Helium atom in strong magnetic fields: An application of the configuration-interaction method with Hylleraas-Gaussian basis

Xiaofeng Wang, Jijun Zhao, and Haoxue Qiao
Department of Physics, Wuhan University, Wuhan 430072, China
(Received 9 July 2009; revised manuscript received 20 September 2009; published 30 November 2009)

In this work, we apply approximate expansions of Gaussian-type geminals of r_{12} to replace the integer and half-integer powers of r_{12} in Hylleraas-Gaussian basis, and use a full configuration-interaction method to calculate the energies of $^1 0^+$, $^1(-1)^+$, and $^1(-2)^+$ states for helium atom in magnetic fields between 0 and 100 a.u. Compared to the configuration-interaction method with Gaussian basis, at least 1×10^{-4} improvement in the precision of energies has been made when calculated mean value of r_{12} is less than 5.67 a.u. and more than 5×10^{-4} improvement in precision of results has been achieved when calculated mean value of r_{12} is less than 2.41 a.u. The ground-state energy of helium atom in our calculation is −2.903 715 5 in the absence of magnetic field. This work presents a general method which can attain high precise ground and low-lying states energies in the whole field regime and is hopeful to be extended to more complex atomic and molecular systems (lithium, beryllium, and H_2, etc.).

DOI: 10.1103/PhysRevA.80.053425 PACS number(s): 32.60.+i, 32.30.−r, 32.70.−n

I. INTRODUCTION

Since the 1970s, researchers are dedicated to apply various numerical methods to the studies of the properties of atomic and molecular systems in strong magnetic fields. One of their purposes is to explain the spectra from white dwarfs and neutron stars, which have magnetic fields of 10^2-10^5 T [1] and 10^7-10^9 T [2], respectively. The studies of atomic and molecular systems under such extreme circumstance also have theoretical significance. This situation cannot be dealing with general perturbation method because the Coulomb force and the Lorentz force are of comparable strengths. The different symmetries of Coulomb interaction and magnetic field make it difficult for a method to yield considerable precision in both the weak side and the strong side of the whole field region simultaneously.

Most of the early works were focused on the hydrogen atom in magnetic fields (see Refs. [3,4] for a detailed work). As the second-most abundant element in the universe and the simplest multielectron atomic system, the helium's properties in magnetic fields also have been studied by many research groups. Applying a correlation function Monte Carlo method, Jones *et al.* presented the excited-state energies of spin-polarized helium atom in the field region of $B=0-8$ a.u. (1 a.u. corresponds to 2.35×10^5 T) [5]. In Ref. [6], Jones *et al.* calculated more excited-state energies of helium atom in magnetic fields up to 800 a.u. using a Hartree-Fock self-consistent field method. More recently, through computing the two-dimensional Hartree-Fock partial differential equations, Thirumalai *et al.* calculated the energies of the $1s_0 2p_{-1}$, $1s_0 3d_{-2}$, and $1s_0 2p_0$ states for helium atom in strong magnetic fields up to 80 a.u. [7]. Braun *et al.* combined the hyperspherical close coupling and finite element method and calculated the low-lying *S*- and *P*-states energy levels of helium atom in the field region of $B=0-1.0$ a.u. [8], their results were of high precision but only in the weak magnetic-field regime. Using Hylleraas-like explicitly correlated functions, Scrinzi calculated some bound-state energies of helium atom in magnetic fields up to 1 a.u. [9] and the precision of their results was even higher than Braun's results while extent the field region to intermediate fields. Hesse *et al.* extended the Lagrange-mesh method which can achieve high precise energies for helium atom in zero magnetic field to the weak and intermediate magnetic fields case [10]. Hesse's results in the region of $B=0-1.0$ a.u. are of the highest precision but the stability of the results gets worse in the region of $B>1.0$ a.u.. Applying a full configuration-interaction (CI) method using Gaussian-type basis functions with cylindrical symmetry, Becken *et al.* carried out detailed works in the calculation of the energy levels involving the helium ground state and some low-lying states in the field region of $B=0-100$ a.u. [11–13], their results in weak magnetic fields were worse than the related results calculated by Braun, Scrinzi, or Hesse due to the approximately spherical symmetry of the atomic system in weak field regime.

In our previous work [14], using incomplete Hylleraas-Gaussian-type basis functions only including even powers of interelectronic distance r_{12}, we calculated the energies for $^1 0^+$, $^1(-1)^+$, and $^1(-2)^+$ states of helium atom in magnetic fields of $B=0-100$ a.u. and attained better results compared to the similar full CI method using Gaussian-type basis functions [11–13]. Because of the difficulty to get precise numerical solution of the integral $\int \phi_{ij}^* \frac{r_{12}^{2n+1}}{r_1} \phi_{kl} d\vec{r}_1 d\vec{r}_2$ (ϕ_{ij} and ϕ_{kl} are two-particle Gaussian basis) corresponding to the matrix elements of the electron-nuclear Coulomb interaction in cylindrical coordinates, this initial work did not include the odd powers of r_{12} in the basis functions and could not yield the precision expected in the whole field region especially in zero and weak magnetic fields. In this work, we include r_{12}^1 and $r_{12}^{1/2}$ in Hylleraas-Gaussian-type basis functions. We use not explicit r_{12}^1 and $r_{12}^{1/2}$ but the approximate expansions of Gaussian-type geminals of r_{12}. It can be considered as a simple extension of the full CI method using Gaussian-type basis functions and it also provides a general method dealing with the factors of r_{12} (integer or half integer) in Hylleraas-Gaussian-type basis functions.

II. THEORY AND METHOD

Within the frame of infinite-nuclear-mass approximation, the nonrelativistic Hamiltonian of Helium-like atomic system in a magnetic field pointing in the positive-z direction reads in atomic units

$$H=\sum_{i=1}^{2}\left[\frac{1}{2}\left(p_i+\frac{1}{2}\mathbf{B}\times\mathbf{r_i}\right)^2-\frac{Z}{r_i}\right]+\frac{1}{r_{12}}+BS_z, \tag{1}$$

where Z is the nuclear charge. The magnetic field is measured by the parameter $\gamma=B/B_0$ with $B_0=2.35\times10^5$ T.

The upper bounds to energies of the helium atom in magnetic fields are obtained by solving the Schrödinger equation using the Rayleigh-Ritz variational method. The trial wave function for singlet states has the form

$$\Psi(1,2)=\sum_{ij}c_{ij}r_{12}^{n}\phi_{ij},\left(n=0,\frac{1}{2},1,\frac{3}{2},2,\cdots\right),$$

$$\phi_{ij}=[f_i(\rho_1,\varphi_1,z_1)g_j(\rho_2,\varphi_2,z_2)+f_i(\rho_2,\varphi_2,z_2)g_j(\rho_1,\varphi_1,z_1)]\frac{\alpha(1)\beta(2)-\alpha(2)\beta(1)}{\sqrt{2}}, \tag{2}$$

where α and β represent the spinor indices. f and g are one-particle Gaussian bases introduced by Aldrich and Greene [15]

$$\phi_i(\rho,\varphi,z)=\rho^{n_{\rho i}}z^{n_{zi}}e^{-\alpha_i\rho^2-\beta_i z^2}e^{im_i\varphi},$$

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

$$n_{zi}=\pi_{zi}+2l_i,\quad l_i=0,1,2,\ldots\quad\text{with}\quad \pi_{zi}=0,1, \tag{3}$$

where α_i, β_i are positive nonlinear variational parameters obtained by the one-particle optimization procedure for H and He^+ and the direct two-particle optimization procedure for He in a specific magnetic field.

In the absence of magnetic field, the kinetic energy operator $\frac{1}{2}\Sigma_{i=1}^{2}p_i^2$ in Hamiltonian can be written as follow in r_1, r_2, and r_{12} coordinates [16]

$$\frac{1}{2}\sum_{i=1}^{2}p_i^2=-\frac{1}{r_1}\frac{\partial}{\partial r_1}-\frac{1}{r_2}\frac{\partial}{\partial r_2}-\frac{1}{2}\frac{\partial^2}{\partial r_1^2}-\frac{1}{2}\frac{\partial^2}{\partial r_2^2}-\frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}-\frac{\partial^2}{\partial r_{12}^2}-\frac{1}{2}\frac{r_{12}^2+r_1^2-r_2^2}{r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}-\frac{1}{2}\frac{r_{12}^2+r_1^2-r_2^2}{r_1r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}. \tag{4}$$

In the limiting case of $r_1=r_2, r_{12}\to0$, the kinetic-energy operator is simplified and the Schrödinger equation in the absence of magnetic field comes to a second-order differential equation of r_{12}

$$\left(-\frac{d^2}{dr_{12}^2}-\frac{2}{r_{12}}\frac{d}{dr_{12}}+\frac{1}{r_{12}}\right)\psi(r_{12})=0. \tag{5}$$

The solution of wave function can be expended as the series of r_{12}

$$\psi(r_{12})=1+\frac{r_{12}}{2}+\frac{r_{12}^2}{12}+\frac{r_{12}^3}{144}+\frac{r_{12}^4}{2880}+O(r_{12})^5. \tag{6}$$

So the most two important terms are the terms include r_{12}^0 and r_{12}^1. The r_{12}^1 in the trial wave function in Eq. (2) is replaced by an approximate expansion of Gaussian-type geminals of r_{12} [17]

$$r_{12}^n\approx\sum_{\nu}b_\nu(1-e^{-\tau_\nu r_{12}^2}),\left(n=\frac{1}{2},1,\frac{3}{2},2,\cdots\right). \tag{7}$$

This is a powerful step to overcome the difficulty in the derivation of matrix elements of the electron-nuclear Coulomb interaction mentioned in the introduction part. As the half-integer power has a contribution to the precision of results [18], we also include $r_{12}^{1/2}$ in the Hylleraas-Gaussian basis, which has a similar approximate expansion to r_{12}. The other integer or half-integer power of r_{12}, which can be expressed by the product of the approximate expansions of $r_{12}^{1/2}$ and r_{12}^1, are not used in this work respect to the linear dependences of large number of basis functions. In our procedure

TABLE I. Energy convergence of $1\ ^1\!0^+$ state for helium atom at $\gamma=0,1,10$ a.u..

	$\gamma=0$ a.u.		$\gamma=1$ a.u.		$\gamma=10$ a.u.	
Configurations	No. of total terms	$E(1\ ^1\!0^+)$	No. of total terms	$E(1\ ^1\!0^+)$	No. of total terms	$E(1\ ^1\!0^+)$
0^+0^+	1132	−2.90364855	450	−2.73008479	450	3.06452521
0^-0^-	1775	−2.90367449	650	−2.73017307	650	3.06387495
$1^+(-1)^+$	2418	−2.90370919	850	−2.73026642	850	3.06373782
$1^-(-1)^-$	2926	−2.90371137	1050	−2.73026852	1050	3.06371853
$2^+(-2)^+$	3434	−2.90371487	1250	−2.73027405	1250	3.06369592
$2^-(-2)^-$	3582	−2.90371520	1348	−2.73027415	1450	3.06369568
$3^+(-3)^+$	3730	−2.90371552	1446	−2.73027451	1650	3.06369319
$3^-(-3)^-$					1750	3.06369057
$3^-(-3)^-$					1850	3.06369002

TABLE II. Energy convergence of $1\ ^1(-1)^+$ and $1\ ^1(-2)^+$ states for helium atom at $\gamma=0$ a.u..

Configurations	No. of total terms	E($1\ ^1(-1)^+$)	Configurations	No. of total terms	E($1\ ^1(-2)^+$)
$0^+(-1)^+$	450	−2.12382269	$0^+(-2)^+$	1600	−2.05561791
$0^-(-1)^-$	650	−2.12382741	$(-1)^+(-1)^+$	2400	−2.05561962
$1^+(-2)^+$	850	−2.12383403	$0^-(-2)^-$	2850	−2.05561967
$1^-(-2)^-$	1050	−2.12383429	$(-1)^-(-1)^-$	3300	−2.05561975
$2^+(-3)^+$	1250	−2.12383453	$1^+(-3)^+$	3500	−2.05561983

to determine the fit parameters of b_ν and τ_ν, about 1000 points in the region of $0<r_{12}\leq 20$ are used and the points in the region of r_{12} tending to zero have the denser mesh and larger weights. The expansions in Eq. (7) only add $e^{-\tau_\nu r_{12}^2}$ terms to the general Gaussian basis, so the derivations of the matrix elements with the Gaussian basis can be extended easily to this Hylleraas-Gaussian basis case.

The spectroscopic notation $\nu^{2S+1}M^{\Pi_z}$ are used in this work to label the states of the helium atom in a magnetic field, here ν stands for the degree of excitation.

III. RESULTS AND DISCUSSIONS

In our calculation, the nonrelativistic ground-state energy of helium atom is −2.903 7155 in the absence of magnetic field. Compared to −2.903 473 [14] (computed by the full CI method with incomplete Hylleraas-Gaussian basis including r_{12}^0 and r_{12}^2) and −2.903 351 [11] (computed by the full CI method with Gaussian basis), our result is much closer to −2.903 724 377 034 119 598 305 calculated by Drake *et al.* [19]. Table I presents the energy convergence of $1\ ^10^+$ state for helium atom while including more and more configurations in the trial wave functions at a magnetic field strength of 0, 1, and 10 a.u. respectively. The Hylleraas-Gaussian basis is more efficient in strong magnetic fields due to its cylindrical symmetry, and the contributions of configurations with high angular moments increases while increasing the magnetic field strength. Table II shows the energy convergence of $1\ ^1(-1)^+$ and $1\ ^1(-2)^+$ states in the absence of magnetic field. The $[0^+,(-1)^+]$ and $[0^+,(-2)^+]$ configurations have the biggest contributions to the total energies of $1\ ^1(-1)^+$ and $1\ ^1(-2)^+$ states, respectively, the including of other configurations only improve the precision of the results at the fifth or sixth decimal places.

Because of the field-dependent kinetic energy, the total energies of all singlet states are monotonically increasing while increasing the field strength. Table III–V presents the total energies of $^10^+$, $^1(-1)^+$, and $^1(-2)^+$ states, respectively, and the average values of r_{12} are also listed. For $1\ ^10^+$ state

TABLE III. Total energies E of $1\ ^10^+$ and $2\ ^10^+$ states for helium atom as a function of magnetic field strength γ. The numbers in the parentheses are not the general uncertainties of the results but the last one or two digitals varied when we add more terms to the trial wave function, while the other numbers are invariant by including more configurations and increasing the number of terms for each configuration.

	$1\ ^10^+$					$2\ ^10^+$			
γ	E	$E_{\text{lit[14]}}$	$E_{\text{lit[11]}}$	E_{lit}	$\bar{r}_{12}$	E	$E_{\text{lit[14]}}$	$E_{\text{lit[11]}}$	E_{lit}
0	−2.90371(55)	−2.903473	−2.903351	−2.90372 [a]	2.9352	−2.14597(30)	−2.145951	−2.145912	−2.14597 [a]
				−2.903724[b]					−2.145974 [b]
0.01	−2.90368(98)	−2.903451		−2.903704[b]	2.8446	−2.14570(10)	−2.145683		−2.145706 [b]
0.02	−2.90362(75)	−2.903386	−2.903270	−2.903645[b]	2.8444	−2.14490(39)	−2.144883	−2.144852	−2.144913 [b]
0.05	−2.90321(06)	−2.902966			2.8435	−2.13964(78)	−2.139616		
0.1	−2.90172(63)	−2.901479		−2.901740[b]	2.8403	−2.12354(80)	−2.123512		2.123553[b]
0.2	−2.89581(59)	−2.895499		−2.89583 [a]	2.8281	−2.07648(01)	−2.076450		−2.07650 [a]
0.5	−2.85621(41)	−2.855906	−2.855859		2.7580	−1.90873(11)	−1.908712	−1.908671	
1	−2.73027(45)	−2.730015	−2.729508	−2.73038 [a]	2.6049	−1.61789(78)	−1.617892	−1.617870	−1.61787 [b]
				−2.730373[b]					
2	−2.33052(60)	−2.330270	−2.329780	−2.33065 [b]	2.3331	−0.97585(27)	−0.975874	−0.975861	
5	−0.57573(84)	−0.575411	−0.574877	−0.5755 [b]	1.8691	1.25234(89)	1.252364	1.252363	
10	3.06369(00)	3.064202	3.064582		1.5251	5.39320(13)	5.393203	5.3932	
20	11.26608(89)	11.266617	11.267051		1.2297	14.24897(66)	14.249009	14.248991	
50	38.07548(59)	38.07607	38.07632		0.9262	42.20752(37)	42.207553	42.20751	
100	84.91769(79)	84.918049	84.918313		0.7545	90.18069(59)	90.180739	90.18069	

[a]A. Scrinzi [9].
[b]M. Hesse and D. Baye [10].

TABLE IV. Total energies E of $1\ ^1(-1)^+$ and $2\ ^1(-1)^+$ states for helium atom as a function of magnetic field strength γ.

	$1\ ^1(-1)^+$					$2\ ^1(-1)^+$			
γ	E	$E_{\text{lit[14]}}$	$E_{\text{lit[12]}}$	E_{lit}	$\bar{r}_{12}$	E	$E_{\text{lit[14]}}$	$E_{\text{lit[12]}}$	E_{lit}
0	−2.12383(45)	−2.123801	−2.123774	−2.12384[a]	10.2827	−2.05514(05)	−2.055131	−2.055124	−2.05514[a]
				−2.12379[b]					
0.01	−2.12850(62)	−2.128490		−2.12848[b]	10.2491	−2.05835(67)	−2.058360		
0.02	−2.13260(02)	−2.132561	−2.132539	−2.13254[b]	10.1611	−2.05864(46)	−2.058629	−2.058622	
0.05	−2.14154(40)	−2.141515			9.6944	−2.05037(75)	−2.050363		
0.1	−2.14850(23)	−2.148464		−2.14846[b]	8.8196	−2.02987(56)	−2.029861		
0.2	−2.14525(73)	−2.145196		−2.14527[a]	7.5385	−1.98779(18)	−1.987779		−1.98828[a]
0.5	−2.07740(21)	−2.077346	−2.077302		5.7072	−1.84328(85)	−1.843347	−1.843343	
1	−1.88517(89)	−1.885011	−1.884875	−1.88573[a]	4.4835	−1.56568(11)	−1.565704	−1.565692	
2	−1.36949(22)	−1.369122	−1.368986		3.4791	−0.93051(93)	−0.930512	−0.930508	
5	0.61849(53)	0.619038	0.619265		2.4839	1.29150(86)	1.291508	1.291512	
10	4.50007(51)	4.500762	4.500982		1.9353	5.42806(64)	5.428068	5.428064	
20	13.00950(23)	13.010161	13.010551		1.5220	14.27981(75)	14.279840	14.279839	
50	40.33857(35)	40.339265	40.339488		1.1268	42.23365(77)	42.233622	42.233602	
100	87.670230(1)	87.670794	87.671288		0.9108	90.20361(66)	90.203624	90.203618	

[a]A. Scrinzi [9].
[b]M. Hesse and D. Baye [10].

the total energy raises from −2.903 715 5 at $\gamma=0$ a.u. to 84.917 697 9 at $\gamma=100$ a.u., and the average value of r_{12} for $1\ ^1 0^+$ state decreases from 2.9352 to 0.7545 a.u. The relative small interelectronic distance makes the method with Hylleraas-Gaussian basis more efficient. Compared to the related data calculated by the full CI method with Gaussian basis [11], our results of $1\ ^1 0^+$ state are about 3.6×10^{-4} lower in the zero and weak magnetic fields, and $6.1-9.6\times10^{-4}$ lower in intermediate and strong magnetic fields. Compared to the results in our previous work [14], our energies of $1\ ^1 0^+$ state are $2.4-5.8\times10^{-4}$ lower in the whole field region due to the including of odd and half-integer powers of r_{12}. Our results are very close to the results in Refs. [9,10] by methods in spherical coordinates, and have better convergence in strong magnetic fields attributed to the cylindrical symmetry of Hylleraas-Gaussian basis.

In the $^1(-1)^+$ and $^1(-2)^+$ cases, the correlation between electrons is not as strong as that in the $^1 0^+$ case especially in weak magnetic fields, so the results by full CI method with Gaussian basis [12,13] are much closer to the results by

TABLE V. Total energies E of $1\ ^1(-2)^+$ and $2\ ^1(-2)^+$ states for helium atom as a function of magnetic field strength γ.

	$1\ ^1(-2)^+$					$2\ ^1(-2)^+$	
γ	E	$E_{\text{lit[14]}}$	$E_{\text{lit[11]}}$	$E_{\text{lit[9]}}$	$\bar{r}_{12}$	E	$E_{\text{lit[11]}}$
0	−2.055619(8)	−2.055619	−2.055619	−2.05562	21.0279	−2.03127(89)	−2.031279
0.01	−2.06430(43)	−2.064304			20.4871	−2.03659(77)	
0.02	−2.07072(73)	−2.070727	−2.070739		19.3691	−2.03635(13)	−2.036364
0.05	−2.08184(67)	−2.081843			16.2989	−2.02863(84)	
0.1	−2.08744(06)	−2.087439			13.3052	−2.01278(20)	
0.2	−2.07938(23)	−2.079374		−2.07949	10.4516	−1.97343(77)	
0.5	−2.00092(04)	−2.000892	−2.000873		7.3953	−1.83016(89)	−1.830171
1	−1.79907(02)	−1.798998	−1.798963	−1.80500	5.6789	−1.55316(36)	−1.553161
2	−1.27276(45)	−1.272606	−1.272473		4.3833	−0.91884(77)	−0.918836
5	0.73380(73)	0.734027	0.734276		3.1227	1.30136(72)	1.301338
10	4.63570(36)	4.636247	4.636327		2.4137	5.43565(95)	5.435657
20	13.17371(42)	13.174041	13.174417		1.8681	14.28387(69)	14.283868
50	40.55810(80)	40.558421	40.558628		1.3439	42.22475(60)	42.224693
100	87.94916(39)	87.949409	87.949762		1.0599	90.11899(91)	91.119604

methods in spherical coordinates than the $^1 0^+$ case [9,10]. While increasing the field strength directed at z, the distribution of electron density will be constricted into a smaller extent in z as well as the xy plane. Therefore, our upper bound energies of $1\ ^1(-1)^+$ and $1\ ^1(-2)^+$ states for helium atom also have reasonable improvement over corresponding results by full CI method with Gaussian basis [12,13] and with incomplete Hylleraas-Gaussian basis [14]. In the weak field region, our results of $1\ ^1(-1)^+$ state are only about 6.0×10^{-5} lower than the related results in Ref. [12], about $1.0–5.0 \times 10^{-4}$ lower in the field region of $0.5 \leq \gamma \leq 2$ a.u. and about $7.6–10.5 \times 10^{-4}$ lower in the field region of $2 < \gamma \leq 100$ a.u.. Compared to energies of $1\ ^1(-1)^+$ states in our previous work [14], our results are about $1.6–5.1 \times 10^{-5}$ lower in the field region of $0 \leq \gamma \leq 0.5$ a.u., and about $1.6–6.9 \times 10^{-4}$ lower in the field region of $0.5 < \gamma \leq 100$ a.u..

For the $1\ ^1(-2)^+$ case, all the methods come to same results at $\gamma=0$ a.u. because the correlation between electrons is relative small. Our data is even worse than the corresponding data of Becken *et al.* [13] at $\gamma=0.02$ a.u. possibly due to different optimization strategy. While increasing the field strength, the priority of the Hylleraas-Gaussian basis over the Gaussian basis becomes more and more obvious. Compared to the related data in Ref. [13], our data is only about 4.7×10^{-5} lower at $\gamma=0.05$ a.u. and about $1.0–7.0 \times 10^{-4}$ lower in the field region $0.5 < \gamma \leq 100$ a.u.. Compared to the data by the full CI method with incomplete Hylleraas-Gaussian basis [14], the results in this work are about $3.2 \times 10^{-7}–8.3 \times 10^{-6}$ lower in the field region of $0 \leq \gamma \leq 0.2$ a.u., $2.8–7.2 \times 10^{-5}$ lower in the field region of $0.5 \leq \gamma \leq 1$ a.u., and $1.5–5.4 \times 10^{-4}$ lower in the field region of $2 \leq \gamma \leq 100$ a.u..

In Ref. [14] we mainly discussed the priority of the incomplete Hylleraas-Gaussian basis over the Gaussian basis, and drew an initial conclusion that the incomplete Hylleraas-Gaussian basis is more efficient when the average value of r_{12} is less than 4.5 a.u. In this work, we also focus on the comparison between the Hylleraas-Gaussian basis and the Gaussian basis. As the average value of $\bar{r}_{12}$ for $1\ ^1 0^+$ state is relative small ($\bar{r}_{12} \leq 2.9357$ a.u.), more than 1×10^{-4} improvement in the precision of energies has been made in the whole field regime. In $^1(-1)^+$ state and $^1(-2)^+$ state, more than 1×10^{-4} improvement has been achieved when $\gamma \geq 0.5$ a.u. ($\bar{r}_{12} \leq 5.7072$) and $\gamma \geq 1.0$ a.u. ($\bar{r}_{12} \leq 5.6789$), respectively. For the three states concerned here, more than 5×10^{-4} improvement has been maintained when $\gamma \geq 1.0$ a.u. ($\bar{r}_{12} \leq 2.6049$), $\gamma \geq 5.0$ a.u. ($\bar{r}_{12} \leq 2.4839$), and $\gamma \geq 10.0$ a.u. ($\bar{r}_{12} \leq 2.4137$), respectively. So we can draw the final conclusion than more than 1×10^{-4} improvement has been achieved when $\bar{r}_{12}$ is less than 5.67 a.u. and more than 5×10^{-4} improvement has been achieved when $\bar{r}_{12}$ is less than 2.41 a.u.

IV. CONCLUSION

By including the approximate expansions of r_{12}^1 and $r_{12}^{1/2}$ terms in the Hylleraas-Gaussian basis, the precision of helium ground and low-lying states energies has been improved significantly in the whole field region, and the limitation of incomplete Hylleraas-Gaussian basis applied in our recent paper [14] has been surpassed. Most of our results have improvement at 10^{-4} order in precision compared to the results of full CI method with Gaussian basis or with incomplete Hylleraas-Gaussian basis, especially when the electrons are restricted in small spatial extent in a strong magnetic field. As the linear dependences of large number of basis functions prevent the further improvement of precision, to develop a technique about the parameters optimizing and choosing should be helpful. The efficiency of the approximate expansions of r_{12}^n also should be further studied to apply this method to other more complicated atomic or molecular systems.

All our computational work has been carried out on a personal computer with $2.66\text{G} \times 4$ CPU and 6 GB RAM.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China under Grant No. 10874133.

[1] J. C. Kemp, J. B. Swedlund, J. D. Landstreet, and J. R. P. Angel, Astrophys. J. **161**, L77 (1970).
[2] J. Truemper, W. Pietsch, C. Reppin, W. Voges, R. Staubert, and E. Kendziorra, Astrophys. J. **219**, L105 (1978).
[3] H. Ruder, G. Wunner, H. Herold, and F. Geyer, *Atoms in Strong Magnetic Fields* (Springer, Berlin, 1994).
[4] P. Schmelcher and W. Schweizer, *Atoms and Molecules in Strong External Fields* (Springer, Berlin, 1998).
[5] M. D. Jones, G. Ortiz, and D. M. Ceperley, Phys. Rev. E **55**, 6202 (1997).
[6] M. D. Jones, G. Ortiz, and D. M. Ceperley, Phys. Rev. A **59**, 2875 (1999).
[7] A. Thirumalai and J. S. Heyl, Phys. Rev. A **79**, 012514 (2009).
[8] M. Braun, W. Schweizer, and H. Elster, Phys. Rev. A **57**, 3739 (1998).
[9] A. Scrinzi, Phys. Rev. A **58**, 3879 (1998).
[10] M. Hesse and D. Baye, J. Phys. B **37**, 3937 (2004).
[11] W. Becken, P. Schmelcher, and F. K. Diakonos, J. Phys. B **32**, 1557 (1999).
[12] W. Becken and P. Schmelcher, J. Phys. B **33**, 545 (2000).
[13] W. Becken and P. Schmelcher, Phys. Rev. A **63**, 053412 (2001).
[14] X. F. Wang and H. X. Qiao, Phys. Rev. A **77**, 043414 (2008).
[15] C. Aldrich and R. L. Greene, Phys. Status Solidi **93**, 343 (1979) b.
[16] E. A. Hylleraas, Z. Phys. **54**, 347 (1929).
[17] B. J. Persson and P. R. Taylor, J. Chem. Phys. **105**, 5915 (1996).
[18] H. M. Schwartz, Phys. Rev. **103**, 110 (1956).
[19] G. W. F. Drake, M. M. Cassar, and R. A. Nistor, Phys. Rev. A **65**, 054501 (2002).