

Saddle-point complex-rotation method for resonances

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A new procedure is suggested to improve the convergence of the complex-rotation method. Calculations are carried out for the He $2s2s$ 1S and $2s2p$ 1P resonances. With a relatively small and simple wave function, one obtains a width which is stable to six digits over a wide range of rotational angles and nonlinear parameters. The results are compared with those of the most accurate theoretical calculations and experiments. The feasibility of applying this method to more complicated systems as well as multichannel problems is also discussed.

The method of complex rotation¹ has generated considerable interest in the past several years. The advantage of this method is that the resonance energy and width of a scattering resonant state can be computed with square-integrable basis functions. This is an extremely attractive feature which has spurred many intensive efforts in applying this method to atomic and molecular systems.² However, poor convergence has been the main obstacle for wide range applications. For example, for a two-electron system, Hylleraas basis functions ranging from 125 to 1200 terms have been used to achieve convergent results.³⁻⁵ Very limited accurate results have been published beyond the two-electron system. Another feature in the conventional complex-rotation method is that the physical solution is mingled with a large number of unphysical solutions. Unless one knows the resonance position before the calculation, it is difficult to sort out the true resonance from among the large number of solutions, especially when the convergence is poor. This seriously limits the ability of the method to "predict" resonances. Junker and Huang⁶ and Rescigno *et al.*⁷ have shown that since the resonant wave function is an analytic function, much of the instability in the complex eigenvalue that results from rotating the Hamiltonian can be eliminated by using basis functions that are functions of $re^{i\theta}$. Although much attention has been given to the convergence of the complex eigenvalue with respect to different forms for the "open-channel" component of the wave function, and with various correlated target functions,^{8,6} less attention has been given to the "closed-channel" component. The degree to which the complex eigenvalue can converge to the true resonant energy depends on how complete the basis

functions are for describing the closed-channel component. In this work we start our complex-rotation calculation with a set of optimized basis functions representing the closed channel that have been predetermined by the saddle-point technique.⁹

Recently, the saddle-point technique has been developed to calculate the energy of a closed-channel resonance.⁹ Extensive applications have been carried out which show that it is highly accurate and a fast convergent method.^{10,11} The greatest strength of the saddle-point technique is its ability to predict Feshbach resonances. Since spurious solutions are removed by directly building the proper vacancies into the wave function, the energies obtained below a corresponding threshold are all physical resonances. The maximum-minimum principle upon which this method is based allows the nonlinear parameters in the basis functions to be optimized, so that each resonance can be represented with a relatively compact wave function. The one shortcoming of this method is that it does not give the width of a resonance directly without including the open-channel segment explicitly, and this may also introduce a small "shift" from the saddle-point energy to the true resonance position. The inclusion of this nonsquare-integrable component, however, would increase the computational difficulties substantially. By combining the saddle-point technique with the complex-rotation method this shortcoming can be avoided.

Part of the convergence problem associated with the conventional complex-rotation method has been previously corrected for by understanding the analytic properties of the resonant wave function.^{6,7} One can also understand this problem from the viewpoint of optimized basis functions in a varia-

tional calculation.

Let us consider an N -particle Hamiltonian

$$H(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = H(R_N, \Omega_N), \quad (1)$$

where R_N represents the set of radial coordinates r_1, r_2, \dots, r_N , and Ω_N represents the angular coordinates collectively. Assume that an eigenfunction of this H can be efficiently expanded in terms of a basis set $\phi_j(R_N, \Omega_N)$, so that only a limited number of terms need be used to give an accurate representation of the eigenfunction and eigenvalue. This limited number of ϕ_j , is, of course, far from being a complete set. If we begin to rotate the Hamiltonian, i.e.,

$$H = H(R_N e^{i\theta}, \Omega_N), \quad (2)$$

where $R_N e^{i\theta}$ implies that each radial coordinate r_j takes the form $r_j e^{i\theta}$, then this new Hamiltonian is very different from Eq. (1), and the corresponding eigenfunction is also changed substantially even though the eigenvalue is supposed to remain the same. The nonlinear parameters in ϕ_j which are most suitable for the solution of $H(R_N, \Omega_N)$ may not be suitable for that of $H(R_N e^{i\theta}, \Omega_N)$. Since the ϕ_j are far from a complete set, the corresponding roots of the secular equation become unstable, resulting in poor convergence.

It is easy to recover this convergence if one rotates the basis functions ϕ_j with H , i.e.,

$$\phi_j = \phi_j(R_N e^{i\theta}, \Omega_N). \quad (3)$$

In this case one finds that the eigenvalue E is invariant as H rotates. If E is real before the rotation, it remains real when H rotates. No imaginary part will appear as a result of this rotation, i.e., the

$$\Psi(R_N e^{i\theta}, \Omega_N) = \sum_j C_j \phi_j(R_N e^{i\theta}, \Omega_N) + A \sum_{i,k} d_{ik} \psi_i(R_{N-1} e^{i\theta}, \Omega_{N-1}) u_k(\vec{r}_N). \quad (5)$$

With this Ψ , the width and shift are calculated from the secular equation that results from

$$\delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0. \quad (6)$$

Note that the unconjugated $e^{i\theta}$ is used in the complex conjugated wave function.

To test our procedure, we carried out calculations for the He $2s2s \ ^1S$ and $2s2p \ ^1P$ resonances. The ϕ_j are the same configuration basis functions as those of Ref. 10. The $1s$ vacancy orbital is also of the same form. The optimized nonlinear parameter q

width does not come out.

It is well known that the width of a resonance is the result of the coupling between the closed- and open-channel components of the resonant wave function.^{12,13} For narrow resonances, this coupling is very weak. The resonant wave function can then be approximated by the closed-channel component and the resonance energy is largely determined by this component. Based on these considerations, we propose a saddle-point complex-rotation method as follows.

We first solve the resonance problem in the real space with the saddle-point technique. This allows us to obtain a highly accurate and relatively compact basis set ϕ_j with optimized nonlinear parameters. We then add to this function the open-channel segment. The total wave function is then given by

$$\psi(\vec{R}_N) = \sum_j C_j \phi_j(\vec{R}_N) + A \sum_{i,k} d_{ik} \psi_i(\vec{R}_{N-1}) u_k(\vec{r}_N). \quad (4)$$

Here C_j and d_k are the linear parameters, ψ_i are the open-channel target states, and A is the antisymmetrization operator. The angular coupling in the second term of Eq. (4) is suppressed. It is understood that if in the LS coupling scheme Ψ takes a set of good quantum number L, M, S , and S_z , then the target state and the u_k will couple in such a way that the correct angular and spin quantum numbers will be obtained.

The u_k in Eq. (4) form a one-dimensional complete set. The nonlinear parameters in this set can be chosen when a particular calculation is carried out.

When H rotates through an angle θ , we adjust Eq. (4) as follows:

in the vacancy orbital is $q = 1.994$ for the $2s2p \ ^1P$. For the closed-channel component of this resonance, we used a five-partial-wave—47-term-wave function, the saddle-point energy calculated from this basis set is $-0.692\ 620\ 4$ a.u. ψ_i is the ground state of He^+ . If we choose

$$u_k(r) = r^k e^{-\beta r}, \quad (7)$$

the open-channel component becomes

$$\Psi_{\text{open}} = A \left[\psi_{1s}(\vec{r}_1) \sum_{k=1}^K d_k r_2^k e^{-\beta r_2} Y_{10}(\hat{r}_2) \right]. \quad (8)$$

TABLE I. Convergence of the width Γ of $\text{He}2s2p^1P$ as a function of rotation angle θ (in rad) and nonlinear parameter β using the saddle-point complex-rotation method; here y is given in the body of the table, where $\Gamma=(0.00138697+y\times 10^{-8})$ a.u., e.g., if $y=2$, $\Gamma=0.00138699$ a.u. K is the number of terms used in the open-channel wave function.

	β	θ						
		0.2	0.3	0.4	0.5	0.6	0.7	0.8
$K=14$	1.0	-987	-56	-8	-16	-46	-135	-76
	1.5	-476	-19	-1	0	-1	-2	+24
	1.75	-183	-8	-1	0	0	0	+6
	2.00	+506	+20	0	0	0	0	-23
	2.25	-492	-19	-2	-1	0	+8	+64
	2.5	+574	+14	-1	-1	-6	-15	-29
	3.0	+50	+85	+19	+3	+6	-20	-79
	3.5	-1320	-4	+21	+30	+61	+75	+36
$K=19$	1.5	-96	+53	-9	-6	0	-1	41
	1.75	-42	-5	-1	0	1	-1	0
	2.0	+29	+2	0	0	0	0	-5
	2.25	+27	+3	0	0	0	+1	+19
	2.5	+27	-2	0	0	0	-2	-45
	3.0	-287	-10	-1	-1	-1	+4	+55
	3.5	-169	-28	0	+1	-7	-34	-104
	4.0	73	48	+17	+16	+15	-10	-79

If Eq. (8) is substituted into Eqs. (5) and (6), with the rotated H , one obtains the complex energy eigenvalue. This energy is very stable over a wide range of rotation angles θ and nonlinear parameters β . For example, if we use 14 u_k 's ($K=14$), the real

part of the energy is stable to about seven or eight digits. The imaginary part which gives the width of the resonance is also stable. Table I demonstrates the convergence of the width for the 14- and 19-term calculations. Both calculations give a con-

TABLE II. Convergence of the width Γ of $\text{He}2s2s^1S$ as a function of rotation angle θ (in rad) and nonlinear parameter β using the saddle-point complex-rotation method; here y is given in the body of the table, where $\Gamma=(0.0046051+y\times 10^{-7})$ a.u., e.g., if $y=2$, $\Gamma=0.0046053$ a.u. $K+1$ is the number of terms used in the open-channel wave function.

	β	θ					
		0.2	0.3	0.4	0.5	0.6	0.7
$K=14$	1.0	220	25	5	0	-18	-47
	1.25	167	2	1	1	1	2
	1.5	104	4	1	0	0	0
	1.75	-1076	-2	0	0	0	0
	2.0	-102	-5	0	0	0	-3
	2.5	-270	-16	1	-2	-6	18
	3.0	-3	24	23	17	-50	-346
	3.5	775	28	7	131	293	406
$K=19$	1.5	-44	63	4	2	-4	17
	1.75	-78	-5	1	0	0	0
	2.0	-36	-5	0	0	0	0
	2.25	-1	2	0	0	0	1
	2.5	53	18	0	0	0	-4
	2.75	-12	-1	-1	0	2	-2
	3.0	74	2	0	0	2	21
	3.5	126	-2	5	-3	-32	-40

TABLE III. Comparison of energies and width of $2s2s\ ^1S$ and $2s2p\ ^1P$ resonances of helium (in eV).

		Energy	Width	Authors
$2s2p\ ^1P$	Theory	60.1456	0.0371	Ho ^a 161-term Hylleraas function, complex-rotation method
		60.1450	0.0363	Bhatia and Temkin ^b 84-term Hylleraas function plus static exchange
		60.1463	0.0388	Burke and Taylor ^c close-coupling plus correlation
		60.1486	0.03736	This work, configuration-interaction function, saddle-point complex-rotation method
	Expt.	60.13±0.015	0.038±0.0004	Madden and Codling, ^d optical-absorption experiment
$2s2s\ ^1S$	Theory	57.848	0.1235	Ho ^a
		57.8435	0.125	Bhatia and Temkin ^b
		57.8473	0.124	Burke and Taylor ^c
		57.8483	0.124 68	This work
	Expt. ^g	57.82±0.04	0.138±0.015	Hicks and Comer ^e scattering experiment
		57.78±0.03	0.138±0.015	Gelebart <i>et al.</i> ^f scattering experiment

^aReference 3.

^bReference 14.

^cReference 15.

^dReference 18.

^eReference 16.

^fReference 17.

^gBoth experiments are calibrated with $2s2p\ ^1P$ He at 60.13 eV.

verged width of 0.001 386 97 a.u. and a converged resonant energy of $-0.692\ 877\ 7$ a.u. Compared with the saddle-point energy, it is shifted by $-0.000\ 257\ 3$ a.u., or $-0.007\ 00$ eV. This shift agrees with the shift of $-0.007\ 13$ eV calculated by Bhatia and Temkin.¹⁴ A test calculation is also carried out for the $2s2s\ ^1S$ of helium. In this case $q=1.92$. A four-partial-wave-45-term closed-channel wave function gives a saddle-point energy of $-0.777\ 851$ a.u. If we couple this with a 15-term open-channel component we obtain a resonance energy of $-0.777\ 839$ a.u. and a width of 0.004 6051 a.u. If the open-channel component is extended to 20 terms, the same result is again obtained. The convergence behavior for the width is shown in Table II, again, the result is stable over a wide range of θ and β .

It should be pointed out here that the converged width in Tables I and II is with respect to the par-

ticular closed-channel wave function used. Therefore, if the saddle-point solution is further improved, the corresponding result for the width may also change slightly. For example, if we extend the saddle-point solution for $2s2p\ ^1P$ to 73 terms, the saddle-point energy becomes $E=0.692\ 773$ a.u. and we find $E_{\text{res}}=-0.693\ 024$ a.u. and $\Gamma=0.001\ 373\ 1$ a.u. The width is reduced by about 1%. If we extend the $2s2s\ ^1S$ closed-channel wave function to 78 terms, $E=-0.777\ 882$ a.u., we find $E_{\text{res}}=-0.777\ 858$ a.u. and $\Gamma=0.004\ 570\ 7$ a.u. The width is reduced by about 0.5%. These results agree quite well with the accurate theoretical calculations in the literature.^{3,14,15} A comparison of the accurate theoretical and experimental results for these two resonances calculated here is given in Table III. It appears that the widths of the $2s2s\ ^1S$ calculations agree extremely well despite the fact that very different theoretical methods and wave

functions are used. But these results lie on the low side of the quoted experimental width which is also very consistent among the different scattering experiments. It is not clear whether this discrepancy between theory and experiment is due to the way experimental widths are determined.^{16,17}

By contrast, the calculated widths for the $1P^o$ resonance agree very well with the optical-absorption experiment of Madden and Codling¹⁸ in which a detailed line-profile analysis has been made. However, the calculated energy positions are higher than the quoted experimental position by 0.015 to 0.019 eV. The experimental uncertainty is given to be 0.015 eV. Since this experimental result has been used for calibrating many scattering experiments,^{16,17} it would be highly desirable if the experimental uncertainty could be reduced and the disagreement between theory and experiment be resolved.

The method used here bears some similarity with that used by Junker and Huang⁶ except that we propose the use of an optimized closed-channel basis set with the proper vacancies built in and a different

type of basis function is used for the outgoing particle wave function. By taking these procedures, this method can predict resonances rather accurately.

The calculations we carried out in this work are for helium. It is used because accurate theoretical and experimental results are available to access the effectiveness of the method. However, the advantage of this method is mainly for more complicated N -particle systems where a conventional complex-rotation calculation becomes impractical. Instead of using an N -dimensional complete set, the method suggested here advocates the use of a one-dimensional complete set for one particle, namely, the outgoing particle. All other nonlinear parameters are predetermined before the complex rotation is made. This should greatly enhance the applicability of the complex-rotation method.

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