Hyperspherical approach to the calculation of few-body atomic resonances

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Direct solution of the Schrödinger equation for the doubly excited resonant $^1S^e$ state of the helium atom is obtained with the help of the complex rotation method (which reduces the resonance problem to that of bound states with complex energy) and the correlation function hyperspherical harmonic (CFHH) method. In the CFHH method the solution is a product of a correlation function and a smooth factor expanded into hyperspherical harmonic functions. Given a proper correlation function, chosen from physical considerations, the method generates resonant wave functions, accurate in the whole range of interparticle distances. Since the method is nonvariational no stabilization procedure is needed. The calculated energy and width are shown to be strictly independent of the angle of complex rotation, hence there is no need for the angle optimization procedure as well. The results are compared with variational and other precise computations. [S1050-2947(97)03602-0]

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Resonances are common phenomena in all branches of physics. They play a significant role in different low-energy scattering cross sections, such as in electron-atom and electron-molecular scattering processes as well as in positron-atom scattering and in photoionization. Doubly excited two-electron resonances, for example, apart from their theoretical importance as the simplest few-body resonant systems, are of interest for atomic processes in fusion plasmas [1] as well as for beam foil spectroscopy [2,3], electron impact [4], and single-collision beam [5] experiments and for charge-exchange processes [6–8] between heliumlike atoms and multicharged ions. During the past 20 years the calculation of these atomic resonances has been performed by a variety of methods, among them the close-coupling approximation [9], the Feshbach projection operator formalism [10,11], the multiconfiguration Hartree-Fock method [12], and the hyperspherical coordinate method [13]. Most of the recent resonance computations [13–18] are, however, made with the use of the complex coordinate rotation method, based on the dilatation analytic continuation [19–21]. Such computations were pioneered by Nuttall and co-workers [22–24] and developed further in numerous papers by different authors (see, for example, reviews of Ho [25] and Reinhardt [26] and references therein).

The advantage of the complex coordinate rotation $\mathbf{r}_i \rightarrow \mathbf{r}_i e^{i\theta}$ is that it transforms the continuum resonance wave function to the normalizable wave function of the bound state. The computation of the non-normalizable resonance wave functions thus becomes unnecessary, which bring great simplifications. Furthermore, the resonance wave function could be now obtained by a simple modification of existing bound-state codes mostly based on the variational ansatz (formulated for the complex Hamiltonian by Herzenberg and Mandl [27]). Bound and resonant states thus are treated on the same footing and the accurate results, normally obtained

for few-body bound states by variational method, become available now also for few-body resonant states.

The use of the variational approach for the calculation of resonance wave function means, however, the necessity of guessing the mathematical form of the wave function, which can result in a low-quality wave function even in cases where hundreds of variational parameters generate extremely precise energies [28]. Theoretically, variational wave functions are accurate only in the region where the probability density is high [29]. The analytical structure of three-body wave functions calculated variationally is therefore uncertain, since inclusion or omission of logarithmic terms, or negative powers of interparticle distances in case, for example, of bound states, has a negligible effect on the value of the variational energy [28,30]. A variational function coincides with the precise one only on the average and could wildly or even infinitely deviate from it locally [31]. These local discrepancies could lead to wrong estimates of expectation values of different operators that have significant contributions from the regions of the configuration space where the deviations occur. This could result, in principle, in an error in estimate of relativistic, finite-size, and QED effects for both resonant and bound states.

One has to stress, however, that modern variational calculations use a sufficiently complete set of a few hundred or even a few thousand basis functions of appropriate symmetry and therefore, in practice, some of the conclusions of Bartlett, Gibson, and Dunn [31], which were based on calculations with only a six-term wave function, are no longer relevant. In particular, the present variational calculations of atomic resonances [14–16,18] give very accurate and reliable results for energies as well as other quantities. Nevertheless, an independent nonvariational corroboration of their results would be of value. A careful verification of the currently accepted theoretical values of these parameters could be done using the direct solution of the complex rotated Schrödinger equation by the correlation function hyperspherical harmonics (CFHH) method unifying the correlation function approach [32] with the hyperspherical harmonic method (see the reviews in [33] and references therein).

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TABLE I. Energies of the ground state of the helium atom (a.u.) calculated for the dilatation parameter $\theta=0.4$ rad. The results are for the infinite mass of the helium nucleus. K_m is the maximum global angular momentum and $N=(K_m/4+1)^2$ is the number of hyperspherical functions included and coupled equations solved. The number of digits indicates the numerical precision of calculated values. The results for the correlation parameters $\gamma=2$ and $\delta=0$ in Eq. (4) corresponding to the cusp parametrization are displayed in the first line of each entry, while the results for the independent-particle parametrization $\gamma=2\sqrt{-E}$ and $\delta=0$ are displayed in the second line.

K_m	N	$-E_r$	$\Gamma/2$
4	4	2.907 574 78	0.000 000 00
		3.060 143 74	0.000 000 00
8	9	2.902 332 03	0.000 000 00
		3.011 942 95	0.009 703 26
12	16	2.903 880 66	0.000 000 00
		2.964 006 11	0.002 367 89
16	25	2.903 548 75	0.000 000 00
		2.935 259 10	0.000 208 95
20	36	2.903 737 33	0.000 000 00
		2.923 645 24	0.000 022 22
24	49	2.903 680 37	0.000 000 00
		2.916 516 67	0.000 001 52
28	64	2.903 723 44	0.000 000 00
		2.912 735 44	0.000 000 15

TABLE II. Dependence of the resonance energy E_r and of the width, calculated with the independent-particle correlation factor on the dilatation parameter θ for different numbers of the hyperspherical basis states.

θ	K_m	E_r	$\Gamma/2$
0.10	4	−0.777 580 72	0.002 236 79
0.20	4	−0.777 580 72	0.002 236 79
0.30	4	−0.777 580 72	0.002 236 79
0.40	4	−0.777 580 72	0.002 236 79
0.50	4	−0.777 581 17	0.002 237 00
0.10	8	−0.790 688 50	0.009 451 67
0.20	8	−0.790 688 50	0.009 451 67
0.30	8	−0.790 688 50	0.009 451 68
0.40	8	−0.790 688 50	0.009 451 68
0.50	8	−0.790 688 50	0.009 451 67
0.60	8	−0.790 688 50	0.009 451 68
0.70	8	−0.790 688 50	0.009 451 66
0.80	8	−0.790 688 50	0.009 451 68
1.00	8	−0.790 688 50	0.009 451 67
0.10	20	−0.775 796 35	0.002 214 27
0.20	20	−0.775 796 49	0.002 214 39
0.30	20	−0.775 796 49	0.002 214 40
0.10	24	−0.776 166 68	0.002 241 29
0.20	24	−0.776 166 48	0.002 241 01
0.30	24	−0.776 166 48	0.002 241 02
0.10	28	−0.776 441 11	0.002 256 27
0.20	28	−0.776 441 11	0.002 256 27
0.30	28	−0.776 441 11	0.002 256 28
0.20	36	−0.776 936 26	0.002 267 66
0.30	36	−0.776 936 26	0.002 267 67

The CFHH method [33–35] provides a very accurate *direct* solution of the Schrödinger equation for different three-body systems. Given the proper correlation function, chosen from physical considerations, the CFHH method provides analytically correct wave functions, accurate in the whole range of interparticle distances, including coalescence points, which leads, in turn, to precise estimates of the expectation values of the Hamiltonian and of different functions of interparticle distances. To date, the accuracy of the CFHH method has been verified for ground ($1\,^1S$), first excited ($2\,^1S$), and highly excited ($3\,^1S-5\,^1S$) states of one heavy and two light particles, such as the helium atom, as well as for the ground states of mesomolecular $pp\mu$, $dd\mu$, $dt\mu$, and $tt\mu$ systems containing one light and two heavy particles and for the ground state of the positronium negative ion $e^-e^-e^+$ (also denoted Ps$^-$) consisting of particles of equal masses. It was shown [33–35] that the direct bound-state solution of the Schrödinger equation obtained by the CFHH method yields precision comparable to that obtained previously only by elaborate variational calculations. With 225 hyperspherical harmonic functions, up to nine significant figure precision were obtained for the energies of the ground and excited states of the helium atom and of the positronium ion. The wave functions for the whole range of the interparticle distances and different expectation values for these systems have about six significant figure precision and the overall and local quality of the corresponding wave functions is very high. Relativistic and QED corrections calculated by using a direct solution of the Schrödinger equation for the $2\,^1S$ excited state of the helium atom obtained with the CFHH method confirmed that the discrepancy between theory and experiment is not a result of our inaccurate knowledge of the

helium wave functions, but is rooted in our inadequate knowledge of the QED operators.

The complex rotation method is most successful in the calculation of atomic and molecular resonances since for particles interacting with Coulomb forces, the kinetic- and potential-energy operators in the Hamiltonian H simply scale as $\exp(-2i\theta)$ and $\exp(-i\theta)$, respectively,

$$H_\theta = Te^{-2i\theta} + Ve^{-i\theta}. \tag{1}$$

In this paper, which is our first attempt to calculate resonances by direct solution of the complexly rotated Schrödinger equation, we present the results of CFHH calculations of the position and the width of the lowest $^1S^e$ helium resonance. We compare our results with previous computations of the doubly excited helium states that were performed by the close-coupling approximation [9], the Feshbach projection operator formalism [10,11], as well as the hyperspherical coordinates method [13] and the complex coordinate rotation method [14–18].

The spectrum of the rotated Hamiltonian (1) has the following features [19–26]: (i) the position of the bound-state poles remains unchanged; (ii) the cuts are rotated downward of the real axis by an angle 2θ; (iii) a resonant pole is exposed by the cuts once the rotational angle θ is greater than $\beta/2$, where β is the phase of the pole

TABLE III. Energy and width of the $^1S^e$ state of the helium atom (a.u.). The first two columns correspond to the eigenvalue of the Hamiltonian, while the third and fourth columns display its expectation value. The other notations are the same as in Table I. The last lines of the table display the results of calculations performed by the close-coupling approximation [9], the Feshbach projection operator formalism [10,11] the hyperspherical coordinates method [13], and the complex coordinate rotation method [14–18]. The last two lines are the results of two experiments [36,37] that measured the positions and lifetimes of the $^1S^e$ helium resonance.

K_m	$-E_r$	$\Gamma/2$	$-E_r$	$\Gamma/2$
8	0.778 239 52	0.005 269 18		
12	0.787 546 41	0.002 986 05		
16	0.781 962 56	0.002 172 34		
20	0.779 818 12	0.002 240 00	0.777 395	0.002 236 1
24	0.779 048 69	0.002 248 84		
28	0.778 479 60	0.002 259 90	0.777 801 533	0.002 273 004
32	0.778 296 96	0.002 261 92		
36	0.778 105 17	0.002 266 23	0.777 848 732	0.002 271 317
40	0.778 050 72	0.002 266 73		
44	0.777 974 14	0.002 268 59	0.777 860 427	0.002 270 900
48	0.777 955 40	0.002 268 71	0.777 863 624	0.002 270 787
56	0.777 913 64	0.002 269 61	0.777 865 632	0.002 270 720
64	0.777 893 50	0.002 270 06	0.777 866 534	0.002 270 690
72	0.777 883 03	0.002 270 29	0.777 866 984	0.002 270 675
extrapolated			0.777 867 6	0.002 270 65
Reference				
[9]			0.777 8	0.002 29
[10]			0.778 035	0.002 295
[11]			0.778 41	0.002 27
[13]			0.777 35	0.002 205
[14]			0.777 868	0.002 265
[15]			0.777 858	0.002 285 35
[16]			0.777 872	0.002 27
[17]			0.777 868	0.002 270 5
[18]			0.777 867 636	0.002 270 653
[52]			0.778 164±0.001 47	0.002 536±0.000 276
[53]			0.779 634±0.001 10	0.002 536±0.000 276

$$E=E_r-i\frac{\Gamma}{2}=|E|e^{-i\beta}, \qquad (2)$$

whose real and imaginary parts correspond to the resonance energy E_r and width Γ, respectively, and its position remain unchanged with a further increase of the angle θ; (iv) the rotated resonant wave function is asymptotically convergent, decaying exponentially with an overall oscillatory factor.

The complex resonance energy E is obtained by solving the Schrödinger equation for bound states with the rotated Hamiltonian (1). In the CFHH method [33–35] one writes the complexly rotated resonance wave function as a product of two factors

$$\psi=\chi\phi, \qquad (3)$$

where χ is the ''correlation function'' and ϕ is expanded in the usual hyperspherical harmonic (HH) functions (which are eigenfunctions of the angular part of kinetic-energy operator T_Ω) with complex coefficients depending on radius. If the correlation function χ is chosen to describe the important physical features of ψ (such as cusps or asymptotics), the

convergence of the HH expansion for ϕ should be rapid. Since the height of the centrifugal potential barrier determined by the eigenvalues $K(K+4)$ of the operator T_Ω increases quadratically with grand orbital quantum momentum $K=0,1,2,\ldots$ (which is the analog of orbital quantum number L in the two-body case), for bound states the contributions of higher K are expected to be negligible beyond some $K=K_m$, which is called the maximal global angular momentum. The expansion of the wave function, therefore, may be truncated at this K_m, leading to a finite system of the differential equations in ρ. This is the only approximation in the hyperspherical harmonics method, which is, in addition, well under control since a comparison of calculated values for subsequent K_m allows for an exact estimate of the errors. The resonance solution for ϕ is sought as the bound-state solution of the Schrödinger equation with the complexly rotated Hamiltonian (1) in the usual HH method, except that the potential V is replaced by an effective velocity-dependent potential V',

$$V'=V-\frac{1}{2}\frac{\nabla^2\chi}{\chi}-(\nabla\ln\chi)\nabla. \qquad (4)$$
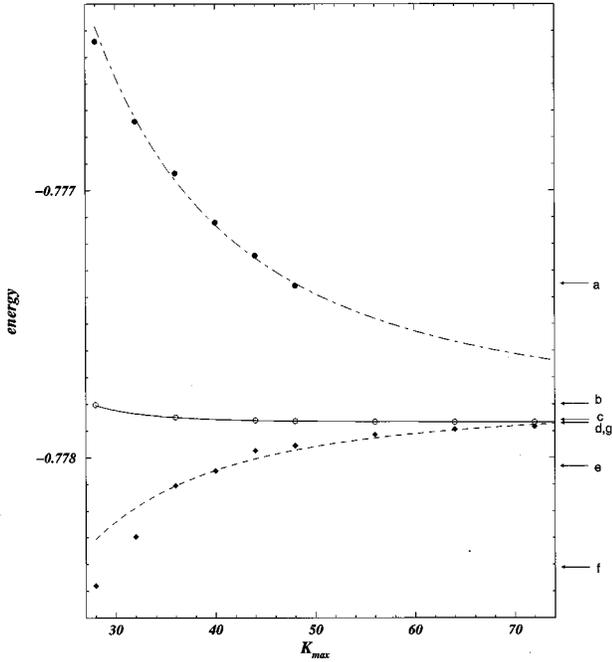
FIG. 1. Dependence of a resonance energy eigenvalue on K_m for the cusp parametrization (dashed line) and for the independent-particle parametrization (dot-dashed line). The solid line displays the K_m dependence of an expectation value of the resonance energy for the cusp parametrization. The position of arrows, denoted by a; b; c; d; e; f; and g; corresponds to resonance positions calculated in Refs. [13;9;15;14,16;10;11;17,18], respectively.

Here ∇ is the six-dimensional gradient operator and V is a sum of the pair Coulomb potentials.

In the computation of the $^1S^e$ helium resonance representing a doubly excited state it is natural to use the same correlation factor as for the helium atom. The simplest correlation factor for the helium atom is given by [33–35]

$$\chi = \exp(f),$$

where f is a spatially symmetric linear correlation function

$$f = -\gamma(r_{13} + r_{23}) - \delta r_{12}. \tag{5}$$

Here particle 3 is the helium nucleus, whose mass M, for the sake of a comparison with the previous calculations, is presumed infinite.

We have used two choices of the parameter γ, namely, $\gamma = 2$ and $2\sqrt{-E}$, corresponding to cusp [33–35] and independent-particle parametrizations, respectively. The first choice is the consequence of the Kato cusp condition, while the second choice corresponds to the model in which two uncorrelated $2s$ electrons interacting with a nucleus with effective screened charge Z_{eff} have energy $E = -Z_{\text{eff}}^2/4$ and a wave function $\exp[-Z_{\text{eff}}(r_{13} + r_{23})] = \exp[-2\sqrt{-E}(r_{13} + r_{23})]$. In both cases, since electrons in doubly excited states are located rather far from one another, we neglected their correlation, setting $\delta = 0$.

The results of computations are displayed in Tables I–III and in Fig. 1. The values in Table I show the change of the position of the pole corresponding to the ground state as a result of the complex rotation by an angle $\theta = 0.4$ rad. One
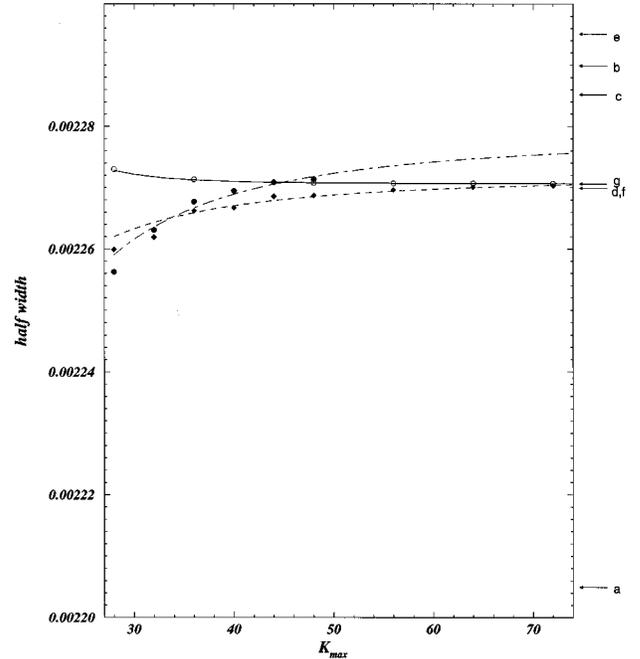
FIG. 2. Same as in Fig. 1, but for the width.

sees that in case of the cusp parametrization the pole for all K_m remains strictly on the real axis. In the case of the independent-particle parametrization the width for small K_m is nonzero but disappears with increasing number of the hyperspherical basis functions. It is in agreement with the fact that the cusp correlation factor describes the physics of the ground state much better than the independent-particle correlation factor that is derived under the assumption that both electrons are in the $2s$ state. The dependence of the energy and the width calculated with the independent-particle correlation factor on the dilatation parameter θ for different numbers of the hyperspherical basis states is displayed in Table II. The table shows that the results of calculations are independent of the rotation angle, that is, provided the rotation is large enough for resonant poles to be exposed by the cuts, the numerical procedure is stable and the results are not affected by choice of a specific rotation angle. We found that the stability increases with an increase of K_m. A similar numerical stability with respect to the rotation angle was registered also by Lindroth [17]. The calculations were done with $\theta = 0.2$ and 0.4 for the cusp and independent-particle parametrizations, respectively. They are displayed in Table III, where the results of variational and other precise computations are also given. Theoretically [34], the complex energy eigenvalue $E(K_m)$ should converge as $1/K_m^2$, which is indeed the case as one can see from the dashed and dot-dashed lines of the form $A + B/K_m^2$ on Figs. 1 and 2, fitted to the calculated complex energy eigenvalues by the least-squares method

$$\sum_{K_m} K_m^6 \left[E(K_m) - \left(A + \frac{B}{K_m^2} \right) \right]^2 = \min. \tag{6}$$

The weight factor K_m^6 in the sum stresses the better accuracy of eigenvalues for higher K_m.

The accuracy of the CFHH results is significantly increased by using our solution of the complex Schrödinger equation as a trial function for the Rayleigh-Ritz variational principle (modernized for complex Hamiltonians by Herzenberg and Mandl [27]), which is stationary with respect to changes in the trial wave function. Such a method of improving the precision of the energy values has proved to be extremely useful in the bound-state CFHH calculations [33–35]. The corresponding computations for the cusp parametrization that we found most rapidly convergent are displayed in third and fourth columns of Table III. The numerical precision of the presented results is around eleven significant figures, so our numerical errors are less than the errors due the to the truncation of the basis set at $K = K_m$, which could be estimated by the comparison of the values for the subsequent K_m. One can see that the final accuracy of the expectation values of energy and width in the third and fourth columns of Table III, derived by a comparison of the results for $K_m = 72$ and 64, is six significant figures for the energy and seven significant figures for the width, judging by a comparison of expectation values for $K_m = 64$ and 72. We represented these results also by a solid curve of the form $A + B/K_m^5$ (since expectation values theoretically [34] should converge as $1/K_m^5$) in Figs. 1 and 2, fitted to the calculated complex expectation values by the least-squares method with the same weight factor K_m^6. We have tried the weight factors K_m^8, K_m^{10}, and K_m^{12} as well in order to check the stability of our interpolation procedure. Values of A obtained for the different weights that are extrapolated values corresponding to $K_m = \infty$ are displayed in Table IV. From this table one deduces that the extrapolated value of the energy (width), which is independent of extrapolation procedure with accu-

TABLE IV. Extrapolated values E_{ext} and $\Gamma_{\text{ext}}/2$ of expectation values of energy and width for different extrapolation procedures. The n in the first column denotes a power used in the weight factor K_m^n; a value of K_m in the second column corresponds to the last value of K_m in Table III taken into account in extrapolation procedure.

n	K_m	$-E_{\text{ext}}$	$\Gamma_{\text{ext}}/2$
6	64	0.777 867 649	0.002 270 649
6	72	0.777 867 604	0.002 270 652
8	72	0.777 867 585	0.002 270 653
10	72	0.777 867 566	0.002 270 655
12	72	0.777 867 551	0.002 270 656

racy of seven (eight) figures, equals 0.777 867 6 (0.002 270 65) a.u. These values of energy and width agree well with the most accurate previous computation of Buergers, Wintgen, and Rost [18].

Summing up, we calculated the $^1S^e$ resonance of the helium atom by combining the complex rotation and the correlation function hyperspherical harmonic methods. It is a direct computation of the resonances with the CFHH method. The method generates resonant wave functions, accurate in the whole range of interparticle distances. Since the method is nonvariational no stabilization procedure is needed. The calculated energy and width are shown to be strictly independent of the angle of complex rotation, hence there is no need for the angle optimization procedure as well. The accuracy of the results is high and they agree excellently with most accurate recent computation of Buergers, Wintgen, and Rost [18].

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