procedure works for N open channels, consider $\Gamma^{(n)}(\epsilon^{(n)},\tau,\mathcal{U})$ computed from $\Phi^{(n)}$, $n=1, \ldots, N+1$, where n distinguishes the stable roots obtained from different diagonalizations. Equations (3.17) and (3.18) show that all the $\Gamma^{(n)}$ become equal as τ and $\mathcal{U}_t$ take on the values Δ_γ and $\mathfrak{U}_{t\gamma}$, respectively. As a result, the N unknowns Δ_γ and $\mathfrak{U}_{t\gamma}$, $t=1, \ldots, N-1$, may be determined from the equations

$$\sqrt{\Gamma^{(1)}}(\Delta_\gamma,\bar{\mathfrak{U}}_\gamma) = \sqrt{\Gamma^{(2)}}(\Delta_\gamma,\bar{\mathfrak{U}}_\gamma) = \cdots = \sqrt{\Gamma^{(N+1)}}(\Delta_\gamma,\bar{\mathfrak{U}}_\gamma) \ . \quad (3.19)$$

Since $\mathfrak{U}$ is an orthogonal matrix $\mathfrak{U}_{N\gamma}$ is determined by the normalization condition

$$\sum_{t=1}^{N} \mathfrak{U}_{t\gamma}^2 = 1 \ . \quad (3.20)$$

In general, eliminating $\mathfrak{U}_{t\gamma}$, $t=1, \ldots, N$, from Eqs. (3.19) and (3.20) gives an Nth-order equation whose solutions are the potential-scattering eigenphases Δ_γ, $\gamma=1, \ldots, N$. If Eq. (3.10) rigorously holds, then the matrix $\mathfrak{U}$ obtained from Eqs. (3.19) will be orthogonal. Since in practice this is rarely the case, one has two options available—either to work with a nonorthogonal $\mathfrak{U}$, i.e., a nonunitary $\mathcal{S}^p$, or to force the orthogonality by relaxing some of the conditions in Eqs. (3.19). As we shall see for the model calculations presented in Sec. IV, the second method appears to give the better results.

In order to derive explicit expressions for E_r and Γ_γ, $\gamma=1, \ldots, N$, one must assume a specific functional form for χ_E which is regular at the origin and which is consistent with Eq. (3.13). Here we choose the lth partial wave of χ_E to be the expression in Eq. (3.13) multiplied by a function $f(r)$ with the properties $f(0)=0$ and $f(r)\approx 1$, $r \geq R$. The algebraic manipulations outlined in Appendix B give the following simple results:

$$\Gamma_\gamma^{1/2} = \textstyle\sum_t \mathfrak{U}_{t\gamma}(S_t\cos\Delta_\gamma + C_t\sin\Delta_\gamma), \quad \gamma=1, \ldots, N \quad (3.21)$$

$$E_r = \epsilon + \textstyle\sum_\gamma \frac{1}{2}\Gamma_\gamma^{1/2}\sum_t (S_t\sin\Delta_\gamma - C_t\cos\Delta_\gamma)\,\mathfrak{U}_{t\gamma} \ , \quad (3.22)$$

$$d_\alpha/d_\beta = (C_\alpha + iS_\alpha)/(C_\beta + iS_\beta) \ . \quad (3.23)$$

For a given Φ, the quantities S_t and C_t are defined by the equations

$$S_t = (4\mu/\hbar^2 k_t)^{1/2}\int_0^\infty dr\, d\vec{r}_0\, R_l(r,\vec{r}_0)(H_{\rm rad}-\epsilon) \times f(r)\phi_t(\vec{r}_0)\sin(k_t r - l\pi/2) \quad (3.24)$$

and

$$C_t = (4\mu/\hbar^2 k_t)^{1/2}\int_0^\infty dr\, d\vec{r}_0 R_l(r,\vec{r}_0)(H_{\rm rad}-\epsilon) \times f(r)\phi_t(\vec{r}_0)\cos(k_t r - l\pi/2) \ , \quad (3.25)$$

where

$$\langle \vec{r},\vec{r}_0|\,\Phi\rangle = r^{-1}R_l(r,\vec{r}_0)Y_{lm}(\hat{r}).$$

It is worthwhile to point out that the partial widths given in Eq. (3.21) describe the decay of the resonance into the eigenchannels of $\mathcal{S}^p$. Whenever it is desirable to determine the physical widths defined in Eq. (3.3), one may calculate them from the expression

$$\tilde{\Gamma}_\alpha = \Big|\sum_{\gamma=1}^{N} e^{i\Delta_\gamma}\,\Gamma_\gamma^{1/2}\,\mathfrak{U}_{\alpha\gamma}\Big|^2 \ , \quad (3.26)$$

which is obtained by applying the inverse of the transformation in Eq. (3.4) to $\langle \Phi HP\tilde{\psi}_{E\alpha}\rangle$.

Finally, we note that, in contrast to previous theories,[8] our expression for the "energy-shift," or Eq. (3.22), does not require the evaluation of integrals involving principal-value Green's functions. Also, the ratios of the coefficients d_α computed from Eq. (3.23) allow one to construct, apart from an over-all normalization constant, the particular solution $\Psi_{E\beta}$ [Eq. (2.2)] which the square-integrable function Φ approximates.

IV. APPLICATION TO MODEL PROBLEM

The model problem to be examined here simulates electron-target scattering in which excitation to the target's first excited state is energetically allowed. In direct analogy with the model in Paper II, we consider the scattering of a projectile from a fictitious target which consists of exactly three bound states with energies E_t $(t=1, 2, 3)$. If $H=-d^2/dx^2+H_0(y)+\mathcal{U}(x,y)$ is the complete Hamiltonian of the system, and $\{\phi_t\}$ represents the target states satisfying $H_0\phi_t=E_t\phi_t$, then a particular solution of $(E-H)\Psi_E=0$ can be written as

$$\Psi_{E\beta}=\sum_{t=1}^{3}\phi_t(y)G_t(x) \quad . \tag{4.1}$$

Writing Schrödinger's equation in matrix form, the projectile functions G_t satisfy[15]

$$\sum_{t=1}^{3}\left[\left(E-E_s+\frac{d^2}{dx^2}\right)\delta_{st}-V_{st}(x)\right]G_t(x)=0, \qquad s=1,2,3 \tag{4.2}$$

where

$$V_{st}(x)=\int \phi_s(y)\,\mathcal{U}(x,y)\,\phi_t(y)\,dy \quad .$$

The matrix elements V_{st} are taken to be square wells of height λ_{st} $(=\lambda_{ts})$ and width a. If V_{33} is sufficiently negative to hold a bound state, resonances associated with the third target state will occur.

For a total energy E satisfying $E_1<E_2<E<E_3$, each function G_t is a particular combination of two linearly independent solutions $F_{t\alpha}$ of Eq. (4.2), i.e.,

$$G_t(x)=\sum_{\alpha=1}^{2} b_\alpha F_{t\alpha}(x) \quad . \tag{4.3}$$

The choice of eigenphase normalization gives linearly independent solutions (denoted by $\alpha=1$ and $\alpha=2$) with asymptotic forms

$$F_{t\alpha}=k_t^{-1/2}\mathcal{W}_{t\alpha}(\sin k_t x+\tan\delta_\alpha\cos k_t x), \quad t=1,2 \tag{4.4a}$$

$$F_{3\alpha}=C_\alpha e^{-\kappa_3 x} \quad . \tag{4.4b}$$

Here $k_t^2=E-E_t$, $t=1,2$, and $\kappa_3^2=E_3-E$.[15]

For the two-channel case, the orthogonal $\mathcal{W}$ matrix may be parametrized in terms of a mixing parameter ω, e.g.,

$$\mathcal{W}=\begin{pmatrix}\cos\omega & -\sin\omega\\ \sin\omega & \cos\omega\end{pmatrix} . \tag{4.5}$$

The scattering information is contained in the three real energy-dependent quantities δ_1, δ_2, and ω, from which the S matrix is readily constructed. Specifically, if $\mathcal{D}$ is the diagonal matrix with nonzero elements $e^{2i\delta_\alpha}$, then $\mathcal{S}=\mathcal{W}\mathcal{D}\mathcal{W}^\dagger$.

The exact solution of Eqs. (4.2) is straightforward. A transformation of these equations gives three uncoupled sixth-order differential equations for $F_{t\alpha}$, $t=1,2,3$. Using the requirement $F_{t\alpha}(0)=0$, the solutions $F_{t\alpha}$ for $x<a$ may be written

$$F_{t\alpha}(x)=\sum_{i=1}^{3}A_{ti}^{\alpha}\sin\xi_i x \quad . \tag{4.6}$$

The constants A_{2i}^{α} and A_{3i}^{α} depend explicitly on A_{1i}^{α} and ξ_i. The quantities ξ_i may be determined by solving the algebraic equations that result from substituting Eq. (4.6) into the sixth-order equations. Connection of the logarithmic derivatives of $F_{t\alpha}$ in Eqs. (4.4) and (4.6) at $x=a$ yields A_{1i}^{α} $(i=1,2,3)$ and $\delta_\alpha(E)$ for $\alpha=1,2$. Finally, ω may be found by setting the ratio $F_{1\alpha}(a)/F_{2\alpha}(a)$ in Eq. (4.4) equal to the corresponding ratio in Eq. (4.6) for either $\alpha=1$ or 2.

Before discussing the extraction of resonance parameters from the exact values of $\delta_1(E)$, $\delta_2(E)$, and $\omega(E)$, a remark should be made concerning the labeling of δ_α. From the $\mathcal{W}$ matrix in Eq. (4.5) one can see that interchanging the labels in δ_α (i.e., the columns in $\mathcal{W}$) is equivalent to taking $\omega'=\omega\pm\pi/2$. If the coupling between channels occurs mainly through resonance, then at energies far from E_r, ω is either near zero or near $\pi/2$. By labeling δ_α for $E\ll E_r$ so that ω is near zero, δ_α corresponds physically to the phase shift which goes with k_α, i.e., asymptotically for $E\ll E_r$:

$$F_{\alpha\alpha}\simeq k_\alpha^{-1/2}(\sin k_\alpha x+\tan\delta_\alpha\cos k_\alpha x)$$

and

$$F_{t\alpha}\simeq 0, \quad t\neq\alpha \quad .$$

We shall adopt this convention for the mixing parameter ω throughout the calculation.

In the eigenphase representation, the resonance parameters consist of the energy E_r, the potential eigenphases Δ_α, the partial widths $\Gamma_\alpha(\alpha=1,2)$, and the potential mixing parameter ρ at energy $E=E_r$. The first five satisfy a relationship with each $\delta_\alpha(E)$ similar to the Breit-Wigner form for elastic scattering[14]:

$$E-E_r=\tfrac{1}{2}\{\Gamma_1\cot[\Delta_1-\delta_\alpha(E)]+\Gamma_2\cot[\Delta_2-\delta_\alpha(E)]\}, \qquad \alpha=1,2 \quad . \tag{4.7}$$

For a given set of parameters E_t and λ_{st} defining the model problem, $\delta_\alpha(E)$ [along with $\omega(E)$] were

found for an energy range exhibiting resonance behavior. We calculated the quantities Γ_α and Δ_α at $E=E_r$ by fitting the exact $\delta_\alpha(E)$ to Eqs. (4.7), in which Δ_α were taken to vary quadratically with energy. The quantity ρ, which is related to the background $\mathfrak{U}$ matrix

$$\mathfrak{U}=\begin{pmatrix}\cos\rho & -\sin\rho\\ \sin\rho & \cos\rho\end{pmatrix} ,$$

is determined from the parametrization of the S matrix in terms of Γ_α, Δ_α, and $\mathfrak{U}$ given in Eq. (3.12). From the relationship

$$\tan\omega=\frac{\mathcal{S}_{22}-\mathcal{S}_{11}\pm[(\mathcal{S}_{22}-\mathcal{S}_{11})^2+4\mathcal{S}_{12}^2]^{1/2}}{2\mathcal{S}_{12}} \qquad (4.8)$$

one finds, after straightforward algebra, that ρ satisfies

$$\tan\omega=\frac{-\alpha\cos2\rho-\beta\sin2\rho\pm(\alpha^2+\beta^2)^{1/2}}{\alpha\sin2\rho-\beta\cos2\rho} , \qquad (4.9)$$

where $\alpha=(E-E_r)\sin(\Delta_1-\Delta_2)+\frac{1}{2}(\Gamma_2-\Gamma_1)\cos(\Delta_1-\Delta_2)$ and $\beta=(\Gamma_1\Gamma_2)^{1/2}$. The sign of the root in Eqs. (4.8) and (4.9) is chosen to be consistent with the ordering of δ_α already discussed. From this point on, we shall let Δ_α and ρ denote their respective values at $E=E_r$.

Often the physical widths $\tilde{\Gamma}_\alpha$, defined in Eq. (3.3), are of greater interest than the partial widths Γ_α. Once the resonance parameters Γ_α, Δ_α, and $\mathfrak{U}$ are known, $\{\tilde{\Gamma}_\alpha\}$ may be determined from Eq. (3.26). In this work, we shall calculate both sets of partial widths.

In order to examine both narrow and broad resonances, we varied the strength of the coupling between the closed and open channels, i.e., λ_{t3} for $t=1,2$, while holding the other parameters fixed. Specifically, with $E_1=0$, $E_2=75$, $E_3=100$, $\lambda_{11}=10$, $\lambda_{22}=2$, $\lambda_{33}=-16$, and $a=1$, four sets of coupling were treated in detail. Table I lists the values of λ_{st}, $s\neq t$, used in the four calculations which we shall call A, B, C, and D. We note that the well $V_{33}(x)$ has a bound state located at $E_b=-9.8765$ which is responsible for the occurrence of a compound-state resonance in this model. Throughout the calculations we used a small value for the coupling λ_{12} in order to keep the contribution from background scattering small.

TABLE I. Strengths of the couplings between channels used in the model calculations.

Model calculation	λ_{12}	λ_{13}	λ_{23}
A	0.1	1.0	0.1
B	0.1	10.0	0.1
C	0.1	10.0	1.0
D	0.1	10.0	5.0

We apply the stabilization method to the model problem in a manner analogous to the elastic case treated in Paper II. Referring the reader to Sec. III of Paper II for the details, we briefly remark that the basis functions are of the form $\phi_t(y)u_m(x)$ ($t=1,2,3$ and $m=1,\ldots,M_t$), where the functions $u_m(x)$ are the odd harmonic-oscillator functions with a frequency of 30.[15] The Hamiltonian matrix consists now of nine blocks, each of dimension $M_s\times M_t$ ($s,t=1,2,3$) and is of total dimension $M_0=M_1+M_2+M_3$. The diagonalization of H yields M_0 roots ϵ_j and M_0 orthonormal eigenfunctions Φ_j, each of which has the form

$$\Phi_j=\sum_{t=1}^{3}\phi_t(y)Z_t(x) . \qquad (4.10)$$

The functions $Z_t(x)$ are just linear combinations of the basis elements u_m, $m=1,\ldots,M_t$, as given in Eq. (2.5).

Before making a detailed comparison between the exact results and those obtained with the stabilization method, we discuss briefly the stabilization property of certain roots observed in the model calculations. Because $G_3(x)$ is itself a square-integrable function for $E<E_3$, the roots ϵ_j below E_3 (and corresponding eigenfunctions Φ_j) are not sensitive to changes in M_3, provided the basis $\{\phi_3u_m\}$, $m=1,\ldots,M_3$ is sufficiently large to span the range of the potential. For example, for model calculation B a change of M_3 from 30 to 35 affected the stable root by only $10^{-4}\%$. As a result, M_3 was held fixed at 35 throughout the calculations. Figure 1 shows the intersections of two perpendicular planes with the two-dimensional surfaces representing the roots as functions of M_1 and M_2 for model calculation B. The behavior shown is typical for all sets of couplings considered. The reader is reminded that stability of a root occurs when the corresponding surface has a plateau. With M_2 held fixed, several roots—in particular, those with large expansion coefficients $c_{m2}^{(j)}$—were stable with respect to changing M_1; similarly, the roots with large $c_{m1}^{(j)}$ were stable as only M_2 was varied. But only one root below, E_3 was stable with respect to variation of both M_1 and M_2; this is the stable root which represents the resonance. From the corresponding eigenfunction Φ_j we hope to extract resonance information.

A given diagonalization of H yields, for each root ϵ_j, an approximation to a particular solution of $(\epsilon_j-H)\Psi_{\epsilon_j}=0$, in accordance with Eqs. (4.1) and (4.3). To evaluate how accurately $Z_t(x)$ approximates $G_t(x)$, we must first determine the coefficients $b_\alpha(\alpha=1,2)$ which define G_t in terms of the exact solutions $F_{t\alpha}(x)$. In actuality, only the ratio b_2/b_1 is required since Φ_j approximates Ψ_{ϵ_j} only within an over-all normalization factor. In a

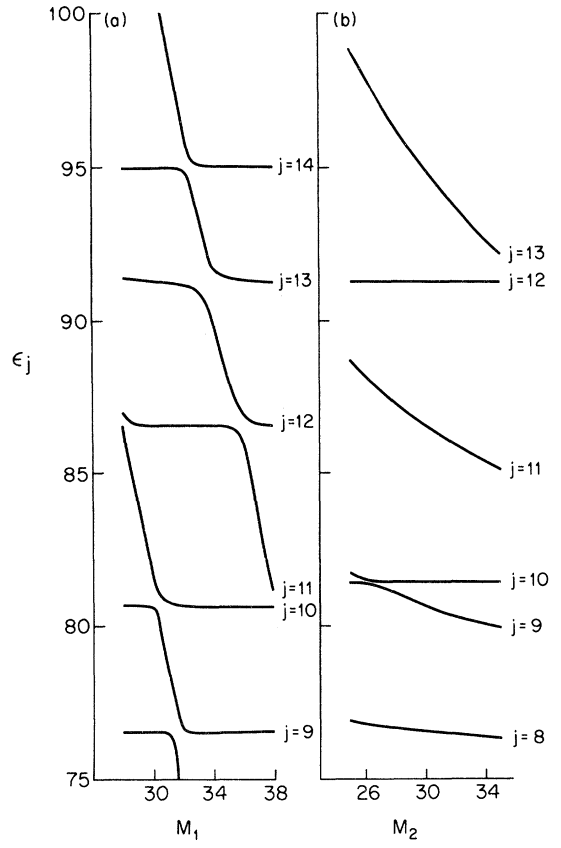

FIG. 1. Variation of the eigenvalues ϵ_j with open-channel basis size M_t, $t=1,2$, for model calculation B: (a) M_1 is varied for $M_2=30$, (b) M_2 is varied for $M_1=30$. In both (a) and (b), $M_3=35$.

manner analogous to the derivation of Eq. (3.23) for the complex coefficients d_α in S matrix representation, we find eventually that the appropriate real quantity is given by

$$\frac{b_2}{b_1}=\sum_{t=1}^{2} \mathfrak{u}_{t2}\, C_t \Big/ \sum_{t=1}^{2} \mathfrak{u}_{t1} C_t \,, \tag{4.11}$$

where C_t is defined in Eq. (3.25).

Figures 2 and 3 show a comparison of the functions $Z_t(x)$ associated with two roots ϵ_j and the exact $G_t(x)$ evaluated at energies $E=\epsilon_j$ in the case of intermediate couplings B. In Fig. 2 we have plotted the functions associated with the root in the stable region; in Fig. 3 are the functions for a root far from E_r. From these results it appears that the conclusions drawn in Paper II are equally valid for the inelastic case. First, the square-integrable functions Φ_j approximate the exact solutions at $E=\epsilon_j$, both on and off resonance; and, second, the eigensolutions which appear in a particular diagonalization are those for which the open-channel functions Z_1 and Z_2 go to zero near nodes in the exact G_1 and G_2, respectively.

Equipped with good approximations to the resonance state, we are ready to use the method developed in Sec. III to calculate the resonance parameters.

Before one can calculate the integrals required in Eq. (3.14), one must choose a functional form for χ_E, which is zero at the origin and which is consistent with Eq. (3.13). To satisfy the first requirement, we considered two possibilities: multiplication of the entire asymptotic expression in Eq. (3.13) by $f(x)=1-e^{-\xi x^2/2}$, as was done in the elastic case and also in Sec. III of this paper; or multiplication of only the cosine terms in Eq. (3.13) by the same $f(x)$. For the inelastic case, the first alternative gave a greater dependence on ξ than was seen in Paper III. Adoption of the second alternative essentially removed the sensitivity of the calculated quantities on ξ; and hence, in the model

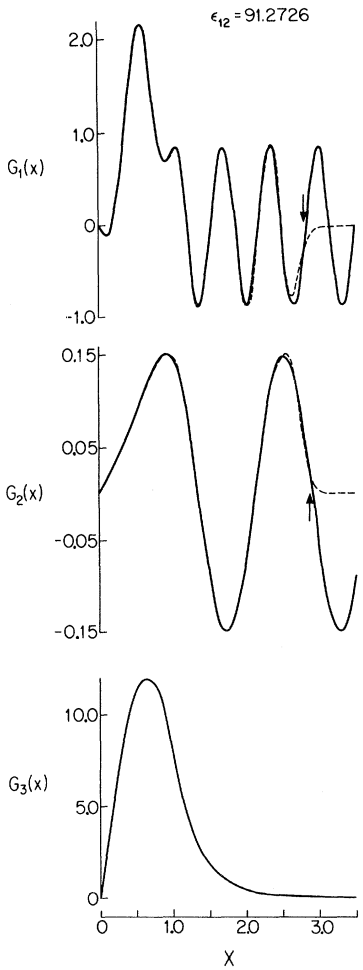

FIG. 2. Comparison of approximate functions Z_t (dashed line) with exact functions G_t (solid line) for the stable root ϵ_{12} resulting from the diagonalization with $M_1=30$, $M_2=31$, $M_3=35$ in model calculation B. Arrows indicate channel radii r_{M_t} [see Eq. (3.4) in Paper II].

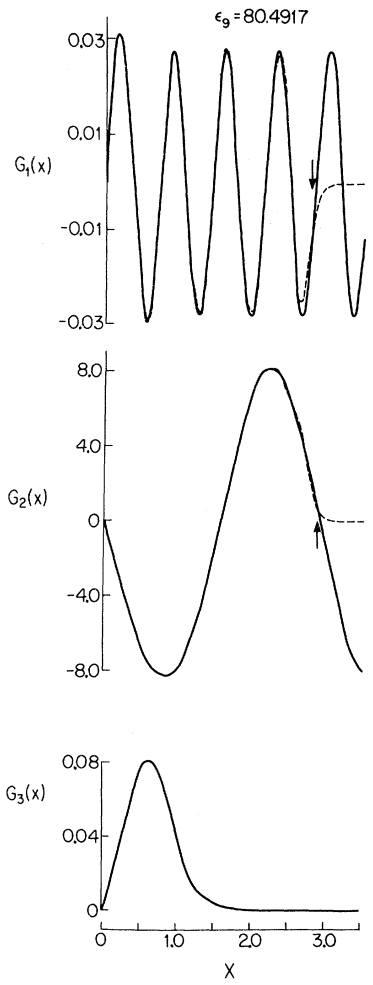

FIG. 3. Comparison of approximate functions Z_t (dashed line) with exact functions G_t (solid line) for an off-resonant root, ϵ_9, resulting from the same diagonalization as is described for Fig. 2. Arrows indicate channel radii r_{M_t} [see Eq. (3.4) in Paper II].

calculations reported here, we have used the following form[16] for $\chi_{\epsilon\alpha}$:

$$\chi_{\epsilon\alpha}=\pi^{-1/2}e^{i\Delta_\alpha}\sum_{t=1}^{2}\phi_t(y)k_t^{-1/2}\times[\sin k_t x\cos\Delta_\alpha+f(x)\cos k_t x\sin\Delta_\alpha]\mathfrak{U}_{t\alpha}\ , \quad (4.12)$$

where $\epsilon=k_t^2+E_t$, $t=1,2$. To be consistent with Eq. (4.12), we have set $f=1$ in the expression for S_t [Eq. (3.24)], while we have used $f(x)=1-e^{-\xi x^2/2}$ with $\xi=5$ in C_t [Eq. (3.25)].

Equation (3.21) gives the partial widths $\Gamma_\alpha^{(n)}$ calculated from the eigenvector $\Phi^{(n)}$ associated with a stable root $\epsilon^{(n)}$. (Here we reintroduce the superscript n to distinguish the stable roots obtained from different diagonalizations.) In terms of Δ_α and ρ, we have, for the two-channel case,

$$(\Gamma_1^{(n)})^{1/2}=\cos\rho[S_1^{(n)}\cos\Delta_1+C_1^{(n)}\sin\Delta_1]+\sin\rho[S_2^{(n)}\cos\Delta_1+C_2^{(n)}\sin\Delta_1]\ , \quad (4.13a)$$

$$(\Gamma_2^{(n)})^{1/2}=-\sin\rho[S_1^{(n)}\cos\Delta_2+C_1^{(n)}\sin\Delta_2]+\cos\rho[S_2^{(n)}\cos\Delta_2+C_2^{(n)}\sin\Delta_2]\ . \quad (4.13b)$$

An approximate value of E_r may be calculated from Eq. (3.22) for each root. For a given set of three stable roots ($n=1,2,3$), Δ_1, Δ_2, and ρ may be determined from Eqs. (3.19). Elimination of ρ gives Δ_1 and Δ_2; from them two values of ρ, viz., ρ_1 and ρ_2, respectively, result. If the results were exact, one would obtain

$$\rho_2=\rho_1+\pi/2\ , \quad (4.14)$$

in accordance with the orthogonality of the matrix $\mathfrak{U}$. The extent to which Eq. (4.14) is satisfied provides some measure of the accuracy of the approximations being made. In line with our convention for small background scattering, Δ_α will be so ordered that ρ_1 is nearer zero than $\pi/2$.

If Eq. (4.14) is satisfied only approximately, two possible approaches to the calculation of Γ_α emerge. If one requires that both partial widths be independent of n, i.e., that Eqs. (3.19) hold rigorously for $n=1,2,3$, then Γ_α must be computed from Δ_α and ρ_α, $\alpha=1,2$. In this case, one obtains a nonorthogonal matrix $\mathfrak{U}$:

$$\mathfrak{U}=\begin{pmatrix}\cos\rho_1 & \cos\rho_2\\ \sin\rho_1 & \sin\rho_2\end{pmatrix} \quad (4.15)$$

and the total width Γ is not preserved as one transforms from the partial widths $\{\Gamma_\alpha\}$ to the physical widths $\{\tilde{\Gamma}_\alpha\}$.

Alternatively, one may choose to ensure the orthogonality of $\mathfrak{U}$, i.e., the unitarity of $\mathcal{S}^p$. In this case, $\rho=\rho_1$, *or* $\rho=\rho_2-\pi/2$ must be consistently used in Eqs. (4.13) and also in Eq. (3.26) in the computation of $\{\tilde{\Gamma}_\alpha\}$. Thus, with unitarity preserved, one obtains two sets of results for $\{\Gamma_\alpha\}$. For $\rho=\rho_1$, $\Gamma_1^{(n)}$ is independent of n because ρ_1 is consistent with Δ_1, while three different $\Gamma_2^{(n)}$ result. On the other hand, for $\rho=\rho_2-\pi/2$, three different $\Gamma_1^{(n)}$ result while $\Gamma_2^{(n)}$ is independent of n. In this work, whenever a given ρ_α is used, we take Γ_β, $\beta\neq\alpha$, to be the average of $\Gamma_\beta^{(n)}$ over the three values of n, and compute the standard deviation σ_α of $\Gamma_\beta^{(n)}$ from the average value. We remark that σ_1 and σ_2 would be identically zero if Eq. (4.14) were rigorously satisfied.

In all of these approaches, dependence on n persists in the calculation of E_r [Eq. (3.22)], and E_r is taken to be the average of the three values obtained from the triplet of roots.

For each of the model calculations, we have taken four stable roots (denoted by $n=1,2,3,4$) and computed the resonance parameters from the four

TABLE II. Dependence of the computed widths on the method employed to determine the background parameters and, for each, dependence on the triplet of stable roots used for model calculation C. Method (i): unitary $\mathfrak{U}$ with $\rho=\rho_1$; method (ii): unitary $\mathfrak{U}$ with $\rho=\rho_2-\pi/2$; method (iii): nonunitary $\mathfrak{U}$ [Eq. (4.15)].

Method	Triplet[a]	ρ	Γ_1	Γ_2	$\tilde{\Gamma}_1$	$\tilde{\Gamma}_2$	Γ	σ_α
Exact	...	0.0076	0.1477	0.1044	0.1459	0.1062	0.2521	...
(i)								
	1, 2, 3	0.0832	0.1620	0.0827	0.1428	0.1019	0.2447	0.010
	1, 2, 4	0.0841	0.1627	0.0826	0.1433	0.1020	0.2453	0.012
	1, 3, 4	0.0566	0.1555	0.0893	0.1424	0.1024	0.2448	0.009
	2, 3, 4	0.0572	0.1558	0.0890	0.1425	0.1023	0.2448	0.010
(ii)								
	1, 2, 3	0.0040	0.1408	0.1030	0.1398	0.1040	0.2438	0.007
	1, 2, 4	−0.0074	0.1378	0.1062	0.1395	0.1045	0.2440	0.005
	1, 3, 4	−0.0080	0.1384	0.1055	0.1403	0.1036	0.2439	0.003
	2, 3, 4	−0.0222	0.1344	0.1090	0.1396	0.1038	0.2434	0.007
(iii)								
	1, 2, 3	...	0.1620	0.1030	0.1598	0.1250	0.2848[b]	...
	1, 2, 4	...	0.1627	0.1062	0.1635	0.1288	0.2923	...
	1, 3, 4	...	0.1555	0.1055	0.1570	0.1200	0.2770	...
	2, 3, 4	...	0.1558	0.1090	0.1610	0.1239	0.2849	...

[a]The four stable roots were obtained from the diagonalization H with the following basis sets: $M_1=36$, $M_2=31$ for $n=1$; $M_1=36$, $M_2=32$ for $n=2$; $M_1=37$, $M_2=30$ for $n=3$; $M_1=37$, $M_2=31$ for $n=4$. For all n, $M_3=35$.

[b]In method (iii) we take $\Gamma=\tilde{\Gamma}_1+\tilde{\Gamma}_2\neq\Gamma_1+\Gamma_2$.

triplets available in this set of roots. For each triplet we have various results from the unitary and nonunitary prescriptions. Table II shows a detailed comparison of the resulting widths for model calculation C. In general, the variation of E_r with n or ρ_α was very slight (less than 0.02%) and therefore is not shown. From Table II several trends are apparent, and we comment in advance that the same trends carried over to the other three model calculations.

First, when unitarity is preserved, the dependence on which ρ (ρ_1 or ρ_2) is used is much less for the total width Γ and the physical widths $\tilde{\Gamma}_\alpha$ than for the partial widths Γ_α. In addition, as we carry out the calculation for a different triplet of roots, still keeping unitarity, we see that Γ and $\tilde{\Gamma}_\alpha$ are only weakly sensitive to the triplet of roots used. In general, the ρ_α for which σ_α is smaller yields more accurate values for Γ_1 and Γ_2, apparently because ρ_α itself is more accurate. On the other hand, when the $\mathfrak{U}$ matrix in Eq. (4.15) is nonorthogonal, i.e., when $\mathcal{S}^p$ is nonunitary, the total, as well as the partial, widths are sensitive to which triplet is used—an undesirable outcome for a method which expects equally valid results from any roots, provided that they are stable and obtained from a sufficiently large basis.

With the conclusion that an orthogonal $\mathfrak{U}$ matrix is essential, we have adopted the following procedure for approximating the resonance parameters. After choosing a set of (four) stable roots, calculations are made from every available triplet of roots. For a given triplet, we compute the resonance parameters twice using two values for ρ, and choose the results obtained with the ρ_α for which σ_α is smaller. From the resonance parameters calculated from all of the (four) triplets, we take those for which σ_α is smallest to be our final results.[17] In Table III, we show a comparison of the exact and approximate resonance parameters for model calculations A, B, C, and D. In addition, to give an indication of the relative insensitivity of the results to roots, we show the average of the four sets of resonance parameters computed from the different triplets of roots.

As was seen in the elastic-model problem, the results are excellent for small couplings and decrease in accuracy as the couplings are increased. Even for large couplings it appears that this method is capable of predicting good values for the resonance energy and potential eigenphases, while providing reasonable estimates of the decay widths.

V. DISCUSSION

From the results presented in Sec. IV we may draw the following conclusions concerning the stabilization method as applied to inelastic scattering. When the exact H is diagonalized in a large enough set of square-integrable basis functions, the resulting eigenfunctions are good approximations, apart from a normalization constant, to particular combinations of the exact linearly inde-

TABLE III. Comparison of the exact and approximate resonance parameters for all four cases of couplings considered. For each model calculation, the first row gives the exact values, the second the final results obtained as described in the text (i.e., corresponding to the smallest σ_α), and the third the values averaged over the four triplets of roots used.

		Δ_1	Δ_2	ρ	Γ_1	Γ_2	$\tilde{\Gamma}_1$	$\tilde{\Gamma}_2$	Γ	E_r
A[a]										
	exact	−0.5655	−0.2362	−0.004 17	0.001 043	0.001 529	0.001 053	0.001 519	0.002 572	90.1364
	best σ	−0.5665	−0.2356	−0.004 19	0.001 042	0.001 529	0.001 052	0.001 519	0.002 571	90.1366
	av	−0.5665	−0.2359	−0.004 06	0.001 043	0.001 529	0.001 053	0.001 519	0.002 572	90.1366
B										
	exact	−0.4688	−0.2243	−0.003 25	0.1443	0.001 498	0.1444	0.001 406	0.1458	91.2694
	best σ	−0.4697	−0.2237	−0.004 83	0.1423	0.001 522	0.1424	0.001 387	0.1438	91.2698
	av	−0.4674	−0.2197	−0.005 53	0.1423	0.001 539	0.1424	0.001 384	0.1438	91.2700
C										
	exact	−0.4683	−0.2064	0.0076	0.1477	0.1044	0.1459	0.1062	0.2521	91.3794
	best σ	−0.4623	−0.2166	−0.0080	0.1384	0.1055	0.1403	0.1036	0.2439	91.3802
	av	−0.4622	−0.2199	−0.0084	0.1379	0.1059	0.1398	0.1040	0.2438	91.3802
D										
	exact	−0.4580	0.0911	0.0570	0.2266	0.8857	0.1853	0.9270	1.1123	93.7033
	best σ	−0.4559	0.0639	0.0736	0.2002	0.7276	0.1545	0.7733	0.9278	93.6959
	av	−0.4510	0.0783	0.0509	0.1862	0.7467	0.1549	0.7780	0.9329	93.7037

[a]See Table I for the couplings used in each model calculation.

pendent solutions at energies equal to the corresponding eigenvalues in both the resonant and nonresonant regions. The eigenvalues and the coefficients defining the particular solutions are determined by the requirement that the open-channel functions have nodes at the channel radii defined by the one-particle basis sets in terms of which the open-channel functions are expanded. The eigenfunctions Φ associated with stable roots represent the resonance state. The decay widths of the resonance are calculated as the off-diagonal elements of H between Φ and continuum functions representing the background scattering. The potential scattering parameters, i.e., $\mathcal{S}^p$, which specify these continuum functions, may be determined by the requirement that several good Φ give the same partial widths. It is necessary to use this criterion in such a way that a unitary background S matrix results in order to obtain accurate values for the widths.

We conclude with a few remarks about the observed decrease in the accuracy of the computed widths with increasing coupling, i.e., for broader resonances. We believe that, because we have used adequate basis sets, this trend is due solely to the approximation embodied in Eq. (3.10). The assumption that Φ is proportional to the exact solution in the region where the amplitude of Φ is not negligible allows one to replace the background scattering solution $P\psi_E^+$ by its asymptotic form in the expression for the width. As Figs. 2 and 3 show, this approximation is quite accurate, at least for the basis sets employed in the present calculations. As a result, we suspect that it is not Φ itself but rather the proportionality constant between Φ and $\Psi_{E\beta}$ given in Eq. (3.10) which becomes less accurate as Γ becomes larger. This conclusion is supported by the observation that the method appears to give more accurate values for the ratio $\tilde{\Gamma}_2/\tilde{\Gamma}_1$, which does not depend on the proportionality constant, than the partial widths themselves. For example, for model calculation D, the approximate value of $\tilde{\Gamma}_2/\tilde{\Gamma}_1$ is 5.03, compared with the exact value 5.00. Clearly, this is a much better agreement than that found for the physical widths in Table III. It is encouraging that the proposed method gives accurate estimates of $\tilde{\Gamma}_\alpha/\tilde{\Gamma}_\beta$ or the branching ratios $\tilde{\Gamma}_\alpha/\Gamma$ even when it underestimates the partial widths in case of broad resonances.

We note that both in the elastic case treated in Paper III and the inelastic case studied here, the computed total widths, as well as the physical partial widths, are always smaller than the corresponding exact values. This trend, which may be a special property of the model considered, is presently under investigation.

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APPENDIX A

In order to derive Eq. (3.16), one needs to eval-

uate $\langle \Psi_{\epsilon\beta}(H-\epsilon)\chi_\epsilon \rangle$ in terms of the resonance parameters. We integrate by parts twice to find that

$$\langle \Psi_{\epsilon\beta}(H-\epsilon)\chi_\epsilon\rangle = \langle \chi_\epsilon (H-\epsilon)\Psi_{\epsilon\beta}\rangle^* - \frac{\hbar^2}{2\mu}\left[\int d\vec{r}_0\left(\Psi^*_{\epsilon l}\frac{\partial\chi_{\epsilon l}}{\partial r} - \chi_{\epsilon l}\frac{\partial\Psi^*_{\epsilon l}}{\partial r}\right)\right]_0^R , \quad \text{(A1)}$$

where $\Psi_{\epsilon l}$ and $\chi_{\epsilon l}$ are the lth partial waves of $\Psi_{\epsilon\beta}$ and χ_ϵ, respectively. The first term on the right-hand side of Eq. (A1) is of course zero. If the point R is beyond the range of interactions, one can evaluate the surface term using the asymptotic forms in Eqs. (3.11) and (3.13) to obtain

$$\langle \Psi_{\epsilon\beta}(H-\epsilon)\chi_\epsilon\rangle = i(2\pi)^{-1}\textstyle\sum_t \mathcal{U}_t \sum_\alpha d^*_\alpha(\delta_{\alpha t} - \mathcal{S}^*_{t\alpha}e^{2i\tau}) . \quad \text{(A2)}$$

Substituting Eq. (3.12) for $\mathcal{S}_{t\alpha}$ and then rearranging Eq. (A2), one gets

$$\langle \Psi_{\epsilon\beta}(H-\epsilon)\chi_\epsilon\rangle = (2\pi)^{-1}(\epsilon - E_r - i\Gamma/2)^{-1} \times \{i(\epsilon - E_r - i\Gamma/2)[\textstyle\sum_\alpha d^*_\alpha \mathcal{U}_\alpha - \sum_\omega (\sum_\alpha d^*_\alpha \mathcal{U}_{\alpha\omega})(\sum_t \mathcal{U}_t \mathcal{U}_{t\omega})\, e^{2i(\tau-\Delta_\omega)}] + e^{2i\tau}(\textstyle\sum_\omega\sum_t \mathcal{U}_t\mathcal{U}_{t\omega}e^{-i\Delta_\omega}\Gamma_\omega^{1/2})(\sum_\gamma\sum_\alpha d^*_\alpha \mathcal{U}_{\alpha\gamma}e^{-i\Delta_\gamma}\Gamma_\gamma^{1/2})\} . \quad \text{(A3)}$$

Because $\mathcal{U}$ is a real orthogonal matrix, the following identity holds:

$$\mathcal{U}_\alpha = \textstyle\sum_t \delta_{t\alpha}\mathcal{U}_t = \sum_t(\sum_\omega \mathcal{U}_{\alpha\omega}\mathcal{U}_{t\omega})\mathcal{U}_t . \quad \text{(A4)}$$

Using Eq. (A4) one can simplify the first term in the curly brackets of Eq. (A3) to obtain

$$\langle \Psi_{\epsilon\beta}(H-\epsilon)\chi_\epsilon\rangle = (2\pi)^{-1}(\epsilon - E_r - i\Gamma/2)^{-1} \times \{2(\epsilon - E_r - i\Gamma/2)\textstyle\sum_\omega(\sum_\alpha d^*_\alpha \mathcal{U}_{\alpha\omega})(\sum_t \mathcal{U}_t\mathcal{U}_{t\omega})e^{i(\tau-\Delta_\omega)}\sin(\tau-\Delta_\omega) + e^{2i\tau}(\textstyle\sum_\omega\sum_t \mathcal{U}_t\mathcal{U}_{t\omega}e^{-i\Delta_\omega}\Gamma_\omega^{1/2})(\sum_\gamma\sum_\alpha d^*_\alpha \mathcal{U}_{\alpha\gamma}e^{-i\Delta_\gamma}\Gamma_\gamma^{1/2})\} . \quad \text{(A5)}$$

Finally, substitution of Eq. (A5) into Eq. (3.15) yields Eq. (3.16).

APPENDIX B

Substitution of the explicit expression for χ_ϵ [Eq. (3.13) multiplied by $f(r)$] into Eq. (3.14) gives

$$\Gamma(\epsilon,\tau,\mathcal{U})^{1/2} = \textstyle\sum_t \mathcal{U}_t(S_t\cos\tau + C_t\sin\tau) , \quad \text{(B1)}$$

where the integrals S_t and C_t are defined in Eqs. (3.24) and (3.25). To obtain Eq. (3.21) for Γ_γ, one simply lets $\tau = \Delta_\gamma$ and $\mathcal{U}_t = \mathcal{U}_{t\gamma}$, $t = 1, \ldots, N$, and then substitutes Eq. (3.18) for the left-hand side of Eq. (B1).

The derivation of Eq. (3.22) for E_r and Eq. (3.23) for d_α/d_β requires that the expressions for S_t and C_t be in terms of the resonance parameters. These may be obtained by setting equal the right-hand side of Eq. (B1) and the right-hand side of Eq. (3.16). Using the fact that $\sin\tau$ and $\cos\tau$ are linearly independent and that the equality must hold for any $\mathcal{U}_t$ subject to $\sum_{t=1}^N \mathcal{U}_t^2 = 1$, one obtains

$$S_t = \textstyle\sum_\omega \mathcal{U}_{t\omega}e^{-i\Delta_\omega} \times [\Gamma_\omega^{1/2} - 2D(\epsilon - E_r - i\Gamma/2)\sin\Delta_\omega\sum_\alpha d^*_\alpha(\epsilon)\mathcal{U}_{\alpha\omega}] \quad \text{(B2)}$$

and

$$C_t = \textstyle\sum_\omega \mathcal{U}_{t\omega}e^{-i\Delta_\omega} \times [i\Gamma_\omega^{1/2} + 2D(\epsilon - E_r - i\Gamma/2)\cos\Delta_\omega\sum_\alpha d^*_\alpha(\epsilon)\mathcal{U}_{\alpha\omega}] , \quad \text{(B3)}$$

where D is defined with Eq. (3.16). If one substitutes Eqs. (B2) and (B3) into the right-hand side of Eqs. (3.22) and (3.23), then the repeated use of the relationship

$$\textstyle\sum_t \mathcal{U}_{t\omega}\mathcal{U}_{t\gamma} = \delta_{\omega\gamma}$$

verifies the expressions for E_r and d_α/d_β.

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[16]Recalculation of E_r, Γ, and δ_p with Eq. (4.12) for the elastic case gave improved results for the two smaller couplings. The following values should be compared with the average values found in Table I of Ref. 5: $\lambda_{12} = 1$: $E_r = 90.1347$, $\Gamma = 0.001472$, $\delta_p = -0.2719$; $\lambda_{12} = 10$: $E_r = 91.2162$, $\Gamma = 0.1692$, $\delta_p = -0.1856$; $\lambda_{12} = 20$: $E_r = 94.3809$, $\Gamma = 0.7377$, $\delta_p = 0.0469$.
[17]Two remarks of caution are in order. First, when one partial width is significantly larger than the other (and if the background scattering is small), it turns out that severe cancellation may result in the calculation of either ρ_1 or ρ_2, so that $\rho_2 - \rho_1$ may be far from $\pi/2$. This effect was seen in model calculation *B*; however, as Table III partially indicates, the results obtained from the ρ_α with smaller σ_α are not affected by this difficulty. Second, extreme cancellation was seen when the three roots used were so similar that $S_t^{(n)}$ and $C_t^{(n)}$ ($t = 1, 2$) were close for all three values of n. This occurred when one of the open-channel M_t (M_1 or M_2) was the same for all three roots used. In this work, the triplets were chosen to avoid this difficulty.

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Si $K\alpha$ X-Ray Spectrum Produced by 30-MeV Oxygen Bombardment*

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$K\alpha$ x-rays of Si were produced by 30-MeV oxygen bombardment on a Si wafer. Nine $K\alpha$ lines are observed with an energy resolution of 2.5 eV at energies of 1739.78 ($K\alpha_{1,2}$), 1750.8 ± 0.5 ($K\alpha_3$), 1753.1 ± 0.6 ($K\alpha_4$), 1762.6 ± 0.5 ($K\alpha_5$), 1766.4 ± 0.6 ($K\alpha_6$), 1775.3 ± 0.6, 1778.8 ± 0.5, 1794.2 ± 0.6, and 1809.7 ± 0.8 eV. The intensity pattern is very nearly symmetric and the envelope approximately Gaussian. The energies of these lines are found to agree with Hartree-Fock-Slater calculated energies for $K\alpha$ transitions from Si atoms with initial configurations $(1s)^{-1}(2p)^{-n}$ for $n = 0$, 1, 2, 3, 4, and 5.

I. INTRODUCTION

Characteristic x rays produced by bombarding targets with heavy ions at MeV energies have produced x-ray spectra unlike any previously seen with other means of excitation.[1-6] The K and L x-ray lines obtained with high-resolution Si (Li) detectors are shifted to energies higher than those excited by other than high-energy heavy-ion bombardment. These energy shifts are attributed to a high probability of multiple inner-shell ionization created by atom-ion collisions.[2] Two recent experiments[7,8] using high-resolution crystal spectrometers have resolved some of the structure in the uncharacteristic $K\alpha$ spectra. In the case of Al plus 5-MeV N^+ beams,[7] six $K\alpha$ lines are observed. One of these lines is the normal $K\alpha_{1,2}$ line whereas the other lines agree with Hartree-Fock-Slater (HFS) calculated ($1s \rightarrow 2p$) transition energies for the five possible initial configurations $(1s)^{-1}(2p)^{-n}$, where $n = 1$, 2, 3, 4, and 5. The production of ($2s$) holes is not manifested in the spectra as distinct peaks due to large Coster-Kronig widths which transfer ($2s$) holes to the ($2p$) shell[9] before a $K\alpha$ event can occur. The observed intensity pattern is nearly symmetric and the envelope nearly Gaussian. In the case of Fe plus 30-MeV O^{5+} beams[8] only three lines were observed corresponding to $1s \rightarrow 2p$ transitions from initial configurations $(1s)^{-1}(2p)^{-n}$, where $n = 0$, 1, 2. Additional m-shell vacancies are deduced in the latter work.

In the present experiment 30-MeV O^{5+} bombardments on Si are used to observe the Si $K\alpha$ spectrum with an over-all resolution full width at half-maximum (FWHM) of ~2.5 eV. At this bombarding energy the observed spectrum is very similar to that given in Ref. 7. Multiplet structure is observed for three of the $K\alpha$ peaks so that a total of nine