

# Resonances by the complex coordinate method with Hermitian Hamiltonian.

## II. Error estimates

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Using the Hermitian representation of the complex coordinate method that recently has been developed (Ref. 1), error estimates for the approximate resonance position and width are calculated. We prove here that for a given estimate of the resonance position and width the *exact* solution is embedded in the surface of a crescent being part of an annular ring whose inner and outer radii can be obtained by variational calculations. An illustrative numerical example is presented.

### I. INTRODUCTION

The complex coordinate method,<sup>2</sup> in spite of its successful application to atomic and molecular resonances, has two mainly numerical difficulties that arise from the fact that the complex-rotated Hamiltonian  $\hat{H}_\theta$  is a non-Hermitian operator:

(1) The spectrum of the complex-rotated Hamiltonian may be incomplete<sup>3,4</sup> such that one of the eigenfunctions is "defective" in the sense that  $\int \psi^2 d\tau = 0$ . Within the finite matrix Hamiltonian approach one can always find at least one rotational angle for which the matrix is defective.<sup>4</sup>

(2) The complex-variation principle, unlike the conventional one, is a stationary principle rather than a minimum principle for either the resonance position or width.<sup>3,5</sup>

To avoid the formal and computational difficulties which rise from the possibility that the spectrum of  $\hat{H}_\theta$  is incomplete a new variational method was proposed by Certain.<sup>6(a)</sup> In this method the resonance state is obtained by solving variational functions for the amplitude and the phase of the complex wavefunction. However, new types of basis sets are required.

Recently,<sup>1</sup> a new representation of the complex-coordinate method has been given, in which the resonance position  $E_r$  and width  $-2E_i$  are variational parameters of an Hermitian Hamiltonian,  $\hat{\mathcal{H}}^2(\theta, E_r, E_i)$  such that

$$\hat{\mathcal{H}}^2 \phi = \lambda^2 \phi; \quad \phi = \begin{pmatrix} \phi_i \\ \phi_r \end{pmatrix}, \quad (1)$$

where

$$\hat{\mathcal{H}}^2(E_r, E_i) = \hat{H}_0 + E_i \hat{H}_1 + E_r \hat{H}_2 + E_i^2 + E_r^2, \quad (2)$$

$$\hat{H}_0 = \hat{H}(\mathbf{r} \exp i\theta), \quad (3)$$

$$\hat{H}_1 = \text{RE}(\hat{H}_\theta),$$

$$\hat{H}_2 = \text{IM}(\hat{H}_\theta)$$

and

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$$\hat{H}_0 = \begin{pmatrix} \hat{H}_r^2 + \hat{H}_i^2 & [\hat{H}_i, \hat{H}_r] \\ [\hat{H}_r, \hat{H}_i] & \hat{H}_r^2 + \hat{H}_i^2 \end{pmatrix},$$

$$\hat{H}_1 = \begin{pmatrix} -2\hat{H}_i & 0 \\ 0 & -2\hat{H}_r \end{pmatrix},$$

$$\hat{H}_2 = \begin{pmatrix} -2\hat{H}_r & 0 \\ 0 & -2\hat{H}_i \end{pmatrix}. \quad (4)$$

The new Hamiltonian  $\hat{\mathcal{H}}^2$  is Hermitian (and real) and its lowest eigenvalue  $\lambda^2$  is the variance of  $\hat{H}_\theta$ , i.e.,

$$\lambda^2 = \langle \phi_r + i\phi_i | (\hat{H}_\theta - E)^+ (\hat{H}_\theta - E) | \phi_r + i\phi_i \rangle. \quad (5)$$

The exact resonance position  $E_r$  (exact) and width  $-2E_i$  (exact) are the variational parameters in Eq. (1) for which

$$\lambda^2 = 0. \quad (6)$$

The purpose of this paper is to show how the resonance position and width can be obtained by solving real and Hermitian eigenvalue problem and to show how maximum information on the location of the resonance can be obtained by using the error estimate for the resonance position and width, obtained recently in Ref. 8. We show here that:

(a) the *exact* position and width of the resonance is a point on the surface of an annular ring.

The outer radius of the annular ring has been proven<sup>8</sup> to be

$$\lambda_0^2 = \langle \chi_r + i\chi_i | (\hat{H}_\theta - E)^+ (\hat{H}_\theta - E) | \chi_r + i\chi_i \rangle, \quad (7)$$

where

$$E = \langle \chi_r + i\chi_i | \hat{H}_\theta | \chi_r + i\chi_i \rangle \quad (8)$$

is the center of the annular ring, and the complex function  $\chi$  is a variational estimate of the exact eigenfunction of the complex but Hermitian operator

$$(\hat{H}_\theta - \tilde{E})^* (\hat{H}_\theta - \tilde{E}) \quad (9)$$

with an estimate of the resonance location  $\tilde{E} = \tilde{E}_r + i\tilde{E}_i$ . It has been shown<sup>8</sup> that

$$(\Delta E_i^c)^2 + (\Delta E_r^c)^2 \leq \lambda_0^2, \quad (10)$$

where  $\Delta E_i^c$  and  $\Delta E_r^c$  are the deviations from the exact position and width, defined as

$$\Delta E_r^c = E_r(\text{exact}) - E_r,$$

$$\Delta E_i^c = E_i(\text{exact}) - E_i. \quad (11)$$

The inner radius of the annular ring is  $\lambda$  [defined in Eqs. (1) and (5)], provided that the energy  $E$  entering these equations satisfy Eq. (8). Then, one has

$$(\Delta E_r^c)^2 + (\Delta E_i^c)^2 \geq \lambda^2, \quad (12)$$

which can be considered as generalization of the result obtained in Ref. 1 for imaginary part only.<sup>7</sup>

The meaning of the above introduced radii  $\lambda$  and  $\lambda_0$  composing the annular ring is following:  $\lambda_0$  gives the actual error estimate,<sup>8</sup> i.e., tells us where the resonance is, whereas  $\lambda$  tells us where the resonance is *not*.

(b) The best error estimate of a given stage of calculation is the area of a crescent, obtained from the intersection of two annular rings with different origins.

A proof of Eq. (12) is given in Sec. III, whereas the relation of the eigenvalue of  $\hat{\mathcal{H}}^2(E_r, E_i)$  [Eq. (1)] to the variance defined in Eq. (5) is given in the next section. In Sec. IV, an illustrative numerical example is presented.

## II. THE VARIANCE OF $\hat{H}_\theta$

The operator  $(\hat{H}_\theta - E) * (\hat{H}_\theta - E)$  can be split into the real and imaginary parts such that<sup>1</sup>

$$(\hat{H}_\theta - E) * (\hat{H}_\theta - E) = (\hat{H}_r - E_r)^2 + (\hat{H}_i - E_i)^2 + i[\hat{H}_r, \hat{H}_i]. \quad (13)$$

Therefore,

$$(\hat{H}_\theta - E) * (\hat{H}_\theta - E) | \phi_r + i \phi_i \rangle$$

can be rewritten and replaced by

$$\begin{pmatrix} (\hat{H}_r - E_r)^2 + (\hat{H}_i - E_i)^2 & [\hat{H}_r, \hat{H}_i] \\ [\hat{H}_r, \hat{H}_i] & (\hat{H}_r - E_r)^2 + (\hat{H}_i - E_i)^2 \end{pmatrix} \times \begin{pmatrix} \phi_i \\ \phi_r \end{pmatrix} \equiv \hat{\mathcal{H}}^2 \phi, \quad (14)$$

and from Eqs. (1)–(5) we see that  $\lambda^2$  is also the eigenvalue of the complex but Hermitian operator  $(\hat{H}_\theta - E) * (\hat{H}_\theta - E)$ . From the Hellman–Feynman theorem,<sup>9</sup> one can show that the lowest eigenvalue of  $\hat{\mathcal{H}}^2$  gets a minimal value  $\lambda^2$  if

$$E_r + iE_i = \langle \phi_r + i\phi_i | \hat{H}_\theta | \phi_r + i\phi_i \rangle. \quad (15)$$

Therefore,  $\lambda_0^2$  is the variance of  $\hat{H}_\theta = \hat{H}_r + i\hat{H}_i$  [ $\sigma(E)$  in the notation used in Ref. 8 and 5]

$$\sigma(E) \equiv \lambda^2 = \langle \phi_r + i\phi_i | \hat{H}_\theta - \langle \hat{H}_\theta \rangle * (\hat{H}_\theta - \langle \hat{H}_\theta \rangle) | \phi_r + i\phi_i \rangle. \quad (16)$$

## III. IMPROVEMENT OF ERROR ESTIMATES FOR THE RESONANCE POSITION AND WIDTH

In the following, we will demonstrate that the error estimate obtained in Ref. 8 (disk with the radius  $\lambda_0$  in the complex plane) can be improved by introducing a new concept<sup>7</sup> of the inner radius, which satisfies the inequality (12). Thus, the error estimate is reduced from a circle to a smaller area of an annular ring which is defined by inner and outer radii  $\lambda$  and  $\lambda_0$ , respectively.

### A. Proof that $(\Delta E_r^c)^2 + (\Delta E_i^c)^2 \geq \lambda^2$

On the basis of the proof given in the previous section, Eq. (1) can be rewritten such that

$$\sigma = \langle \phi | \hat{\mathcal{H}}^2(E_r + \Delta E_r, E_i + \Delta E_i) | \phi \rangle. \quad (17)$$

$E_r$  and  $E_i$  are the approximated resonance position and width and are held fixed, whereas  $\Delta E_r$  and  $\Delta E_i$  are the two variable in the Hamiltonian. If  $\Delta E_r = \Delta E_r^c$  and  $\Delta E_i = \Delta E_i^c$  [see Eq. (11)] then,

$$\begin{aligned} E_i + \Delta E_i^c &= E_i(\text{exact}), \\ E_r + \Delta E_r^c &= E_r(\text{exact}). \end{aligned} \quad (18)$$

Equations (18) can be satisfied if  $\phi$  is optimized in a complete variational space and then

$$|\phi\rangle = |\psi_{\text{exact}}\rangle, \quad (19)$$

and, therefore,

$$\sigma = 0. \quad (20)$$

By substituting Eqs. (18)–(20) in Eq. (17), we obtain:

$$\begin{aligned} 0 &= \langle \psi_{\text{exact}} | \hat{\mathcal{H}}^2(E_r, E_i) | \psi_{\text{exact}} \rangle + \Delta E_i^c \langle \psi_{\text{exact}} | \hat{H}_1 | \psi_{\text{exact}} \rangle \\ &+ \Delta E_r^c \langle \psi_{\text{exact}} | \hat{H}_2 | \psi_{\text{exact}} \rangle + (\Delta E_i^c)^2 + (\Delta E_r^c)^2 \\ &+ 2E_r \Delta E_r^c + 2E_i \Delta E_i^c, \end{aligned} \quad (21)$$

$\Delta E_i^c$  and  $\Delta E_r^c$  can be obtained by the following variational calculations: For any values of  $\Delta E_r$  and  $\Delta E_i$ ,  $|\phi\rangle$  is optimized to yield a minimal value of  $\sigma$ . From the Hellman–Feynman theorem,<sup>9</sup> we get that

$$\begin{aligned} \frac{d\sigma}{d\Delta E_i} &= \left\langle \phi_{\text{opt}} \left| \frac{\partial \hat{\mathcal{H}}^2}{\partial \Delta E_i} \right| \phi_{\text{opt}} \right\rangle \\ &= 2\Delta E_i + \langle \phi_{\text{opt}} | \hat{H}_1 | \phi_{\text{opt}} \rangle + 2E_i, \end{aligned} \quad (22)$$

$$\begin{aligned} \frac{d\sigma}{d\Delta E_r} &= \left\langle \phi_{\text{opt}} \left| \frac{\partial \hat{\mathcal{H}}^2}{\partial \Delta E_r} \right| \phi_{\text{opt}} \right\rangle \\ &= 2\Delta E_r + \langle \phi_{\text{opt}} | \hat{H}_2 | \phi_{\text{opt}} \rangle + 2E_r. \end{aligned} \quad (23)$$

$\Delta E_i^c$  and  $\Delta E_r^c$  are the values for which the global minima of  $\sigma$  at  $\sigma = 0$  is obtained, i.e.,

$$\left. \frac{d\sigma}{d\Delta E_i} \right|_{\Delta E_i^c} = 0, \quad (24)$$

$$\left. \frac{d\sigma}{d\Delta E_r} \right|_{\Delta E_r^c} = 0,$$

and then

$$\begin{aligned} |\phi_{\text{opt}}\rangle &= |\psi_{\text{exact}}\rangle \\ \sigma &= 0. \end{aligned} \quad (25)$$

By substituting Eqs. (24) and (25) in Eqs. (22) and (23) one can get that

$$E_i + \Delta E_i^c = -\frac{1}{2} \langle \psi_{\text{exact}} | \hat{H}_1 | \psi_{\text{exact}} \rangle \quad (26)$$

and

$$E_r + \Delta E_r^c = -\frac{1}{2} \langle \psi_{\text{exact}} | \hat{H}_2 | \psi_{\text{exact}} \rangle. \quad (27)$$

The following equality is obtained by substituting Eqs. (26) and (27) into Eq. (21),

$$(\Delta E_i^c)^2 + (\Delta E_r^c)^2 = \langle \psi_{\text{exact}} | \hat{\mathcal{H}}^2(E_r, E_i) | \psi_{\text{exact}} \rangle. \quad (28)$$

Since  $E_r \neq E_r(\text{exact})$  and  $E_i \neq E_i(\text{exact})$ , then

$$\hat{\mathcal{H}}^2(E_r, E_i) \phi = \lambda^2 \phi, \quad (29)$$

where  $\lambda^2 \neq 0$  and  $\phi = \psi_{\text{exact}}$ . Consequently, on the basis of the variational principle, it is clear that

$$\lambda^2 \leq \langle \psi_{\text{exact}} | \hat{\mathcal{H}}^2(E_r, E_i) | \psi_{\text{exact}} \rangle. \quad (30)$$

From Eq. (28) and Eq. (30) the desired inequality (12) is obtained. If  $\Delta E_r^c = 0$  and  $E_i = 0$  then valuable information can be extracted from Eq. (12), since the lower bound for the width of the resonance (proved in Ref. 1) is obtained,

$$|E_i(\text{exact})| \geq \lambda. \quad (31)$$

Since  $E_i < 0$  (the resonance width,  $\Gamma$ , is equal to  $-2E_i$ ) then,

$$E_i(\text{exact}) < \lambda \quad (32)$$

and

$$\Gamma(\text{exact}) \geq 2\lambda. \quad (33)$$

One should observe, that the last inequality (33), being a consequence of inequality (30), builds only for  $\lambda^2$  being the exact solution of the eigenvalue equation (29). That implies a limitation on the practical utility of the inequality given in Eq. (12), since if  $\lambda$  is to be obtained from the matrix eigenvalue problem, one has

$$\mathcal{H}^2(E_r, E_i)C = \lambda_{\text{var}}^2 C, \quad (34)$$

where  $\lambda_{\text{var}}^2 \geq \lambda^2$ .

However, as will be shown in Sec. IV, if calculations are carried out within a large enough basis set then adequate approximation to  $\lambda^2$  can be obtained and the inequality proved above can actually sharpen the error estimate given in Eq. (10). In connection with the numerical calculations, it should be stressed that although the validity of the inequality (12) depends on the numerical accuracy of  $\lambda^2$ , the validity of the error estimate given by Eq. (10) does not depend on the quality of the variational calculation.

### B. Error estimates given by an annular ring in the $E_r - E_i$ plane

The error estimates can be reduced from an annular ring to the area of a crescent obtained from the intersection of two annular rings with different origins which are obtained by solving Eq. (1). In the iteration procedure (described more explicitly in Sec. IV A) from given initial  $E_r^{(j)}$  and  $E_i^{(j)}$  one calculates  $\lambda^{(j)}$  according to Eq. (29), and then proceeds to obtain  $E_r^{(j+1)}$ ,  $E_i^{(j+1)}$  and  $\lambda_0^{(j+1)}$ , according to Eqs. (7) and (8), so that

$$\lambda_0^{(j)} = \lambda^{(j-1)} - (E_r^{(j)} - E_r^{(j-1)})^2 - (E_i^{(j)} - E_i^{(j-1)})^2. \quad (35)$$

Since  $(\lambda^{(j)})^2$  is the lowest eigenvalue of  $(\hat{H}_\theta - E) * (\hat{H}_\theta - E)$  (see Sec. II) and  $\lambda_0^{(j)}$  is not [see Eq. (7)], then it is clear from the variational principle that

$$\lambda^{(j)} < \lambda_0^{(j)}. \quad (36)$$

Therefore, the exact resonance position and width is a point  $[E_r(\text{exact}), E_i(\text{exact})]$ , located on an annular ring in the  $E_r - E_i$  plane. The origin of the annular ring,  $(E_r^{(j)}, E_i^{(j)})$ , is given by the estimates of the resonance position and width which satisfy Eq. (8). The inner and the outer radii of the annular ring are  $\lambda^{(j)}$  and  $\lambda_0^{(j)}$ , respectively.

From Eq. (35) and the inequality (36), one obtains that

$$\lambda^{(j)} < \lambda_0^{(j)} < \lambda^{(j-1)}. \quad (37)$$

Note that in the present notation,  $\lambda^{(j)}$  and  $\lambda_0^{(j)}$  belong to different iterations, since  $\lambda_0^{(j)}$  is obtained from  $\lambda^{(j-1)}$  without solving a new eigenvalue problem, and to get  $\lambda^{(j)}$  one must solve a new eigenvalue problem the radii  $\lambda_0^{(j)}$  and  $\lambda^{(j)}$  are associated with two circles which have the same origins  $(E_r^{(j)},$

$E_i^{(j)})$ . However,  $\lambda_0^{(j)}$  and  $\lambda^{(j-1)}$  are associated with circles which do not have the same origin.

This behavior of the outer radius,  $\lambda_0^{(j)}$ , and the inner radius,  $\lambda^{(j)}$ , of the annular rings in the iteration process are illustrated in the numerical results presented in Figs. 4 and discussed in the next section. In each  $j$  step of the iteration procedure the values of  $\lambda^{(j)}$  and  $\lambda_0^{(j)}$  are reduced and a new estimate of the resonance position  $E_r^{(j)}$  and width  $-2E_i^{(j)}$  are obtained. Since those values of the resonance position and width  $(E_r^{(j)}, E_i^{(j)})$  are taken as the origin of the annular ring  $D^{(j)}$  then the origin of  $D^{(j)}$  is changed in each iteration and the exact solution is a point on the surface,  $S$ , obtained from the overlap of the shifted annular rings. Such that,

$$S = D^{(1)} \cap D^{(2)} \dots \cap D^{(j)}.$$

Naturally, for a given iteration the "crescent type" estimate given by the surface "S" is better than the "annular type" estimate implied by Eq. (36), since the former is always a subset of the latter.

## IV. AN ILLUSTRATIVE NUMERICAL EXAMPLE

In this section, the procedure of calculating the resonance position and width and its corresponding error estimates, by the complex coordinate method with Hermitian Hamiltonian is illustrated. As an example, we shall study here the one-dimensional model Hamiltonian:

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dX^2} + \left( \frac{1}{2} X^2 - 0.8 \right) \exp(-0.1X^2) + 0.8, \quad (38)$$

whose potential exhibits the predissociation resonances analogous to those found in diatomic molecules, and which was used previously to illustrate the variational calculations by the complex-coordinate method.<sup>3</sup> The computations are carried out by using two basis sets constructed of even-tempered Gaussians

$$\{\phi_i = \exp(-\epsilon^{i-1} X^2)\}.$$

The smaller basis is constructed out of 20 functions,  $N = 20$ , where the nonlinear parameter  $\epsilon$  was optimized and was found to be  $\epsilon = 0.45$ . In large basis set calculations,  $N = 100$ ,  $\epsilon$  was taken to be 0.75. This large basis set can be referred to as a "complete" one since the resonance position and width obtained by the complex coordinate method<sup>10(a)</sup> are in agreement to six digits with the accurate results previously obtained by numerical integration of the complex-rotated Riccati equation.<sup>10(b)</sup>

### A. Resonances by the complex coordinate method with Hermitian Hamiltonian

The outline of the computational procedure is as follows:

(1) Calculation of the matrix elements of the Hermitian Hamiltonian  $\{\langle i | \hat{\mathcal{H}}^2 | j \rangle\}$  which are defined in Eq. (4). The matrix elements of  $\hat{H}_1$  and  $\hat{H}_2$  can be evaluated analytically for any fixed rotation angle  $\theta$ . However, the matrix elements  $\langle i | \hat{H}_0 | j \rangle$  can also be obtained either by a numerical integration or by using the approximate resolution of identity:

$$1 \cong \sum_{k=1}^l |k\rangle \langle k|, \quad (39)$$

where

$$\{|k\rangle, k = 1, \dots, l\}$$

is a large enough basis set. In such a case  $\langle i|\hat{H}_0|j\rangle$  can be evaluated since

$$\langle i|\hat{A}\hat{B}|j\rangle \cong \sum_{k=1}^l \langle i|\hat{A}|k\rangle \langle k|\hat{B}|j\rangle,$$

where  $\hat{A}$  and  $\hat{B}$  are either the real or imaginary parts of the complex rotated Hamiltonian  $\hat{H}_\theta$ .

(2) Optimization of  $E_r$  and  $E_i$  to yield a minimal value of  $\lambda^2$  which is the lowest eigenvalue of  $\mathcal{H}^2$ . From the Hellman-Feynman theorem one can get that a local minimum of  $\lambda^2$  is obtained if,

$$E_r = -\frac{1}{2} \langle \phi | \hat{H}_2 | \phi \rangle \quad (40)$$

and

$$E_i = -\frac{1}{2} \langle \phi | \hat{H}_1 | \phi \rangle. \quad (41)$$

Therefore, the iterative procedure can be used for the optimization of, <sup>2</sup> i.e.,

$$\begin{aligned} \mathcal{H}_{j+1}^2 &= H_0 + E_r^{(j)} H_1 + E_i^{(j)} H_2 + (E_r^{(j)})^2 + (E_i^{(j)})^2, \\ \mathcal{H}_{j+1}^2 C_{j+1} &= \lambda_{j+1}^2 C_{j+1}, \end{aligned} \quad (42)$$

and in the next step of the iteration

$$\begin{aligned} E_r^{(j+1)} &= -\frac{1}{2} C_{j+1} H_2 C_{j+1}, \\ E_i^{(j+1)} &= -\frac{1}{2} C_{j+1} H_1 C_{j+1}. \end{aligned} \quad (43)$$

The initial estimate of the resonance position  $E_r^{(0)}$  is obtained from stabilization calculations, where  $E_i^{(0)} = 0$ .

(3) Optimized  $\theta$  is obtained by carrying out  $\theta$ -trajectory calculations. The resonance is associated with the stationary solution for which<sup>3,11</sup>

$$\frac{\partial E_r}{\partial \theta} = 0 \quad \text{and} \quad \frac{\partial E_i}{\partial \theta} = 0. \quad (44)$$

It should be stressed that for any given basis set

$$\{|i\rangle, i = 1 \dots N\},$$

large enough  $l$  should be used in order to satisfy Eq. (39). If for example,  $l = N$ , where  $N$  is the dimension of the matrices  $H_r$  and  $H_i$  (note that the dimension of the matrices  $H_0$ ,  $H_1$  and  $H_2$  is  $2N$ ) then the iterative procedure presented above is another computational method of obtaining the complex eigenvalues of the matrix

$$H_\theta = H_r + iH_i.$$

As convergence is achieved

$$\lim_{j \rightarrow \infty} \lambda_j^2 = 0!$$

Consequently, if  $l = N$  the resonance position and width obtained by this method are exactly the same as the matrix eigenvalue which are obtained by solving the complex matrix eigenvalue problem

$$H_\theta D = (E_r + iE_i)D.$$

However, if  $l \gg N$ , then  $\lambda$  approaches zero only as  $N$  is increased and the optimized  $E_r$  and  $E_i$  converge to the exact values.

In Fig. 1, the results of the Holøien-Midtal stabilization<sup>12</sup> calculations with 20 basis functions are presented. The

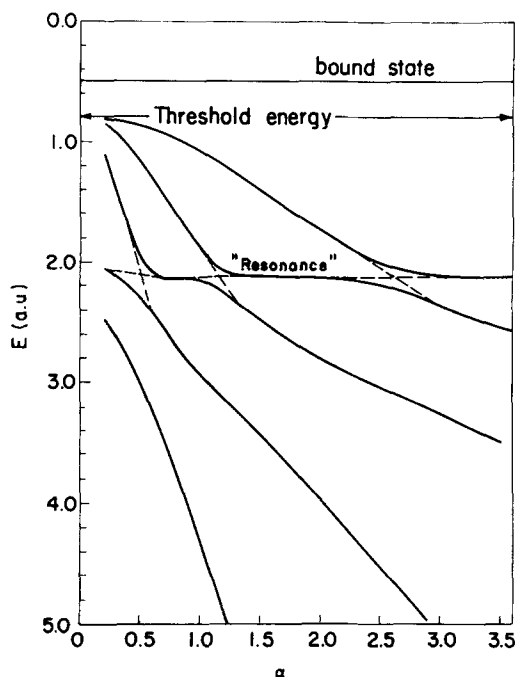


FIG. 1. Stabilization plot of  $E(\alpha)$ .  $\alpha$  is a real scaling factor. The dashed lines indicate the avoiding crossings which give rise to the "plato" associated with the resonance state.

internal coordinate  $X$  in the Hamiltonian was scaled by the real factor  $\alpha$ . For  $\alpha = 1.8$  one of the eigenvalues is stabilized at  $E \approx 2.12$ . This value was used as the initial estimate for the resonance position in the iterative procedure described above. In the calculation of the matrix elements of the square operator,  $\hat{H}^2$ ,  $\hat{H}_i^2$ ,  $\hat{H}_i \hat{H}_r$ , and  $\hat{H}_r \hat{H}_i$  in Eq. (39) was taken to be 100. The iterations were carried out until convergence to within six digits of  $E_r$  and  $E_i$ . The results as functions of  $\theta$  are presented in Fig. 2(a). The estimate of the resonance position  $E_r = 2.12805$  and width  $-2E_i = 0.02545$ , are obtained for  $\theta_{\text{opt}} = 0.36$ .

The convergence of the iterative computations is very rapid. The results given in Fig. 2(b) show that the resonance position and width obtained after the first iteration do not deviate much from the final results.

As discussed above these values are different from the estimates of the resonance position  $E_r = 2.13036$  and width  $-2E_i = +0.03006$ , which are obtained by solving the complex eigenvalue problem

$$H_\theta D = (E_r + iE_i)D,$$

or, alternatively, by taking  $N = l = 20$  in the iterative procedure presented here. [The results of the  $\theta$ -trajectory calculations for the case  $N = l = 20$  are shown in Fig. 2(c).]

## B. Error estimates by the complex coordinate method with Hermitian Hamiltonian

The error estimates of the resonance position and width are obtained from the variance of  $\hat{H}_\theta$ . As it has already been discussed before<sup>5,8</sup> it is not necessarily true that smaller variance is obtained for the variational function which yields a better estimate of the resonance in position and width. Therefore, it might happen that within the finite matrix Ha-

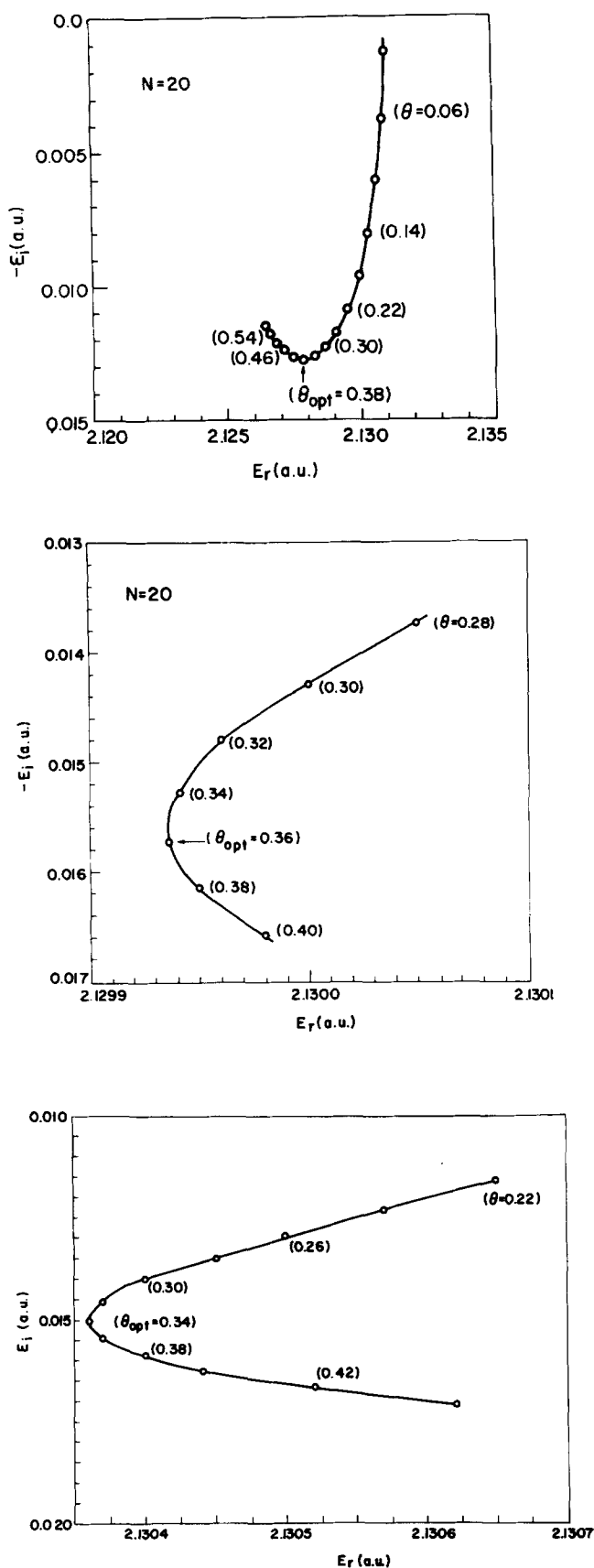


FIG. 2.  $\theta$  trajectory for the predissociation resonance with the optimum scale  $\alpha = 1.8$ , obtained with 20 Gaussians basis. (a) By the Hermitian representation of the complex coordinate method—upon convergence. (b) By the Hermitian representation of the complex coordinate method—first iteration. (c) By the complex coordinate method (i.e., by solving the complex non-Hermitian eigenvalue problem).

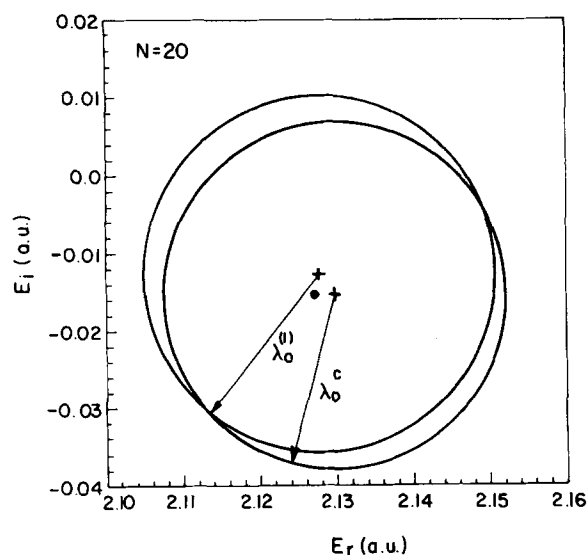


FIG. 3. Error estimates obtained by the Hermitian representation of the complex coordinate method with 20 Gaussians basis.  $\lambda_0^{(1)}$  stands for the error estimate (outer radius) obtained in the first iteration of the calculations, where  $\lambda_0^c$  is the value obtained on convergence.

miltonian approximation a good estimate of the resonance position and lifetime is obtained. Although the corresponding error estimate,  $\lambda_0$  is quite poor, such an example is illustrated in the results presented in Fig. 3. For  $N = 20$  the estimate of the resonance position and width was obtained as discussed above in Sec. IV A (denoted by the cross in Fig. 3). The deviation of  $E_r$  and  $E_i$  from the exact solution (the latter is denoted by the black point in Fig. 3) is small in comparison with the error estimate obtained from the first iteration [c.f. Eq. (42)]. However, for a large enough basis set  $N = 100$  the error estimate  $\lambda_0^{j+1}$  becomes smaller and the  $\lambda^{j+1}$  which is obtained by solving Eqs. (42) reduces the error estimate from a full disc in the complex plane to the smaller area of a crescent. The center of the annular ring is  $(E_r^{(j)}, E_i^{(j)})$  obtained in the  $j$ th iteration where its inner and outer radii are  $\lambda^{j+1}$  and  $\lambda_0^{(j+1)}$ , respectively. Figures 4 show how the error estimates are consequently reduced in the process of iteration. After completion of each iteration the exact result is contained in the crescent area. Comparing two consecutive iterations confines the exact result to the area of a crescent. We note that the relatively large area of the first annular ring is heavily reduced to a small crescent area after the second iteration, obtained after the second, third, etc., iterations, and illustrate clearly how the error estimates shrink to zero as the variational resonance position and width approach the exact values.

## V. DISCUSSION

The calculation of the predissociation resonance position and width by the Hermitian representation of the complex coordinate method that has been recently developed<sup>1</sup> is illustrated here for a simple one-dimensional model Hamiltonian. Under the approximation of  $\langle \hat{H}^2 \rangle = \langle \hat{H} \rangle^2$  the solution obtained by the Hermitian representation of the complex coordinate method is identical to the variational

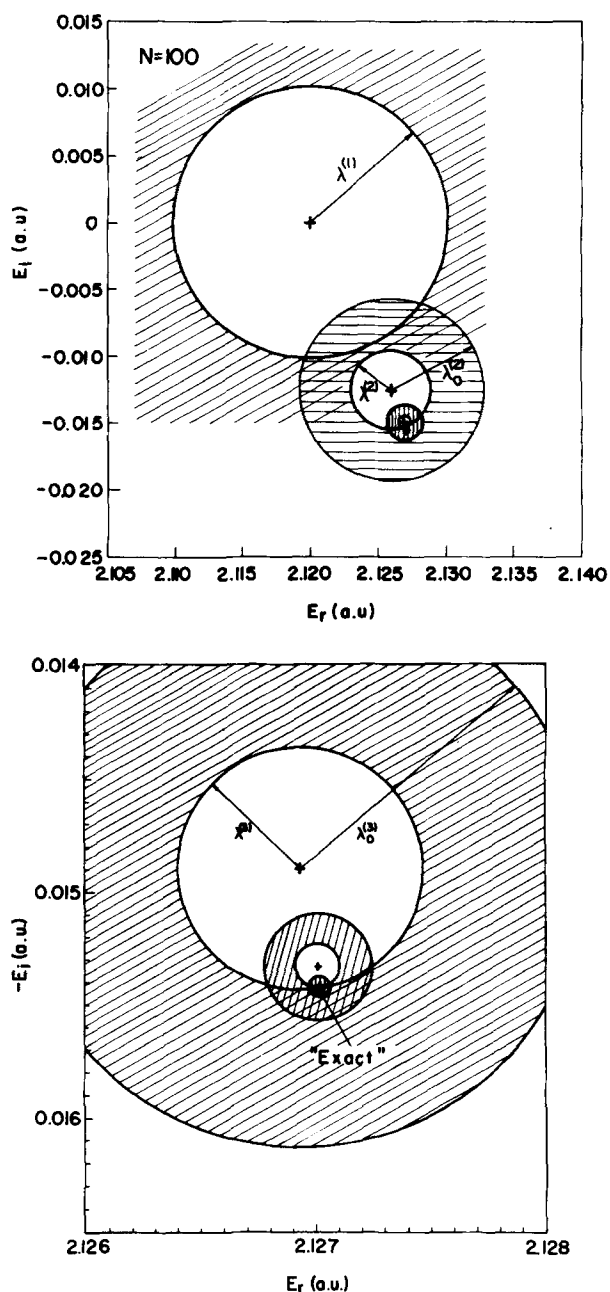


FIG. 4. Error estimates obtained by the Hermitian representation of the complex coordinate method with 100 Gaussians basis. The "+" signs indicate the estimate of the resonance position and width in each iteration. The resonance is located within the dashed area. The intersection of the dashed areas gives the optimal estimate of the resonance location. (a) Results obtained through the first three steps of the iteration procedure. (b) Results obtained throughout iterations three to six. The largest annular ring on this figure is repeated from Fig. 4(a) where it appears as the smallest annular ring.

solution which is obtained by solving the complex eigenvalue problem

$$\mathcal{H}_\theta D = (E_r + iE_i)D.$$

The numerical advantage of the new method in such a case,

is in the truncation of the length of the numerical calculations. The resonance position and width can be estimated by calculating the lowest eigenvalue and the corresponding eigenvector of an Hermitian (and real) matrix Hamiltonian only [i.e., the first iteration,  $j = 0$ , in the computational procedure described in Eqs. (42) and (43)]. If the matrix elements  $\langle H^2 \rangle$  are accurately evaluated, then the variational values of the resonance position and width obtained by the Hermitian representation of the complex coordinate method can differ from the variational solutions obtained by solving the complex eigenvalue problem. It is proved here that for the variational solution

$$((E_r(\text{var}), E_i(\text{var})),$$

obtained by the Hermitian representation of the complex coordinate method the inequality,

$$(E_r(\text{exact}) - E_r(\text{var}))^2 + (E_i(\text{exact}) - E_i(\text{var}))^2 \geq \lambda^2$$

is satisfied where  $\lambda^2$  can be estimated by an accurate variational calculation. This result which is a generalization of the inequality condition proved in Ref. 1, together with the error estimate for the resonance position and width proved in Ref. 8 yield an improvement of the latter. We show here that the exact solutions ( $E_r$  and  $E_i$ ) is a point on an annular ring. In the iterative computational procedure (described in Sec. IV A and illustrated by the results presented in Figs. 4) smaller and smaller annular rings of decreasing size with different origin are obtained. Therefore, the exact solution is a point on the area obtained from the overlap of the shifted annular rings, and a minimal error estimates of the resonance position and width for a given basis set are obtained.

#### ACKNOWLEDGMENT

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