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Complex-coordinate calculation of ${}^1D^e$ resonances using Hylleraas functions

A. K. Bhatia
Laboratory for Astronomy and Solar Physics, NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771

Y. K. Ho
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803-4001

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The method of complex-coordinate rotation is used to calculate the lowest-lying ${}^1D^e$ resonances below the $n=2$ and 3 hydrogen thresholds. Hylleraas functions with up to $N=1230$ terms are used. Resonance parameters for the $n=2$ resonance are determined as $E=-0.255\,873\,7\pm1\times10^{-6}$ Ry and $\Gamma=0.000\,633\,4\pm2\times10^{-6}$ Ry. The resonance parameters for the $n=3$ resonance are determined as $E=-0.131\,906\,6\pm1\times10^{-6}$ Ry and $\Gamma=0.003\,316\pm2\times10^{-6}$ Ry.

There has been continuous interest in accurate calculations of resonances in e^--H scattering. Calculations of resonances below the $n=2$ hydrogen threshold are of particular interest since accurate results could be used for benchmark purposes for other calculations. Three methods have been used for accurate calculations for the $n=2$ resonances. There are the Feshbach projection-operator method,[1] the method of complex-coordinate rotation,[2] and a recent R-matrix (including contributions from a continuum) calculation.[3] In particular, it is found that the resonance parameters for the lowest ${}^1S^e$ and ${}^3P^o$ resonances agree very well among these calculations.[3] In the complex-coordinate-rotation calculation and the Feshbach projection-operator calculation, elaborate Hylleraas-type wave functions were used. It seems now that the resonance parameters for the ${}^1S^e$ and ${}^3P^o$ resonances are accurately known.[4] For the ${}^1D^e$ resonance, Hylleraas-type wave functions have not been used in complex-coordinate calculations. For a strongly correlated lower-lying doubly excited resonance such as the $n=2$ ${}^1D^e$ state, the use of Hylleraas functions would provide an accurate treatment when r_{12} terms are explicitly included. This work provides such a calculation. The most general two-electron D-state wave function of even parity[5] is given by

$$\Phi(r_1,r_2)=(f+\tilde{f})[-\mathcal{D}_2^{0+}(\theta,\phi,\psi)+\sqrt{3}(\cos\theta_{12})\mathcal{D}_2^{2+}(\theta,\phi,\psi)]+(f-\tilde{f})\sqrt{3}\sin\theta_{12}\mathcal{D}_2^{2-}(\theta,\phi,\psi)$$
$$+(g+\tilde{g})[-\cos\theta_{12}\mathcal{D}_2^{0+}(\theta,\phi,\psi)+\sqrt{3}\mathcal{D}_2^{2+}(\theta,\phi,\psi)]\ ,$$

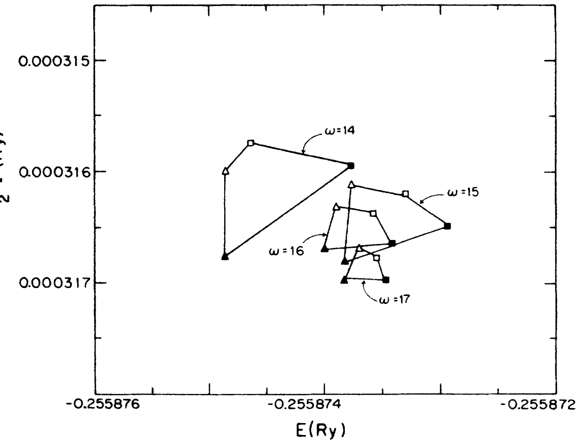

FIG. 1. The $n=2$ ${}^1D^e$ resonance eigenvalue is plotted as a function of θ and N, and for two nonlinear parameters. △: $\alpha=\beta=0.42$, $\theta=0.35$. ▲: $\alpha=\beta=0.42$, $\theta=0.40$. □: $\alpha=\beta=0.45$, $\theta=0.35$. ■: $\alpha=\beta=0.45$, $\theta=0.40$.

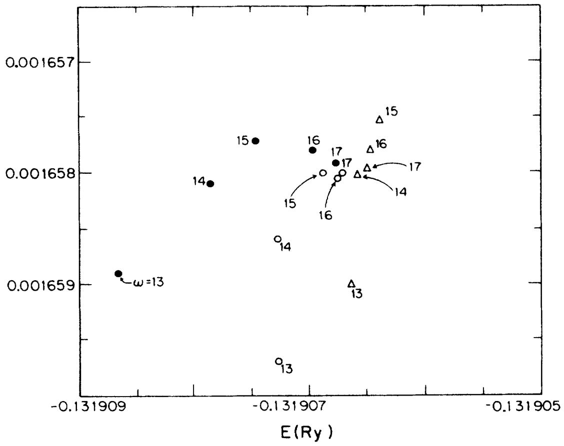

FIG. 2. The $n=3$ ${}^1D^e(1)$ resonance eigenvalue is plotted as a function of θ and N, and for two nonlinear parameters. ○: $\alpha=\beta=0.40$, $\theta=0.35$. △: $\alpha=\beta=0.40$, $\theta=0.40$. ●: $\alpha=\beta=0.42$, $\theta=0.35$.

TABLE I. Stabilized behaviors for the lowest $^1D^e$ resonance in e^--H scattering below the $n=2$ hydrogen threshold.

		$\alpha=\beta=0.42$				$\alpha=\beta=0.45$			
		$\theta=0.35$		$\theta=0.40$		$\theta=0.35$		$\theta=0.40$	
ω	N	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)
10	322	−0.255 886 5	0.000 311 2	−0.255 883 5	0.000 313 0				
11	406	−0.255 881 7	0.000 314 4	−0.255 880 1	0.000 316 1	−0.255 883 1	0.000 312 8	−0.255 879 1	0.000 309 8
12	504	−0.255 876 0	0.000 314 4	−0.255 875 6	0.000 316 4	−0.255 875 8	0.000 314 4	−0.255 873 8	0.000 313 6
13	616	−0.255 875 0	0.000 314 3	−0.255 874 7	0.000 315 5	−0.255 874 9	0.000 313 7	−0.255 873 3	0.000 313 6
14	744	−0.255 874 9	0.000 316 0	−0.255 874 9	0.000 316 8	−0.255 874 6	0.000 315 7	−0.255 873 8	0.000 316 0
15	888	−0.255 873 7	0.000 316 1	−0.255 873 8	0.000 316 8	−0.255 873 3	0.000 316 2	−0.255 872 9	0.000 316 5
16	1050	−0.255 873 9	0.000 316 3	−0.255 874 0	0.000 316 7	−0.255 873 6	0.000 316 4	−0.255 873 4	0.000 316 7
17	1230	−0.255 873 7	0.000 316 7	−0.255 873 8	0.000 316 9	−0.255 873 5	0.000 316 8	−0.255 873 5	0.000 316 9

TABLE II. Comparison of the $n=2$ $^1D^e(1)$ resonance in e^--H scattering. Result relative to the ground state of H using 1 Ry = 13.605 698 eV (see Ref. 7).

	Complex-coordinate rotation[a]	R matrix[b]	Feshbach projection[c]
E (eV)	10.124 36 ±0.000 014	10.1252	10.1243
Γ (eV)	0.008 62 ±0.000 027	0.008 81	0.010

[a] Present calculation; Hylleraas functions.

[b] 3 state + CI including continuum (Ref. 3).

[c] Hylleraas wave functions with polarized-orbital nonresonant continuum (Ref. 9).

TABLE III. Stabilized behaviors for the lowest $^1D^e$ resonance in e^--H scattering below the $n=3$ hydrogen threshold.

		$\alpha=\beta=0.40$				$\alpha=\beta=0.42$			
		$\theta=0.35$		$\theta=0.40$		$\theta=0.35$		$\theta=0.40$	
ω	N	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)	E (Ry)	$\frac{1}{2}\Gamma$ (Ry)
10	322	−0.131 943 4	0.001 669 9	−0.131 960 4	0.001 157 87	−0.131 966 9	0.001 747 7	−0.132 161 7	0.001 664 7
11	406	−0.131 916 5	0.001 661 3	−0.131 907 4	0.001 648 3	−0.131 935 5	0.001 670 8	−0.131 944 3	0.001 621 8
12	504	−0.131 910 2	0.001 661 3	−0.131 909 2	0.001 660 4	−0.131 914 5	0.001 661 3	−0.131 908 4	0.001 653 0
13	616	−0.131 907 4	0.001 659 7	−0.131 906 6	0.001 659 0	−0.131 908 7	0.001 658 9	−0.131 906 6	0.001 657 8
14	744	−0.131 907 3	0.001 658 6	−0.131 906 6	0.001 658 0	−0.131 907 9	0.001 658 1	−0.131 907 3	0.001 657 4
15	888	−0.131 906 9	0.001 658 0	−0.131 906 4	0.001 657 5	−0.131 907 5	0.001 657 7	−0.131 907 1	0.001 656 9
16	1050	−0.131 906 7	0.001 658 0	−0.131 906 5	0.001 657 8	−0.131 906 9	0.001 657 8	−0.131 906 7	0.001 657 5
17	1230	−0.131 906 6	0.001 658 1	−0.131 906 5	0.001 658 0	−0.131 906 7	0.000 657 9	−0.131 906 6	0.001 657 9

TABLE IV. Comparison of the $n=3$ $^1D^e(1)$ resonance in e^--H scattering.

	Complex-coordinate rotation[a] (Hylleraas functions)	Complex-coordinate rotation[b] (CI functions)	Close coupling[c] (18 state)	Close coupling[d] (14 state)
E_r (Ry)	−0.131 906 6±0.000 001 0	−0.1319	−0.131 91	−0.1318
Γ (Ry)	0.003 316±0.000 002	0.0032	0.003 27	0.003 24

[a] Present calculation.

[b] Reference 12.

[c] Reference 10.

[d] Reference 11.

where $\mathcal{D}$ are the rotational harmonics, depending on the symmetric Euler angles θ,ϕ,ψ.[5] The trial radial functions f and g are the Hylleraas form and are given by

$$f(r_1,r_2,r_{12})=e^{-\alpha r_1-\beta r_2}r_2^2\sum_{l,m,n\geq 0}^{N/2}C_{lmn}^{(1)}r_1^l r_2^m r_{12}^n\ ,$$

$$g(r_1,r_2,r_{12})=e^{-\alpha r_1-\beta r_2}r_1 r_2\sum_{l,m,n\geq 0}^{N/2}C_{lmn}^{(2)}r_1^l r_2^m r_{12}^n\ .$$

It is implied that

$$\tilde{f}(r_1,r_2,r_{12})=f(r_2,r_1,r_{12})$$

and

$$\tilde{g}(r_1,r_2,r_{12})=g(r_2,r_1,r_{12})\ ,$$

with $\omega \leq l+m+n$, and ω a positive integer, or zero.

Resonance positions and widths are to be calculated by the method of complex-coordinate rotation.[6] The theoretical aspects of the complex-coordinate-rotation method were discussed in previous publications[2,6] and will not be repeated here. The resonance parameters, both resonance positions and widths, are deduced from conditions that the discrete complex eigenvalue is stabilized with respect to the nonlinear parameters in the wave functions and with respect to θ, the so-called rotational angle of the complex transformation $r \rightarrow r\exp(i\theta)$. Calculations for different expansion lengths are repeated so that convergence behaviors can be examined.

In order to examine the convergence behaviors for the stabilized complex eigenvalues and estimate uncertainties for the resonance parameters, we examine the complex eigenvalue for different sets of values of α, β, N, and θ. Table I shows the convergency behavior for the lowest $^1D^e$ resonance for two sets of nonlinear parameters ($\alpha=\beta$). The number of terms in the wave function are examined from $N=322$ ($\omega=10$) to $N=1230$ ($\omega=17$), with $\theta=0.35-0.40$.

We also plot the resonance eigenvalues for $N=744$ ($\omega=14$) to $N=1230$ ($\omega=17$) functions as θ changes. Figure 1 shows these plots for two different nonlinear parameters. Based on the results shown in Table I and Fig. 1, we estimate the resonance parameters for the $n=2$ $^1D^e$ resonance in e^--H scattering as $E=-0.255\,873\,7 \pm 0.000\,001\,0$ Ry and $\Gamma/2=0.000\,316\,7\pm0.000\,001\,0$ Ry. Converted into eV with Ry$=13.605\,698$ eV,[7] the resonance would lie at $10.124\,36\pm1.4\times10^{-5}$ eV. It should be mentioned that our calculation does not provide a variational bound on the eigenvalues, and the error estimates are deduced from the stabilization behaviors. A variational bound theorem on complex resonant eigenvalues has recently been developed.[8] It would be of interest to use the method to calculate resonances in H^-. However, the method may not be so straightforward to apply to real atomic systems since it requires calculations of matrix elements for the square of the Hamiltonian H.

We compare our results in Table II with a recent R-matrix calculation,[3] and with an earlier Feshbach projection-operator calculation with Hylleraas wave functions and a polarized orbital nonresonant continuum.[7] It is seen that the R-matrix resonant position lies at a higher position by a small but significant amount. In referring to Fig. 1, the R-matrix result would be $E=-0.255\,81$ Ry, and lies outside the scale of the figure. It is noted that the results in Ref. 3 were obtained with the fixed radius of $R=25$ a.u. to ensure that the 1s, 2s, and 2p hydrogen states were fully included in the internal region. It seems that contributions from the 3d (and higher L states) to this doubly excited $^1D^e$ state are also of importance. By forcing the R-matrix radius at $R=25$ a.u., the wave packet that represents the resonance state would therefore be pushed inward to have a higher amplitude. This would lead to a higher energy for the resonance. It is hence of interest to investigate changes of the resonance position when the radius R in the R-matrix calculations is increased.

In this work we also calculate the lowest $^1D^e$ resonance associated with the $n=3$ hydrogen threshold. Using the complex-coordinate-rotation method, calculations of multichannel resonances is as straightforward as calculations for resonances below the $n=2$ threshold. Convergence behaviors for this resonance are shown in Table III, in which two sets of nonlinear parameters are used ($\alpha=\beta=0.40$ and $\alpha=\beta=0.42$). In Table III we also calculate $\theta=0.35-0.40$ with $N=322$ ($\omega=10$) terms to $N=1230$ ($\omega=17$) terms. Convergence behaviors for this resonance are also shown in Fig. 2. We plot the resonance eigenvalues from $N=616$ ($\omega=13$) terms to $N=1230$ ($\omega=17$) terms. Judging from the results shown in Table III and Fig. 2, we assign resonance parameters for the lowest $^1D^e$ resonance below the $n=3$ hydrogen threshold as $E=-0.131\,906\,6\pm0.000\,001\,0$ Ry and a total width of $\Gamma=2\times(0.001\,680\pm0.000\,001)$ Ry. We show our results in Table IV together with other calculations for this resonance.

In comparing with the algebraic close-coupling calculations[10,11] and with another complex-coordinate-rotation rotation calculation[12] in which configuration-interaction-type (CI-type) wave functions are used, it is seen that agreements are quite good. It is believed that the present complex-coordinate-rotation calculation with Hylleraas-type wave functions is more accurate than the previous calculation with CI functions.

In summary, we have calculated the lowest $^1D^e$ resonances below the $n=2$ and 3 thresholds using a method of complex-coordinate rotation. Results obtained with the use of Hylleraas functions are believed to be of high accuracy. This work should serve as a useful reference for other investigations.

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