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Citation: Chin. Phys. B, 2021, 30 (**2**): 023101. DOI: 10.1088/1674-1056/abc156
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Complex coordinate rotation method based on gradient optimization*

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(Received 23 August 2020; revised manuscript received 22 September 2020; accepted manuscript online 15 October 2020)

In atomic, molecular, and nuclear physics, the method of complex coordinate rotation is a widely used theoretical tool for studying resonant states. Here, we propose a novel implementation of this method based on the gradient optimization (CCR-GO). The main strength of the CCR-GO method is that it does not require manual adjustment of optimization parameters in the wave function; instead, a mathematically well-defined optimization path can be followed. Our method is proven to be very efficient in searching resonant positions and widths over a variety of few-body atomic systems, and can significantly improve the accuracy of the results. As a special case, the CCR-GO method is equally capable of dealing with bound-state problems with high accuracy, which is traditionally achieved through the usual extreme conditions of energy itself.

Keywords: complex coordinate rotation method, resonant state, metastable state, gradient optimization

PACS: 31.10.+z, 31.15.–p, 34.80.–i **DOI:** 10.1088/1674-1056/abc156

1. Introduction

Resonant states play an important role in atomic, molecular, and nuclear physics and have a long history of research, such as doubly-excited states in two-electron systems,[1,2] Efimov states in weakly bound few-body systems,[3,4] resonance phenomena under Debye plasma environment,[5] four-body resonant states in positronium hydride[6] and positron-helium,[7] resonances in positron scattering by atoms and molecules,[8] metastable states in antiprotonic helium $\bar{p}^4He^+$,[9–11] and resonance phenomena in nuclear physics.[12,13]

There exist many theoretical methods for studying resonant states. In early years, the S-matrix[14] and R-matrix[15] theories were used to solve resonant problems. In 1970s, the method of complex coordinate rotation (CCR) was mathematically established,[16] and was first used in studies of scattering involving three charged particles by Raju and Doolen.[17] After that, the CCR method was further developed to calculate atomic resonant states by Ho.[18] From then on, the CCR method has been widely adopted as a powerful tool for investigating resonant states in atoms and molecules, including its application to high-precision antiprotonic helium spectrum.[10,11] On the other hand, Feshbach in 1962[19] formulated a general theory for studying resonances, where the wave function space is partitioned into closed- and open-channel segments. The hyperspherical close-coupling method, developed by Lin[20] in 1984 to calculate doubly-excited states, was applied to positron–atom scattering.[21] Recently, the stabilization method combined with hyperspherical coordinates and B-spline expansion was applied to positron–atom scattering by Han and co-workers.[22] Among these methods, both the CCR method and the closed-channel approximation of the Feshbach theory can reach high precision for long-lived metastable states with small widths, such as 10^{-11} atomic units in $\bar{p}^4He^+$ decaying via a radiative channel.[9] However, an Auger-dominated state in $\bar{p}^4He^+$ is usually short-lived and possesses a width larger than 10^{-10} atomic units,[9] such as the ($N = 31$, $L = 30$) state, where N and L are, respectively, the principal and total angular momentum quantum numbers. The accuracy of the closed-channel approximation of the Feshbach theory is limited by the width of a resonant state,[23] whereas the accuracy of the CCR method can go beyond this limit,[10] making the CCR method more suitable for short-lived metastable states.

Since the variational approach using Hylleraas- or Sturmian-type basis sets has been proven to be effective in dealing with atomic or molecular few-body systems, it is natural to combine these basis sets with the CCR method,[24–27] and solve resonance problems variationally. However, due to the lack of extreme theorem for a resonance state, historically it is common practice in using the CCR method that the nonlinear variational parameters in the trial wave function are optimized through repeated trial and error manual adjustment,

*Project supported by the National Natural Science Foundation of China (Grant Nos. 91636216, 11974382, and 11474316), the Chinese Academy of Sciences Strategic Priority Research Program (Grant No. XDB21020200), and by the YIPA Program. ZCY acknowledges the support of NSERC, SHARCnet, and ACEnet of Canada.

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which could become extremely laborious and inefficient, especially for a high-dimensional parameter space. In this work, we propose a novel approach of complex coordinate rotation based on the gradient optimization (CCR-GO). The advantage of the CCR-GO method over the existing resonance methods is that it does not require manual adjustment of nonlinear parameters in the wave function; instead, a mathematically well-defined optimization path can be followed, leading to a resonance pole quickly. Our method will be tested for various three-body atomic systems.

2. Computational method

In the method of complex coordinate rotation,[18] under the radial coordinate transformation $r \to r\exp(\mathrm{i}\theta)$, the original Hamiltonian of the system $\hat{H} = \hat{T} + \hat{V}$, where $\hat{T}$ and $\hat{V}$ are, respectively, the kinetic and potential energy operators, is transformed into

$$\hat{H} \to \hat{H}(\theta) = \hat{T}\exp(-2\mathrm{i}\theta) + \hat{V}\exp(-\mathrm{i}\theta), \tag{1}$$

where the rotational angle θ is assumed to be real and positive. According to the Balslev–Combes theorem,[16] in the complex energy plane, for sufficiently large θ this transformation rotates the continuum spectrum of $\hat{H}$ to "expose" the resonant poles around the thresholds from the unphysical sheet to physical sheet of the Riemann surface, and the bound state poles remain unchanged on the negative side of the real axis. The eigenenergies can be obtained by solving the following complex eigenvalue problem:

$$\hat{H}(\theta)\Psi_\theta = E\Psi_\theta, \tag{2}$$

where the eigenfunction Ψ_θ is square integrable and the corresponding discrete complex eigenvalue $E = E_\mathrm{r} - \mathrm{i}\Gamma/2$ defines the position E_r and the width Γ of a resonance. By choosing a basis set $\{\psi_n, n = 1,\ldots,\mathcal{N}\}$ in an $\mathcal{N}$-dimensional Hilbert space, the complex eigenvalue problem (2) can be converted to the following generalized algebraic complex eigenvalue problem:

$$\boldsymbol{H}(\theta)\Psi_\theta = E\boldsymbol{O}\Psi_\theta, \tag{3}$$

where $\boldsymbol{H}(\theta)_{ij} = \langle\psi_i|\hat{H}(\theta)|\psi_j\rangle$ are the $\mathcal{N}\times\mathcal{N}$ Hamiltonian matrix elements and $\boldsymbol{O}_{ij} = \langle\psi_i|\psi_j\rangle$ are the overlap matrix elements. Since a resonance wave function is square integrable, the rotated Hamiltonian $\hat{H}(\theta)$ holds the complex variational principle that makes the complex energy eigenvalue stationary, although not necessarily extreme, with respect to any parameter ξ in the wave function, such as the rotational angle θ, or a nonlinear parameter in a Hylleraas basis set, or the box size of a B-spline basis set, i.e.,

$$\partial_\xi E \equiv \frac{\partial E}{\partial \xi} = 0 \tag{4}$$

at a resonance pole. This expression can be understood as a stability condition for a resonant energy, which of course also applies to any bound state as a special case. Since we do not have the extreme theorem for a resonance energy E in general, instead of dealing with E itself, we focus on $|\partial_\xi E|$ and minimize it by varying ξ, due to the obvious fact that $|\partial_\xi E| \geq 0$. This is the essence of our CCR-GO method. To be specific, let us consider a three-body Coulombic system, such as Ps^-, H^-, He, and $\bar{\mathrm{p}}^4\mathrm{He}^+$. After eliminating the center of mass coordinates, a three-body problem is reduced to a quasi two-body one with $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ being their position vectors relative to the third particle. In order to solve the complex eigenvalue problem (2), we use two types of basis sets. The first one consists of Hylleraas functions with real nonlinear parameters α and β,

$$\{r_1^\ell r_2^m r_{12}^n \mathrm{e}^{-\alpha r_1 - \beta r_2}\mathcal{Y}^{LM}_{\ell_1\ell_2}(\hat{r}_1,\hat{r}_2)\}, \tag{5}$$

where $\mathcal{Y}^{LM}_{\ell_1\ell_2}(\hat{r}_1,\hat{r}_2)$ is the angular momenta (ℓ_1,ℓ_2)-coupled spherical harmonics to form a common eigenstate of L^2 and L_z. It is noted that a proper symmetrization of the final wave function is implied for a system containing two identical particles. The possible values of ℓ_1 and ℓ_2 are those fulfilling $\ell_1+\ell_2 = L$ for a state of natural parity $(-1)^L$ or $\ell_1+\ell_2 = L+1$ for a state of unnatural parity $(-1)^{L+1}$. Each configuration (ℓ_1,ℓ_2) has its own set of nonlinear parameters. In order to enhance the rate of convergence, we may further divide the most important configuration into more sub-groups each having different set of nonlinear parameters. The basis set is generated by including all terms such that $\ell+m+n \leq \Omega$ with integer Ω controlling the size of the basis set. More information about the construction of basis sets can be found in Refs. [23,32]. This type of basis set has been widely applied to three-body atomic and molecular systems, such as helium,[32] the hydrogen molecular ions,[33] and antiprotonic helium.[23] The second type of basis set consists of Hylleraas basis functions containing complex nonlinear parameters,

$$\{r_1^\ell r_2^m r_{12}^n\, \mathrm{e}^{-(\alpha+\mathrm{i}\mu)r_1-(\beta+\mathrm{i}\nu)r_2-(\gamma+\mathrm{i}\sigma)r_{12}}\mathcal{Y}^{LM}_{\ell_1\ell_2}(\hat{r}_1,\hat{r}_2)\}, \tag{6}$$

where α, β, γ, μ, ν, and σ are real. It is noted that, with nonzero imaginary parts of nonlinear parameters in the basis set, the wave function is more capable of describing the asymptotic behavior of a resonance state; it can also be more flexible to reflect molecular characteristics for some exotic systems, such as $\bar{\mathrm{p}}^4\mathrm{He}^+$.[11]

In our CCR-GO approach, we try to minimize either

$$f_1(\mathcal{P}) = |\partial_\theta E| \tag{7}$$

or

$$\begin{aligned} f_2(\mathcal{P}) = {} & |\partial_\theta E| + |\partial_\alpha E| + |\partial_\beta E| + |\partial_\gamma E| \\ & + |\partial_\mu E| + |\partial_\nu E| + |\partial_\sigma E|, \end{aligned} \tag{8}$$

where $\mathcal{P} \equiv (\theta, \alpha, \beta, \gamma, \mu, \nu, \sigma)$ aggregates all variational parameters, such as the rotational angle θ and the nonlinear parameters α, β, γ, μ, ν, and σ that appear in Eq. (6), for example. The optimization procedure for minimizing $f_1(\mathcal{P})$ or $f_2(\mathcal{P})$ can be done iteratively from step k to step $k+1$: $[\mathcal{P}]_k \to [\mathcal{P}]_{k+1}$, where the initial values of optimization parameters, as well as the search directions and steps for each parameters, are determined by the Broyden–Fletcher–Goldfarb–Shanno algorithm,[34] or the quasi-Newton method. In particular, the search directions are directly related to the following vectors:

$$\boldsymbol{g}_1(E) = \nabla f_1(\mathcal{P}), \quad \boldsymbol{g}_2(E) = \nabla f_2(\mathcal{P}), \tag{9}$$

where $\nabla = (\partial_\theta, \partial_\alpha, \partial_\beta, \partial_\gamma, \partial_\mu, \partial_\nu, \partial_\sigma)$ is the gradient operator in the full parameter space. It is noted here that, for an efficient search of a resonant state, the rotational angle term $|\partial_\theta E|$ must be included in the optimization procedure, whereas the other parameters can sometimes be optional except for some broad resonant states.

3. Results and discussion

For the purpose of demonstrating the effectiveness of our optimization technique, figure 1 shows the convergence pattern for the lowest S-wave resonant state in Ps^- using only one set of nonlinear parameters in Eq. (6), with the initial values $\theta = \alpha = \beta = \gamma = \mu = \nu = \sigma = 0.2$ and the size of basis set $\mathcal{N} = 252$. One can see from the figure that, starting from the same initial point, the two optimization paths based on $\boldsymbol{g}_1(E)$ and $\boldsymbol{g}_2(E)$ approach each other rapidly around the resonant pole after about 9 iterations. Of course, further iterations are needed if one wishes to obtain higher accuracy, as shown in Table 1. It is noted that, since the resonance width of this state is relatively small, the searching process is less sensitive to the initial values of nonlinear parameters and the searching paths. For narrow resonant states, the optimization of nonlinear parameters can be performed firstly to minimize the real energy eigenvalue when $\theta = 0$. After this process, the results are only limited by the width of the resonant states.[23] These optimized parameters as the initial values of CCR-GO implementation can avoid the spurious solutions efficiently and converge to the right results. The prior optimization of real energy can also reduce the computation load and enhance the rate of convergence. However, for a resonant state of broad width, the above strategy for searching the initial values is invalid due to the shallower minimum in parameter space. Thus, manual adjustment of the initial nonlinear parameters is required to approach the true lowest position through minimizing the energy derivations as small as possible. It is advisable to use the more demanding condition $\boldsymbol{g}_2(E)$ to do searching, instead of $\boldsymbol{g}_1(E)$ which is difficult to trap the iteration of parameters into the shallower minimum. It is also noted that our CCR-GO method is applicable not only to resonant states, but also to bound ones. Figure 2 shows two optimization paths determined by $\boldsymbol{g}_1(E)$ and $\boldsymbol{g}_2(E)$ for locating the ground state of helium, with the initial values $\theta = \alpha = \beta = \gamma = \mu = \nu = \sigma = 0.2$ and the size of basis set $\mathcal{N} = 252$. The ground-state energy, thus obtained after 30 iterations, is accurate to about 9 digits.

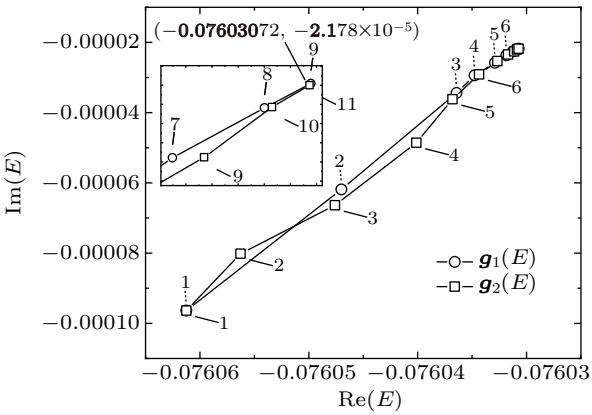


Fig. 1. Two optimization paths based on $\boldsymbol{g}_1(E)$ and $\boldsymbol{g}_2(E)$ for the lowest resonant state $^1S^e$ in Ps^- below the Ps ($N = 2$) threshold, with the size of basis set $\mathcal{N} = 252$. The inset is an enlarged view of the paths around the convergence point. Atomic units are used.

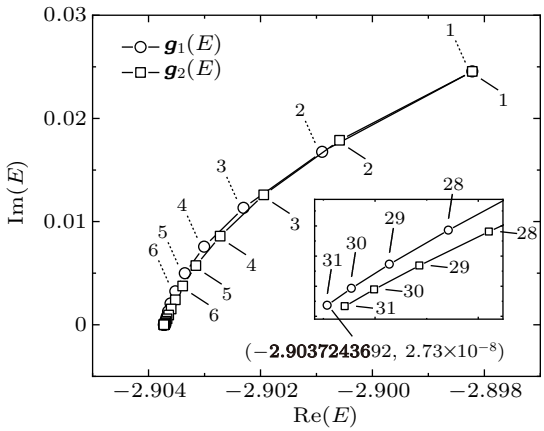


Fig. 2. Two optimization paths based on $\boldsymbol{g}_1(E)$ and $\boldsymbol{g}_2(E)$ for the ground state of helium, with the size of basis set $\mathcal{N} = 252$. The inset is an enlarged view of the paths around the convergence point. Atomic units are used.

Table 1 lists the resonance positions and widths using the CCR-GO method for some representative Coulombic systems, including the weakly-bound Ps^- and H^-, the tightly-bound He, and the exotic quasi-molecule $\bar{p}^4He^+$, with the angular momentum quantum number L ranging from 0 to 30 and the resonance width ranging from 10^{-2} to 10^{-9} atomic units. For the $^3P^o(1)$ state in helium, the possible angular momentum values (ℓ_1, ℓ_2) for two electrons are $(1,0)$ and $(0,1)$, and each configuration has five sub-groups each having different set of nonlinear parameters. For the $^1D^e(1)$ state in helium, the possible angular momentum values (ℓ_1, ℓ_2) for two electrons are $(2,0)$, $(1,1)$, and $(0,2)$, and each configuration has two sub-groups. For $\bar{p}^4He^+$, only the parameter Ω of the leading angular momentum component $(\ell_{\bar{p}} = 30, \ell_e = 0)$ is listed, which

has a primary contribution and is divided into four sub-groups for better description of the closed-channel solution. The subsequent configurations $(29,1)$, $(28,2)$, $(27,3)$, and $(26,4)$ are also included to better represent excited electron intermediate states, and electron continuum. It is noted that 49 parameters were optimized simultaneously by gradient in our $\bar{p}^4He^+$ calculation, which is difficult to do through manual adjustment. The initial values were achieved through minimizing the real energy eigenvalue when $\theta = 0$ and the optimization condition $g_1(E)$ was used to do searching in Table 1 except for S-wave shape resonance in H^-. For H^-, the initial parameters were adjusted manually to reduce the energy derivation to less than 0.1, and then the energy derivation was heavily reduced to below 1×10^{-7} after several iterations using optimization condition $g_2(E)$. Also in the table, a comparison is made with some of the best calculations in the literature. One can see from the table that with moderately large sizes of basis sets, our method can not only reproduce but also be capable of significantly improving the previous values for Ps^-, H^-, and He. To our knowledge, our result for $\bar{p}^4He^+$ is the only theoretical value that confirms the Korobov's calculation for both the position and width, although much smaller size of basis set is used in our work. Our calculations show that the Hylleraas basis sets with complex nonlinear parameters are more powerful than those with real ones in achieving higher precision.

Table 1. Resonance parameters $(E_r, \Gamma/2)$ for various three-body Coulombic systems. In the table, $\mathcal{N}$ is the size of basis set controlled by parameter Ω. A comparison with some of the best theoretical results is also presented. Atomic units are used.

Author (year)	Ref.	$\mathcal{N}$	Ω	$-E_r$	$\Gamma/2$
Ps^- $^1S^e$, below Ps ($N=2$) threshold					
Ho (1979)	[28]	161	10	0.076030(1)	0.000021(1)
Li and Shakeshaft (2005)	[26]	10206	26	0.07603044235	0.00002151725
This work[a]		1222	22	0.07603044186(2)	0.00002151695(1)
H^- S-wave shape resonance, above H ($N=2$) threshold					
Bürgers and Lindroth (2000)	[25]	34447	72	0.103035676	0.015627312
Kar and Ho (2012)	[27]	700		0.1030357(50)	0.0156273(50)
This work[a]		1222	22	0.103035677(3)	0.015627312(3)
He $^1S^e(1)$, below He^+ ($N=2$) threshold					
Ho (1981)	[29]	161	10	0.77787	0.00227
Bürgers, Wintgen and Rost (1995)	[30]	24497	64	0.777867636	0.002270653
This work[b]		1925	26	0.7778675(3)	0.0022706(2)
This work[a]		715	18	0.7778676356(3)	0.0022706527(1)
He $^3P^o(1)$, below He^+ ($N=2$) threshold					
Ho (1981)	[29]	165	8	0.7604975	0.0001485
This work[a]		969	16	0.76049238762(3)	0.0001494308(1)
He $^1D^e(1)$, below He^+ ($N=2$) threshold					
Ho and Bhatia (1991)	[31]	1230	17	0.7019457	0.0011811
This work[a]		959	12	0.70194550(1)	0.001181226(3)
$\bar{p}^4He^+$ ($N=31, L=30$)					
Korobov (2014)	[11]	7000		3.67977478748142(4)	4.76010×10^{-9}
This work[a]		2555	16	3.67977478748(1)	$4.754(2)\times10^{-9}$

[a]Basis set Eq. (6) with complex nonlinear parameters.

[b]Basis set Eq. (5) with real nonlinear parameters.

4. Summary

To sum up, we have presented a new approach called the CCR-GO method, which for the first time makes the search for resonance mathematically automated. This is in sharp contrast to the traditional way of manual adjustment of variational parameters. Therefore, our method can greatly improve the search efficiency and search accuracy of resonance poles. Resonance phenomena exist ubiquitously in physics. The significance of our method is by no means limited to few-body atomic systems; it can also be applied in principle to find resonance poles in many areas of physics, including nuclear and elementary particle physics.

Acknowledgment

ZXZ would like to thank V. I. Korobov of JINR for providing his computer codes of complex nonlinear parameters.

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