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Sodium atom in strong magnetic fields: a pseudospectral approach*

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Energies and wavefunctions of low-lying states and Rydberg states for the sodium atom in uniform magnetic fields varying from 0 to 10^5T are calculated using a pseudospectral approach with a model potential in spherical coordinates. The energies are comparable with experimental results as well as those obtained by other calculations. The spectra of oscillator strength are worked out. The evolution of them with the magnetic field is shown.

Keywords: pseudospectral approach, oscillator strength, magnetic fields, sodium atom
PACC: 0365G, 3210R, 3240, 3260V

1. Introduction

The study of atoms in a high uniform magnetic field has aroused experimental and theoretical interest, as has been reviewed in Ref.[1–3]. In addition to its applications to astrophysics, such study is of great theoretical interest in atomic physics because it requires new methods for treating the nonseparability of the Schrödinger equation for electrons in combined Coulomb and uniform magnetic fields.[3,4] When solving the Schrödinger equation for the Na atom, a model potential should be used,[5–7] which has been discussed thoroughly.[8]

Many of the theoretical calculations have been carried out for hydrogen atom,[9–11] helium like atoms[12] and other atoms having sparse electrons.[13–15] In those studies, various methods, such as B-spline approach, Hartree–Fock method, and Slater-type function expansion, etc., were used to solve the problem that variables cannot be separated, since the Coulomb and uniform magnetic fields are combined in the Schrödinger equation.

However, up to now, only a few calculations are concerned with the sodium atom. Liu *et al*[16] calculated the quasi-Landau resonances with even parity and m_l=–2, –1 of sodium in a magnetic field B=4.2T using a model potential introduced by He *et al*,[6] where the eigenfunctions of a free Na atom are taken as the basis of expansion for the magnetized atom (PM method). Rao *et al*[7] calculated the diamagnetic Rydberg spectrum with even parity and m_l=–2 of Na in magnetic fields B=4.1–6.1T by means of combining a variant of the R-matrix method with quantum defect theory and complex coordinates rotation (HDT method) and PM method respectively. Incidentally, they all compared with the experimental results obtained by Castro *et al*[17] in 1980. Note that those calculations were carried out only for Rydberg states of Na.

In this paper, we present a numerical study of sodium atom in uniform magnetic fields, using a pseudospectral method[18–20] incorporating with a model potential[7] in spherical coordinates. Wavefunctions and energies of ground state to Rydberg states are obtained in magnetic fields ranging from 0 to 0.9a.u. (1a.u. equals to 4.7×10^5T, atomic units are used hereafter). The spectra of oscillator strength are calculated, and the contribution of different l components to states is analysed. The results are comparable with those obtained by other methods or experiments, and show that the pseudospectral method has fast convergence and numerical stability.

2.Method

The Schrödinger equation of the sodium atom in arbitrary external magnetic fields in atomic units and

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spherical coordinates can be written as

$$\Big[-\frac{1}{2}\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}+\frac{\hat{L}^2}{2r^2}+V_{Na}^{PM}(r) + \beta(2m_s+m_l)+\frac{1}{2}\beta^2r^2\sin^2\theta\Big]\psi=E\psi, \quad (1)$$

where $V_{Na}^{PM}(r)$ is the so-called model potential of Na atom, its expression is taken as

$$V_{Na}^{PM}(r)=-\frac{1}{4}\{Z_c\exp(-\gamma_1 r)+\gamma_2 r\exp(-\gamma_3 r)+1\}, \quad (2)$$

in which Z_c=10.0, γ_1=7.902, γ_2=23.51, γ_3=2.688,[7] and $\frac{1}{2}\beta^2r^2\sin^2\theta$ is the diamagnetic term, $\beta=B/B_0$, $B_0=4.7\times10^5$T. In the paramagnetic term $\beta(2m_s+m_l)$, m_s is a spin quantum number and m_l is z component of angular momentum l. This term only induces an energy shift of the whole spectrum, as can be seen in the following. For simplicity, this term does not occur in the following expressions, however, in the practical calculations it is really included.

A suitable non-linear mapping is given as

$$r=r(x)=R_0\frac{1+x}{1+2\alpha-x},\quad y=\cos\theta, \quad (3)$$

where $\alpha=R_0/R_{\max}$, R_0 and $R_{\max}$ are mapping parameters, in which $R_{\max}$ denotes the maximum of r (i.e. a cutoff in the radial orientation), and the x and y are in the range of [–1,1]. Defining

$$F(x,y,\varphi)=\psi[r(x,),\theta,\varphi]r(x)/\sqrt{r'(x)}, \quad (4)$$

the Schrödinger equation Eq.(1) can be transformed into the symmetric form

$$\Big[-\frac{1}{2}\frac{1}{r'^2(x)}\frac{\partial^2}{\partial x^2}+\frac{\hat{L}^2}{2r^2(x)}+V_{Na}^{PM}(x) + \frac{1}{2}\beta^2r^2(x)(1-y^2)\Big]F(x,y,\varphi)=EF(x,y,\varphi). \quad (5)$$

Then the wavefunction $F(x,y,\varphi)$ can be separated into $\Psi(x,y)$ and $\Phi(\varphi)$, that is, $F(x,y,\varphi)=\Psi(x,y)\Phi(\varphi)$, so the corresponding quantum number m_l is a good quantum number. It follows, what needs to be calculated is the wavefunction $\Psi(x,y)$.

With pseudospectral method, as discussed particularly in Ref.[20], the wavefunction can be expressed as

$$\Psi(x,y)=\sum_{i=1}^{N_1-1}\sum_{j=1}^{N_2+1}f_i(x)g_j(y)\,\Psi(x_i,y_j), \quad (6)$$

where

$$f_i(x)=\frac{1}{N_1(N_1+1)P_{N_1}(x_i)}\frac{(x^2-1)P'_{N_1}(x)}{x-x_i}, \quad (7)$$

$$g_j(y)=\frac{1}{P'_{N_2+1}(y_j)}\frac{P_{N_2+1}(y)}{y-y_j}, \quad (8)$$

and $P_N(x)$ is the Legendre polynomial, $\{x_i\}$ and $\{y_i\}$ stand respectively for the zeros of $P'_{N-1}(x)$ and $P_{N_2+1}(y)$. $f_i(x)$ and $g_j(y)$ have the properties

$$f_i(x_j)=\delta_{ij},\quad g_j(y_k)=\delta_{jk}. \quad (9)$$

Substituting Eq.(6) for Eq.(5), it leads to a general eigenvalue problem as the following expressions including the symmetry

$$\begin{aligned}&W(N_1,x_I)W(N_2,y_J)r'^2(x)\\ &\times\sum_{i=1}^{N_1-1}\sum_{j=1}^{N_2+1}\hat{H}(x,y)f_i(x)g_j(y)\,\Psi(x_i,y_j)|_{x=x_I,y=y_J}\\ =&\varepsilon_{IJ}W(N_1,x_I)W(N_2,y_J)r'^2(x)\\ &\times\sum_{i=1}^{N_1-1}\sum_{j=1}^{N_2+1}f_i(x)g_j(y)\,\Psi(x_i,y_j)|_{x=x_I,y=y_J}, \quad (10)\end{aligned}$$

where $W(N_1,x_I)$ and $W(N_2,y_J)$ are the weights on the grid points $\{x_i\}$ and $\{y_j\}$,

$$W(N_1,x_I)=\frac{2}{N_1(N_1+1)}\frac{1}{[P_{N_1}(x_I)]^2}, \quad (11)$$

$$W(N_2,y_J)=\frac{2}{(1-y_J^2)[P'_{N_2+1}(y_J)]^2}. \quad (12)$$

Eq.(10) can be expressed in $[(N_1-1)(N_2+1)]\times[(N_1-1)(N_2+1)]$ matrix form

$$AC=EBC, \quad (13)$$

where E is the eigenvalue, C is the wavefunction, and the matrix elements are presented as

$$\begin{aligned}A_{ij,IJ}=&\Big[\frac{1}{6}\frac{N_1(N_1+1)}{1-x_i^2}+\frac{r'^2(x_i)}{r^2(x_i)}\frac{(N_2+1)(N_2+2)}{6}\\ &+r'^2(x_i)V_{Na}^{PM}(x_i)+\frac{r'^2(x_i)}{r^2(x_i)}\frac{1}{3(y_i^2-1)}\Big]\\ &\times W(N_1,x_i)W(N_2,y_j)\delta_{iI}\delta_{jJ}\\ &+(-1)^{i+I}W(N_2,y_j)\sqrt{W(N_1,x_i)W(N_1,x_I)}\\ &\times\frac{1}{(x_i-x_I)^2}\delta_{jJ}\xi(i,I)+(-1)^{j+J}W(N_1,x_i)\\ &\times\sqrt{(1-y_j^2)(1-y_J^2)}\frac{r'^2(x_i)}{r^2(x_i)}\frac{1}{(y_j-y_J)^2}\\ &\times\sqrt{W(N_2,y_j)W(N_2,y_J)}\delta_{iI}\xi(j,J)\\ &+\Big[\frac{1}{2}\beta^2r^2(x_i)r'^2(x_i)(1-y_j^2)\\ &+\frac{m^2}{2r^2(x_i)}\frac{r'^2(x_i)}{(1-y_j^2)}\Big]\\ &\times W(N_1,x_i)W(N_2,y_j)\delta_{iI}\delta_{jJ}, \quad (14)\end{aligned}$$

$$B_{ij,IJ} = r'^2(x_i)W(N_1, x_i)W(N_2, y_J)\delta_{iI}\delta_{jJ}, \quad (15)$$

where

$$\xi(n,m) = \begin{cases} 1, & n \neq m, \\ 0, & n = m. \end{cases} \quad (16)$$

3. Results and discussions

The wavefunctions obtained by the present method are numerical values on grid points. In the calculations, an appropriate number of grids points, i.e., $N_1 - 1$=100, $N_2 + 1$=40, has been chosen after trials. It is worth pointing out that the points in the present method are very sparse comparing with other grid point methods. In order to obtain accurate result for low-lying states and Rydberg states, we optimized the value of R_0 as R_0=100a.u. and $R_{\max}$ as $R_{\max}$=4000a.u. Let the magnetic fields be parallel to the z-axis, then z component of angular momentum l, m_l, is a good quantum number. Now, the data with m_l=0 has already been obtained and will be analysed in the following.

Table 1. The energies (in a.u.) of sodium in the absence of magnetic field. In each group, the first row of the table refers to our results; the calculations by Chu *et al*[22] are listed in the second row, the experimental results in the same reference are listed in the third row and the data from NIST are listed in the lowest row.

	l/n	3	4	5	6	7	8	9	10
Ours	0	−0.1888494	−0.0716703	−0.0376281	−0.0231545	−0.0156751	−0.0113122	−0.0085468	−0.0066843
[22]		−0.1888621	−0.0715793	−0.0375849	−0.0231323	−0.0156623	−0.0113043	−0.0085415	−0.0066806
[22]		−0.1888621	−0.0715792	−0.0375850	−0.0231322	−0.0156623	−0.0113042	−0.0085415	−0.0066805
NIST		−0.1888576	−0.0715775	−0.0375841	−0.0231317	−0.0156619	−0.0113040	−0.0085413	−0.0066804
Ours	1	−0.1115200	−0.0510219	−0.0292447	−0.0189481	−0.0132713	−0.0098114	−0.0075377	−0.0059859
[22]		−0.1115498	−0.0509354	−0.0291959	−0.0189202	−0.0132542	−0.0098003	−0.0075390	−0.0059805
[22]		−0.1115500	−0.0509352	−0.0291950	−0.0189195	−0.0132536	−0.0097998	−0.0075391	−0.0059790
NIST		−0.1115604	−0.0509382	−0.0291962	−0.0189138	−0.0132539	−0.0098000	−0.0075398	−0.0059803
Ours	2	−0.0559778	−0.0314987	−0.0201445	−0.0139670	−0.0102623	−0.0078524	−0.0062013	−0.0050209
[22]		−0.0559387	−0.0314419	−0.0201051	−0.0139517	−0.0102444	−0.0078399	−0.0061922	−0.0050142
[22]		−0.0559375	−0.0314426	−0.0201061	−0.0139526	−0.0102452	−0.0078405	−0.0061928	−0.0050149
NIST		−0.0559362	−0.0314419	−0.0201059	−0.0139523	−0.0102450	−0.0078402	−0.0061927	−0.0050148
Ours	3	−0.0312514	−0.0200012	−0.0138897	−0.0102047	−0.0078129	−0.0061732	−0.0050002	
[22]		−0.0312681	−0.0200107	−0.0138956	−0.0102085	−0.0078155	−0.0061750	−0.0050016	
[22]		−0.0312685	−0.0200109	−0.0138956	−0.0102085	−0.0078156	−0.0061751	−0.0050015	
NIST		−0.0312682	−0.0200105	−0.0138953	−0.0102083	−0.0078154	−0.0061750	−0.0050014	
Ours	4	−0.0200000	−0.0138889	−0.0102041	−0.0078125	−0.0061728	−0.0050000		
[22]		−0.0200023	−0.0138904	−0.0102051	−0.0078132	−0.0061733	−0.0050004		
[22]		−0.0200024	−0.0138904	−0.0102051	−0.0078132	−0.0061733	−0.0050004		
NIST		−0.0200019	−0.0138902	−0.0102049	−0.0078131	−0.0061732	−0.0050003		

Energies of ground and some excited states in absence of magnetic field are calculated and listed in Table 1. Also in this table, the calculations and experiments carried out by Chu *et al*[22] are shown as well as the data obtained from "NIST (National Institute of Standards and Technology) Atomic Spectra Database Levels Data Na I". Generally speaking, all the results are closed to each other. Although the model potential[7] used here is simple and cannot accurately describe the potential that the valence electron of Na atom really feels, the potential is good enough to describe properties of the Na atom in uniform magnetic fields and is convenient for calculations. As shown in the table, the energies are similar to those of hydrogen atom,[9−11] except for s and p states due to the strong influence of the core of Na atom. The energies of s and p states are lower than those of the hydrogen atom.

Table 2. The lowest three energies of m_l=0 states with even or odd parity in different magnetic fields.

β	$1\left(1-\frac{1}{2}\right)_0^+$	$2\left(1-\frac{1}{2}\right)_0^+$	$3\left(1-\frac{1}{2}\right)_0^+$	$1\left(1-\frac{1}{2}\right)_0^-$	$2\left(1-\frac{1}{2}\right)_0^-$	$3\left(1-\frac{1}{2}\right)_0^-$
0	−0.18885	−0.07167	−0.05598	−0.11152	−0.05102	−0.03125
0.001	−0.18984	−0.07263	−0.05695	−0.11251	−0.05198	−0.03216
0.002	−0.19082	−0.0735	−0.05786	−0.11349	−0.05285	−0.03292
0.005	−0.19369	−0.07565	−0.06026	−0.11632	−0.05499	−0.03452
0.007	−0.19553	−0.07672	−0.06158	−0.11813	−0.05608	−0.03519
0.01	−0.19821	−0.07788	−0.06315	−0.12073	−0.05733	−0.03575
0.02	−0.20632	−0.07978	−0.06463	−0.12849	−0.0598	−0.03556
0.03	−0.21329	−0.08163	−0.06015	−0.13504	−0.06139	−0.03509
0.04	−0.21924	−0.08386	−0.05155	−0.14063	−0.06273	−0.03514
0.05	−0.22429	−0.08597	−0.04455	−0.14546	−0.06392	−0.03540
0.06	−0.22857	−0.08781	−0.04524	−0.14969	−0.06498	−0.03571
0.07	−0.23217	−0.08937	−0.04584	−0.15341	−0.06591	−0.03601
0.08	−0.23519	−0.09067	−0.04633	−0.15673	−0.06674	−0.03629
0.09	−0.2377	−0.09175	−0.04673	−0.1597	−0.06748	−0.03655
0.1	−0.23976	−0.09262	−0.04706	−0.16237	−0.06814	−0.03678
0.15	−0.2452	−0.09472	−0.04782	−0.17256	−0.07057	−0.03763
0.2	−0.2457	−0.09428	−0.04755	−0.17938	−0.0721	−0.03809
0.3	−0.24208	−0.09046	−0.04547	−0.18793	−0.07385	−0.03809
0.4	−0.23943	−0.08708	−0.04289	−0.19325	−0.0748	−0.03696
0.5	−0.23965	−0.08545	−0.04026	−0.19714	−0.07542	−0.03483
0.6	−0.24212	−0.08501	−0.03743	−0.20036	−0.07584	−0.03182
0.7	−0.24599	−0.08518	−0.03432	−0.20324	−0.07613	−0.02811
0.8	−0.25066	−0.08562	−0.0309	−0.20594	−0.0763	−0.0238
0.9	−0.25577	−0.08616	−0.02717	−0.20855	−0.07634	−0.01901

In Table 2, the lowest three energies of m_l=0 states with even or odd parity in different magnetic fields are shown. The states are labelled as $n(m_s)^\pi_{m_l}$, where π is the parity, n is the ordering number of state with fixed m_s, m_l and π, the bigger n, the higher the energy. The energies of $1\left(-\frac{1}{2}\right)_0^-$, $2\left(-\frac{1}{2}\right)_0^-$, $1\left(-\frac{1}{2}\right)_0^+$ and $2\left(-\frac{1}{2}\right)_0^+$ decrease with the increasing magnetic fields up to 1 a.u., the states $3\left(-\frac{1}{2}\right)_0^-$ and $3\left(-\frac{1}{2}\right)_0^+$ decrease first with β in the β domain from 0 to 0.2 a.u. and then turn to rise with increasing magnetic field. The above phenomena are easy to understand. Three terms, i.e., the Coulomb interaction term $V_{Na}^{PM}(r)$, the paramagnetic term $-\beta(2m_s+m_l)$ and the diamagnetic term $\frac{1}{2}\beta^2 r^2\sin^2\theta$, are contained in the Hamiltonian of system (see Eq.(1)). The paramagnetic term is a linear term, which decreases with the increasing β, and the diamagnetic term increases with the increasing β due to its dependence on the square of β. However, when β is small, the linear term is dominant, the energy decreases with the increasing β. When β becomes larger, the diamagnetic term will over take the paramagnetic term, and then the energies turn to rise (e.g., $3\left(-\frac{1}{2}\right)_0^-$ and $3\left(-\frac{1}{2}\right)_0^+$). Nevertheless, $1\left(-\frac{1}{2}\right)_0^-$, $2\left(-\frac{1}{2}\right)_0^-$, $1\left(-\frac{1}{2}\right)_0^+$ and $2\left(-\frac{1}{2}\right)_0^+$ decrease along with the in-

creasing β, this is because the states are strongly affected by the Coulomb attraction of the core.

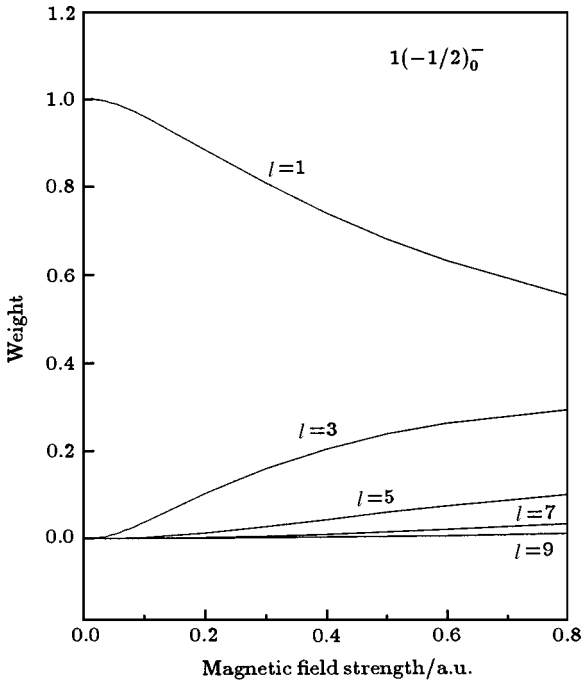


Fig.1. The contributions of each l component to the $1\left(1-\frac{1}{2}\right)_0^-$ state as a function of magnetic field.

Contributions of different l components to states are analysed. The state $1\left(-\frac{1}{2}\right)_0^-$ is taken as an example. The weight of l=1 component is 1 and all the others are zero in the absence of magnetic field (see Fig.1). This is because, when β=0 the potential is an isotropic central potential, l is a good quantum number and the l=1 component is indeed an eigenstate of the Hamiltonian. In the magnetic field, the isotropic central potential is destroyed, angular quantum number l is no longer a good quantum number; various l components with some weight are therefore mixed with each other in a state with certain parity, and the mixture of various l components is enhanced with the increasing of β. This can be seen in Fig.1.

For all those states that range from low-lying states to Rydberg states in Na, the spectra of their oscillator strength to the ground state $1\left(-\frac{1}{2}\right)_0^+$ in different cases of magnetic fields are shown in Figs.2 and 3. Looking over the figures, one finds that, the higher the energy of the state, the smaller the oscillator strength, and such variation trend is strong. When β=0, there are only some main lines with large height and big spacing. However, when the magnetic field is taken into account, the main lines occur accompanied by some small lines and meanwhile the height of the main lines recedes. When β increases, the number and height of the small lines become larger in contrast to the lowered main lines. This is easily understood. As mentioned before, the mixture of various l components is enhanced with the increasing of β, that is, more additional components appear with closer weights. Thus, the previously forbidden transitions among different components due to the selection rules now occur in the magnetic field. This leads to the occurrence of the small lines. Similarly, components of both the excited states and the ground state change with increasing magnetic field, and accordingly, due to the existence of the selection rules transitions among more different components are forbidden. This results in decreasing oscillator strength (i.e. the height of main lines).

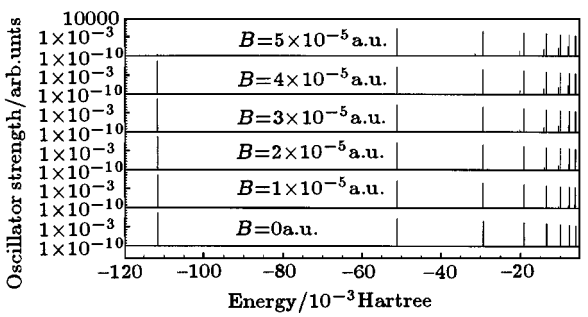


Fig.2. The spectra of oscillator strength of Na in a series of magnetic fields from 0 to 5×10^{-3} a.u. (from excited states to the ground state, the magnetic quantum number m_l=0).

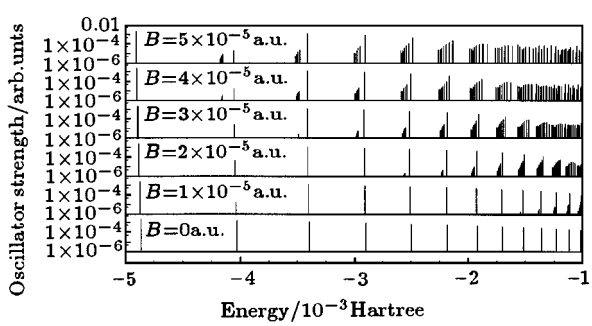


Fig.3. Same as fig. 2.

Incidentally, the present pseudospectral method[20] is also a grid point method. It needs only sparse points to describe the wavefunctions of an atom, because the grid points are Gauss collocation points. The model potential approach with the simpler form[7] is valid in description of Na atom and very convenient for calculations. As one can see, for all

those states concerned, i.e., from the low-lying states to the Rydberg states, the present approach with the simple model potential is reasonable and effective.

In summary, we have calculated the energies and the spectra of oscillator strength of Na atom in the magnetic field in the frame of our pseudospectral approach with the simple model potential. Comparisons of the energies with those obtained by other methods and experimental results are made. It is found that all of them are close to each other. Contributions of different l components to the states were analysed. With increasing magnetic field, the mixture of different l components is enhanced. This leads to the evolution of the spectra of oscillator strength with the magnetic field.

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