Resonance of hydrogen and lithium atoms in parallel magnetic and electric fields

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We apply the complex absorbing potential method to study the resonances of the ground state of hydrogen atom and the low-lying $2S$ and $2P$ $(m=0)$ states of lithium atoms in parallel magnetic and electric fields. The behavior of resonance parameters for the ground state of hydrogen atoms in parallel magnetic and electric fields are consistent with those obtained by other methods. We then discuss the extension of the present method to study the resonant low-lying states of lithium atoms.

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The method of complex absorbing potential (CAP) has been proven to be a powerful tool for locating resonances in atomic scattering problems [1,2]. More recently, this method has been extended for dealing with atomic field ionization processes [3,4]. In these cases the bound state atomic levels are broadened and shifted and the energy eigenvalues are expressed as $E=E_{\rm res}-i\Gamma/2$, where $E_{\rm res}$ would give the resonance energy, and Γ is the level width defining the ionization probability of the atom.

Up to now, most of the studies are concerned with the case of a pure electric field (see [3] and [4] for references). A few, such as those of Refs. [5–10] have considered the cases of pure magnetic fields, and the resonant states in these cases have been studied by the complex coordinate [6], the R-matrix method combined with the quantum-defect theory [11], and the adiabatic coupled channel method [12]. The similar calculational procedures have also been used to obtain the properties of the resonant states of hydrogen atoms in parallel magnetic and electric fields [13–16]. Johnson *et al.* [13] have studied the problem by both a large order perturbation theory and the complex scaling method based on the method introduced by Reinhardt [17] and Chu [18]. More recently, Rao and Li [15] have presented their numerical studies on the behaviors of resonance states of a hydrogen atom in parallel magnetic and electric fields by a complex scaling plus B-spline method. Seipp *et al.* [19] have applied the combination of the R-matrix method and the complex-coordinate method to investigate resonances in sodium atom under external parallel electric and magnetic fields.

It is the purpose of the present report to discuss the extension of the CAP method to study the resonances of the hydrogen and lithium atoms in parallel magnetic and electric fields. This work has been facilitated by recent works [3,4] where the CAP method has been successfully applied to study the resonances of the hydrogen and lithium atoms in an electric field.

The Hamiltonian of the system, with both of the external magnetic and electric fields in the direction of z axis (in atomic units), can be written as

$$H=H_0(\beta)+Fr\cos\theta+V, \tag{1}$$

where

$$H_0(\beta)=-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}+\frac{1}{2}\beta^2r^2\sin^2\theta+\beta L_z \tag{2}$$

is the free electron Zeeman-Hamiltonian and θ is the angle between the radius vector and the field. In Eqs. (1) and (2), β is the magnetic field strength in atomic units with 1 a.u. $\approx 4.7\times10^5$ T, F is the electric field strength in atomic units with 1 a.u. $\approx 5.142\times10^9$ V cm^{-1}, V is the Coulomb potential, and L_z is the z component of the angular momentum operator. Since the total Hamiltonian commutes with L_z, the paramagnetic term, which introduces only a global energy shift, can be considered separately.

In the present work we carry out a theoretical investigation on these resonance states by employing the CAP method. Here an artificial complex absorbing potential $-i\eta W(r)$ is added to the original Hamiltonian leading to an effective Hamiltonian, $H(\eta)=H-i\eta W(r)$, where η denotes the CAP strength. If one chooses a suitable form of the CAP, it generates an absorbing region where the wave packets are damped. As a result, the wave functions become square integrable, and the complex eigenvalues $E_{\rm res}$ are obtained in a single diagonalization. The complex resonance energy is given by $E_{\rm res}=E_r-i\Gamma/2$, where Γ is the resonance width, and E_r is the resonance energy.

In order to perform the linear variational calculations we have choosen the orthonormal Laguerre type basis

$$\Phi_{nlm}=C_{nlm}r^{l+1}e^{\lambda r/2}L_n{}^{2l+2}(\lambda r)Y_{lm_1}(\theta,\phi), \tag{3}$$

where $n=0,1,2,...,N-1$, and C_{nlm} is the normalization constant. N is the number of basis functions per l value.

In spherical coordinate, $H(\eta)$ becomes a block diagonal matrix in the absence of an external field. In our calculations each block is taken of dimension N and the number of blocks have been restricted to $(l_{\rm max}+1)$, where $l_{\rm max}$ is the maximum value of the angular momentum used in a given calculation. To obtain the spectral distribution of the effective Hamiltonian we perform calculations with $N=30$, and $l_{\rm max}$ ranging from 24 to 29. The complex eigenvalues, those representing the resonance states, are found to have η dependence. Hence we adopt a stabilization method that the pronounced minimum of $|\eta(dE_i/d\eta)|$ identifies the optimal value of η, and the eigenvalue E_i obtained for that parameter

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TABLE I. Complex eigenvalue representing the shifted and broadened ground state of hydrogen as a function of external electric and magnetic field strengths.

		Present calculations CAP method		Other methods	
β^2 (a.u.)	F (a.u.)	E_{res} (a.u.)	$\Gamma/2$ (a.u.)	E_{res} (a.u.)	$\Gamma/2$ (a.u.)
0.00	0.040	−0.503 771	0.1958×10^{-5}	−0.503 771[a]	0.1964×10^{-5}
				−0.503 771 591 013 5[b]	$0.194\,635\,00\times10^{-5}$
0.00	0.080	−517 564	0.2266×10^{-2}	−0.517 560[a]	0.2269×10^{2}
				−0.517 560 616 888[b]	$0.226\,982\,875\times10^{-2}$
0.00	0.100	−0.527 412	0.7270×10^{-2}	−0.527 418[a]	0.7269×10^{-2}
2.5×10^{-3}	0.040	−0.501 206	0.8960×10^{-6}	−0.501 206[a]	0.8957×10^{-6}
				−0.501 206 356 2[b]	$0.895\,759\times10^{-6}$
2.5×10^{-3}	0.080	−0.514 712	0.1944×10^{-2}	−0.514 690[a]	0.1933×10^{-2}
				−0.514 690 932 2[b]	$0.193\,358\,900\times10^{-2}$
2.5×10^{-3}	0.100	−0.524 658	0.6534×10^{-2}	−0.524 599[a]	0.6639×10^{-2}
				−0.524 600[c]	$0.663\,92\times10^{-2}$
1.0×10^{-2}	0.040	−0.493 846	0.1770×10^{-6}	−0.493 846[a]	$0.175\,7\times10^{-6}$
1.0×10^{-2}	0.060	−0.498 68	0.8160×10^{-4}	−0.498 687[a]	$0.818\,4\times10^{-4}$
1.0×10^{-2}	0.100	−0.516 426	0.5097×10^{-2}	−0.516 338[a]	$0.512\,5\times10^{-2}$
				−0.516 339[c]	$0.512\,55\times10^{-2}$

[a]CR method, present calculations.
[b]Rao and Li [15].
[c]Ivanov [16], not including the linear term in order to have the same notation as ours.

defines the closest approximation to the exact complex resonance energy E_{res} [1–4,20].

We first discuss the feasibility of the CAP method for studying the ground state resonances of H atom in parallel electric and magnetic fields. In this case, $V(r)$ is taken as $-1/r$ as usual. CAP is taken to be $W(r)=r^6$. The field range is chosen as $0.025\leqslant F\leqslant 0.1$, and $0.0\leqslant\beta^2\leqslant 0.02$, and λ is taken to be 1.0. Results are tabulated in Table I. For a pure electric field, we see that over the tabulated field range our results agree well with the results obtained by the complex rotation (CR) method [21]. Thus the CAP results are reasonably good over the above field range. In Fig. 1 we have plotted the electric field effects on the ground state energy of H atom at different magnetic field strengths. It shows that in the region considered for the ground resonance, the increase of the magnetic field strength increases the ground state energy. In Fig. 2, we have plotted the behavior of the autoionization width of ground resonance of H atom in parallel electric and magnetic fields. It shows that the width of the resonance decreases with the increase of the magnetic field strength. The stronger the magnetic field is, the more stable the ground state. Figure 1 shows that the evolutions of E_{res} with the field strength F for different values of β are almost parallel. At a fixed electric-field strength, the magnetic field pushes the energy level up. From Fig. 2 we can see that the effect on the width of the resonance depends approximately on the factor β/F. The results are consistent with others [15,16].

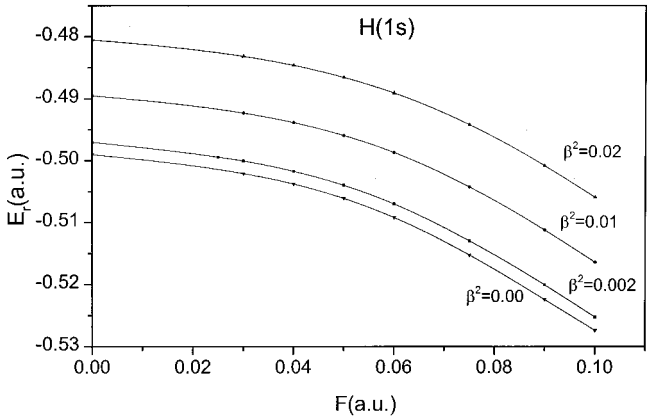

FIG. 1. Electric and magnetic field effects on the resonance energy E_{res} of the ground state of hydrogen atom are shown as functions of F for different values of β^2 (in a.u.).

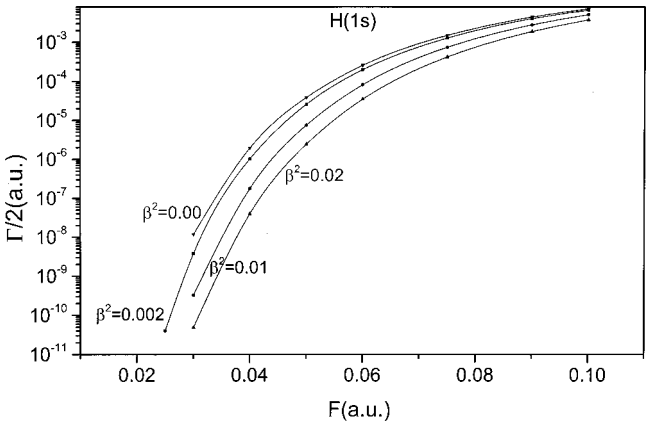

FIG. 2. Electric and magnetic field effects on $\Gamma/2$, with Γ being the field ionization width of the ground state of hydrogen atom, are shown as functions of F for different values of β^2 (in a.u.).

TABLE II. Complex eigenvalue representing the shifted and broadened $2S$ state of lithium as a function of external electric and magnetic field strengths.

		CAP (present)		Others	
β^2 (a.u.)	F (a.u.)	E_{res} (a.u.)	$\Gamma/2$ (a.u.)	$\Gamma/2$ (a.u.)	
0.000	0.006	−0.201 092 85[a]	0.885×10^{-8}	0.54×10^{-8} [b]	
0.000	0.008	−0.203 419 04[a]	0.148×10^{-5}	0.2062×10^{-5} [b]	0.19×10^{-5} [c]
0.000	0.015	−0.217 542 82[a]	0.176×10^{-2}	0.1966×10^{-2} [b]	0.198×10^{-2} [c]
0.002	0.008	−0.192 590 88	0.7147×10^{-7}		
0.002	0.012	−0.199 200 24	0.8735×10^{-4}		
0.002	0.016	−0.208 732 33	0.1382×10^{-2}		
0.010	0.010	−0.163 305 17	0.6370×10^{-6}		
0.010	0.014	−0.169 430 84	0.1152×10^{-3}		
0.010	0.018	−0.179 756 90	0.1279×10^{-2}		
0.020	0.010	−0.128 476 86	0.1690×10^{-6}		
0.020	0.012	−0.132 276 34	0.5974×10^{-5}		
0.020	0.016	−0.141 636 78	0.2817×10^{-3}		

[a]Taken from Ref. [3].
[b]Reference [25].
[c]Reference [24].

We now apply this method to the Li atom. Our interest in such a study has been spurred on by the increasing importance of developing new computational techniques in the area of resonance calculations to produce fruitful results in atomic collision processes. Although the exact description of $V(r)$ in the case of Li atom is a difficult task, we use a model potential to represent the interaction between the inner core electrons with the outside valance electron, and $V(r)$ is taken as $V(r)=-z/r+V_m(r)$, where Z is the nuclear charge of the Li atom, and $V_m(r)$ a model potential of the form

$$V_m(r)=2/r-2/r\,(1+\alpha r)e^{-2\alpha r}, \tag{4}$$

where α is the parameter describing the effective charge of the $1s^2$ core. A qualitative justification for such a choice of potential is well described in Ref. [22].

We use the same basis set and the same CAP as above and perform the calculation to find the spectral distribution of the effective Hamiltonian of the Li atom. We focus our attention on the lowest S, and P states. Calculations have been performed with $N=30$, l_{max} ranging from 24 to 29 and $\lambda=1.0$. The parameter α is found to be 1.6559, obtained by fitting the exact energy of the $2S$ ground state of the Li atom. Tables II and III summarize the results for the $2S$ and $2P$ states, respectively. Up to now, results on the low-lying resonances of lithium atom in the combination of electric and magnetic fields have not been reported to our knowledge.

TABLE III. Complex eigenvalue representing the shifted and broadened $2P$ state of lithium as a function of external electric and magnetic field strengths.

		CAP (present)		Others	
β^2 (a.u.)	F (a.u.)	E_{res} (a.u.)	$\Gamma/2$ (a.u.)	$\Gamma/2$ (a.u.)	
0.000	0.0025	−0.130 373[a]	0.427×10^{-9}	0.442×10^{-6} [b]	$\sim0.1\times10^{-9}$ [c]
0.000	0.0035	−0.130 896[a]	0.552×10^{-6}	0.234×10^{-5} [b]	0.811×10^{-6} [c]
0.000	0.0070	−0.136 287[a]	0.379×10^{-2}	0.422×10^{-2} [b]	0.4204×10^{-2} [c]
0.002	0.004	−0.121 044 25	0.1317×10^{-7}		
0.002	0.006	−0.122 366 31	0.7655×10^{-4}		
0.002	0.010	−0.127 513 94	0.8551×10^{-2}		
0.010	0.006	−0.092 727 85	0.6068×10^{-6}		
0.010	0.009	−0.093 716 24	0.6078×10^{-3}		
0.010	0.012	−0.094 578 29	0.6092×10^{-2}		
0.020	0.008	−0.064 951 62	0.1623×10^{-4}		
0.020	0.010	−0.064 653 29	0.4734×10^{-3}		
0.020	0.012	−0.064 368 34	0.2622×10^{-2}		

[a]Taken from Ref. [3].
[b]Reference [24].
[c]Reference [25].

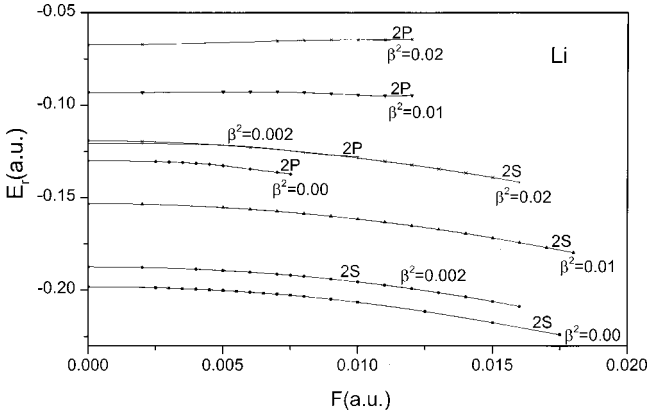

FIG. 3. Electric and magnetic field effects on the resonance energy E_{res} of the $2S$ and $2P$ states of Li atom are shown as functions of F for different values of β^2 (in a.u.).

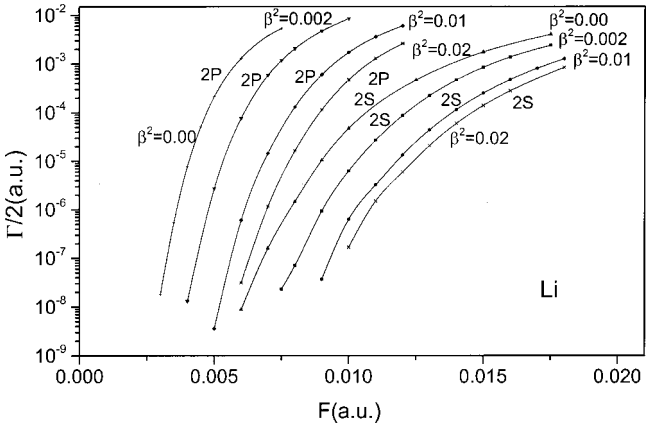

FIG. 4. Electric and magnetic field effects on $\Gamma/2$, with Γ being the field ionization width of the $2S$ and $2P$ states of Li atom, are shown as functions of F for different values of β^2 (in a.u.).

The high Rydberg states of Li in parallel electric and magnetic fields have been investigated by Cacciani *et al.* [23]. As for pure electric-field effects ($\beta=0$), Nicolaides and Themelis in a series of publications [24–26] have reported results for low-lying Li states obtained from the state-specific complex eigenvalue Schrödinger equations (CESE). Some quantitative differences for results between the CAP method and those of CESE do exist. The differences become more pronounced at the low-field region. It seems that an independent investigation on the low-lying Li states to shed light on the discrepancy between the CAP and CESE results is needed.

Figure 3 shows our results for the changes of the resonance energies for the $2S$ and $2P$ states as functions of F when different values of β are used. For a given β, the energies are shifted downward by the external electric field. The downward shifts of the resonance energies are found to occur for all the magnetic field strengths being considered here. For the $2P$ state, we have dealt with the $m=0$ component only. Figure 4 shows the autoionization widths for the $2S$ and $2P(m=0)$ states as functions of F for different values of β. For a given β and for the range of electric field strengths considered in this paper, the autoionization width increases rapidly for increasing F. The behavior is very similar to the hydrogenic system. When the magnetic field is increased, the width starts to decrease and tries to neutralize the effect of the electric field. It indicates the possible stabilization of an autoionization atom under the influence of an external magnetic field. When the external magnetic field is turned on, the electrons are confined to a region further away from the potential barrier. Therefore it would require a longer time for the electron to tunnel out of the barrier, resulting in a decrease of the width for increased magnetic field strength. Overall, the behaviors of resonances of Li atoms in parallel electric and magnetic field are similar to those of the hydrogen system. Our present results also indicate that the autoionization in the case of lithium atoms starts at a lower field value than that of the hydrogenic system. Studies on the evolution of higher resonances in parallel electric and magnetic field would be of interest.

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