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Extensions of the complex-coordinate method to the study of resonances in many-electron systems

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Difficulties in the straightfoward application of the complex-coordinate method to the calculation of resonance states in many-electron systems are examined. For the case of shape resonances, it is shown that many of these difficulties can be avoided by using complex coordinates only after reduction of the system to an effective one-electron problem. Further simplifications are achieved by the use of an inner-projection technique to facilitate the computation of the complex Hamiltonian matrix elements. The method is first illustrated by application to a model-potential problem. Its suitability for studying many-electron problems is demonstrated by calculation of the position and width of a low-energy $^2P^o$ shape resonance in Be^-. We discuss the modifications necessary to study core-excited (Feshbach) resonances.

I. INTRODUCTION

The calculation of the positions and widths of atomic and molecular autoionizing states continues to be a problem of considerable interest. In the case of molecules, resonance parameters can be used to model a variety of important processes such as dissociative attachment, associative, and Penning ionization.[1]

While resonance effects can be studied theoretically by solution of the scattering equations and a search for the characteristic rapid variation of the cross section in the vicinity of a resonance, such an approach frequently involves calculations over a fine energy mesh and the possibility of missing narrow resonances. Furthermore, in the case of molecules, such detailed calculations are beset with numerous computational difficulties and, in many cases, are beyond the scope of present computer capabilities. This has led many investigators to search for direct methods of evaluating resonance parameters.

The stabilization method[2] is perhaps the simplest of these approaches and makes use of the fact that a resonance wave function is often localized, i.e., has large amplitude in a region close to the target center and is thus well represented by an expansion in terms of square-integrable functions. While the stabilization method is quite successful in finding the position of narrow resonance states, it becomes more difficult to apply in the case of broad resonances where the wave functions are not necessarily well localized. Furthermore, the stabilization method does not provide a rigorous prescription for finding the resonance width, except in special cases.[3]

Another frequently used technique is based on a projection operator formalism, originally introduced by Feshbach.[4] This approach provides a "golden-rule-like" formula for the width involving a matrix element of the Hamiltonian between a resonance wave function $Q\psi$ (which can be calculated by the stabilization method, for example) and a background continuum function $P\psi$.[5] The principle difficulty with this method is that the projection operators become difficult to evaluate in many-electron problems when multiconfiguration wave functions are used. Furthermore, rigorous evaluation of the background function $P\psi$ is equivalent to solving the full scattering problem and hence further approximations, such as the use of unperturbed wave functions or the expansion of $P\psi$ in terms of normalizable functions, are often required to make the problem tractable.[6]

A third approach to the study of autoionizing states is provided by the use of complex coordinates to analytically continue the Hamiltonian into the complex plane. While such techniques have been known for some time as a formal tool for extending the region of analyticity of the S matrix,[7] complex-coordinate techniques have more recently been used as the basis for new computational developments as well.[8] The method is based on the analytic properties of the Hamiltonian under the dilatation transformation $r \to re^{i\theta}$. For a suitable class of analytic potentials, this transformation has the following effect on the spectrum of H (Ref. 9): (i) The eigenvalues corresponding to bound states of H are not effected by the transformation. (ii) The branch cuts associated with the continuous spectrum of H are rotated into the lower-half E plane (assuming $0<\theta<\frac{1}{2}\pi$) by an angle -2θ. (iii) Resonance or Siegert states exposed by the rotation of the branch cut correspond to discrete, normalizable states of the Hamiltonian $H(re^{i\theta})$. Thus the problem of finding resonance states is reduced to that of finding the square-integrable (complex) states of the rotated Hamiltonian $H(re^{i\theta})$.

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The use of complex coordinates is deceptively attractive in its simplicity, since it reduces the problem of finding many-electron resonance states to the solution of an algebraic eigenvalue problem to which the well-established techniques of bound-state configuration interaction can in principle be applied. Indeed, the method has been very successful in various applications to problems involving two-electron atoms.[8] However, efforts to extend the method to many-electron systems have been hampered by problems of slow convergence. A recent attempt to apply this method to study a three-electron resonance was only partially successful.[10]

The slow convergence of the complex-coordinate method when applied to many-electron problems has never been adequately discussed. Such a discussion is given in Sec. II B in terms of a simple physical argument. We also suggest a method for removing these difficulties which is illustrated by calculations on a model-potential problem. To demonstrate the applicability of the method to many-electron problems, we calculate the position and width of a $^2P^o$ shape resonance in Be$^-$.

We should like to point out that a method similar to that discussed here has recently been formulated by Junker and Huang[11] and successfully applied to the $(1s2s2p)\,^2P^o$ resonance in He$^-$. The reader is encouraged to consult these papers for further details.

II. THEORETICAL FORMULATION

A. Potential scattering

For simplicity, we first consider a single-particle potential-scattering problem for which the radial Schrödinger equation is (in a.u.).

$$\left(-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}+V(r)-E\right)\phi(r)=0\,. \qquad (1)$$

We wish to consider the properties of this equation under the transformation $r\rightarrow re^{i\theta}$. If $\phi_b(r)$ is a bound state of (1) with eigenvalue E, then the requirement that E be unchanged under the dilatation transformation means that the corresponding solution of the rotated Schrödinger equation apart from a normalization constant is simply $\phi_b(re^{i\theta})$. In particular, we note that a bound state of (1), which has a simple exponential behavior for large r, picks up an oscillatory character under coordinate rotation:

$$\psi_b(r\,\exp(i\theta))\sim\exp[-i(\sin\theta)(2E)^{1/2}r]\times\exp[-(\cos\theta)(2E)^{1/2}r]\,. \qquad (2)$$

If one attempts to solve for the bound eigenfunctions of H by an expansion in a set of basis functions $\{\chi_i(r)\}$ and applications of the standard Rayleigh-Ritz variational method, one finds that, whereas $\phi_b(r)$ may be accurately approximated in terms of a few real Slater-type or Gaussian basis functions, a larger set will be required to achieve comparable accuracy in the determination of $\phi_b(re^{i\theta})$ because of the oscillatory nature of the function. One can, of course, expand $\phi_b(re^{i\theta})$ in terms of the complex set of functions $\{\chi_i(re^{i\theta})\}$, but this simply undoes the dilatation transformation and gives back a real set of eigenvalues which are independent of θ.

Now consider a continuum state of H. For large r, the wave function will have the form

$$\phi_k(r)\sim[F(k)e^{-ikr}+F(-k)e^{ikr}]\,, \qquad (3)$$

where $F(k)$ is the Jost function.[12] Resonance or Siegert states will occur at those complex values of k in the lower-half plane where the Jost function vanishes. At these points, the asymptotic wave function will only contain outgoing waves. If we consider such a state with momentum $k=|k|e^{-i\alpha}$, then it is clear from Eq. (3) that for rotation angles $\theta>\alpha$, $\phi_k(re^{i\theta})$ will decay exponentially. However, the same considerations of the convergence to be expected in a conventional basis-set expansion apply equally to the resonance and bound-state cases, since the states we are attempting to calculate will oscillate as a function of r with an overall exponential decay.

Before concluding this section, we wish to point out that, in using the complex-coordinate method, we require matrix elements of the rotated Hamiltonian:

$$\langle\phi_i|H(re^{i\theta})|\phi_j\rangle=\int_0^\infty\phi_i^*(r)H(re^{i\theta})\phi_j(r)\,dr\,. \qquad (4)$$

If we carry out the integration in Eq. (4) along a rotated contour and then make the simple change of variable $r\rightarrow re^{i\theta}$, we obtain

$$\langle\phi_i|H(re^{i\theta})|\phi_j\rangle=e^{-i\theta}\int_0^\infty\phi_i^*(re^{+i\theta})H(r)\phi_j(re^{-i\theta})\,dr\,. \qquad (5)$$

For this simple case, we see that the rotated-coordinate method is equivalent to a calculation of matrix elements of the real Hamiltonian $H(r)$ using the complex basis $\{e^{-i\theta/2}\phi_i(re^{-i\theta})\}$.[13] It is this identity that will allow us to make progress in the solution of many-electron problems.

B. Many-electron problem

We consider the elastic scattering of an electron by a many-electron target which is described by a ground-state wave function $\Psi_0(r_1,\ldots,r_N)$. We assume that there is an energy range over which the incident electron can be temporarily captured into an autoionizing negative ion state. For simplicity we only consider shape resonances which can occur in symmetries where the effective potential seen by the incident electron contains a barrier. For certain values of the initial momentum, the electron can tunnel through the barrier into an attractive potential well and be temporarily trapped in a pseudo-bound-state. We are not considering Feshbach resonances which are associated with virtual excitation of the target. The modifications necessary to treat these types of resonances will be mentioned in the concluding remarks.

The elastic wave function for the $N+1$ particle system is antisymmetric under interchange of the coordinates of any pair of electrons. As any one coordinate becomes large, the wave function has the asymptotic form

$$\Psi(r_1,\ldots,r_{N+1}) \xrightarrow[r_i\to\infty]{} \Psi_0(\cdots r_{i-1}, r_{i+1}\cdots) \times[A(k)e^{-ikr_i}+A(-k)e^{ikr_i}]. \quad (6)$$

Note that we have suppressed any dependence of the wave function on angular coordinates and, for simplicity, assumed it to be a function of radial coordinates only. This is only done for purposes of keeping the notation simple.

A resonance state of the many-electron system corresponds to a complex value of k for which the coefficient $A(k)$ in Eq. (6) vanishes. Such a state will be square integrable when evaluated at complex values of r_i for which $|\arg(r_i)|>|\arg(k)|$. Formally, such states can be obtained by transforming all the radial coordinates and looking for the discrete, normalizable eigenvectors of the Hamiltonian $H(r_1e^{i\theta},\ldots,r_{N+1}e^{i\theta})$. From a practical viewpoint we can see that this expansion will be slowly convergent from the following considerations.

Suppose that the ground state of the target is well described by a Hartree-Fock, single Slater determinant:

$$\Psi_0(r_1,\ldots,r_N)\sim\mathcal{A}(\phi_1(r_1)\cdots\phi_N(r_N)). \quad (7)$$

After coordinate rotation, the wave function which gives the same value for the Hartree-Fock energy is simply that given in Eq. (7) with all the coordinates replaced by $r_ie^{i\theta}$. To represent this function accurately in terms of real Slater functions, it is necessary to expand each orbital in (7) in terms of a new one-particle basis. This amounts to doing a full configuration-interaction expansion just to obtain the Hartree-Fock energy and is clearly impossible for systems containing more than two or three electrons. It is easy to see from the discussion of Sec. II A that in the independent-particle model, the period of oscillation for fixed θ will be proportional to the square root of the orbital binding energy, and hence that the tight core orbitals will be the most difficult to represent in a basis set. This is disconcerting since one would hope that it would be a good approximation to describe the core electrons in an independent-particle model, since they contribute minimally to low-energy resonance formation.

Consideration of the asymptotic form of the $(N+1)$-electron wave function given in Eq. (6) shows that it is only necessary to make the coordinate dependence of a single-electron complex in order to render the solution square integrable. Recalling the discussion at the end of Sec. II A, we see that this can be accomplished by using $(N+1)$-electron configurations of the form

$$\chi_i(r_1,\ldots,r_{N+1})=\mathcal{A}(\Psi_0(r_1,\ldots,r_N)e^{-i\theta/2}\phi_i(re^{-i\theta})) \quad (8)$$

to expand the wave function. Because of the antisymmetrizer in Eq. (8), these configurations are in general nonorthogonal. Furthermore, although we have assumed that $\Psi_0(r,\ldots,r_N)$ is a single-determinantal wave function for the purposes of this discussion, we see that this is by no means necessary in actual computations, as Ψ_0 can be an arbitrarily complex multiconfiguration wave function.

This procedure is not equivalent to computation with the usual complex many-electron Hamiltonian. It does, however, correspond to an analytic continuation of the effective one-body Hamiltonian one obtains by first integrating over the coordinates of the target electrons. Because of the need for antisymmetrizing the entire wave function, this effective Hamiltonian must necessarily be nonlocal. The advantage of this approach is that the accuracy achieved in the original specification of Ψ_0 is maintained in the resonance computations, since complex basis functions are only used to expand the open-channel one-particle function.

There is one additional approximation we should like to discuss. Consider a matrix element of H between two configurations of the kind used in Eq. (8):

$$\langle\chi_i|H|\chi_j\rangle=e^{-i\theta}\int\mathcal{A}(\phi_1^*(r_1)\cdots\phi_N^*(r_N)\phi_i^*(r_{N+1}e^{i\theta}))H(r_1,\ldots,r_{N+1})\,\mathcal{A}(\phi_1(r_1)\cdots\phi_N(r_N)\phi_j(r_{N+1}e^{-i\theta}))dr_1\cdots dr_{N+1}. \quad (9)$$

If the Hamiltonian is first projected onto a real set of $N+1$ electron configurations $\Gamma_i(r_1, \ldots, r_{N+1})$,

$$H \sim \sum_{k,l} \Gamma_k^*(r_1, \ldots, r_{N+1}) H_{kl} \Gamma_l(r_1, \ldots, r_{N+1}) , \quad (10)$$

then we can approximate the matrix element in Eq. (9) as

$$\langle \chi_i | H | \chi_j \rangle = \sum_{ijkl} \langle \chi_i | \Gamma_k \rangle H_{kl} \langle \Gamma_k | \chi_j \rangle . \quad (11)$$

The simplifying feature of this approximation is that complex orbitals are only used in the evaluation of an overlap matrix.[14] The fundamental one- and two-electron matrix elements used in the evaluation of the Hamiltonian in Eq. (10) are all performed using real functions. From a more practical viewpoint, this means that we can calculate the Hamiltonian matrix elements using standard bound-state codes without modification, an important consideration in calculations on complex atoms where the evaluation, transformation, and storage of large numbers of two-electron integrals is a limiting factor. This is especially true in molecular applications. The evaluation of complex overlap integrals is by contrast a relatively simple task.

III. APPLICATIONS

A. Model problem

The complex-basis-function technique is first illustrated by application to a model problem involving s-wave scattering from the potential

$$V = V_0 r^2 e^{-r} . \quad (12)$$

This same problem has been studied previously by Bain, Bardsley, Junker, and Sukumar using complex-coordinate methods.[10] Our purpose in reexamining the problem here is to illustrate the inner-projection technique discussed in Sec. II.

The s-wave Hamiltonian, $-\frac{1}{2}(d^2/dr^2) + V(r)$, is first projected onto a set of N square-integrable real functions, $\{\chi_n\}$. These are chosen to be normalized Laguerre functions,

$$\chi_n(r) = \frac{\lambda^{3/2} r}{[(n+1)(n+2)]^{1/2}} L_n^2(\lambda r) e^{-\lambda r/2} , \quad (13)$$

which are equivalent to the functions used by Bain *et al.* in their trial function A.[10] We then chose a basis set of M complex functions with which to diagonalize the projected Hamiltonian. For this purpose, we have used the same type of Laguerre functions given by Eq. (13), with λ replaced by $\lambda e^{-i\theta}$. As previously discussed, the final computation of the Hamiltonian matrix only involves evaluation of the complex overlap matrix elements

$$S_{mn} = \frac{\lambda^3 e^{-i3\theta/2}}{[(m+1)(m+2)(n+1)(n+2)]^{1/2}} \times \int_0^\infty r^2 L_m^2(\lambda r) L_n^2(\lambda r e^{-i\theta}) \, dr , \quad (14)$$

in terms of which the Hamiltonian is written,

$$\underline{H}^\theta = \underline{S}^\dagger \cdot \underline{H} \cdot \underline{S} , \quad (15a)$$

with

$$H_{ij} = \langle \chi_i | H | \chi_j \rangle . \quad (15b)$$

For a value of $V_0 = 7.5$, Bain *et al.* find, by direct integration, a shape resonance with a position E of 3.426 39 a.u. and a width Γ of 0.025 55 a.u., which can be associated with a complex eigenvalue of the rotated Hamiltonian at $E - \frac{1}{2} i \Gamma$. It is not our purpose here to study exhaustively the convergence of the expansion as the scaling parameter λ, the rotation angle, and the number of functions are independently varied. This has already been done by Bain *et al.* What we have found in our studies is that their results can be reproduced essentially exactly, provided that the number of functions N used in the inner projection of the Hamiltonian is greater than the number of complex functions M used in the outer projection. This of course is not surprising since the inner-projection technique simply invokes closure in inserting a quasicomplete set of states into the calculation of an $M \times M$ matrix. For this approximation to be valid, it is necessary that the inner set be essentially complete over the region spanned by the outer set. In our calculations, we found this condition to be well met as long as we choose $N > M + 2$. We emphasize that our only criterion of success here is the accuracy of the computed resonance eigenvalue and

TABLE I. Position and width of s-wave resonance for model potential $V(r) = 7.5 r^2 e^{-r}$ as a function of rotation angle. Results are given for a basis of 20 Laguerre functions of the type $r L_n^2(\lambda r) e^{-\lambda r/2}$ used to expand the Hamiltonian. Fifteen such functions with r replaced by $r e^{-i\theta}$ are used in the formation of the complex Hamiltonian. For these calculations, $\lambda = 8$. The exact answer is $E = 3.4264$, $\Gamma = 0.025 55$.

Rotation angle (deg)	Energy (a.u.)	Width (a.u.)
5	3.4240	0.026 96
10	3.4262	0.025 58
15	3.4264	0.025 42
20	3.4264	0.025 52
25	3.4264	0.025 54
30	3.4264	0.025 56
35	3.4264	0.025 78
40	3.4264	0.008 46

TABLE II. Dependence of model-problem resonance parameters on the number of real functions used to represent the Hamiltonian. In these calculations, 18 complex functions are employed with a rotation angle of 15° and $\lambda = 8$.

N	Energy (a.u.)	Width (a.u.)
12	3.4028	0.000 05
15	3.4139	0.014 68
18	3.4236	0.023 96
20	3.4264	0.025 51
22	3.4264	0.025 50
25	3.4264	0.025 52
30	3.4264	0.025 55
35	3.4264	0.025 55
40	3.4264	0.025 55

that we are not concerned with other properties of the matrix.

Some typical results are presented in Table I, where we show the behavior of the resonance parameters as the rotation angle is varied. For these calculations, the values of M and N were 15 and 20, respectively. The scaling exponent λ was taken to be 8. The accuracy achieved in these calculations is comparable to that obtained by Bain *et al.*, who used the same expansion parameters.

In Table II we show how, for a given complex basis, the computed resonance energy depends on the number of functions used in the inner projection. For these calculations, 18 complex functions were used with $\lambda = 8$ and the rotation angle was 15°. We see that the results rapidly converge as soon as N is increased beyond 18, as expected.

B. $^2P^o$ shape resonance in Be

Electron scattering by the group IIA and IIB metal vapors has been the subject of recent experimental work.[15] The elastic cross sections for these systems show broad resonance behavior at low energy, which has been ascribed to the formation of short-lived $^2P^o$ negative-ion states. These atoms all have (ns^2) closed-shell ground states, so that the resonance states could be associated with a negative ion of the configuration $(ns^2np)\,^2P^o$. Atomic Be is unfortunately not among those systems that have been studied, but it would be expected to show the same type of behavior.

In all of our calculations, we have considered the attachment of a p electron to a ground-state Be atom that is described by a simple Hartree-Fock wave function. While it is true that use of a more elaborate target function or an attempt to include polarization effects may well have an effect on the position and width of the resonance, we wished to confine our attention to a model that we could also solve numerically. We did have access to a numerical Hartree-Fock program[16] and, as we will show, the low-energy phase shifts obtained in this manner are entirely consistent with the results obtained using the rotated-coordinate procedure.

We begin with a self-consistent-field wave function for the $(1s^2 2s^2)\,^1S^e$ state of Be. For this purpose, we use the $5s$ set of Slater functions given by Clementi.[17] The Hartree-Fock energy of Be in this basis is $-14.573\,01$ a.u. For the Be$^-$ calculations, this basis is augmented with an additional set of 14 p functions. The calculations reported here were performed with Slater functions whose parameters are given in Table III. We wish to point out, however, that equivalent results were obtained in calculations using different sets of functions.

We next form a matrix representation of the five-electron Hamiltonian using all configurations of the form

$$\Gamma_n(r_1, \ldots, r_5) = \mathcal{A}(\phi_{1s}(r_1)\alpha_1\phi_{1s}(r_2)\beta_2\phi_{2s}(r_3) \times \alpha_3\phi_{2s}(r_4)\beta_4\phi_{np}(r_5)\alpha_5)\,. \quad (16)$$

In Eq. (15), ϕ_{1s} and ϕ_{2s} are the Hartree-Fock orbitals of neutral Be. The $\{\phi_{np}\}$ constitute an orthornormal set and are formed by ordering the Slater functions according to the magnitude of their orbital exponents and sequentially Gramm-Schmidt orthogonalizing them starting with the tightest function. Thus ϕ_{np} is a function containing n modes and spans a larger region of r space than ϕ_{n-1p}.

TABLE III. Slater orbital parameters used in Be$^-$ calculations. Numbers refer to basis functions of the type $r^n e^{-\alpha r} Y_{lm}(\hat{r})$.

Orbital	n	l	α
S_1	1	0	3.5297
S_2	1	0	6.4072
S_3	2	0	1.1956
S_4	2	0	3.2341
S_5	2	0	0.8198
P_1	2	1	5.0
P_2	2	1	4.2
P_3	2	1	3.4
P_4	2	1	2.6
P_5	2	1	1.8
P_6	2	1	1.0
P_7	2	1	0.787
P_8	2	1	0.620
P_9	2	1	0.487
P_{10}	2	1	0.384
P_{11}	2	1	0.302
P_{12}	2	1	0.237
P_{13}	2	1	0.186
P_{14}	2	1	0.147

The complex-coordinate configurations are then chosen as

$$\chi_n(r_1, \ldots, r_5) = \mathcal{A}(\phi_{1s}(r_1)\alpha_1\phi_{1s}(r_2)\alpha_2\phi_{2s}(r_3) \times \alpha_3\phi_{2s}(r_4)\beta_4\phi_{np}(r_5e^{-i\theta})\alpha_5). \qquad (17)$$

We use fewer functions in this second expansion than we do in the original specification of H, for the reasons discussed in Sec. III A. Furthermore, because of the way in which the functions are orthogonalized, it is most reasonable to delete functions from the end of the list.

The results of a series of calculations using 10 complex orbitals are shown in Fig. 1. The real and imaginary parts of an eigenvalue which is clearly a resonance is plotted as a function of rotation angle. We note that this root is quite stationary over the broad range of rotation angles $50° < \theta < 80°$. This behavior contrasts sharply with that of other nonresonant roots which show no sign of stability as the rotation angle is varied. A typical nonresonant trajectory is also shown in Fig. 1 for comparison.

The complex root shown in Fig. 1 stabilizes at a value of (−14.5450, −0.0205) a.u. When referenced to the Hartree-Fock energy of Be calculated in our basis, this corresponds to a resonance position of 0.76 eV and width of 1.11 eV or a k value of (0.250, −0.082) a.u. We have also evaluated the p-wave-continuum Hartree-Fock functions of Be numerically, and in Fig. 2 we have plotted the $l = 1$ phase shift as a function of incident energy. The phase shift is seen to rise rapidly from threshold to a value near $\frac{1}{2}\pi$ and then decrease slowly. It is difficult to obtain a meaningful fit of this data with a Breit-Wigner form, since the resonance is extremely broad and occurs at a low energy where the background phase shift is also varying rapidly. It is possible, however, to use the effective-range formula to obtain the desired resonance parameters, as suggested by Henry, Burke, and Sin Fai Lam.[18]

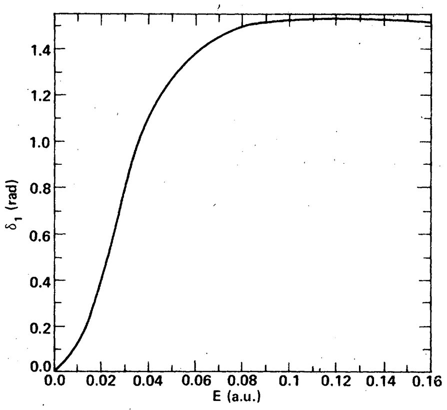

FIG. 2. Numerical p-wave phase shifts for $e^- +$ Be in the static-exchange approximation.

In the absence of polarization terms, the low-energy p-wave phase shifts will possess the behavior given by

$$k^3 \cot\delta = -1/a + \tfrac{1}{2}\rho k^2 , \qquad (18)$$

where a is the scattering length and ρ is the effective range.[19] This formula should also be valid for complex k near zero energy. Now, as Henry *et al.*[18] point out, at a resonance the T matrix, which we write as

$$T_l(k) \sim e^{i\delta}\sin\delta = \frac{1}{\cot\delta - 1} , \qquad (19)$$

has a simple pole so that $\cot\delta = i$. Thus the resonance corresponds to that value of k for which

$$k^3 i = -1/a + \tfrac{1}{2}\rho k^2 . \qquad (20)$$

If we now substitute the value of k obtained in our

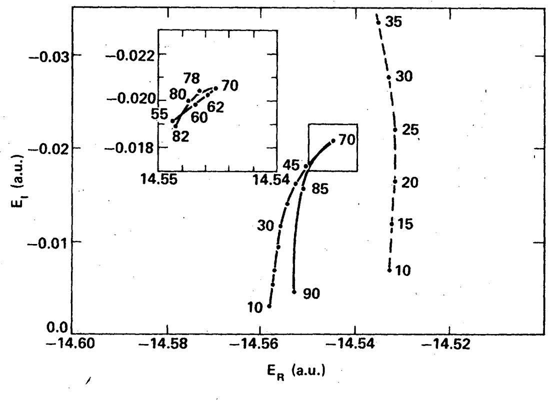

FIG. 1. Behavior of the Be⁻ resonance eigenvalue as a function of rotation angle (solid line + insert). Shown for comparison is the trajectory of a nonresonant root (dashed line).

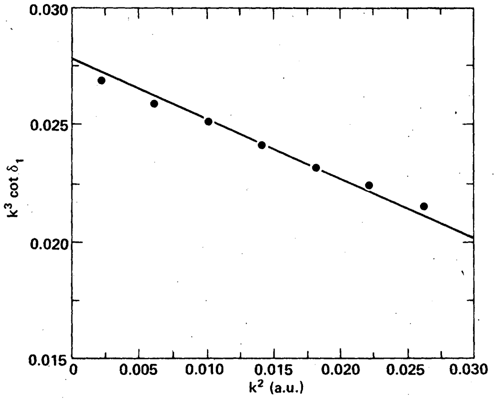

FIG. 3. Numerically obtained values of $k^3 \cot\delta$ vs k^2 (dotted curve) and the theoretical curve obtained using the computed complex value of k and Eqs. (18) and (20) of the text (solid curve).

complex-coordinate calculations [$k = (0.250, -0.082)$] into Eq. (20), we obtain values for a and ρ of -33.97 and -0.521, respectively. In Fig. 3, we plot the numerically obtained values of $k^3 \cot\delta$ vs k^2 along with the values obtained using our values of a and ρ in Eq. (18). The agreement between the two sets of data is seen to be quite good and shows that the resonance energy given by the complex-coordinate technique is, in fact, the correct one for this frozen-core model.

IV. CONCLUSION

We have argued that the slow convergence experienced in straight forward application of the complex-coordinate method to many-electron problems is associated with the use of square-integrable functions to expand oscillatory core orbitals and have shown how a modified complex basis function technique can be used to sidestep this problem. We have outlined a method for using complex basis functions in the calculation of shape resonances in many-electron atoms and applied it to study on autoionizing $^2P^o$ state of Be . In this approach, the $(N+1)$-electron Hamiltonian is reduced to an effective one-body problem by integrating over the coordinates of the target wave function. Complex basis functions are only used in calculating matrix elements of this one-body operator.

The approach we have used calls for a coordinate rotation in the basis functions referring to a single active electron. While we have only illustrated the case of elastic-shape resonances in this paper, it should be clear that the same techniques can also be applied to core-excited Feshbach resonances. Such states can be idealized as being formed when a bound target electron is excited into an unoccupied orbital, thereby providing the energy required for the temporary capture of a second electron. The configurations necessary to describe such states correspond to virtual excitation into closed channels and can certainly be included within the framework we have suggested. If the total energy of the system is high enough to allow for decay of the resonance into excited target states plus a free electron, we have to extend the asymptotic form of the wave function [Eq. (6)] to include all such open channels. The technique of using configurations with a single complex orbital simply allows one to render the open-channel parts of the resonance wave function square integrable. The closed-channel components of the wave function, which decay exponentially even for real r, could in principle be described by a set of purely real configurations. The use of a single rotated orbital in all configurations would then be more a matter of convenience than necessity.

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