# Accurate calculations of the helium atom in magnetic fields*

Zhao Ji-Jun(赵继军), Wang Xiao-Feng(王晓峰), and Qiao Hao-Xue(乔豪学)†

*Department of Physics, Wuhan University, Wuhan* 430072, *China*

(Received 9 June 2010; revised manuscript received 2 July 2010)

The $1^1 0^+$, $1^1(-1)^+$and $1^1(-2)^+$ states of the helium atom in the magnetic field regime between 0 and 100 a.u. are studied using a full configuration-interaction (CI) approach. The total energies, derivatives of the total energy with respect to the magnetic field and ionisation energies are calculated with Hylleraas-like functions in spherical coordinates in low to intermediate fields and Hylleraas–Gaussian functions in cylindrical coordinates in intermediate to high fields, respectively. In intermediate fields, the total energies and ionisation energies are determined in terms of Hermite interpolation, based on the results obtained with the two above-mentioned basis functions. Calculations show that the current method can produce lower total energies and larger ionisation energies, and make the two ionisation energy curves obtained with the two above-mentioned basis functions join smoothly in intermediate fields. Comparisons are also made with previous works.

**Keywords:** strong magnetic field, helium atom, total energy, ionisation energy
**PACC:** 3120T, 3130, 3260V

## 1. Introduction

The problem of atoms in strong magnetic fields is a fascinating subject which has attracted much interest of both experimentalists and theorists for the past three decades. The motivation in this area arises from several sources. On the one hand, this is due to the astrophysical discovery of strong magnetic fields on the surfaces of white dwarfs ($10^2$–$10^5$ T) and neutron stars ($10^7$–$10^9$ T).[1–3] On the other hand, the complex properties of atoms under these extreme conditions are of immediate interest from a pure theoretical point of view. In addition, the observations of excitons with small effective masses and large dielectric constants in semiconductors,[4,5] which result in very large effective magnetic fields, give additional impetus for this subject.

However, it is quite complicated to study the electronic structure of atoms in the presence of a magnetic field. In a weak magnetic field which can be treated as a perturbation, the wave function can be expanded in terms of spherical harmonics. And in a very strong magnetic field where Lorentz forces dominate, the wave function can be expanded in terms of Landau-like orbitals. But in the strong magnetic field where Lorentz and Coulomb forces are of nearly equal importance, neither of them can be treated as a perturbation. Hence, it is necessary to develop non-perturbative techniques to solve this problem. Here $\beta_Z$ can be used to characterise three different regimes of strength: the low (weak, $\beta_Z < 10^{-3}$), the intermediate (strong, $10^{-3} \leq \beta_Z \leq 1$), and the high (very strong, $\beta_Z > 1$), regimes where $\beta_Z = B/2B_0Z^2$, $B_0 = 2.35 \times 10^5$ T, and $Z$ is the charge of the atomic nucleus.

So far, considerable effort has been devoted to the theoretical investigations of atoms in magnetic fields with arbitrary strength. Rosner *et al.*[6,7] have done detailed work on the spectrum of the hydrogen atom in magnetic fields up to $4.7 \times 10^8$ T, which has been successfully applied to the identification of the observed spectra from many magnetic white dwarfs. Kravchenko *et al.*[8,9] presented accurate results for the hydrogen atom in magnetic fields up to $9.4 \times 10^8$ T with an accuracy of $10^{-12}$. In view of this, the issue of the hydrogen atom over a wide range of magnetic fields can be considered to be completely solved. In spite of this great success, there were also a large number of magnetic white dwarfs whose spectra remain unexplained or could not be completely accounted for with hydrogen atom. It is thus essential to acquire extensive and accurate data of energy levels and resulting transition wavelengths of multielectron atoms subjected to strong magnetic fields. Hence, the re-

*Project supported by the National Natural Science Foundation of China (Grant No. 10874133).
†Corresponding author. E-mail: qhx@whu.edu.cn
© 2010 Chinese Physical Society and IOP Publishing Ltd

search emphasis of atoms under these extreme conditions focused on the next lightest element, neutral helium. In contrast to the hydrogen atom, the problem of the helium atom is much more intricate because of the occurrence of the electron–electron repulsion. Even so, there exist a number of investigations on helium atoms in the literature. Thurner *et al.*[10] gave the energies of several triplet excited states of helium atoms for magnetic field strengths in the range $4.7 \times 10^1$ to $4.7 \times 10^8$ T. Furthermore, they presented a consistent correspondence diagram between the low field and high field domains for the first time. Employing a Hartree–Fock method, Jones *et al.*[11] studied the ground state and some low-lying excited states of the helium atom in low to intermediate fields, but the accuracy of their results is not very high.[11] With Hylleraas-like explicitly correlated functions, Scrinzi calculated the bound-state energies of the helium atom and gave more accurate energy levels in intermediate magnetic fields.[12] Hesse and Baye studied the helium atom in intermediate magnetic fields with the Lagrange-mesh method, combining simplicity and accuracy.[13] Adopting a full CI approach which is based on a nonlinearly optimised anisotropic Gaussian basis set, Becken *et al.*[14−16] have investigated the electronic structure of the helium atom in strong magnetic fields. With the help of these accurate data, Jordan *et al.*[17,18] have proved that the mysterious absorption edges of the magnetic white dwarf GD229, which were unexplained for almost 25 years, should be attributed to helium at a magnetic field of about 50000 T. Recently, using Hylleraas–Gaussian basis functions, Wang *et al.* calculated the energies of the ground state and some low-lying excited states of the helium atom embedded in a strong magnetic field and attained more accurate results compared to the similar method with Gaussian basis functions.[19,20]

In this work, we study the helium atom in a magnetic field with spherical wave function in low to intermediate fields and cylindrical wave function in intermediate to high fields, respectively. In view of the results calculated with the two above-mentioned basis functions in intermediate fields are less accurate, we use the Hermite interpolation and obtain lower total energies in this regime. And then the larger ionisation energies are calculated by the use of the obtained total energies above. Atomic units are used throughout unless otherwise stated.

## 2. Method

We assume that the nuclear mass is infinite and the magnetic field is in the $z$ direction. Under such circumstances, cylindrical symmetry is maintained and the square of the total spin $S^2$, the $z$-component $S_z$ of the total spin, the $z$-component $L_z$ of the total angular momentum and the $z$-component $\Pi_z$ of the total parity remain conserved quantities. Hence there are four good quantum numbers $S$, $M_S$, $M$ and $\Pi_z$ which characterise the different eigenstates of helium.

In spherical coordinates, the nonrelativistic Hamiltonian of a helium atom in a uniform magnetic field is expressed as

$$H = \sum_{i=1}^{2}\left[-\frac{1}{2}\nabla_i^2 - \frac{2}{r_i} + \frac{1}{8}\gamma^2 r_i^2 \sin^2\theta_i\right] + \frac{1}{r_{12}} + \frac{\gamma}{2}\left(L_z + 2S_z\right). \tag{1}$$

The magnetic field parameter is $\gamma = B/B_0$. The trial wave function for singlet states is expanded in the form

$$\Psi(1,2) = \sum_{L=0}^{L_{\max}} \sum_{l_1=0}^{l_{1\max}} \sum_{i=l_1}^{i_{\max}} \sum_{j=l_2}^{j_{\max}} \sum_{k=0}^{k_{\max}} a_{ijk}^{Ll_1l_2}\left(1+P_{12}\right) r_1^i r_2^j r_{12}^k \mathrm{e}^{-ar_1-br_2} Y_{l_1l_2}^{LM}\left(\boldsymbol{r}_1,\boldsymbol{r}_2\right), \tag{2}$$

where $Y_{l_1l_2}^{LM}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is a vector-coupled product of spherical harmonics for the two electrons and $P_{12}$ is permutation operator. Electron correlation is explicitly included in the interelectron distance $r_{12}$. Based on a semiempirical rule, $l_1$, $l_2$ are chosen so that $l_1 + l_2 = L$. The nonlinear parameters $a$ and $b$ are optimised for each $L$, $l_1$, and magnetic field. When choosing parameters in Eq. (2), we follow the following rule[21]

$$i + j + k + |i-j|\,\delta_{k0} \le p. \tag{3}$$

Hylleraas-like function is used to expand the wave function for low to intermediate field strengths. It is a strong tool to treat electron correlation.[22,23] At low field strengths it is particularly efficient.

In cylindrical coordinates, the nonrelativistic Hamiltonian can be written as

$$H = \sum_{i=1}^{2} -\frac{1}{2}\left[\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\rho_i\frac{\partial}{\partial\rho_i}\right) + \frac{1}{\rho_i^2}\frac{\partial^2}{\partial\phi_i^2} + \frac{\partial^2}{\partial z_i^2}\right] + \sum_{i=1}^{2}\left[-\frac{2}{\sqrt{\rho_i^2+z_i^2}} + \frac{1}{8}\gamma^2\rho_i^2\right] + \frac{\gamma}{2}\left(L_z+2S_z\right) + \frac{1}{\sqrt{\rho_1^2+\rho_2^2-2\rho_1\rho_2\cos\left(\varphi_1-\varphi_2\right)+\left(z_1-z_2\right)^2}}. \tag{4}$$

Then the trial wave function for singlet states can be expanded as

$$\Psi\left(1,2\right) = \sum_{ijn} c_{ij} r_{12}^n \left[f_i\left(\rho_1,\varphi_1,z_1\right) g_j\left(\rho_2,\varphi_2,z_2\right) + f_i\left(\rho_2,\varphi_2,z_2\right) g_j\left(\rho_1,\varphi_1,z_1\right)\right] \times \frac{\alpha\left(1\right)\beta\left(2\right)-\alpha\left(2\right)\beta\left(1\right)}{\sqrt{2}}, \tag{5}$$

where $\alpha$ and $\beta$ represent the spinor indices. And $f$ and $g$ are one-particle anisotropic Gaussian basis functions[14]

$$\Phi_i\left(\rho,\varphi,z\right) = \rho^{n_{\rho i}} z^{n_{zi}} \mathrm{e}^{-\alpha_i\rho^2-\beta_i z^2} \mathrm{e}^{\mathrm{i}\, m_i\varphi}, \tag{6}$$

where $\alpha_i$ and $\beta_i$ are positive nonlinear variational parameters obtained through the one-particle optimisation procedure for the H atom and the $He^+$ ion, and the direct two-particle optimisation procedure for the He atom at a given field strength. The parameters $n_{\rho i}$ and $n_{zi}$ obey the following restrictions:[14]

$$n_{\rho i} = |m_i| + 2k_i, \quad k_i = 0,1,2,\ldots$$

with $m_i = \ldots,-2,-1,0,1,2,\ldots,$

$$n_{zi} = \pi_{zi} + 2l_i, \quad l_i = 0,1,2,\ldots$$

with $\pi_{zi} = 0,1.$

The $r_{12}^n$ term in Eq. (5) is replaced by an approximate expansion of Gaussian-type geminals[24]

$$r_{12}^n \approx \sum_{\upsilon=0} b_\upsilon \left(1-\mathrm{e}^{-\tau_\upsilon r_{12}^2}\right), \left(n=0,\frac{1}{2},1,\ldots\right). \tag{7}$$

By way of this powerful step, the derivations of the matrix elements with the Gaussian basis can be extended easily to the Hylleraas–Gaussian basis case. Hylleraas–Gaussian function is used to expand the wave function for intermediate to high field strengths. At high field strengths it is more efficient.

Upper bounds to energies of the helium atom in magnetic fields are obtained with the Rayleigh–Ritz variational method. In order to label the states of the helium atom at a specific magnetic field, we exploit the standard spectroscopic notation $\upsilon^{2S+1}M^{\Pi_z}$. In the notation, $\upsilon$ stands for the degree of excitation.

# 3. Results

The total energies and derivatives of the total energy of $1^1 0^+$, $1^1(-1)^+$and $1^1(-2)^+$ states have been calculated as functions of magnetic field with two kinds of basis functions. The obtained results are presented in Tables 1–3. However, it should be pointed out that the results presented in the tables are the most part of the data calculated with Hylleraas-like function and Hylleraas–Gaussian function for field strengths from $\gamma = 0$ to $\gamma = 10$ and from $\gamma = 0.1$ to $\gamma = 100$, respectively. Moreover, a comparison with other works in the literature is performed.

Table 1 presents the results of $1^1 0^+$ state. Our energies are compared with the most accurate available results. The energy of $1^1 0^+$ state of the helium atom in the absence of magnetic field is –2.903724374, which is very close to –2.903724377034119598305 obtained by Drake *et al.*[25] Since Hesse *et al.*'s results[13] are rounded, one cannot come to a conclusion that their values for field strengths $\gamma = 0.02$ and $\gamma = 0.1$ are lower than ours. Furthermore, our energy at $\gamma = 0.8$ is lower than theirs. Besides, our calculations with Hylleraas-like function have seven significant digits identical with those of Scrinzi, and are consistently lower than those obtained in our previous work with Hylleraas–Gaussian function from $\gamma = 0$ to $\gamma = 0.8$.[20] In addition, through further optimisation of the nonlinear variational parameters mentioned above, the total energies of $1^1 0^+$ state are recalculated with Hylleraas–Gaussian function. Compared to our previous work, our results are about $8.7 \times 10^{-6}$ to $9.5 \times 10^{-5}$ lower between $\gamma = 1$ and $\gamma = 50$. Apart form $\gamma = 1$ and $\gamma = 2$, our values are lower than the available theoretical data.[12,13] The derivatives of the total energy with respect to the magnetic field, which can be obtained by the Hellman–Feynman theorem

$$\frac{\partial E}{\partial\gamma} = \left\langle \Psi \left| \frac{\partial H}{\partial\gamma} \right| \Psi \right\rangle, \tag{8}$$

are provided in the eighth column of Table 1.The last column in Table 1 provides the values for the identical one-electron ionisation threshold of $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states in terms of the scaling rule[14]

$$T\left(\gamma\right) = \gamma - 4E\left(H,\gamma/4\right), \tag{9}$$

where the binding energy of ground state of hydrogen $E\left(H,\gamma/4\right)$ can be obtained from Ref. [8]. And then the one-electron ionisation energies $I\left(\gamma\right)$ of $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states can be obtained from the one-electron ionisation threshold $T\left(\gamma\right)$ by subtracting the corresponding total energies $E\left(\gamma\right)$ in Tables 1–3, respectively.

**Table 1.** Total energy $E$ and derivative of the energy $\mathrm{d}E/\mathrm{d}\gamma$ of $1^1 0^+$ state and one-electron ionisation threshold $T$ as functions of magnetic filed strength $\gamma$. The energy values given in the literature are included for comparison.

| $\gamma$ | $E(1^1 0^+)$ | $E^{[20]}$ | $E^{[19]}$ | $E^{[14]}$ | $E^{[12]}$ | $E^{[13]}$ | $\mathrm{d}E/\mathrm{d}\gamma$ | $T$ |
|---|---|---|---|---|---|---|---|---|
| | | | | Hylleraas-like function | | | | |
| 0 | –2.903724374 | –2.9037155 | –2.903473 | –2.903351 | –2.90372 | –2.903724 | 0.000 | –2.000 |
| 0.001 | –2.903724173 | | | | | | 0.000397827 | –1.999499938 |
| 0.002 | –2.903723576 | | | | | | 0.000795654 | –1.998999750 |
| 0.005 | –2.903719398 | | | | | | 0.001989116 | –1.997498438 |
| 0.008 | –2.903711641 | | | –2.903340 | | | 0.003182532 | –1.995996000 |
| 0.01 | –2.903704480 | –2.9036898 | –2.903451 | | | –2.903704 | 0.003978101 | –1.994993750 |
| 0.02 | –2.903644813 | –2.9036275 | –2.903386 | –2.903270 | | –2.903645 | 0.007955154 | –1.989975001 |
| 0.05 | –2.903227357 | –2.9032106 | –2.902966 | | | | 0.019869592 | –1.974843777 |
| 0.08 | –2.902453100 | | | –2.902083 | | –2.902453 | 0.031737483 | –1.959600176 |
| 0.1 | –2.901739559 | –2.9017263 | –2.901479 | | | –2.901740 | 0.039610410 | –1.949375430 |
| 0.2 | –2.895835116 | –2.8958159 | –2.895499 | | –2.89583 | | 0.078244375 | –1.897506827 |
| 0.5 | –2.856237306 | –2.8562141 | –2.855906 | –2.855859 | –2.85623 | | 0.182410623 | –1.734628064 |
| 0.8 | –2.788425996 | | | –2.787556 | –2.78842 | –2.788425 | 0.266479607 | –1.561526260 |
| | | | | Hylleraas–Gaussian function | | | | |
| 1 | –2.7303464 | –2.7302745 | –2.730015 | –2.729508 | –2.73038 | –2.730373 | 0.312982810 | –1.440989741 |
| 2 | –2.3306211 | –2.3305260 | –2.330270 | –2.329780 | | –2.33065 | 0.470160829 | –0.788842154 |
| 5 | –0.5757771 | –0.5757384 | –0.575411 | –0.574877 | | –0.5755 | 0.663587509 | 1.456132354 |
| 8 | 1.5457109 | | | | | | 0.742130995 | 3.911144369 |
| 10 | 3.0636148 | 3.0636900 | 3.064202 | 3.064582 | | | 0.774024780 | 5.609851957 |
| 20 | 11.2660802 | 11.2660889 | 11.266617 | 11.267051 | | | 0.852655853 | 14.47840453 |
| 50 | 38.0754611 | 38.0754859 | 38.076070 | 38.076320 | | | 0.918816034 | 42.45369075 |
| 80 | 66.0122130 | | | | | | 0.940839386 | 71.13840594 |
| 100 | 84.9176979 | 84.9176979 | 84.918049 | 84.918313 | | | 0.949205697 | 90.43945348 |

**Table 2.** Total energy $E$ and derivative of the energy $\mathrm{d}E/\mathrm{d}\gamma$ of $1^1(-1)^+$ state as functions of magnetic filed strength $\gamma$. The energy values given in the literature are included for comparison.

| $\gamma$ | $E(1^1(\text{-}1)^+)$ | $E^{[20]}$ | $E^{[19]}$ | $E^{[15]}$ | $E^{[12]}$ | $E^{[13]}$ | $\mathrm{d}E/\mathrm{d}\gamma$ |
|---|---|---|---|---|---|---|---|
| | | | | Hylleraas-like function | | | |
| 0 | –2.123843084 | –2.1238345 | –2.123801 | –2.123774 | –2.12384 | –2.12379 | –0.500 |
| 0.001 | –2.124339943 | | | | | | –0.493719532 |
| 0.002 | –2.124830524 | | | | | | –0.487441980 |
| 0.005 | –2.126264648 | | | | | | –0.468655720 |
| 0.008 | –2.127642587 | | | | | | –0.449998113 |
| 0.01 | –2.128530235 | –2.1285062 | –2.128490 | | | –2.12848 | –0.437666862 |
| 0.02 | –2.132605335 | –2.1326002 | –2.132561 | –2.132539 | | –2.13254 | –0.377975993 |
| 0.05 | –2.141574199 | –2.1415440 | –2.141515 | | | | –0.227680726 |
| 0.08 | –2.146690537 | | | –2.146622 | | –2.14663 | –0.119357863 |
| 0.1 | –2.148506030 | –2.1485023 | –2.148464 | | | –2.14846 | –0.064026251 |
| 0.2 | –2.145276349 | –2.1452573 | –2.145196 | | –2.14527 | | 0.107446353 |
| 0.5 | –2.077467794 | –2.0774021 | –2.077346 | –2.077302 | –2.07755 | | 0.308835382 |
| 0.8 | –1.969699746 | | | –1.969560 | –1.97011 | | 0.400740045 |
| | | | | Hylleraas–Gaussian function | | | |
| 1 | –1.8852381 | –1.8851789 | –1.885011 | –1.884875 | –1.88573 | | 0.443472020 |
| 2 | –1.3695270 | –1.3694922 | –1.369122 | –1.368986 | | | 0.572283939 |
| 5 | 0.6184424 | 0.6184953 | 0.619038 | 0.619265 | | | 0.724738932 |
| 8 | 2.8974184 | | | | | | 0.787717969 |
| 10 | 4.5000003 | 4.5000751 | 4.500762 | 4.500982 | | | 0.813444603 |
| 20 | 13.0094863 | 13.0095023 | 13.010161 | 13.010551 | | | 0.877339673 |
| 50 | 40.3384976 | 40.3385735 | 40.339265 | 40.339488 | | | 0.931692669 |
| 80 | 68.5974871 | | | | | | 0.949925462 |
| 100 | 87.6702246 | 87.6702301 | 87.670794 | 87.671288 | | | 0.956904622 |

Table 2 lists the results for $1^1(-1)^+$ state. For $\gamma = 0$, the energy of $1^1(-1)^+$ state is in good agreement with the result of Drake and Yan,[26] which is –2.123 843 086 4. For field strengths from $\gamma = 0$ to $\gamma = 0.8$, our results, as compared with the reference values, are generally lower. But, the energies at $\gamma = 0.5$ and $\gamma = 0.8$, respectively, are a bit higher than those given by Scrinzi.[12] Besides, our recalculations with Hylleraas–Gaussian function are about $5.5\times10^{-6}$ to $7.6\times10^{-5}$ lower than our previous work.[20] Apart from $\gamma = 1$, the recalculations are lower than any data published. Moreover, the last column in Table 2 gives the derivatives of the energy.

Table 3 presents the results for $1^1(-2)^+$ state. Our field-free energy is slightly higher than the value –2.556 207 328 of Drake *et al.*[26] By comparison, the accuracy of our energy is higher than that of the available data[14,19,20] for $\gamma = 0$ to $\gamma = 0.8$. But, for $\gamma = 0.2$ and $\gamma = 0.8$, Scrinzi's results are considerably lower than our values. Additionally, our recalculations with Hylleraas–Gaussian function improve our previous work[20] by about $1.4\times10^{-6}$ to $1.9\times10^{-4}$. And they are systematically lower than the energies of Becken and Schmelcher[16] but still higher than the energy of Scrinzi for $\gamma = 1$. Finally, the last column in Table 3 gives the derivatives of the energy.

**Table 3.** Total energy $E$ and derivative of the energy $\mathrm{d}E/\mathrm{d}\gamma$ of $1^1(-2)^+$ state as functions of magnetic filed strength $\gamma$. The energy values given in the literature are included for comparison.

| $\gamma$ | $E(1^1(-2)^+)$ | $E^{[20]}$ | $E^{[19]}$ | $E^{[16]}$ | $E^{[12]}$ | $\mathrm{d}E/\mathrm{d}\gamma$ |
|---|---|---|---|---|---|---|
| | | | Hylleraas-like function | | | |
| 0 | –2.055620730 | –2.0556198 | –2.055619 | –2.055619 | –2.05562 | –1.000 |
| 0.001 | –2.056607215 | | | | | –0.972982128 |
| 0.002 | –2.057566726 | | | | | –0.946073585 |
| 0.005 | –2.060285568 | | | | | –0.867021503 |
| 0.008 | –2.062773127 | | | –2.062771 | | –0.792204350 |
| 0.01 | –2.064310299 | –2.0643043 | –2.064304 | | | –0.745409936 |
| 0.02 | –2.070740958 | –2.0707273 | –2.070727 | –2.070739 | | –0.551605872 |
| 0.05 | –2.081864221 | –2.0818467 | –2.081843 | | | –0.235939844 |
| 0.08 | –2.086454269 | | | –2.086450 | | –0.084816760 |
| 0.1 | –2.087465703 | –2.0874406 | –2.087439 | | | –0.019685904 |
| 0.2 | –2.079392682 | –2.0793823 | –2.079374 | | –2.07949 | 0.154339694 |
| 0.5 | –2.000922970 | –2.0009204 | –2.000892 | –2.000873 | | 0.334985702 |
| 0.8 | –1.886843468 | | | –1.886749 | –1.89021 | 0.417578087 |
| | | | Hylleraas–Gaussian function | | | |
| 1 | –1.7990808 | –1.7990702 | –1.798998 | –1.798936 | –1.80500 | 0.457818705 |
| 2 | –1.2727659 | –1.2727645 | –1.272606 | –1.272473 | | 0.580645129 |
| 5 | 0.7337602 | 0.7338073 | 0.734027 | 0.734276 | | 0.729677722 |
| 8 | 3.0258306 | | | | | 0.791598139 |
| 10 | 4.6357002 | 4.6357036 | 4.636247 | 4.636327 | | 0.816906961 |
| 20 | 13.1736803 | 13.1737142 | 13.174041 | 13.174417 | | 0.879763427 |
| 50 | 40.5579160 | 40.5581080 | 40.558421 | 40.558628 | | 0.933156589 |
| 80 | 68.8554798 | | | | | 0.950990001 |
| 100 | 87.9491624 | 87.9491639 | 87.949409 | 87.949762 | | 0.957878834 |

The one-electron ionisation energy of $1^1(-2)^+$ state as a function of magnetic field is displayed in Fig. 1. The energies are calculated using Hylleraas-like function or Hylleraas–Gaussian function. Figure 1 shows that the ionisation energies increase monotonically with increasing field strength. But there exists a gap between the two ionisation energy curves obtained using the two different basis functions above, respectively, from $\gamma = 10$ to $\gamma = 20$. Actually, the gap has already existed between the two ionisation energy curves for $\gamma < 10$. Furthermore, there also exists a crossing at a certain field strength which is determined in Fig. 2. Figure 2 shows the difference between the two ionisation energy curves. At $\gamma \approx 0.52$, the two ionisation energy curves experience a crossing. These phenomena reflect the fact that the ionisation ener-

gies obtained with Hylleraas-like function are larger for $\gamma < 0.52$, while those obtained with Hylleraas–Gaussian function are lareger for $\gamma > 0.52$. Obviously, due to the same one-electron threshold employed at a given field stength in calculating the two ionisation energy curves, the total energy obtained with Hylleraas-like function is lower for $\gamma < 0.52$, while that obtained with Hylleraas–Gaussian function is lower for $\gamma > 0.52$.

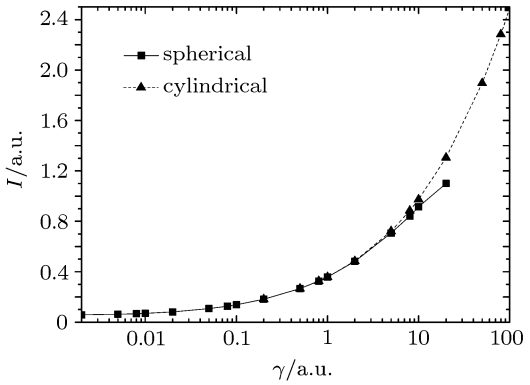



**Fig. 1.** The ionisation energies of $1^1(-2)^+$ state versus magnetic field strength, obtained with Hylleraas-like function in spherical coordinates and Hylleraas–Gaussian function in cylindrical coordinates, respectively.

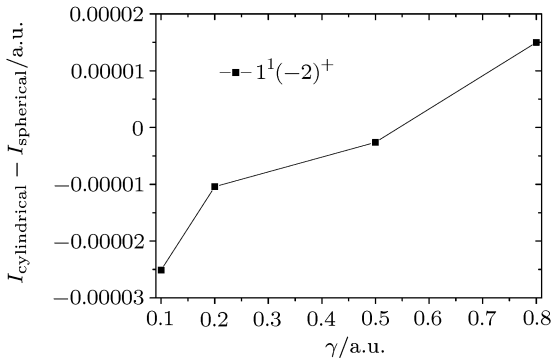



**Fig. 2.** The difference between the ionisation energy obtained with Hylleraas–Gaussian function in cylindrical coordinates and that obtained with Hylleraas-like function in spherical coordinates.

Theoretically, it is well known that spherical wave function is appropriate in the low field regime and cylindrical wave function is more appropriate in the high field regime. So the ionisation energies of the helium atom obtained with the two different basis functions above, respectively, are smaller than the accurate values in the intermediate field regime. In order to estimate the total energies and the ionisation energies, and make a smooth connection between the two ionisation energy curves obtained with the two different basis functions above, respectively, in this regime, we present a method based on Hermite interpolation. Adopting the total energies and derivatives of the energy at $\gamma = 0.1$ and $\gamma = 0.8$, we can estimate the total energies of $1^1(-2)^+$ state for $0.1 < \gamma < 0.8$. At $\gamma = 0.1$, the energy and derivative of the energy obtained with Hylleraas-like function are –2.087465703 and –0.019685904, respectively. At $\gamma = 0.8$, the energy and derivative of energy obtained with Hylleraas–Gaussian function are –1.8868586 and 0.418489714, respectively. In Table 4, the total energies and the values from reference papers are given. It is clear that the results calculated by Hermite interpolation are lower than the energies of Scrinzi.[12] However, Scrinzi's results are considerably lower than our values in Table 3 and other reference data. Hence, some researchers suggest that Scrinzi's values are systematically too low, most probably due to numerical errors.[15,27] Nevertheless, we deduce that Scrinzi's results for $0.1 < \gamma < 0.8$ are likely correct. Additionally, we also calculate the ionisation energies of $1^1(-2)^+$ state with the total energies obtained by Hermite interpolation. The ionisation energies are illustrated graphically in Fig. 3. It shows that the calculated ionisation energies are larger than those obtained with Hylleraas-like function and Hylleraas–Gaussian function, respectively.

**Table 4.** Total energies $E$ of $1^1(-2)^+$ state obtained by Hermite interpolation and the results of Scrinzi for comparison.

| $\gamma$ | $E$ | $E^{[12]}$ |
|---|---|---|
| 0.2 | –2.0829240 | –2.07949 |
| 0.4 | –2.0411842 | –2.03308 |
| 0.5 | –2.0082560 | |
| 0.6 | –1.9701356 | –1.96735 |

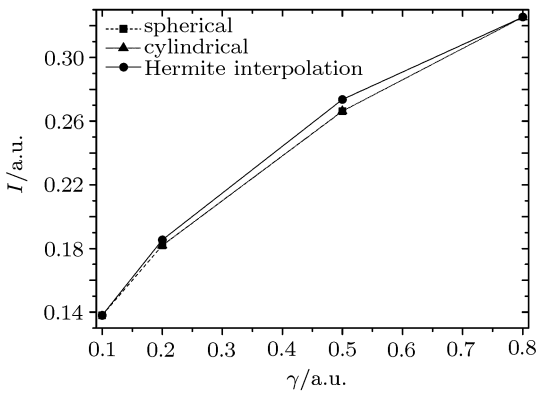



**Fig. 3.** The ionisation energies of $1^1(-2)^+$ state obtained with Hylleraas-like function in spherical coordinates, Hylleraas–Gaussian function in cylindrical coordinates and Hermite interpolation, respectively.

Similarly, exploiting the same method as the above, the $1^1 0^+$and $1^1(-1)^+$ states in the intermediate field regime are also analysed. In Figs. 4 and 5, the ionisation energies of $1^1 0^+$and $1^1(-1)^+$ states for $1 < \gamma < 5$ and $0.2 < \gamma < 1$, respectively, are displayed.

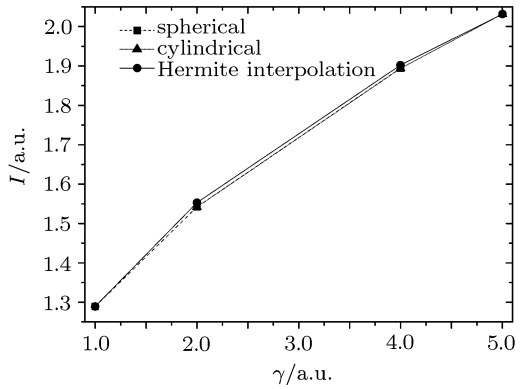



**Fig. 4.** The ionisation energies of $1^1 0^+$ state obtained with Hylleraas-like function in spherical coordinates, Hylleraas–Gaussian function in cylindrical coordinates, and Hermite interpolation, respectively.

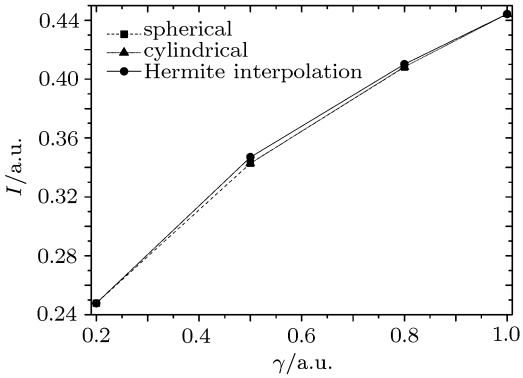



**Fig. 5.** The ionisation energies of $1^1(-1)^+$ state obtained with Hylleraas-like function in spherical coordinates, Hylleraas–Gaussian function in cylindrical coordinates, and Hermite interpolation, respectively.

From these two figures, we can see that the ionisation energies calculated by Hermite interpolation are always lareger than those obtained with the two different basis functions above. For $1^1 0^+$ state, it should be added that the total energy and derivative of energy obtained with Hylleraas-like function at $\gamma = 1$ are –2.730379161 and 0.312841919, respectively.

## 4. Conclusions

In the present work, we have investigated the helium atom in a magnetic field. Based on a CI method, we calculate the total energies, derivatives of the total energy with respect to the magnetic field, and ionisation energies of $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states with Hylleraas-like function in low to intermediate fields and Hylleraas–Gaussian function in intermediate to high fields. High accuracy results are obtained in low and high fields, due to the two basis functions taking into consideration electron correlation. Our results confirm that Hylleraas-like function is particularly efficient in the low field regime, while Hylleraas–Gaussian function is more efficient in the high field regime. But in intermediate fields, both of the two different basis functions produce low accuracy results. To estimate the total energies and ionisation energies, and make a smooth connection between the two ionisation energy curves obtained with the two different basis functions in the intermediate field regime, we present a method in terms of Hermite interpolation. With the aid of this approach, we obtain lower total energies and larger ionisation energies in this regime.

## References

[1] Ostriker J P and Hartwick F D A 1968 *Astrophys. J.* **153** 797

[2] Kemp J C, Swedlund J B, Landstreet J D and Angel J R P 1970 *Astrophys. J.* **161** L77

[3] Trumper J, Pietsch W, Reppin C, Voges W, Staubert R and Kendziorra E 1978 *Astrophys. J.* **219** L105

[4] Elliott R J and Loudon R 1960 *J. Phys. Chem. Solids* **15** 196

[5] Wan Y, Ortiz G and Phillips P 1995 *Phys. Rev. Lett.* **75** 2879

[6] Rosner W, Wunner G, Herold H and Ruder H 1984 *J. Phys.* B: *At. Mol. Phys.* **17** 29

[7] Ruder H, Wunner G, Herold H and Geyer F 1994 *Atoms in Strong Magnetic Fields* (Berlin: Springer)

[8] Kravchenko Y P, Liberman M A and Johansson B 1996 *Phys. Rev.* A **54** 287

[9] Kravchenko Y P, Liberman M A and Johansson B 1996 *Phys. Rev. Lett.* **77** 619

[10] Thurner G, Korbel H, Braun M, Herold H, Ruder H and Wunner G 1993 *J. Phys.* B: *At. Mol. Opt. Phys.* **26** 4719

[11] Jones M D, Ortiz G and Ceperley D M 1996 *Phys. Rev.* A **54** 219

[12] Scrinzi A 1998 *Phys. Rev.* A **58** 3879

[13] Hesse M and Baye D 2004 *J. Phys.* B: *At. Mol. Opt. Phys.* **37** 3937

[14] Becken W, Schmelcher P and Diakonos F K 1999 *J. Phys.* B: *At. Mol. Opt. Phys.* **32** 1557

[15] Becken W and Schmelcher P 2000 *J. Phys.* B: *At. Mol. Opt. Phys.* **33** 545

[16] Becken W and Schmelcher P 2001 *Phys. Rev.* A **63** 053412

[17] Jordan S, Schmelcher P, Becken W and Schweizer W 1998 *Astron. Astrophys.* **336** L33

[18] Jordan S, Schmelcher P and Becken W 2001 *Astron. Astrophys.* **376** 614

[19] Wang X F and Qiao H X 2008 *Phys. Rev.* A **77** 043414

[20] Wang X F, Zhao J J and Qiao H X 2009 *Phys. Rev.* A **80** 053425

[21] Kono A and Hattori S 1984 *Phys. Rev.* A **29** 2981

[22] Şakiroğlu S, Doğan Ü, Yıldız A, Akgüngör K, Epik H, Ergün Y, Sarı H and Sökmen İ 2009 *Chin. Phys.* B **18** 1578

[23] Şakiroğlu S, Akgüngör K and Sökmen İ 2009 *Chin. Phys.* B **18** 2238

[24] Persson B J and Taylor P R 1996 *J. Chem. Phys.* **105** 5915

[25] Drake G W F, Cassar M M and Nistor R A 2002 *Phys. Rev.* A **65** 054501

[26] Drake G W F and Yan Z C 1992 *Phys. Rev.* A **46** 2378

[27] Jones M D, Ortiz G and Ceperley D M 1999 *Phys. Rev.* A **59** 2875