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Resonances of the hydrogen atom in strong parallel magnetic and electric fields

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The behavior of the rsonances of a hydrogen atom in parallel magnetic and electric fields is obtained with a complex scaling plus B-spline method. The resonant parameters E and Γ_0 in an electric field alone are consistent with those obtained by other methods. In a fixed electric field F the widths Γ of both the ground and excited resonances decrease with an increase of the magnetic field B, and the relative variation $(\Gamma-\Gamma_0)/\Gamma_0$ is directly proportional to the ratio of the magnetic-field strength to the electric-field strength. The positions of the resonances, however, are pushed higher by an increasing of magnetic field. The pushing effect is insensitive to the electric-field strength and depends almost entirely on the magnetic-field strength.

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I. INTRODUCTION

Up until now, most of the studies of atoms in parallel magnetic and electric fields are constrained to the domain where the strengths of the fields is so weak that field-ionization effects can be ignored completely. The states can be treated as stable ones. This allows the application of such methods as the semiclassical perturbative treatment [1,2] and group theoretical approach [3] which take advantage of the existence of an approximate constant of motion. When the fields are very strong, the field-ionization effect cannot be ignored. It shifts and broadens the bound-state atomic levels and the energy eigenvalues may be expressed as $E_r = E_{\text{res}} - (i/2)\Gamma$, where E_{res} determines the center of a band into which the level in the parallel magnetic and electric field evolves and Γ is the level width defining the ionization probability of the atom. The field effects drastically increase upon going from one excited level to another. For the field-ionization region, up until now, most of the studies are concerned with the cases of a pure magnetic and a pure electric field.

For the pure electric field, quite different calculation procedures are used to get the properties of resonant states. For example the WKB method [4–6], the Borel summation of the Rayleigh-Schrödinger perturbation series [6–7], the finite basis expansion method [8–11], and the consistent uniform quantum-mechanical approach [12]. For hydrogen atoms in pure magnetic fields, the properties of resonant states were calculated by the complex scaling, the R matrix, and other methods [13–15].

Johnson, Scheibner, and Farrelley [16] studied the ground-state hydrogen atom in parallel electric and magnetic fields by both a large-order perturbation theory and complex scaling based on the method introduced by Reinhardt [17] and Chu [18]. They found that the effect of a sizable magnetic field ($\beta \geq 0.05$) is to decrease the width of the ground state but they did not study the effect of a magnetic field on the excited states of a hydrogen atom in parallel electric and magnetic fields.

In this paper, we present our numerical studies on the evolution of both ground and excited resonances of a hydrogen atom in parallel magnetic and electric fields by a complex scaling plus B-spline method. Our main purpose is to find how the magnetic field modifies the behavior of the resonances in the electric field, especially for the excited states.

II. THEORY AND METHOD

The Hamiltonian for a hydrogen atom subjected to electric and magnetic fields both parallel to the z direction is (in atomic units)

$$H = -\tfrac{1}{2}p^2 - \frac{1}{r} + \beta L_z + \tfrac{1}{2}\beta^2\rho^2 + fz \ , \tag{1}$$

where $\beta = B/B_c$, $B_c = 4.7\times10^5 T$, $f = F/F_c$, $F_c = 5.14\times10^9$ V/cm^{-1}. The nucleus is taken to be dimensionless, of infinite mass and relativistic effects are completely neglected; L_z denotes oz projection of the orbital momentum $\vec{L}$ and ρ the projection of the position vector $\vec{r}$ onto the plane $z=0$. The total Hamiltonian commutes with L_z; therefore, in a subspace with a given m, the paramagnetic term, which introduces only a global energy shift βm, can be disregarded. There exists only one good quantum number m, and the problem is two dimensional and nonseparable.

The complex scaling method has been widely used for resonances in various atomic and molecular structures and processes [19]. Reinhardt [17] diagonalized the complex scaled Stark Hamiltonian of hydrogen with a real L^2

basis set and obtained complex eigenvalues $E_r = E_{\mathrm{res}} - (i/2)\Gamma$. Such a method of directly diagonalizing the complex scaled Hamiltonian with a real L^2 basis set is referred by the author as a direct approach of complex scaling. In contrast to other methods, the direct approach described above needs no explicit consideration of boundary conditions, and with the use of the L^2 basis the boundary condition of square integrability is preserved.

Based on the successful use of the B-spline basis in the hydrogenic Zeeman system [20,21], we have combined the two techniques in an effort to give accurate resonant parameters of the ground and lower excited states of the Stark system over a wide range of electric-field strengths [22]. Now, this method is extended to the calculation of the behavior of resonances of a hydrogen atom in parallel magnetic and electric fields.

A full description of B-spline functions can be found in, e.g., Ref. [23]. Given a knot sequence on the r axis $\{r_1 \le r_2 \le \cdots \le r_N \le \cdots \le r_{N+k}\}$, B-spline functions of order k, $B_{i,k}$ is defined. The $B_{i,k}$ $(i=1,2,\ldots)$ are piecewise polynomials of order $k-1$ localized within $[r_1, r_{N+k}]$, while $B_{i,k}$ is nonvanishing within $[r_i, r_{i+k}]$. The behavior of B-spline functions can be readily adjusted with the knot sequence, viz., the choice of knot point r_i, order k and number of B splines N, which offer a means to optimize the B splines as a basis set to expand the wave functions of one or several states concerned. With such a B-spline basis set, the radial dimension of a field-dressed wave function of a certain state Ψ can be expanded as

$$\Psi_m = \frac{1}{r} \sum_{l=|m|}^{l_{\max}} R_l Y_{lm} \tag{2}$$

(for fixed m and a truncation at $l = l_{\max}$), where $R_l(r)$ is

$$R_l(r) = \sum_i B_{i,k}(r) C_{i,l} \ . \tag{3}$$

The Schrödinger equation reads

$$HC = EBC \ , \tag{4}$$

where B is the overlap matrix of the nonorthogonal B-spline basis. After complex scaling $r \rightarrow re^{i\theta}$, we get an non-Hermitian complex Hamiltonian and a complex Schrödinger equation in matrix notation. The solution of the complex equation yields the complex eigenvalues from which the resonant energy of our interests can be singled out for its distinct imaginary part that is related with the resonant width.

Given the number of B-spline functions N (viz., the size for basis set) and the order k, our knot sequence is so determined that the B-spline basis defined on the knot sequence can best represent the zero-field behavior of the resonant state concerned, in particular the accurate zero-field energy $-1/2n^2$. For example with $N=38$, $k=7$, we adjust the knot sequence so that the B-spline basis for the Stark shifted and the broadened ground state gives zero-field energy of $-\frac{1}{2} + 1 \times 10^{-13}$ a.u. With this basis set, the solution of Eq. (4) can give accurate ground resonance up to the high field range of $f = 2.0$ a.u., then we use the same basis to calculate the energy levels in a pure magnetic field to determine the magnetic-field range in which the accuracy can be maintained. After that, we calculate the ground resonance in parallel magnetic and electric fields in the field range determined by the above procedure. For the $n=10$ states, the knot sequence is readjusted, using the same procedure as described above.

III. RESULTS AND DISCUSSIONS

In the calculations for the ground and the $n=2$ excited resonances, we employ the same knot sequence and hence the same B-spline basis, with $l_{\max} = 12$, $N = 38$. The field range is chosen as $0.03 \le f \le 0.2$, $0.0 \le \beta \le 0.05$ for ground resonance (parabolic number $n=1$, $m=0$, $n_1=0$, $n_2=0$) and $0.005 \le f \le 0.02$, $0.0 \le \beta \le 0.01$ for $n=2$ resonances. For $n=10$ resonance we employ another knot sequence with $l_{\max}=24$, $N=58$, the field range is chosen as $2 \times 10^{-5} \le f \le 4.5 \times 10^{-5}$, $0.0 \le \beta \le 1 \times 10^{-4}$. Results are tabulated in Table I, where results of a pure electric field of some other authors are listed for comparison. With such a basis set, θ trajectories are very stationary, and an accurate complex energy at the stationary point can be obtained.

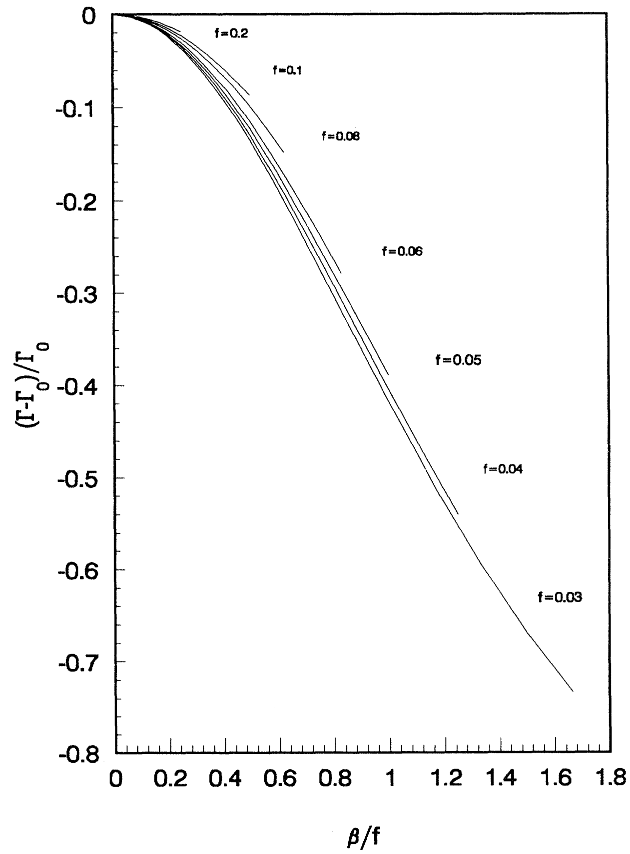

FIG. 1. The evolution of the $[(\Gamma-\Gamma_0)/\Gamma_0]$ of ground resonance of a hydrogen atom with the magnetic-field strength over the electric-field strength.

TABLE I. The evolution of the E_{res} and $\Gamma/2$ for the ground and excited states of a hydrogen atom in parallel magnetic and electric fields. Square brackets denote powers of 10.

State	Quantity	$\beta=0.0$	$\beta=10^{-3}$	$\beta=5\times10^{-2}$
		$f=0.04$		
$n_1=0,n_2=0$	$-E_{\text{res}}$	0.503 771 591 013 5	0.503 770 551 370	0.501 206 356 2
	$-E_{\text{res}}$	0.503 771 591 00[a]		
	$\frac{\Gamma}{2}$	0.194 635 00[−5]	0.194 566 5[−5]	0.895 759[−6]
	$\frac{\Gamma}{2}$	0.194 635 [−5][a]		
		$f=0.08$		
$n_1=0,n_2=0$	$-E_{\text{res}}$	0.517 560 616 888	0.517 559 457 175	0.514 690 932 2
	$-E_{\text{res}}$	0.517 560 617 00[a]		
	$\frac{\Gamma}{2}$	0.226 982 875 [−2]	0.226 968 039 9[−2]	0.193 358 900[−2]
	$\frac{\Gamma}{2}$	0.226 982 877 [−2]		
		$f=0.2$		
$n_1=0,n_2=0$	$-E_{\text{res}}$	0.570 124 88	0.570 124 056 29	0.568 045 897 6
	$\frac{\Gamma}{2}$	0.606 145 5[−1]	0.606 140 917 [−1]	0.594 814 638[−1]
State	Quantity	$\beta=0.0$	$\beta=10^{-3}$	$\beta=10^{-2}$
		$f=0.005$		
$n_1=0,n_2=1$	$-E_{\text{res}}$	1.426 186 076[−1]	1.426 079 644[−1]	1.415 817 9[−1]
	$-E_{\text{res}}$	1.426 186 08[−1]		
	$\frac{\Gamma}{2}$	5.297 223 174[−5]	5.275 310 116[−5]	3.622 265 9[−5]
	$\frac{\Gamma}{2}$	5.297 223 2[−5][b]		
$n_1=0,n_2=0$	$-E_{\text{res}}$	1.120 619 240[−1]	1.120 506 749[−1]	1.109 587 2[−1]
	$-E_{\text{res}}$	1.120 619 24[−1][b]		
	$\frac{\Gamma}{2}$	2.864 684 06[−6]	2.820 209 896[−6]	6.378 513 4[−7]
	$\frac{\Gamma}{2}$	2.864 684[−6][b]		
		$f=0.02$		
$n_1=0,n_2=1$	$-E_{\text{res}}$	2.066 822 362[−1]	2.066 751 798 6[−1]	2.059 766 24[−1]
	$-E_{\text{res}}$	2.066 822 37[−1][b]		
	$\frac{\Gamma}{2}$	3.039 285 5[−2]	3.038 943 263 4[−2]	3.005 607 7[−2]
	$\frac{\Gamma}{2}$	3.039 285 60[−2][b]		
$n_1=1,n_2=0$	$-E_{\text{res}}$	8.898 376 54[−2]	8.897 535 614 9[−2]	8.815 250 7[−2]
	$-E_{\text{res}}$	8.998 378 55[−2][b]		
	$\frac{\Gamma}{2}$	1.544 575 74[−2]	1.543 879 718 0[−2]	1.476 797 8[−2]
	$\frac{\Gamma}{2}$	1.544 575 80[−2][b]		
State	Quantity	$\beta=0.0$	$\beta=10^{-5}$	$\beta=10^{-4}$
		$f=1.4\times10^{-5}$		
$n_1=0,n_2=9$	$-E_{\text{res}}$	7.212 084 47[−3]	7.211 916 89[−3]	7.195 855 76[−3]
	$-E_{\text{res}}$	7.212 084 5[−3][c]		
	$\frac{\Gamma}{2}$	4.007 021 6[−5]	4.004 574 1[−5]	3.784 611 0[−5]
	$\frac{\Gamma}{2}$	4.007 021 6[−5][c]		
$n_1=1,n_2=8$	$-E_{\text{res}}$	6.780 036 12[−3]	6.779 577 06[−3]	6.735 493 46[−3]

TABLE I. (*Continued*).

State	Quantity	$\beta=0.0$	$\beta=10^{-5}$	$\beta=10^{-4}$
	$\frac{\Gamma}{2}$	2.478 737 3[−5]	2.473 255 0[−5]	1.999 453 1[−5]
$n_1=2, n_2=7$	$-E_{\text{res}}$	6.343 873 45[−3]	6.343 187 14[−3]	6.277 299 16[−3]
	$\frac{\Gamma}{2}$	1.314 668 7[−5]	1.308 672 5[−5]	8.286 835[−6]
		$f=2.2\times10^{-5}$		
$n_1=0, n_2=9$	$-E_{\text{res}}$	8.660 579 4[−3]	8.660 451 1[−3]	8.647 923 8[−3]
	$-E_{\text{res}}$	8.660 578[−3][c]		
	$\frac{\Gamma}{2}$	5.329 919 7[−4]	5.329 394 0[−4]	5.279 798[−4]
	$\frac{\Gamma}{2}$	5.329 92[−4][c]		
$n_1=1, n_2=8$	$-E_{\text{res}}$	8.028 665 96[−3]	8.028 308 3[−3]	7.993 273 5[−3]
	$\frac{\Gamma}{2}$	4.674 810 1[−4]	4.673 283 1[−4]	4.528 659[−4]
$n_1=2, n_2=7$	$-E_{\text{res}}$	7.383 110 66[−3]	7.382 558 6[−3]	7.328 252 3[−3]
	$\frac{\Gamma}{2}$	3.977 618 8[−4]	3.975 185 5[−4]	3.744 031[−4]

[a] Reference [8].
[b] Reference [11].
[c] Reference [10].

From Table I, for the pure electric field, we see that over the tabulated field range our results agree well with the most accurate ones by Benassi and Grecchi [8]. This means that our method is reliable and accurate at least over the range concerned. It shows that in the region considered for the ground resonance, the increase of the magnetic-field strength reduces the width of the resonance. The stronger the magnetic field is, the more stable the ground state. This confirms the results by Johnson, Scheibner, and Farrelly [16]. They show that the effect of sizable magnetic fields ($\beta \geq 0.05$) is to decrease the width of the ground resonance of a hydrogen atom in parallel electric and magnetic fields. Our results show that the effect of a magnetic field that is not as strong as in Ref. [16], for instance, $\beta=0.001$, is also to decrease the width. Johnson *et al.* only gave very few figures for the position of the ground resonance of a hydrogen atom and did not give the width of resonance in figures; besides, their results are not very accurate even for the pure electric field. For example, at $f=0.1$, $\beta=0$, they gave $F_{\text{res}}=-0.5396$, but the accurate result is -0.5274.

The factor $\alpha=(\Gamma-\Gamma_0)/\Gamma_0$ can be used to indicate the relative effects of a magnetic field on the width of resonance of an atom in parallel electric and magnetic fields (here Γ_0 is the width of resonance free of magnetic field, and Γ is the width of the same resonance in the same electric field and a magnetic field added in). Figure 1 shows that the relative effect of the magnetic field on the width of resonance depends approximately on the factor β/f (the relative intensity of the magnetic field with respect to the electric one). The bigger the factor is, the greater the relative effects. From Fig. 2, we can see that

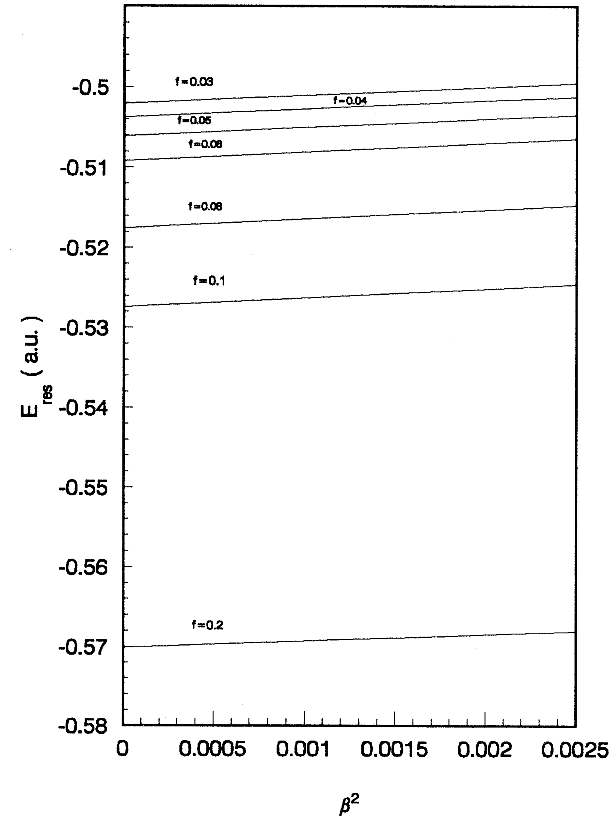

FIG. 2. The evolution of energy level of ground resonance of hydrogen atom with the square of the magnetic field.

at a fixed electric-field strength, the magnetic field pushes the energy level up. The lines used to describe the evolution of $E_{\rm res}$ with β^2 in Fig. 2 are almost parallel. This implies that, unlike the effect on the width, the pushing up effect is insensitive to the electric-field strength but proportional to the square of the magnetic one for a definite state.

For the $n=2$ and $n=10$ states, from Table I we can see that for pure electric fields our results are consistent with the works by Telnov [11] and Kolosov [10], respectively. Careful study of Table I reveals that the evolution pattern is the same as that of the ground resonance. It is also shown in Table I that for the same n manifold, the width of a higher level state is more easily affected by the magnetic field.

Some of the above behaviors of the resonances in parallel electric and magnetic fields can be explained qualitatively as below. The energy levels being pushed up, can be understood from a perturbation point of view, viz., one of the effects of the magnetic field, to the first-order perturbation, is to shift the position up by $\beta^2/2\langle|\rho^2|\rangle$ which is proportional to the square of the magnetic field.

Generally speaking, the widths of resonances in a parallel magnetic and electric field are induced by field ionization which depends on the following factors, the electric- and magnetic-field strengths, the position of the energy level, and the charge distribution of the states considered. The last factor plays a very important role in the excited resonances but makes almost no effect on the ground one. So for excited resonances, the analysis will be more difficult than for the ground one, since the widths depend not only on the level positions but also on the charge distribution of the states considered. For example, in the pure electric field, the width of a higher level state is narrower than that of a lower one in the same n manifold due to the difference between their charge distributions [24]. Our numerical results for resonances in a parallel magnetic and electric field reveal the same pattern that is also due to the charge distribution.

This implies that the ionization rates of the excited states are sensitively affected by their charge distributions whose dependence on the external field needs further investigation.

IV. CONCLUSION

B-spline basis has been shown to be an excellent basis for the direct approach of complex scaling for resonances of a hydrogenic atom in parallel magnetic and electric fields. Accurate complex energies for $n=1$, $n=2$, and $n=10$ resonances are obtained. The results for a pure electric field agree well with existing highly accurate results. The evolution of resonances in parallel magnetic and electric fields is obtained numerically and analyzed theoretically. Further studies for the evolution of higher resonances of hydrogen and non-hydrogen atoms in parallel electric and magnetic field are under way.

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