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Normalization of resonance wave functions and the calculation of resonance widths

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We show that the resonance wave function can be generally thought of as being unit normalized under an appropriate analytic continuation procedure and that, so normalized, the resonance eigenfunctions obtained from a finite-basis-set calculation can be used to evaluate partial widths. Numerical results are given for two model problems.

I. THEORY

There is a vast amount of literature associated with the description of resonance wave functions. Much of this literature has emphasized the similarities between resonance states and bound states. This similarity is reflected in the procedures used to characterize resonances, which are often not those of traditional continuum theory. Indeed, most of the so-called "direct" methods for computing resonance positions and lifetimes,[1] such as complex scaling[2] and other related methods,[3] rely heavily on the computational techniques of conventional bound-state theory.

The resonance energy $\varepsilon_R = E_R - i\Gamma/2$ is generally defined as a pole of the S matrix on a second sheet of the complex energy plane (or, for a single-channel problem, the lower-half k plane with $k=\sqrt{2E}$). In a variety of methods employing complex basis functions, the resonance energy is directly obtained as one of the complex eigenvalues of an analytically continued finite-matrix approximation to the Hamiltonian. The imaginary part of the resonance energy so obtained gives the total width or inverse lifetime against decay of the resonance into all open channels.

However, there is an alternate definition of the resonance width as the modulus squared of a "golden-rule" matrix element of the scattering potential between the resonance wave function and an unperturbed continuum function, evaluated at the same energy.[4] The partial width for decay into asymptotic channel Φ_α, where α stands collectively for all the quantum numbers required to specify the final asymptotic state, is defined by

$$\Gamma_\alpha = |\langle \phi_\alpha | V | \Psi_R \rangle|^2 . \tag{1}$$

These partial widths do not, however, sum to the total width, except in the case of a narrow resonance.[5] For broad resonances, the two definitions are not equivalent.

The locations of the complex poles of the S matrix do not give any information about the partial widths. In two recent studies, however, it was shown how the resonance wave function Ψ_R, obtained either from a complex coordinate[6] or basis-set Siegert[5] calculation, could be used to obtain partial widths via Eq. (1). The normalization of Ψ_R in these studies was fixed by requiring the computed Γ_α to sum to the total width Γ obtained from the complex resonance energy. We have noted,[5] however, that this identity is only valid in the case of a narrow resonance. More recent studies[7] have pointed to the inconsistency of requiring the partial widths to sum to the total width and alluded to an ambiguity in the normalization of Ψ_R. There seems to be some confusion regarding this latter point. Indeed, it has been asserted[6] that the partial widths cannot be evaluated directly from Eq. (1) because the resonance wave function obtained from a finite-basis-set calculation cannot be properly normalized. It is our purpose here to show that this is not the case and that, just as for bound states, the resonance wave functions obtained from a complex-basis-set calculation should be normalized to unity. In other words, the complex-basis-set approach provides the correct analytic continuation of the normalization integral.

As More and Gerjuoy have pointed out,[8] the normalization of the resonance wave function is fixed by its definition in terms of the residue of the Green's function at a resonance pole,

$$|\Psi_R\rangle\langle\tilde{\Psi}_R| = \lim_{E\to\varepsilon_R}(E-\varepsilon_R)G(E) , \tag{2}$$

where the dual function $\langle\tilde{\Psi}_R|$ is in general not simply the complex conjugate of $|\Psi_R\rangle$. For simplicity, consider a single partial wave of a central potential scattering problem, although the results of this section are by no means limited to potential scattering. The resonance wave function Ψ_R in Eq. (2) is not normalizable in the usual sense that the integral

$$\langle\tilde{\Psi}_R|\Psi_R\rangle = \int_0^\infty \tilde{\Psi}_R^*(r)\Psi_R(r)dr \tag{3}$$

is finite, because the asymptotic form of the resonance wave function is

$$\Psi(r) \underset{r\to\infty}{\longrightarrow} A\frac{e^{ik_R r}}{r} \to \infty , \tag{4}$$

where k_R is the resonance momentum and lies in the lower-half k plane.

The point, however, is not whether or not the integral in Eq. (3) can be assigned a finite value. There are any number of ways to render the normalization integral finite, for example regularization[9] (for central potential scattering the radial functions satisfy $\tilde{\Psi}_R^* = \Psi_R$),

$$(\tilde{\Psi}_R, \Psi_R) = \lim_{\varepsilon \to 0} \int_0^\infty e^{-\varepsilon r^2} \tilde{\Psi}_R^*(r) \Psi_R(r) dr \ , \tag{5}$$

or contour distortion

$$(\tilde{\Psi}_R, \Psi_R) = \int_0^\infty \tilde{\Psi}_R^*(re^{i\theta}) \Psi_R(re^{i\theta}) e^{i\theta} dr \tag{6}$$

with $\theta > |\tan^{-1}[\text{Im}(k_R)/\text{Re}(k_R)]|$. Gyarmati and Vertse[10] have shown that all of these methods give the same result, namely the analytic continuation of the result from $\text{Im}(k_R) > 0$ into the lower-half k plane where the physical resonance momentum lies. Thus there is a *unique* analytic continuation which assigns a finite value to the integral in Eq. (3).

The question here is, what is the result if Ψ_R from its definition in Eq. (2) (in terms of the residue of the full Green's function at a pole) is subjected to one of the analytic continuation procedures which renders the normalization integral finite? The answer is suggested by some simple formal manipulations in which it is understood that each matrix element, denoted by $(\tilde{f}, g)$, is defined via one of the valid analytic continuation procedures. First we note that since $G(E)$ satisfies

$$G(E) = G_0(E) + G_0(E) V G(E) \ , \tag{7}$$

taking the residue of both sides of this equation at ε_R as in Eq. (2) gives the condition

$$G_0(\varepsilon_R) V \Psi_R = \Psi_R \ . \tag{8}$$

This is the well-known result that the kernel of the Lippmann-Schwinger equation has a unit eigenvalue at ε_R, because that energy is a discrete eigenvalue of the Hamiltonian.[11] Equation (7) also yields

$$|\Psi_R\rangle\langle\tilde{\Psi}_R| = \lim_{E \to \varepsilon_R} (E - \varepsilon_R)[1 - G_0(E)V]^{-1} G_0(E) \ . \tag{9}$$

Taking the matrix element of this equation with $\tilde{\Psi}_R$ from the left-hand-side and Ψ_R from the right-hand side gives

$$\begin{aligned} (\tilde{\Psi}_R, \Psi_R)(\tilde{\Psi}_R, \Psi_R) &= (\tilde{\Psi}_R, \lim_{E \to \varepsilon_R} (E - \varepsilon_R)[1 - G_0(E)V]^{-1} G_0(E) \Psi_R) \\ &= (\tilde{\Psi}_R, [-dG_0(\varepsilon_R)/d\varepsilon_R V]^{-1} G_0(\varepsilon_R) \Psi_R) \\ &= (\tilde{\Psi}_R, [G_0(\varepsilon_R) G_0(\varepsilon_R) V]^{-1} G_0(\varepsilon_R) \Psi_R) \end{aligned} \tag{10}$$

in a manner analogous to the derivation of Eq. (9.16) in Ref. 11. Replacing Ψ_R in the last line of this equation with $G_0(\varepsilon_R) V \Psi_R$ immediately gives the result

$$(\tilde{\Psi}_R, \Psi_R) = (\tilde{\Psi}_R, \Psi_R)^2 \tag{11}$$

and shows that the analytically continued normalization integral has the value ± 1. We argue here that normalization to $+1$ can be chosen without loss of generality, since the same relations, Eqs. (8)—(11), hold for bound states.

Although this derivation obviously ignores some formal details necessary to make it a rigorous proof, it can be given further support by examining some successful numerical procedures involving analytic continuation for constructing the full Green's function and its matrix elements. Consider for a moment a finite-basis-set calculation employing real basis functions[12] and a real Hamiltonian. The matrix eigenvalues and eigenvectors of the Hamiltonian (E_i, ϕ_i) can be used to construct the following approximation to the full Green's function in the coordinate representation:

$$G(Z) = \sum_i \frac{\phi_i^*(r) \phi_i(r')}{Z - E_i} \ . \tag{12}$$

This representation is only valid in the cut Z plane (the physical plane), excluding the positive real Z axis. To find the complex poles of $G(Z)$, Eq. (3) must be analytically continued from the physical onto the second Riemann sheet. This can be done by either complex scaling the coordinates in the Hamiltonian[2] or by using complex-basis functions with a scalar defined as above.[12,13] In the latter case, the eigenvectors are normalized as

$$(\tilde{\phi}_i, \phi_j) = \int \tilde{\phi}_i^*(r) \phi_j(r) d^3r = \delta_{ij} \ . \tag{13}$$

Note that for a purely radial problem $\tilde{\phi}_i = \phi_i^*$. In either case, the eigenvectors, including the resonance eigenvectors, used to construct Eq. (12) must be taken to be unit normalized. With the resonance wave function so normalized, Eq. (1) can be applied directly to obtain the resonance width.

The resonance eigenvalues are associated with isolated poles of the analytically continued S matrix. The corresponding eigenfunctions of the Hamiltonian, which for a single-channel potential scattering problem behave asymptotically as $e^{(ik_R r)}/r$ with $\text{Im}\, k_R < 0$ and hence increase exponentially for real $r \to \infty$, can nonetheless be unit normalized by analytic continuation. Consider the following example. For analytic potentials, one can obtain an approximation to a resonance eigenvalue by diagonalizing the complex-scaled Hamiltonian $H(re^{i\theta})$ over a set of real orthonormal functions $\{\chi_i(r)\}$. The resonance eigenvector $\sum c_i \chi_i(r)$ is an approximation to the true resonance wave function evaluated at $re^{i\theta}$ and will hence *decrease* exponentially at large r as long as we choose $\theta > |\tan^{-1}(\text{Im}\, k_R / \text{Re}\, k_R)|$. However, we can also think of the set $\{c_i\}$ as expansion coefficients of the exponentially increasing resonance wave function evaluated at real r, which is obtained by diagonalizing the real Hamiltonian over the set of complex functions $\{e^{(-3i\theta/2)} \chi_i(re^{-i\theta})\}$. Both notions are valid since, for analytic potentials at least,

$$\begin{aligned} &\int \chi_i(r) H(re^{i\theta}) \chi_j(r) d^3r \\ &\qquad = e^{-3i\theta} \int \chi_i(re^{-i\theta}) H(r) \chi_j(re^{-i\theta}) d^3r \ . \end{aligned} \tag{14}$$

If the set of functions $\{\chi_i(r)\}$ is orthonormal, then the complex set $\{e^{(-3i\theta/2)}\chi_i(re^{-i\theta})\}$ is normalized as in Eq. (13).

We prefer to think of using complex-basis functions rather than complex scaled Hamiltonians since this picture can be generalized to allow the use of mixed sets of real and complex basis states, normalized as in Eq. (13), and can even be valid for nonanalytic potentials,[13] such as the square well, as long as the analytically continued matrix elements are well defined. In the following section, we will illustrate the previous discussion by considering two examples.

II. EXAMPLES

A. One-term separable potential

The first problem we treat here is one we have considered previously,[5] scattering by a one-term separable potential,

$$V=|\zeta\rangle\lambda\langle\zeta| \tag{15}$$

where we choose

$$\langle r|\zeta\rangle=\exp(-\zeta r)/r\ . \tag{16}$$

This problem has a simple analytic solution[14] which we will discuss first, and can also be conveniently addressed computationally by the method of complex basis functions.

The T operator for this problem is

$$T(E)=|\zeta\rangle\frac{\lambda}{1-\lambda\Delta(E)}\langle\zeta|\ , \tag{17}$$

where

$$\Delta(E)=\langle\zeta|G_0^+(E)|\zeta\rangle=\frac{4\pi}{\zeta}(k+i\zeta)^{-2} \tag{18}$$

and has a pole at $\varepsilon_R=k_R^2/2$ where the denominator of Eq. (17) vanishes,

$$k_R=2(\pi\lambda/\zeta)^{1/2}-i\zeta\ . \tag{19}$$

The resonance wave function can be evaluated from Eq. (2) as the residue of the full Green's function

$$G^+(E)=G_0^+(E)+G_0^+(E)T(E)G_0^+(E)\ , \tag{20}$$

evaluated at $E=\varepsilon_R$. Using Eq. (17) in Eq. (20) gives

$$|\Psi_R\rangle=[-k_R/\Delta'(k_R^2/2)]^{1/2}G_0^+(k_R^2/2)|\zeta\rangle\ , \tag{21}$$

where $\Delta'(k^2/2)$ denotes the derivative of Eq. (18) with respect to k. Note that in Eq. (21) the Green's function is the analytic continuation of $G_0^+(k_R^2/2)$ from the upper- to the lower-half k plane. For the choice of $|\zeta\rangle$ in Eq. (16) the right-hand side of Eq. (21) can be evaluated directly to give the particularly simple result

$$\Psi_R(r)=2[-k_R/\Delta'(k_R^2/2)]^{1/2}\frac{1}{(k_R^2+\zeta^2)}\times\left[\frac{e^{ik_Rr}}{r}-\frac{e^{-\zeta r}}{r}\right]. \tag{22}$$

Thus $\Psi_R(r)$ is indeed proportional to $\exp(ik_Rr)/r$ for large r and diverges as indicated in Eq. (4) since $\mathrm{Im}(k_R)=-i\zeta$. We can nevertheless define its normalization by analytic continuation from the upper-half k plane using either regularization [Eq. (5)] or contour distortion [Eq. (6)]. The reader can easily verify by either means that Ψ_R, given in Eq. (22) from its definition in Eq. (2) in terms of the residue of the Green's function, is unit normalized.

The partial-width matrix element can be computed, even for this single-channel problem, from its definition,[5]

$$\gamma(k)=(2\pi k)^{1/2}(\tilde{\chi}_0(kr),V\Psi_R)\ , \tag{23}$$

where

$$\chi_0(kr)=\left[\frac{2}{\pi}\right]^{1/2}\frac{\sin(kr)}{kr}Y_{00}(\theta,\phi)\ . \tag{24}$$

Only the s-wave free-particle wave function $\chi_0(kr)$ appears in Eq. (23) because there is only s-wave scattering for this potential.[14]

In general the evaluation of Eq. (23) requires that we employ one of the analytic continuation methods to provide the analytic continuation from the upper-half k_R plane. The result in this case can be obtained with or without analytic continuation because of the special relation between the rate of increase of the resonance wave function with r and the rate of decrease of the potential [recall $\mathrm{Im}(k_R)=-i\zeta$]. We find

$$\gamma(k)=\frac{(2kk_R\zeta)^{1/2}(k_R+i\zeta)^{3/2}}{\zeta^2+k^2}\ . \tag{25}$$

As we have shown previously[5] the partial-width matrix element gives the total width Γ from $\mathrm{Im}(\varepsilon_R)$ only in the narrow resonance (Breit-Wigner) limit.

$$\Gamma=4\zeta(\pi\lambda/\zeta)^{1/2}=\lim_{\zeta\to 0}|\gamma(k_R)|^2\ . \tag{26}$$

This problem can also be solved numerically using complex-basis-function techniques. The results of such a computation are illuminating because they show that the unit-normalized resonance wave function from such a calculation can be used to compute the partial-width matrix elements $\gamma(k)$. Since only s-wave scattering occurs for this potential, we can solve the problem completely by diagonalizing the s-wave Hamiltonian in a basis of complex Laguerre functions of the form

$$\phi_n(\alpha,e^{-i\theta},r)=\frac{(\alpha e^{-i\theta})^{3/2}}{[(n+1)(n+2)]^{1/2}}re^{-\alpha e^{-i\theta}r/2}\times L_n^2(\alpha e^{-i\theta}r)\ . \tag{27}$$

Note that these functions are orthonormal as they are written—without any analytic continuation being required to define the normalization integral in Eq. (13). All the matrix elements of the Hamiltonian in this basis can be evaluated with simple analytical formulas or reduced to finite hypergeometric series. This procedure yields an approximate resonance energy and the resulting finite-basis approximation for Ψ_R,

$$\Psi_{\mathrm{res}}(r)=\sum_{n=0}^{N-1}a_n\phi_n(\alpha e^{-i\theta},r)\ , \tag{28}$$

also provides an approximation for the partial-width matrix element,

$$\gamma(k)=(2\pi k)^{1/2}\sum_{n=0}^{N-1} a_n(\tilde{\chi}_0(kr),V\phi_n(\alpha e^{-i\theta},r)) \ . \tag{29}$$

No analytic continuation is required to evaluate the matrix elements in Eq. (29).

Calculations are reported here for values of the potential parameters chosen as $\lambda=0.01$ and $\zeta=0.1$, and for values of the basis-set parameters of $\alpha=1.0$ and $\theta=20°$. In Fig. 1(a) the finite-basis approximation to the resonance wave function from the complex-basis calculation described above is compared with the exact wave function from Eq. (22). These are both eigenfunctions of the real Hamiltonian and the finite-basis-set approximation mimics the exponential increase of the resonance wave function as r increases until the spatial extent of the basis is exceeded.

Nonetheless, Eq. (29) provides a perfectly convergent approximation for $\gamma(k)$ as is shown in Table I. The reason for this somewhat paradoxical result is that interchanging the order of summation and integration in Eq. (29) results in a series representation in which each term is finite, and which, when it converges, must converge to the same result obtained by analytic continuation of the integrand of the original integral. Although we report only calculations on exponentially bounded potentials in this paper, we expect that this procedure will be generally convergent. Additionally we note that the results in Table I illustrate the point that, for finite widths, $2\,\mathrm{Im}(\varepsilon_R) \neq |\gamma(k_R)|^2$.

TABLE I. Results for the separable potential problem from calculations with N Laguerre basis functions. Note that $\Gamma=2\,\mathrm{Im}(\varepsilon_R)=0.224\,199\,64$. See text for values of parameters.

N	ε_R		$\lvert\gamma(k_R)\rvert^2$
5	0.618 921 40	$-0.080\,777\,63i$	0.192 340 76
10	0.626 902 48	$-0.113\,116\,40i$	0.223 173 65
15	0.622 982 68	$-0.112\,422\,85i$	0.220 204 97
20	0.623 294 87	$-0.112\,039\,09i$	0.218 672 87
25	0.623 327 97	$-0.112\,099\,74i$	0.219 013 95
30	0.623 318 08	$-0.112\,101\,12i$	0.219 022 77
35	0.623 318 38	$-0.112\,099\,70i$	0.219 011 19
40	0.623 318 56	$-0.112\,099\,81i$	0.219 012 23
Exact	0.623 318 53	$-0.112\,099\,82i$	0.219 012 39

Figure 1(b) shows the same wave functions appearing in Fig. 1(a) but as functions of $re^{i\theta}$. The resonance wave function is exponentially decreasing for large r along this ray in the complex plane.

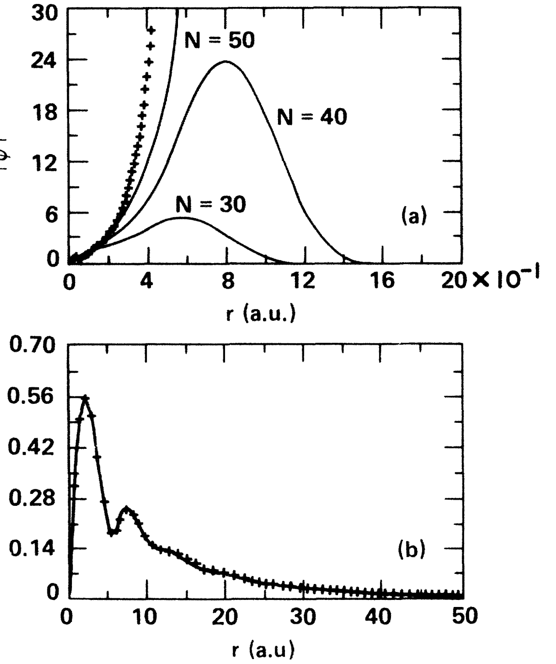

FIG. 1. (a) Convergence of basis representation of resonance wave function in Eq. (28) with increasing basis size. +, exact wave function from Eq. (22). (b) Same as (a), but with all wave functions evaluated at $re^{i\theta}$.

So far we have discussed only results for $\gamma(k)$ evaluated at the resonance momentum. The results of this section also allow us to construct the partial-width matrix elements at other values of k. In particular, it is interesting to study the approximation for the T matrix which is suggested by its partition into resonant, Born, and background contributions. The T matrix is given by

$$\langle \mathbf{k}\,|\,T\,|\,\mathbf{k}\rangle=\langle \mathbf{k}\,|\,V+VG^{+}(E)V\,|\,\mathbf{k}\rangle \tag{30}$$

and Eq. (2) immediately suggests that we write this as

$$\langle \mathbf{k}\,|\,T(E)\,|\,\mathbf{k}\rangle=\langle \mathbf{k}\,|\,V\,|\,\mathbf{k}\rangle+\frac{\langle \mathbf{k}\,|\,V\,|\,\Psi_R\rangle\langle\tilde{\Psi}_R\,|\,V\,|\,\mathbf{k}\rangle}{E-\varepsilon_R}$$
$$+\langle \mathbf{k}\,|\,VG_{\mathrm{BG}}V\,|\,\mathbf{k}\rangle \tag{31a}$$

or

$$T=T_{\mathrm{Born}}+T_{\mathrm{res}}+T_{\mathrm{BG}}\ , \tag{31b}$$

where the last term denotes the residual contribution of the nonresonant parts of the Green's function. Since we have a procedure for calculating the numerator of the resonance term in Eq. (31), we can compute that term and use it to construct an approximation to the T matrix. Note that the matrix elements in the numerator of Eq. (31a) are energy dependent and differ from $\gamma(k)$ given in Eq. (23) only by simple factors.

In Fig. 2 we compare the results for the cross section

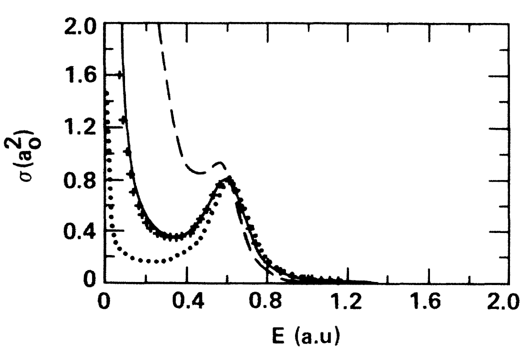

FIG. 2. Cross section (a.u.) for separable potential problem showing resonance feature. +, exact values; dotted line, Breit-Wigner formula; dashed line, $T^{(1)}$; solid line, $T^{(2)}$.

TABLE II. Results for model two-channel problem as a function of basis-set size. The basis-set parameters [Eq. (27)] were $\alpha=1.5$, $\theta=15°$. N refers to the number of functions in each channel.

N	E_R	$\Gamma=2\,\mathrm{Im}(\varepsilon_r)$	$\lvert\gamma_1\rvert^2$	$\lvert\gamma_2\rvert^2$
30	3.665 641 50	0.019 117 686	0.001 043 0	0.018 787
45	3.665 650 53	0.019 111 783	0.001 106 3	0.018 065
55	3.665 650 49	0.019 111 458	0.001 118 3	0.018 118
65	3.665 650 49	0.019 111 458	0.001 116 4	0.018 067
75	3.665 650 49	0.019 111 457	0.001 114 5	0.018 036
85	3.665 650 49	0.019 111 457	0.001 113 8	0.018 026
90	3.665 650 49	0.019 111 457	0.001 113 6	0.018 023

from three approximations for T with the exact results. Those approximations are

$$T^{(1)}=T_{\mathrm{res}}(k)=\frac{\gamma(k)^2/8\pi^2k}{k^2/2-\varepsilon_R}\,, \tag{32}$$

$$T^{(2)}=T_{\mathrm{Born}}(k)+T_{\mathrm{res}}(k)\,, \tag{33}$$

and the Breit-Wigner formula

$$T_{\mathrm{BW}}=-\frac{1}{k4\pi^2}\frac{\Gamma/2}{E-\varepsilon_R}\,. \tag{34}$$

The results in Fig. 2 show that, for this case, $T^{(2)}$ provides a remarkably accurate representation of the cross section over a range of energies, while $T^{(1)}$ gives no improvement over the Breit-Wigner formula. The fact that we can construct these approximations using basis set methods is important, because the off-shell dependence of the T matrix features in a number of applications of scattering theory.

B. Two-channel potential scattering

We have studied a model two-channel problem, previously considered by Noro and Taylor,[6] which consists of the s-wave scattering of a structureless particle by a fictitious target which has only two internal states, labeled by energies E_1 and E_2. The matrix elements of the interaction potential are taken to be

$$V_{\alpha\beta}=\lambda_{\alpha\beta}r^2e^{-r},\quad \alpha=1,2\,. \tag{35}$$

For this study, we chose the target energies to be 0.0 and 0.1 a.u. and we took the potential strengths to be

$$\lambda=\begin{vmatrix}-1.0 & 2.0\\ 2.0 & 7.5\end{vmatrix}\,. \tag{36}$$

The properly normalized radial asymptotic states for this problem are

$$\Phi_\alpha(r)=\frac{2}{(k_\alpha)^{1/2}}\sin(k_\alpha r),\quad k_\alpha=\Big[2(E-E_\alpha)\Big]^{1/2}\,. \tag{37}$$

A complex symmetric matrix representation of the real two-channel Hamiltonian was formed by using in each channel N orthonormal complex-scaled Laguerre functions of the form given in Eq. (27).

The required kinetic- and potential-energy matrix elements can all be computed either from analytic formulas or stable recursion relations. We diagonalized the $2N\times 2N$ matrix of the Hamiltonian for values of N up to 90 and for a range of θ values. A stable resonance state was found whose energy rapidly converges to the value $E=3.66565-i0.009\,555$ with increasing N. The partial widths were evaluated from the integrals

$$\gamma_\alpha=\sum_\beta\lambda_{\alpha\beta}\sum_n c_n^\beta\int_0^\infty\Psi_\alpha(r)r^2e^{-r}\chi_n(r)dr\,, \tag{38}$$

where the resonance wave function has been expanded as

$$\Psi_R=\sum_\beta\sum_n c_n^\beta\chi_n(r)\,. \tag{39}$$

The results for the partial widths, $\Gamma_\alpha=|\gamma_\alpha|^2$, and resonance energy values are summarized in Tables II and III. We note that the resonance energy, which is computed from a variational principle, converges much more rapidly with increasing basis size and is more stable with respect

TABLE III. Results for model two-channel problem as a function of basis-set scaling angle θ for fixed $N=65$. Other parameters as in Table II.

θ (deg)	E_R (a.u.)	$\Gamma=2\,\mathrm{Im}(\varepsilon_R)$	$\lvert\gamma_1\rvert^2$	$\lvert\gamma_2\rvert^2$
1	3.672 646 80	0.020 204 507	0.002 090 1	0.038 081
3	3.666 197 56	0.019 573 740	0.001 202 6	0.019 803
5	3.665 702 32	0.019 142 082	0.001 128 0	0.018 291
10	3.665 650 61	0.019 111 355	0.001 120 0	0.018 126
15	3.665 650 49	0.019 111 458	0.001 116 4	0.018 067
20	3.665 650 49	0.019 111 461	0.001 146 0	0.018 553
22	3.665 650 49	0.019 111 466	0.001 273 1	0.020 687
25	3.665 650 50	0.019 111 473	0.003 195 6	0.053 902

to changes in θ than are the partial widths which are computed from Eq. (1) and which are subject to first-order errors in the resonance wave function.

III. DISCUSSION

We have shown that the proper normalization for the resonance wave function, under the appropriate analytic continuation, is unity, as it is for bound states. This observation allows the calculation of partial resonance widths directly from any discrete basis-set approximation to the resonance state using complex basis functions. The width matrix element may also be evaluated off shell, where the energy of the asymptotic state is not set equal to ε_R. We have indicated one example where this allows one to construct a better approximation to the energy dependence of the cross section than that given by the usual Breit-Wigner approximation. There are also examples from molecular physics where the off-shell energy dependence of the width function can be used to study processes such as vibrational excitation by electron impact and dissociative electron attachment.

The advantage of the present approach of using a properly normalized resonance wave function obtained from a complex-basis-function calculation is that we have an approximation to the exact resonance wave function. We avoid the introduction of projection operators and the calculation of the energy shift needed to compute the resonance energy when a real function is used to approximate the resonance state. We have also avoided the introduction of any finite boundaries or inner channel radii in fixing the normalization of the resonance wave function.

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[11] R. G. Newton, *Scattering Theory of Waves and Particles*, 2nd ed. (Springer-Verlag, Berlin, 1982), pp. 228–238.

[12] By real basis functions we mean, in many instances, real-valued radial basis functions multiplied by complex spherical harmonics. For example, when the problem has spherical symmetry, the Green's function in Eq. (2) is for the radial Schrödinger equation and its analytic continuation to complex values of Z is accomplished by making the radial coordinates complex or using complex radial basis functions. This point is explained fully in Refs. 1 and 2.

[13] T. N. Rescigno and C. W. McCurdy, Phys. Rev. A **31**, 624 (1985).

[14] K. Gottfried, *Quantum Mechanics*, (Benjamin, Reading, PA, 1966), p. 161.