PHYSICAL REVIEW A VOLUME 22, NUMBER 2 AUGUST 1980

Association of resonance states with the incomplete spectrum of finite complex-scaled Hamiltonian matrices

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(Received 26 November 1979)

The incomplete spectrum of finite complex-scaled Hamiltonian matrices H_η is studied. It is pointed out that the occurrence of an incomplete spectrum of complex-scaled Hamiltonians in the finite-element approximation is neither accidental nor rare, and the existence of a defective eigenvector (orthogonal to itself) of H_η can be associated with a complex-stationary point which represents the resonance state. A physical interpretation of the incomplete spectrum (the eigenvalues of a defective Hamiltonian matrix) is given, supported by numerical results for e^--He^+ scattering worked out as an example. The numerical procedure suggested here for the purpose of identifying the resonance state with the eigenvalue associated with the defective eigenvector of H_η, may prove to be not very practical. This is so as long as only relatively small basis sets are used. However, in the finite-element approximation, this procedure does yield a better understanding of the behavior of the resonance solution.

I. INTRODUCTION

The fundamental works of Aguilar, Balslev, Combes, and Simon[1] have provided a mathematical foundation for the description of atomic and molecular[2] resonances by the complex-scaling method.

In the complex-scaling method, the internal coordinates of the Hamiltonian $\hat{H}(\vec{r})$ are complex scaled by $\eta=\exp(-i\theta)$, and thereby a complex Schrödinger equation is obtained,

$$\hat{H}_\eta(\vec{r})\psi_k(\vec{r})=W_k\psi_k(\vec{r})\,, \tag{1}$$

in which $\hat{H}_\eta(\vec{r})=\hat{H}(\vec{r}/\eta)$ and $W_k=(E_r+iE_i)_k$. The effect of the scaling on the spectrum of the Hamiltonian is as follows[1]:

(1) The bound-state energies ($E_r<E^+$, where E^+ is the lowest eigenvalue of the $(n-1)$-particle Hamiltonian, and $E_i=0$) are θ independent.

(2) The continuum-state energies are rotated to the complex plane by varying θ, $E_i=(E_r-E_{\text{thresh}})\tan(2\theta)$.

(3) The resonance states (like the bound state, and unlike the scattering states) are θ independent:

$$\frac{\partial^J W_k}{\partial\eta^J}=0,\ j=1,2,\ldots\,, \tag{2}$$

where $W_k=E_r-\frac{1}{2}i\Gamma$ (E_r and Γ are the resonance position and width, respectively). When the rotation angle θ satisfies

$$\theta\geq\Gamma/[2(E_r-E_{\text{thresh}})]\,, \tag{3}$$

the resonance eigenfunctions become square-integrable functions, and therefore they are isolated from the eigenfunctions corresponding to the continuous spectrum.

If the eigenfunctions of $\hat{H}_\theta$ form a complete set, then the nondegenerate eigenfunctions are complex normalizable[3] and

$$(\psi_k|\psi_k)=\int\psi_k(\vec{r})\psi_k(\vec{r})d\vec{r}\neq 0$$

for all space. Consequently, the resonance function Ψ_r can be expanded in a linear combination of orthogonal basis functions $\{\phi_i\}$ forming a complete set. The linear coefficients $\vec{C}_i$ can be chosen to satisfy the complex-variation (stationary) principle (Ref. 3) $\partial W/\partial C_i=0$, where

$$W=\sum_{i,j}^{\infty}C_iC_jH_{ij}\Big/\sum_{i,j}^{\infty}C_iC_j\,,$$

and

$$H_{ij}=(\phi_i(\vec{r})\,|\,\hat{H}(\vec{r}/\eta)\phi_j(\vec{r}))\,.$$

By truncating the basis set to N basis functions, the original complex Schrödinger equation [Eq. (1)] is transformed into a finite-matrix eigenvalue problem

$$(\underline{H}(\eta)-W_k\underline{I})\vec{C}_k=0,\quad k=1,2,\ldots,N\,. \tag{4}$$

It has generally been assumed that by increasing N, the complex-stationary point $\partial W/\partial\eta\,|\,\eta_0=0$ [see Eq. (2)] will converge to the exact resonance eigenvalues of the Schrödinger equation.[4] However, it is possible to have degenerate poles in the scattering amplitude, so that the resonance eigenfunction is orthogonal to itself, $(\psi_r|\psi_r)=0$.[5] In such a case the complex-variational and other theorems that have been proved for $\hat{H}_\eta(r)$ are not valid anymore.[3]

Actually, any infinitesimal perturbation removes the degeneracy of the poles and the formal difficulty mentioned above disappears. Therefore, it is numerically unlikely to observe this phenomenon (incomplete spectrum because of multiple poles in the scattering amplitude) in a finite-element approximation of the complex-scaled Hamiltonian.[6] Conversely, if a defective eigenvector is observed in a finite-element calculation, it is unlikely to correspond to a true case of degenerate poles in the exact scattering amplitude. In this paper, we study the incomplete spectrum of the complex-scaled Hamiltonians in the finite-element approximation.

In the next section it is shown that for such a complex-scaled Hamiltonian matrix, one can always find at least one scaling parameter η for which the matrix is defective and the spectrum is incomplete. Moreover, the defective eigenvector of $\underline{H}_\eta$ can be associated with the complex-stationary point which represents the resonance state. In Sec. III a physical interpretation of the incomplete spectrum is given. It is suggested that the critical scaling parameter for which a defective eigenvector is obtained may be associated with the critical rotation angle $\theta_c = \Gamma/[2(E_r - E_{\text{thresh}})]$ for which the resonance state is "covered" by the continuum solution (see Eq. 3). The incomplete spectrum of the finite-matrix Hamiltonian associated with the e^--He resonance has been studied as an example.

II. THE SPECTRUM OF THE COMPLEX-SCALED HAMILTONIAN IN MATRIX REPRESENTATION

Let us restrict ourselves to an n-particle Hamiltonian in which the potential $\hat{V}(\vec{r})$ is a homogeneous function of the first order (e.g., the Coulomb potential). For this type of operators the complex-scaled Hamiltonian in a finite-matrix representation can be written as

$$\underline{H}(\eta) = \eta^2 \underline{T} + \eta \underline{V}\,, \tag{5}$$

where

$$\underline{T}(i,j) = \langle \phi_i(\vec{r}) \,|\, \hat{T}(\vec{r}) \phi_j(\vec{r}) \rangle \tag{6}$$

and

$$\underline{V}(i,j) = \langle \phi_i(\vec{r}) \,|\, \hat{V}(\vec{r}) \phi_j(\vec{r}) \rangle \tag{7}$$

are the discretizations of the kinetic- and potential-energy operators $\hat{T}(\vec{r})$ and $\hat{V}(\vec{r})$, respectively, and $\{\phi_i(\vec{r})\}$ are N square-integrable basis functions. The eigenvalues $W_i(\eta), \ldots, W_N(\eta)$ of $\underline{H}(\eta)$ are the solutions of the secular equations

$$(\underline{H}(\eta) - W_i \underline{I})\vec{C}_i = 0, \quad i = 1, \ldots, N\,. \tag{8}$$

Without loss of any generality, we consider the related Hamiltonian[7]

$$\underline{\tilde{H}}(\eta) = \underline{H}(\eta)/\eta = \eta \underline{T} + \underline{V}\,, \tag{9}$$

with

$$W_i(\eta) = \eta \lambda_i(\eta), \quad i = 1, \ldots, N\,. \tag{10}$$

From a physical point of view, the interesting case is when $\underline{TV} \neq \underline{VT}$, and we shall assume that this holds.

Following the result of Motzkin and Taussky,[8] the fact that $[\underline{T}, \underline{V}] \neq 0$ implies that the eigenvectors $\vec{C}_i$ need not be normalizable. For real η each $\lambda_j(\eta)$ is an analytical function of η,[9] and one can analytically parametrize the eigenvector

$$\underline{\tilde{H}}(\eta)\vec{C}_j(\eta) = \lambda_j(\eta)\vec{C}_j(\eta), \quad j = 1, \ldots, N \tag{11}$$

such that

$$\vec{C}_i^T(\eta)\vec{C}_j(\eta) = \delta_{ij} \quad \text{for } \eta = \text{Re}(\eta)\,.$$

However, when η obtains complex value, so that $\underline{H}(\eta)$ is complex symmetric, $\underline{\tilde{H}}(\eta)$ can have an arbitrary Jordan canonical[10] form. We shall call an eigenvalue b of $\underline{\tilde{H}}$ a defective eigenvalue if b is not a simple pole of the resolvent $(\underline{\tilde{H}} - \lambda \underline{I})^{-1}$. That is, for any choice of linearly independent eigenvectors which span the eigenspace corresponding to b, there exists an eigenvector $\vec{C}_b$ such that $\vec{C}_b^T \vec{C}_b = 0$ when $\underline{\tilde{H}}(\eta)\vec{C}_b = \lambda_0 \vec{C}_b$. In that case the set of eigenvectors of $\underline{\tilde{H}}$ does not span the whole space and we say that $\underline{\tilde{H}}$ has an *incomplete spectrum*. Moreover, the Motzkin and Taussky results[11] imply the following theorems.

Theorem 1. If $\underline{T}$ and $\underline{V}$ are $N \times N$ (real or complex) matrices which are similar to diagonal matrices, and $\underline{T}$ and $\underline{V}$ do not commute, *then there exists at least one* η_b (a defective point) *such that* $\lambda_j(\eta_b)$ *is a defective eigenvalue for some* j.

The eigenfunctions $\lambda_j(\eta)$, $j = 1, \ldots, N$ are algebraic functions since they satisfy the equation

$$\det|\underline{\tilde{H}}(\eta) - \lambda_j \underline{I}| = 0\,. \tag{12}$$

Therefore, the $\lambda_j(\eta)$ are analytic in η except at a finite number of points $\eta_1, \ldots, \eta_q$ which are the *branch points* for some eigenvalues; i.e., some $\lambda_j(\eta)$ do not have a Taylor expansion in $(\eta - \eta_b)$ around the branch points η_b. However, $\lambda_j(\eta)$ does have an expansion in $(\eta - \eta_b)^{1/p}$:

$$\lambda_j(\eta) = \sum_{k=0}^{\infty} \alpha_{jk} (\eta - \eta_b)^{k/p}\,, \tag{13}$$

the so-called Puiseux series. Here $p \geq 2$ is some integer which does not exceed the multiplicity of $\lambda_j(\eta_b)$ in the characteristic polynomial [Eq. (12)]. The assumption $[\underline{T}, \underline{V}] \neq 0$ implies that at least one branch point exists when $\underline{T}$ and $\underline{V}$ are constructed from a real basis set [real ϕ_i in Eq. (5)]. Then, we can prove the next theorem.

Theorem 2. When $\underline{T}$ and $\underline{V}$ are $N \times N$ real symmetric matrices and do not commute, then *there exists at least one branch point* η_b *such that*

$$\left.\frac{d\lambda_j(\eta)}{d\eta}\right|_{\eta=\eta_b} = \infty \tag{14}$$

for some j. [Note that the resonance state, by constrast, is a (stationary) point for which $dW/d\eta|_{\eta_{\rm opt}} = d\lambda/d\eta|_{\eta_{\rm opt}} + \lambda_j/\eta_{\rm opt} = 0$.]

Proof. Suppose that for all finite η_b, $\lambda_j'(\eta_b) \equiv \partial\lambda_j/\partial\eta|_{\eta_b}$ is also finite. This means that either η_b is a point analyticity of $\lambda_j(\eta)$, or η_b is a branch point for $\lambda_j(\eta)$ and the coefficients $\alpha_{j'}, \ldots, \alpha_{j(p-1)}$ vanish. Now let us consider $\eta = \infty$. According to Rellich's result[9] each $\lambda_j(\eta)$ is analytic around $\eta = \infty$ and we have the expansion

$$\lambda_j(\eta) = \eta\lambda_j(\underline{T}) + \sum_{k=0}^{\infty} \alpha_{jk}\eta^{-k}, \quad |\eta| > R \tag{15}$$

and

$$\lambda_j'(\infty) = \lambda_j(\underline{T}) .$$

Here $\lambda_j(\underline{T})$ denotes the jth eigenvalue of the kinetic-energy matrix $\underline{T}$. Therefore, the derivative of the multivalued function $\lambda(\eta)$ is bounded on the whole complex plane. The maximum principle implies that each $\lambda_j'(\eta)$ is a constant.[12] (See, for example, Ref. 13 for use of this type of argument.) Consequently, each $\lambda_j(\eta)$ is linear in η but then, by another result of Motzkin and Taussky,[8] $\underline{T}$ and $\underline{V}$ commute, in contradiction with the assumption of $[\underline{T}, \underline{V}] \neq 0$.

It is also possible to show that the branch point η_b which satisfies Eq. (14) must be a defective point. This is a result of the following variational formula.[13]

Theorem 3. Let $\underline{\tilde{H}}(\eta)$ be an analytic symmetric-matrix function on $|\eta - \eta_0| < R$:

$$\underline{\tilde{H}}(\eta) = \sum_{k=0}^{\infty} \underline{h}_k(\eta - \eta_0)^k . \tag{16}$$

Assume that λ_0 is semisimple, namely, that all the Jordan blocks of $\underline{h}_0$ corresponding to $\lambda_0 = \lambda_j(\eta_0)$ are 1×1 (λ_0 is not a defective eigenvalue of $\underline{h}_0$). Then, for any $\lambda_j(\eta)$ we have the Puiseux expansion

$$\lambda_j(\eta) = \lambda_0 + \mu_j(\eta - \eta_0) + \sum_{k=p+1}^{\infty} \alpha_{jk}(\eta - \eta_0)^{k/p}, \quad j = 1, \ldots, m \tag{17}$$

where m is the multiplicity of λ_0 in $\underline{h}_0$.

Let $(\vec{C}_1, \ldots, \vec{C}_m)$ be the eigenvectors of $\underline{h}_0 = \underline{\tilde{H}}(\eta_0)$. Then

$$\underline{h}_0\vec{C}_j = \lambda_0\vec{C}_i$$

and

$$\vec{C}_j^T\vec{C}_k = \delta_{jk}; j,k, \; k = 1, \ldots, m .$$

Then $(\mu_1, \ldots, \mu_m)$ are the eigenvalues of the $m \times m$ matrix, $(\vec{C}_k^T\underline{h}_1\vec{C}_j)$. Thus if η_0 which satisfies Eq. (14) is not defective, then the expansion in Eq. (17) shows that $d\lambda_j(\eta_0)/d\eta = \mu_j$, which contradicts Eq. (14).

However, it may happen that η_0 is a defective point and Eq. (14) does not hold for any j. Moreover, there are cases in which η_0 is a *defective point* but all $\lambda_j(\eta)$ are *analytic* at $\eta = \eta_0$. We shall illustrate such a possibility by giving the following simple example.

Example.

$$\underline{\tilde{H}}(\eta) = \begin{vmatrix} 144(\eta+1) & -108(\eta+1) & -180i \\ -108(\eta+1) & -544(\eta+1) & -240i \\ -180i & -240i & 0 \end{vmatrix} . \tag{18}$$

Then the characteristic polynomial of $\underline{\tilde{H}}(\eta)$ is

$$\lambda[\lambda^2 + 400(1+\eta)\lambda - 90\,000(2+\eta)\eta] , \tag{19}$$

where λ stands for the eigenvalues of H.

Therefore the eigenvalues of $\underline{\tilde{H}}(\eta)$ satisfy

$$\lambda_1(\eta) = 0 , \tag{20}$$

$$\lambda_{2,3}^2 + 400(\eta+1)\lambda_{2,3} - 90\,000(\eta+2)\eta = 0 . \tag{21}$$

Thus, for $\eta = 0$ we have

$$\lambda_1(0) = \lambda_2(0) \tag{22}$$

and

$$\lambda_3(0) = -400 . \tag{23}$$

Obviously in view of Eqs. (21)–(23), $\lambda_2(\eta)$ and $\lambda_3(\eta)$ are analytic at $\eta = 0$. On the other hand, a straightforward calculation shows that the only eigenvector which corresponds to $\lambda_1 = \lambda_2 = 0$ is

$$\vec{C} = (4, -3, -5i), \quad \vec{C}^T\vec{C} = 0 . \tag{24}$$

This shows that $\eta = 0$ is a defective point. Furthermore, since $\partial\lambda/\partial\eta = 0$ for all η, $\eta = 0$ is also a stationary point. This particular example shows that a stationary point $\eta_{\rm opt}$ for which

$$\left.\frac{d\lambda_j(\eta)}{d\eta}\right|_{\eta_{\rm opt}} = 0 , \tag{25}$$

for some j, can also be a defective point at $\eta_b = \eta_{\rm opt}$.

III. THE PHYSICAL INTERPRETATION OF THE INCOMPLETE SPECTRUM OF FINITE-MATRIX HAMILTONIANS

As was discussed in the Introduction, the resonance wave function becomes square integrable when the internal coordinates of the Hamiltonian are complex scaled by $\eta = \exp(-i\theta)$, where $\theta > \theta_c$ and $\theta_c = \frac{1}{2}\Gamma/(E_r - E_{\rm thresh})$. When θ is exactly equal to θ_c the resonance eigenvalue (complex energy,

$E_r - \frac{1}{2}i\Gamma$) is degenerate with the rotating continuum. This is a necessary condition to have a branch point associated with a defective spectrum. However, since the resonance wave function ψ_r and the eigenfunction corresponding to the continuous spectrum ψ_s do not belong to the same class of functions ($\psi_r \in \mathfrak{L}_2$ and $\psi_s \notin \mathfrak{L}_2$), the eigenfunctions ψ_r and ψ_s cannot coalesce at $\theta = \theta_c$ and the spectrum is a complete one.

In contrast with the behavior of the exact solution, when the Hamiltonian is approached by the finite-element method the resonance eigenvalue varies somewhat with θ (though much less than the continuum solutions), and the continuous solutions are described by square-integrable functions. Consequently, for $\theta = \theta_b$ (which approaches the exact θ_c) it is possible that both the eigenvalues and the eigenvectors that represent the resonance and the continuum (scattering) solutions will coalesce in the complex plane to a defective point at

$$\eta_b = \alpha_b \exp(-i\theta_b) . \qquad (26)$$

In other words, *the incomplete spectrum of the model Hamiltonian obtained by the finite-element method may be associated with the critical rotation angle θ_c for which the resonance state is covered by the rotating continuum solution.* We study this possibility for a model Hamiltonian for the ^1S resonance of helium.[14]

For the lowest resonance of helium in the ^1S state the kinetic and the potential matrices $\underline{T}$ and $\underline{V}$ [see Eq. (5)] were constructed by a real basis of 36 Hylleraas-type functions

$$(1+P_{12})r_1^l r_2^m r_{12}^n \exp(-\beta_1 r_1 - \beta_2 r_2) \qquad (27)$$

in which P_{12} permutes the particle labels, r_1 and r_2 are the scalar distances of each electron from the nucleus, and r_{12} is the interelectron distance. The $1, m, n$ are the preselected integers ($0 \leq [1, m, n] \leq 3$) and were ordered by the values of the sum $\omega = 1 + m + n$, up to $N = 36$. The prescale parameters were $\beta_1 = \beta_2 = 1.0$. When the scaling factor in Eq. (5) is $\eta = \alpha \exp(-i\theta)$, then the insensitivity of the resonance eigenvalue to changes in θ is reflected (through the Cauchy-Riemann conditions) in the most-stationary behavior of the eigenvalue of $\underline{H}$ [Eq. (5)] with respect to α, when θ is held fixed (the generalized stabilization method, Ref. 14). In the generalized stabilization method the real and the imaginary parts of the complex eigenvalues of $\underline{H}$ are calculated as a function of $\alpha = |\eta|$. The resonance position and width are determined from those eigenvalues that are only weakly dependent on α (the exact resonance eigenvalue is α independent), in contrast to the case of the scattering states that are strongly α dependent. To arrive at these eigenvalues we hold fixed the rotational angle at a value for which a maximum flatness in the curves of either E_r or E_i vs α is realized. The optimal value of θ, θ_{opt} is obtained subject to the requirement that

$$\left(\frac{\partial E_r}{\partial \alpha}\right)_{\eta_{opt}} = \left(\frac{\partial E_i}{\partial \alpha}\right)_{\eta_{opt}} = 0 , \qquad (28)$$

where $\eta_{opt} = \alpha_{opt} \exp(-i\theta_{opt})$.

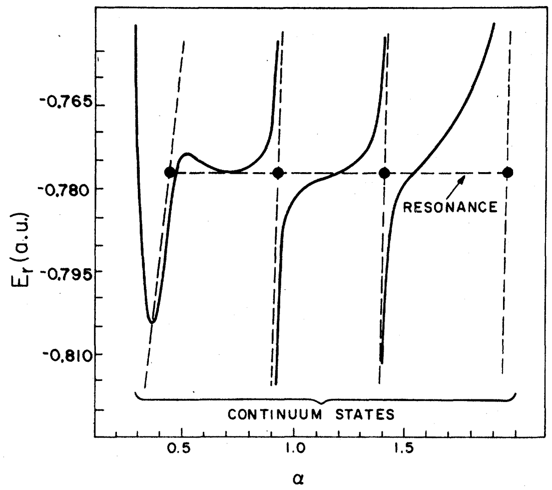

FIG. 1. Stabilization plot of $E_r(\alpha) = \mathrm{Re}[W(\alpha, \theta, N)]$, where $\theta = 0$ and the basis set was composed of $N = 36$ Hylleraas-type functions.

Since the real part of the eigenvalue E_r is less sensitive to variations in θ than the imaginary part E_i, the resonance position can be approximated by the real eigenvalue of the unrotated self-adjoint Hamiltonian $H(\theta = 0)$, which is almost stationary with respect to the variation of the real scaling parameter α (the Holøien-Midtdal procedure[15]). Figure 1 shows such a stabilization plot for helium, clearly indicating the resonance position at approximately −0.777 a.u. This result is in good agreement with the resonance position obtainable from the real part of the complex-stationary points satisfying Eq. (28). The stationary points that represent the resonance solution[16] are given in Table I.

Following the analysis given in the beginning of this section, the resonance position E_r and width

TABLE I. The complex eigenvalues $E_r + iE_i$ at the stationary points $\eta = \alpha_{opt} \exp(-i\theta_{opt})$ (Ref. 16).

α_{opt}	θ_{opt}	$-E_r$	$-E_i$ (10^2)
0.8799	0.2383	0.77767	0.252
1.0677	0.2284	0.77821	0.229
1.2875	0.2266	0.77774	0.259
1.4722	0.0963	0.77782	0.437

$\Gamma = -2E_i$ can also be obtained from the branch point that results from the crossing (in the complex plane) of the curve of the almost-stationary eigenvalue (representing the resonance state) and the family of curves belonging to the eigenvalues that are strongly α dependent (representing the continuous solutions). For $\theta = 0$, this crossing of the curves representing the resonance and scattering eigenvalues is avoided, as can be seen in Fig. 1. Nevertheless, the branch-points positions can be estimated from the values of α associated with the avoided crossing. We therefore would expect the following:

(a) That these branch points will be of order one-half [$P=2$ in Eq. (13)]. Following Theorem 2 in Sec. II, we may assume that $\alpha_{ji} \neq 0$ in Eq. (13), (namely, $\partial w/\partial\eta\,|_{\eta_b} = \infty$).

(b) That the number of the branch points associated with the resonance state (in the finite-matrix-element approximation) is equal to the number of times the continuum solutions cross the resonance eigenvalue (see the dashed lines in Fig. 1). This conjucture is based on the fact that the degeneracy of the resonance state and the scattering state is a necessary condition for obtaining a branch point.

(c) That the values of α for which the branch points may be obtained can be estimated from the positions at which the avoided crossings of the resonance and the continuum solutions take place (see the black dots in Fig. 1).

Following the first argument the energy in the neighborhood of the branch point can be written as

$$W = W_b[(\eta - \eta_b)(\eta - \eta_b^*)]^{1/2} + W(\lambda)\,. \tag{29}$$

The branch point $\eta_b = \alpha_b \exp(-i\theta_b)$ can be obtained[17,18] by expanding W_η in a power series in $(\eta/\alpha_0 - 1)$:

$$W = E_r + iE_i = \sum_{n=0}^{\infty} (\eta/\alpha_0 - 1)^n W^{(n)}\,, \tag{30}$$

where

$$W^{(n)} = [P_{n-2}(\cos\theta_b) - P_n(\cos\theta_b)]/(2n-1)\alpha_b^{n-1} + R^{(n)}\,, \tag{31}$$

in which $P_n(x)$ is a Legendre polynomial and $R^{(n)}$ is a reminder term. By neglecting the $R^{(n)}$ term, Eq. (31) can be rewritten such that[18]:

$$(\alpha_b - 1)^2 = \frac{(n-4)(2n-3)/r_{n-2} - (n-3)(2n-5)/r_{n-1}}{n(2n-5)r_n - (n-1)(2n-3)r_{n-1}}$$

and (32)

$$\cos\theta_b = \frac{(\alpha_b - 1)^2 r_n + (1 - 3/n)/r_{n-1}}{2(\alpha_b - 1)(1 - 3/2n)}\,,$$

where $r_n = W^{(n)}/W^{(n-1)}$. Here $W^{(n)}$ can be calculated by the standard Rayleigh-Schrödinger perturbation theory[19] when the unperturbed Hamiltonian is[20]

$$\underline{H}^{(0)} = \underline{H}(\theta = 0,\ \alpha = \alpha_0) \tag{33}$$

and the perturbation is

$$\underline{H} - \underline{H}^{(0)} = (\eta/\alpha_0 - 1)(2\alpha_0^2 \underline{T} + \alpha_0 \underline{V}) + (\eta/\alpha_0 - 1)^2 \alpha_0^2 \underline{T}\,. \tag{34}$$

By solving Eqs. (32) for different values of α_0, the branch points summarized in Table II were obtained. One can see from these results that our conjectures (b) and (c) were satisfied as well: The number of the branch (and defective) points is found, as was indicated in Fig. 1, and the values of α_b that were obtained from the above branch-point analysis are in good agreement with the estimated values obtained from Fig. 1 (as summarized in Table II). The same phenomena were obtained for a smaller basis set of 20 functions in which $0 \leq [1, m] \leq 2$ and $n = 0$.

The association of the defective point with the resonance state can be also introduced by the θ-trajectory results (see Fig. 2): For a certain value of α, two eigenvalues of $\underline{H}$ approach one another as θ is varied, and these coalesce at the defective point $\theta = \theta_b$. By increasing the value of θ, two branches of eigenvalues are obtained again, where one branch is much more θ dependent than the other one. The branch that represents the continuum spectrum solution is strongly rotated with θ. On the other hand, the branch that is almost θ independent represents the resonance state. As the basis set becomes complete this resonance branch will be closer to the branch point. The distance in the complex plane (L in Fig. 2) between the complex-stationary solution and the defective solution (the branch point) is an indication of the quality of the basis to describe both the resonance and the continuum solutions. Since the real square-integrable basis functions are not well suited to describe the rotating continua, it is not expected that the branch-defective point will give a good approximation to the resonance width. As shown in Tables I and II, the rotation angle θ_b for which the branch point was obtained deviates numerically from the rotation angle $\theta_c \simeq 0.005$ that

TABLE II. The complex eigenvalues $E_r + \frac{1}{2}i\,E_i$ at the defective points $\eta = \alpha_b \exp(-i\theta)$.

α (Fig. 1)	α_b	θ_b	$-E_r$	$-E_i$
0.4	0.44 564	0.13 527	0.75	0.04
0.9	0.92 500	0.02 326	0.78	0.03
1.4	1.40 635	0.01 926	0.78	0.03
2.0	2.05 440	0.03 224	0.74	0.06

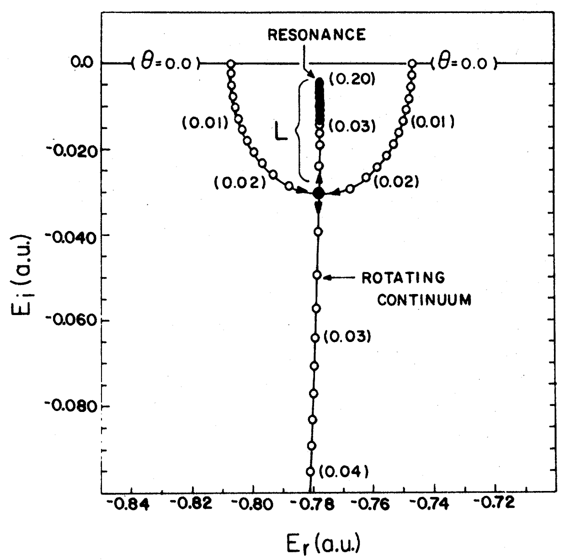

FIG. 2. θ trajectory for fixed $\alpha = 0.925$. The black dot denotes the branch point in which the spectrum is incomplete. Note that the eigenvalues that represent the continuum are more strongly affected by θ than those that represent the resonance. The arrows indicate the direction of motion of the eigenvalues with increasing θ.

should be obtained following the Balslev-Combes theorem.[1]

IV. DISCUSSION

It has already been noted[3] that in the finite-element approximation of the complex-scaling method some numerical and formal difficulties may arise. For a certain value of the complex-scaling parameter η one eigenvector of the non-Hermitian complex-scaled Hamiltonian $\underline{H}_\eta$ is orthogonal to itself (so-called defective eigenvector), giving rise to an incomplete spectrum. We proved here that for *any* matrix representation of the complex-scaled Hamiltonian one can find, at least, one such value of η. It was pointed out that this defective eigenvector can be associated with a complex-stationary point $(\partial/\partial\eta)[(\psi|H|\psi)/(\psi|\psi)] = 0$ that represents the resonance state. Furthermore, the defective point, which is not a stationary solution in the variational space, may be associated with the resonance state as well. The defective point is the branch point obtained whenever the resonance eigenvector and the eigenvectors that represent the continuum as well as their respective eigenvalues coincide. This phenomenon was illustrated here for the e^--He^+ scattering process.

In order to get a proper estimation for the resonance width from the branch-point analysis, the matrix representation of the complex-scaled Hamiltonian should be good enough in describing both those scattering states which are not square-integrable and the resonance state. The latter is square integrable when the complex product rather than the Hermitian product is utilized.

The numerical procedure suggested here may prove to be not very practical; it does, however, yield a better understanding of the behavior of the resonance solution in the finite-element approximation.

ACKNOWLEDGMENTS

This work was supported in part by the National Science Foundation under Grant No. CHE77-1994 and Grant No. MCS 7908323, and by the U. S. Army under Contract No. DAAG29-75-C-0024. One of us (N.M.) welcomes the opportunity to thank Professor J. O. Hirschfelder and all the members of TCI in Madison, Wisconsin for their warm hospitality. Special thanks are due to Professor Phillip Certain and to Professor Frank Weinhold for their constant encouragement, discussions, and patience, and to Dr. Murray Brockman, Dr. Chris Corcoran, and Dr. Jim-Gingi Diamond for the enjoyable scientific discussions we shared.

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[2]See, e.g., C. W. McCurdy and T. N. Rescigno, Phys. Rev. Lett. 41, 1364 (1978); N. Moiseyev and C. T. Corcoran, Phys. Rev. A 20, 814 (1979).

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[4]In this spirit the complex-scaling method was applied to atomic autoionizing resonances. See, for example, the special complex-scaling issue of Int. J. Quantum Chem. 14, No. 4 (1978).

[5]For an example of an incomplete spectrum of a finite complex-symmetric matrix (one eigenvector is orthogonal to itself) see J. H. Wilkinson, *The Algebraic Eigenvalues Problem* (Oxford University Press, New York, 1965), p. 27. The fact that this is also possible for the resonance state was also privately communicated by B. Simon.

[6]The fact that the exact spectrum is incomplete may be indicated by the finite-element methods. As the basis set is increased, the components of the resonance eigenvector would get larger and larger values. This is because an eigenvector $\vec{C}^T\vec{C} = \epsilon^2$ will subsequently be complex normalized by multiplying by the large factor $1/\epsilon$. ϵ does not vanish because of the finite-element approximation, but becomes smaller as $\vec{C}$ approaches the exact eigenfunction.

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New York, 1964), Chap. 9, Sec. 15.
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[13]Reference 12, Chap. 2, Theorem 2.3; S. Friedland, Bol. Soc. Bras. Mat. 9, 13 (1978).
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[20]Note that $\underline{H}^{(0)}$ is a self-adjoint matrix, and the branch point which is associated with the incomplete spectrum of $\underline{H}$ determines the radius of convergence of the Rayleigh-Schrödinger perturbation expansion. For a more detailed discussion see Ref. 18.