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Resonances of a hydrogen atom in strong parallel electric and magnetic fields using B-spline basis sets*

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The B-spline basis set plus complex scaling method is applied to the numerical calculation of the exact resonance parameters $E_{\rm r}$ and $\Gamma/2$ of a hydrogen atom in parallel electric and magnetic fields. The method can calculate the ground and higher excited resonances accurately and efficiently. The resonance parameters with accuracies of $10^{-9}-10^{-12}$ for hydrogen atom in parallel fields with different field strengths and symmetries are presented and compared with previous ones. Extension to the calculation of Rydberg atom in crossed electric and magnetic fields and of atomic double excited states in external electric fields is discussed.

Keywords: hydrogen atom, B-spline, complex scaling method, resonance, parallel electric and magnetic fields

PACC: 2320C, 2570E, 3150, 3345B

1. Introduction

The behaviour of a hydrogen atom in external electric and magnetic fields is a basic quantum mechanical problem, which has been studied over a century due to its fundamental significance. In the past several decades, more attention has been paid to the atom in strong fields, in which the external field cannot be considered as a perturbation. In general, strong field condition can be fulfilled experimentally in the case of Rydberg atom in an external field, where the electric or magnetic force is comparable with or larger than the coulomb interaction between valence electron and atomic core. Due to its important role in understanding classical and quantum correspondence and quantum chaos,[1−5] a large number of experimental and theoretical studies have been carried out for the atom in a pure magnetic field and a combined electric and magnetic fields separately.[6,7] Currently, it is of interest to investigate the Rydberg atom in a combined electric and magnetic field, which provides an ideal system to study high-dimensional chaos dynamics. In a recent experiment, Stania and Walther[8] found that the photoionization cross section of $^{85}{\rm R_b}$ atom in crossed electric and magnetic fields exhibits strong Ericsson fluctuations, a characteristic feature of quantum chaos for open systems. Adopting multichannel quantum defect theory combined large-basis-set complex scaling method with a basis-set size up to 300000, Madronero and Buchleitner performed quantum mechanic calculation of the photoionization cross section for $^{85}{\rm R_b}$ atom in crossed fields[9] and explained quantitatively the experimental observation. Such a large scale calculation can be carried out only on an advanced supercomputer. A more effective method with reduced basis-set size is desirable. It is also urgently needed to investigate the effect of external fields on multi-electron atom.

Another interest in studying an atom in strong fields is aroused by the discovery of huge magnetic fields in the vicinity of magnetic white dwarfs ($B\sim 10^2-10^5$T) and the neutron stars ($B\sim 10^7-10^9$T) in the 1970s.[10,11] Since then, a large number of magnetic white dwarfs and neutron stars have been found at the astronomical observatories, for example, in the Sloan Digital Sky Survey (SDSS).[12] To explain the observed spectra, the accurate spectrum calculation for atom in such a strong field is crucial. So far, there has been made a tremendous success of explaining many absorption features in the spectra of magnetic white dwarf stars. However, there are still a number

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of unexplained and unidentified features in the spectra of some white dwarf stars.[13] One reason is that the additional electric field on the order of $10^{-6} - 10^{-3}$ a.u., where a.u. stands for atomic unit, may come from the discrepancy between observations and calculated data. Attempts to address this problem have been made by several authors.[14−18]

The quantum states of an atom in a combined electric and magnetic field appear as resonant states due to the coupling between the continuum and bound states. Traditional bound-state method adopted in several previous studies is practicable only to narrow resonances but cannot provide any information about lifetime of resonances(see Ref.[15] and references therein). There are well-established methods of dealing with the resonant states. One of the most efficient methods to study resonances is the complex scaling method, or say, complex rotation method. In this method, the radial coordinates are rotated into a complex plane by an angle α ($r \to r\mathrm{e}^{\mathrm{i}\alpha}$). By choosing suitable α, the resonance problem is converted into bound-state one, therefore the calculation is greatly simplified. The details of this method and its application to an atom in external fields can be found in Refs.[19,20]. Another method, named the complex absorbing potential (CAP) method, is also widely used for the study of resonances.[21]

In the complex rotation method, it is important to choose an appropriate basis function. One should take seriously care of the completeness of basis set. In other words, the basis set should be suitable to well representing both bound states and continuum. The B-spline function is a highly localized and flexible function and has been proved to be a good candidate for the high-precision calculation of oscillator strength spectra near the ionization threshold of Rydberg atom in a magnetic field in which continuum contribution cannot be neglected.[22] On the other hand, external fields mix the field-free quantum states. The angular mixing can be described well by combining spherical harmonics with different angular momentum. However, this spherical harmonics expansion is slowly convergent if the mixing is strong. Using the B-spline basis set as an angular basis-set can reduce considerably the basis set dimension, and then accelerate convergence.[23,24] These advantages have been verified further by our recent calculation of electronic structure of hydrogen molecular ion[25] and energy spectra of confined atoms,[26,27] where the quantum systems are far from spherical symmetry.

In the present paper, we extend the bound-state method proposed in Ref.[22] to the study of resonances by combining the complex rotation of coordinates. A hydrogen atom in parallel electric and magnetic fields is adopted as a test system. The validity and efficiency of the method will be evaluated by testing the convergence and comparing our results with the data available in the literature. Some new results for m=1 states in parallel fields are reported. The feasibility of extending the method to the calculation of Rydberg atom in crossed electric and magnetic fields and atomic double excited states in external electric fields is also discussed.

2. Theory and method

We consider a hydrogen atom in parallel electric and magnetic fields. The direction of fields is assumed to be along the z-axis. In spherical coordinates, the non-relativistic Hamiltonian can be written as

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{1}{2}\gamma L_z + \frac{1}{8}\gamma^2 r^2 \sin^2\theta + fr\cos\theta, \quad (1)$$

where the magnetic field strength $\gamma = B/B_0$ with $B_0 \approx 2.35 \times 10^5$T; electric field strength $f = F/F_0$ with $F_0 \approx 5.14 \times 10^9$V/cm; L_z is the z-component of the angular momentum L. In the case of parallel electric and magnetic fields, only magnetic quantum number m is a good quantum number. The paramagnetic term $\frac{1}{2}\gamma L_z$ is a constant and can be dropped. Atomic unit is used throughout this paper.

After complex scaling $r \longrightarrow r\mathrm{e}^{\mathrm{i}\alpha}$, we can obtain a non-Hermitian Hamiltonian

$$\begin{aligned} H^\alpha = &-\frac{\nabla^2}{2}\mathrm{e}^{-2\mathrm{i}\alpha} - \frac{1}{r}\mathrm{e}^{-\mathrm{i}\alpha} \\ &+ \frac{1}{8}\gamma^2 r^2 \sin^2\theta \mathrm{e}^{2\mathrm{i}\alpha} + fr\cos\theta\mathrm{e}^{\mathrm{i}\alpha}. \end{aligned} \quad (2)$$

Let $\xi = \cos\theta$ and separate the axial variable, then the resultant effective Hamiltonian for a given m will be as follows:

$$\begin{aligned} H^\alpha(r,\xi) = &-\frac{\mathrm{e}^{-2\alpha}}{2r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right. \\ &\left. + \frac{\partial}{\partial\xi}(1-\xi^2)\frac{\partial}{\partial\xi} - \frac{m^2}{1-\xi^2}\right] \\ &- \frac{1}{r}\mathrm{e}^{-\mathrm{i}\alpha} + \frac{1}{8}\gamma^2 r^2(1-\xi^2)\mathrm{e}^{2\mathrm{i}\alpha} + fr\xi\mathrm{e}^{\mathrm{i}\alpha}. \end{aligned} \quad (3)$$

We expand the wavefunction of the system in terms of the B-spline-type basis set as

$$\Psi(r,\xi) = \sum_{i=1}^{N_r}\sum_{j=1}^{N_\xi} C_{ij}\frac{B_{i,k_r}(r)}{r}(1-\xi^2)^{\frac{|m|}{2}}B_{j,k_\xi}(\xi), \quad (4)$$

where B_{i,k_r} and B_{j,k_ξ} are radial and angular B-splines, respectively; N_r and k_r denote the size and order of the radial B-splines while N_ξ and k_ξ represent the size and order of the angular B-splines respectively. The details of the definition and application of B-splines may be found in Refs.[22, 28, 29].

The standard variational procedure recast the Schödinger equation into a complex symmetric generalized eigenvalue equation

$$HC = ESC, \tag{5}$$

where H and S are the Hamiltonian and overlap matrix, respectively; $E = E_{\rm res} - {\rm i}\Gamma/2$ is the complex value with the real part, $E_{\rm res}$, being energy position of resonance, and the imagine part, $\Gamma/2$, being the halfwidth of the resonance, which is relevant to ionization rate; C is the combination coefficient corresponding to Eq.(4).

3. Results and discussion

It is known that the wavefunction of hydrogen atom in a uniform electric field can be separated in parabolic coordinates and its quantum states can be denoted as (n_1, n_2, m) with n_1 and n_2 being the node numbers along the two parabolic coordinate directions, respectively. The relation $n_1 + n_2 + |m| + 1 = n$ holds with n being the principal quantum number in spherical coordinates. And for the resonances with the same n and m, n_1 and n_2 can be labelled as $n_1 = 0, 1, 2, \cdots, n - |m| - 1$ and $n_2 = n - n_1 - |m| - 1, n - n_1 - |m| - 2, n - n_1 - |m| - 3, \cdots, 1, 0$ according to the energy levels from low to high. If an additional magnetic field is applied, the exact meanings of n_1 and n_2 will be lost. If the magnetic field strength is not strong enough, we can still label the state with (n_1, n_2, m) as can be done in a pure electric field. This will facilitate the presentation and discussion.

The convergences of the position and width of resonance are dependent on the sizes (N_r and N_ξ) of radial and angular B-splines, radius of box $r_{\rm max}$, rotation angle α and distribution of knot sequence. For the radial B-splines, exponential distribution of knots defined in the region $[0, r_{\rm max}]$ is used. $r_{\rm max}$ is large enough and can be adjusted according to the states of interest to us. A uniform knot sequence of the angular B-spline defined in the region $[-1, 1]$ is adopted. The order $k_r = 7$ and $k_\xi = 7$ of the radial and angular B-splines are used throughout all the calculations. In the practical calculation, the knot sequence of radial B-splines and r_{max} are carefully optimized, so that we can describe best the resonance energies for a ground state and n=2 excited states of the hydrogen atom in a pure magnetic field, then we apply the same knot sequence to the case of parallel electric and magnetic fields. The identification of physical resonances in the present calculating scheme is not straightforward. Only those states with energy position and width unchanged with $r_{\rm max}$ or knot sequence are physical ones.

A large number of convergence tests have been performed for different field values, and for both low-lying and higher-lying states. A typical convergence test is shown in Table 1 for $n_1 = 0, n_2 = 0, m = 0$ state with $\gamma = 0.1$ and $f = 0.2$. It is seen that the convergences with respect to N_r and N_ξ are very fast. Both energy and width are accurate to 10^{-5} when a 20×10 basis set is used. For results obtained by a 30×20 basis set, an accuracy of 10^{-9} is achieved. The results obtained from different values of rotation angle α are different in the last digit for all the basis sets. This means that the resonances are well revealed by the complex rotation and the obtained energies and widths are reliable. It is noted that the non-perturbation calculation of a multi-electron atom in external fields is a challenge to the theory and computation. The fast convergence of the present method shows promise in further applying the method to investigating the effect of external fields on double excited states which is of current interest.[30−33]

In Table 2, we present resonance parameters $E_{\rm r}$ and $\Gamma/2$ for a ground state of the hydrogen atom with m=0. The results in a pure electric field are listed in the first column and compared with those obtained from the previous methods, such as complex-coordinate method,[19,34] recursion method[35] and perturbation method.[36] It is obvious that the accuracy of perturbation method rapidly decreases with the increase of field strength. For example, the accuracy is only 10^{-3} for f=0.2a.u., while our method can still arrive at an accuracy of 10^{-9} at this field strength. Even in the case of parallel electric and magnetic fields, our results can converge at least to nine significant digits compared with the most accurate ones given by Rao and Li.[19]

Table 1. The convergence of the $n_1 = 0, n_2 = 0, m = 0$ resonance of the hydrogen atom for γ=0.1a.u. and f=0.2a.u. The number in the square brackets represents the power of 10.

$N_r \times N_\xi$		$\alpha = 0.4$	$\alpha = 0.5$	$\alpha = 0.6$
20×10	$-E_{\rm r}$	0.568 042	0.568 048	0.568 039
	$\Gamma/2$	5.948 2[−2]	5.948 3[−2]	5.948 6[−2]
30×10	$-E_{\rm r}$	0.568 047 379	0.568 047 377	0.568 047 377
	$\Gamma/2$	5.948 220[−2]	5.948 220[−2]	5.948 220[−2]
30×15	$-E_{\rm r}$	0.568 045 91	0.568 045 91	0.568 045 91
	$\Gamma/2$	5.948 143 9[−2]	5.948 143 9[−2]	5.948 143 8[−2]
30×20	$-E_{\rm r}$	0.568 045 908	0.568 045 906	0.568 045 905
	$\Gamma/2$	5.948 143 7[−2]	5.948 143 7[−2]	5.948 143 6[−2]
40×30	$-E_{\rm r}$	0.568 045 906 07	0.568 045 906 05	0.568 045 906 04
	$\Gamma/2$	5.948 143 623[−2]	5.948 143 623[−2]	5.948 143 622[−2]
50×40	$-E_{\rm r}$	0.568 045 906 07	0.568 045 906 05	0.568 045 906 04
	$\Gamma/2$	5.948 143 623[−2]	5.948 143 623[−2]	5.948 143 621[−2]

Table 2. The evolutions of the $E_{\rm res}$ and $\Gamma/2$ for the ground state of the hydrogen atom for m=0 in parallel magnetic and electric fields. The number in the square brackets represents the power of 10.

quantity	γ=0	γ=2×10^{-3}	γ=2×10^{-2}	γ=0.1
		f=0.04		
$-E_{\rm res}$	0.503 771 591 016	0.503 770 551 37	0.503 667 683 621	0.501 206 356
$-E_{\rm res}$	0.503 771 591 013 5[a]	0.503 770 551 370[a]		0.501 206 356 2[a]
$-E_{\rm res}$	0.503 771 591 013 654 2[f]			0.501 206[i]
$\frac{\Gamma}{2}$	0.194 635 4[−5]	0.194 566 7[−5]	0.187 933[−5]	0.896[−6]
$\frac{\Gamma}{2}$	0.194 635 00[−5][a]	0.194 566 5[−5][a]		0.895 759[−6][a]
$\frac{\Gamma}{2}$	0.194 634 999 5[−5][f]			0.896 0[−6][i]
		f=0.08		
$-E_{\rm res}$	0.517 560 617 007	0.517 559 457 29	0.517 444 691 257	0.514 690 931
$-E_{\rm res}$	0.517 560 616 888[a]	0.517 559 457 175[a]		0.514 690 932 2[a]
$-E_{\rm res}$	0.517 560 50[f]			0.514 712[i]
$\frac{\Gamma}{2}$	0.226 982 878[−2]	0.226 968 043[−2]	0.225 505 183 3[−2]	0.193 358 89[−2]
$\frac{\Gamma}{2}$	0.226 982 875[−2][a]	0.226 968 039 9[−2][a]		0.193 358 900[−2][a]
$\frac{\Gamma}{2}$	0.226 981 5[−2][f]			0.194 4[−2][i]
		f=0.2		
$-E_{\rm res}$	0.570 124 899	0.570 124 070	0.570 041 941	0.568 045 905
$-E_{\rm res}$	0.570 124 88[a]	0.570 124 056 29[a]		0.568 045 897 6[a]
$-E_{\rm res}$	0.570 124 899[c]			
$-E_{\rm res}$	0.570 124 899[d]			
$-E_{\rm res}$	0.570 3[f]			
$\frac{\Gamma}{2}$	0.606 145 5[−1]	0.606 140 871[−1]	0.605 687 15[−1]	0.594 814 37[−1]
$\frac{\Gamma}{2}$	0.606 145 5[−1][a]	0.606 140 917[−1][a]		0.594 814 638[−1][a]
$\frac{\Gamma}{2}$	0.606 145 457[−1][c]			
$\frac{\Gamma}{2}$	0.606 145 46[−1][d]			
$\frac{\Gamma}{2}$	0.606[−1][f]			

[a]Ref.[19], [c]Ref.[35], [d]Ref.[37], [f]Ref.[36], [i]Ref.[21].

To show the validity of the method further, we investigate the higher excited resonances. For n=10 excited resonances, we choose a large basis set rather than adjust the parameters in order to acquire the accurate results. The convergence of every resonance is carefully checked. The largest basis set used is 80×50. We should point out that it takes only several minutes to finish a computing task by using a moderate basis set, which is due to the banded structure of Hamiltonian matrix. The details about the diagonalization procedure can be found in Ref.[22]. This can be considered as one of the advantages of the present method. The resonance parameters of n=10 excited states are presented in Table 3, where the results from Refs.[19, 37] are also listed for comparison. Our results are in agreement with the most accurate ones given by Rao and Li.[19] The accuracies for n=10 states in different electric and magnetic fields are the same as that of the ground state, which can reach at least 10^{-9}.

Table 3. The evolutions of the $E_{\rm res}$ and $\Gamma/2$ for n=10 excited states of the hydrogen atom for m=0 in parallel magnetic and electric fields. The number in the square brackets represents the power of 10.

state	quantity	γ=0	$\gamma=2\times10^{-5}$	$\gamma=2\times10^{-4}$
		$f=1.4\times10^{-5}$		
n_1=0, n_2=9	$-E_{\rm res}$	7.212 084 46[−3]	7.211 916 9[−3]	7.195 855 75[−3]
	$-E_{\rm res}$	7.212 084 47[−3]$^{\rm a}$	7.211 916 89[−3]$^{\rm a}$	7.195 855 76[−3]$^{\rm a}$
	$-E_{\rm res}$	7.212 084 5[−3]$^{\rm d}$		
	$\frac{\Gamma}{2}$	4.007 021[−5]	4.004 574[−5]	3.784 610[−5]
	$\frac{\Gamma}{2}$	4.007 021 6[−5]$^{\rm a}$	4.004 574 1[−5]$^{\rm a}$	3.784 611 0[−5]$^{\rm a}$
	$\frac{\Gamma}{2}$	4.007 021 6[−5]$^{\rm d}$		
n_1=1, n_2=8	$-E_{\rm res}$	6.780 036 11[−3]	6.779 577 05[−3]	6.735 493 44[−3]
	$-E_{\rm res}$	6.780 036 12[−3]$^{\rm a}$	6.779 577 06[−3]$^{\rm a}$	6.735 493 46[−3]$^{\rm a}$
	$\frac{\Gamma}{2}$	2.478 735[−5]	2.473 253[−5]	1.999 450[−5]
	$\frac{\Gamma}{2}$	2.478 737 3[−5]$^{\rm a}$	2.473 255 0[−5]$^{\rm a}$	1.999 453 1[−5]$^{\rm a}$
n_1=2, n_2=7	$-E_{\rm res}$	6.343 873 4[−3]	6.343 187 1[−3]	6.277 299 13[−3]
	$-E_{\rm res}$	6.343 873 45[−3]$^{\rm a}$	6.343 187 14[−3]$^{\rm a}$	6.277 299 16[−3]$^{\rm a}$
	$\frac{\Gamma}{2}$	1.314 66[−5]	1.308 67[−5]	8.286 7[−6]
	$\frac{\Gamma}{2}$	1.314 668 7[−5]$^{\rm a}$	1.308 672 5[−5]$^{\rm a}$	8.286 835[−6]$^{\rm a}$
		$f=2.2\times10^{-5}$		
n_1=0, n_2=9	$-E_{\rm res}$	8.660 579 1[−3]	8.660 451[−3]	8.647 923 5[−3]
	$-E_{\rm res}$	8.660 579 4[−3]$^{\rm a}$	8.660 451 1[−3]$^{\rm a}$	8.647 923 8[−3]$^{\rm a}$
	$-E_{\rm res}$	8.660 578[−3]$^{\rm d}$		
	$\frac{\Gamma}{2}$	5.329 92[−4]	5.329 392[−4]	5.279 796[−4]
	$\frac{\Gamma}{2}$	5.329 919 7[−4]$^{\rm a}$	5.329 394 0[−4]$^{\rm a}$	5.279 798[−4]$^{\rm a}$
	$\frac{\Gamma}{2}$	5.329 92[−4]$^{\rm d}$		
n_1=1, n_2=8	$-E_{\rm res}$	8.028 666 0[−3]	8.028 308 3[−3]	7.993 274[−3]
	$-E_{\rm res}$	8.028 665 96[−3]$^{\rm a}$	8.028 308 3[−3]$^{\rm a}$	7.993 273 5[−3]$^{\rm a}$
	$\frac{\Gamma}{2}$	4.674 81[−4]	4.673 282[−4]	4.528 66[−4]
	$\frac{\Gamma}{2}$	4.674 810 1[−4]$^{\rm a}$	4.673 283 1[−4]$^{\rm a}$	4.528 659[−4]$^{\rm a}$
n_1=2, n_2=7	$-E_{\rm res}$	7.383 110 6[−3]	7.382 558 0[−3]	7.328 252[−3]
	$-E_{\rm res}$	7.383 110 66[−3]$^{\rm a}$	7.382 558 6[−3]$^{\rm a}$	7.328 252 3[−3]$^{\rm a}$
	$\frac{\Gamma}{2}$	3.977 62[−4]	3.975 19[−4]	3.744 032[−4]
	$\frac{\Gamma}{2}$	3.977 618 8[−4]$^{\rm a}$	3.975 185 5[−4]$^{\rm a}$	3.744 03[−4]$^{\rm a}$

$^{\rm a}$Ref.[19], $^{\rm d}$Ref.[37].

The results for the case of m=1 states are shown in Tables 4 and 5, in which n=2,10 excited resonance states are presented respectively. We compare the results obtained in a pure electric field with those available in the literature. For n=2 resonances, our results are in good agreement with those given by Rao[34], Telnov[35] and Kolosov,[37] especially with those presented by Telnov and Kolosov. There exist at least nine significant numbers for our results. While for n=10 resonances, the consistency decreases with the increase of electric field. The results for parallel electric and magnetic fields are new. No such data are available from the literature for comparison. We believe that the data presented in Tables 4 and 5 are accurate to the last digit.

Table 4. The resonance parameters E_0 and $\Gamma/2$ for n=2 excited states of the hydrogen atom for m=1 in parallel magnetic and electric fields. The number in the square brackets represents the power of 10.

state	quantity	γ=0	γ=2×10^{-3}	γ=2×10^{-2}
		f=0.005		
n_1=0, n_2=0	$-E_{\rm res}$	0.127 146 612 704	0.127 133 490 292	0.125 863 685 167
	$-E_{\rm res}$	0.127 146 613[c]		
	$-E_{\rm res}$	0.127 146 612[d]		
	$-E_{\rm res}$	0.127 146 612 714[j]		
	$\frac{\Gamma}{2}$	0.130 764 27[−4]	0.129 522 50[−4]	0.524 402 38[−5]
	$\frac{\Gamma}{2}$	0.130 764 27[−4][c]		
	$\frac{\Gamma}{2}$	0.130 764 272 5[−4][d]		
	$\frac{\Gamma}{2}$	0.130 764 366[−4][j]		
		f=0.02		
n_1=0, n_2=0	$-E_{\rm res}$	0.146 729 380 607	0.146 720 271 646	0.145 814 546 915
	$-E_{\rm res}$	0.146 729 381[c]		
	$-E_{\rm res}$	0.146 729 38[d]		
	$-E_{\rm res}$	0.146 729 461[j]		
	$\frac{\Gamma}{2}$	0.218 536 404 49[−1]	0.218 478 808 73[−1]	0.212 841 811 08[−1]
	$\frac{\Gamma}{2}$	0.218 536 404[−1][c]		
	$\frac{\Gamma}{2}$	0.218 536 4[−1][d]		
	$\frac{\Gamma}{2}$	0.218 535 718[−1][j]		

[c]Ref.[35], [d]Ref.[37], [j]Ref.[34].

From Tables 2 to 5, we can find that the energy increases and the width decreases with the increase of magnetic field in a fixed electric field. It means that the magnetic field makes the resonances more and more stable for states over the field region considered in this paper. Systematic investigation of the effects of parallel electric and magnetic fields needs a large number of data in different electric and magnetic field strengths. Such a compilation of resonant parameters is also useful for the applications in astrophysics, for example, the evaluation of opacity of atmosphere in magnetic white dwarfs.

Table 5. The resonance parameters E_0 and $\Gamma/2$ for n=10 excited states of the hydrogen atom for m=1 in parallel magnetic and electric fields. The number in the square brackets represents the power of 10.

state	quantity	γ=0	γ=2×10^{-5}	γ=2×10^{-4}
		f=1.0×10^{-5}		
n_1=0, n_2=8	$-E_{\rm res}$	6.324 856 721 068[−3]	6.324 571 424 6[−3]	6.297 318 508 505[−3]
	$-E_{\rm res}$	6.324 857[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	5.581 12[−9]	5.541 33[−9]	2.936 23[−9]
	$\frac{\Gamma}{2}$	5.581[−9]$^{\rm h}$		
n_1=1, n_2=7	$-E_{\rm res}$	6.023 885 043 86[−3]	6.023 376 660[−3]	5.974 653 594 46[−3]
	$-E_{\rm res}$	6.023 885 0[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	1.061 27[−9]	1.045 2[−9]	4.181[−10]
	$\frac{\Gamma}{2}$	1.061 3[−9]$^{\rm h}$		
n_1=2, n_2=6	$-E_{\rm res}$	5.721 681 790[−3]	5.721 012 697 13[−3]	5.656 653 891 627[−3]
	$-E_{\rm res}$	5.721 681 79[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	1.61[−10]	1.578 4[−10]	4.7291[−11]
	$\frac{\Gamma}{2}$	1.617 15[−10]$^{\rm h}$		
		f=1.5×10^{-5}		
n_1=0, n_2=8	$-E_{\rm res}$	7.177 032 160[−3]	7.176 716 746 4[−3]	7.146 354 563 493[−3]
	$-E_{\rm res}$	7.155[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	6.397 542 1[−5]	6.391 556 09[−5]	5.851 686 695 3[−5]
	$\frac{\Gamma}{2}$	7.5[−5]$^{\rm h}$		
n_1=1, n_2=7	$-E_{\rm res}$	6.712 370 865[−3]	6.711 791 992 91[−3]	6.655 933 277[−3]
	$-E_{\rm res}$	6.702[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	4.221 193 7[−5]	4.211 814 029[−5]	3.389 813 84[−5]
	$\frac{\Gamma}{2}$	4.5[−5]$^{\rm h}$		
n_1=2, n_2=6	$-E_{\rm res}$	6.241 980 926[−3]	6.241 200 280[−3]	6.165 850 322 378[−3]
	$-E_{\rm res}$	6.238[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	2.442 962 7[−5]	2.432 955 44[−5]	1.603 521 848[−5]
	$\frac{\Gamma}{2}$	2.5[−5]$^{\rm h}$		
		f=2.0×10^{-5}		
n_1=0, n_2=8	$-E_{\rm res}$	8.035 515 476[−3]	8.035 252 72[−3]	8.009 624 766[−3]
	$-E_{\rm res}$	7.75[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	3.551 827 23[−4]	3.550 800 27[−4]	3.454 286 69[−4]
	$\frac{\Gamma}{2}$	9.5[−4]$^{\rm h}$		
n_1=1, n_2=7	$-E_{\rm res}$	7.443 958 975[−3]	7.443 465 950[−3]	7.395 151 973[−3]
	$-E_{\rm res}$	7.20[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	2.958 444 97[−4]	2.956 502 696[−4]	2.773 863 29[−4]
	$\frac{\Gamma}{2}$	8[−4]$^{\rm h}$		
n_1=2, n_2=6	$-E_{\rm res}$	6.837 972 782[−3]	6.837 283 121[−3]	6.769 397 403[−3]
	$-E_{\rm res}$	6.67[−3]$^{\rm h}$		
	$\frac{\Gamma}{2}$	2.347 893 26[−4]	2.345 237 313[−4]	2.096 903 99[−4]
	$\frac{\Gamma}{2}$	4.85[−4]$^{\rm h}$		

$^{\rm h}$Ref.[38].

4. Summary

We have proposed an effective method of calculating the resonance parameters of a hydrogen atom in parallel electric and magnetic fields. B-spline functions have been adopted as both the radial and angular basis sets. The positions and widths of some selected low-lying and higher-lying resonances have been calculated accurately by the complex rotation scheme. The convergence of the method is surprisingly fast. It shows promise in further applying this method to dou-

ble excited states in external fields, which is of great and realistic significance.[30−33] In principle, the extension of present method to Rydberg atom in crossed electric and magnetic fields is straightforward. Considering the banded structure of Hamiltonian, it is not difficult to push the size of basis set up to 10^5 if a parallel algorithm is developed. We emphasize that the using of B-spline as an angular basis function results in considerable reduction of basis-set size, which is crucial to making feasible calculation of problem concerning Rydberg atom in crossed electric and magnetic fields.

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