Calculation of the energy levels of a hydrogen atom in a magnetic field of arbitrary strength by using B splines

Jang-Haur Wang and Chen-Shiung Hsue
Institute of Physics, National Tsing Hua University, Hsinchu, Taiwan 30043, Republic of China
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B splines with carefully adjusted knot sequences are used as basis functions in cylindrical coordinates to calculate the energy levels of the low-lying ($m=0$) states of a hydrogen atom in a uniform magnetic field of arbitrary strength by using the variational method. The strength of the field calculated covers a range from $\gamma=0$ to $\gamma=100\,000$ for the ground state and up to $\gamma=2000$ for the $2s$ and $2p$ states. A precision of up to ten digits in the region of $0\leqslant\gamma\leqslant200$ and up to eight digits for $\gamma>200$ has been maintained for all the results presented. In order to test the applicability of the B splines for the higher excited states, the energy levels of $3s$, $3p$, $3d$, and $4f$ states with $m=0$ in the field region of $0\leqslant\gamma\leqslant10$ have also been calculated. Even though the number of basis sets was kept constant, the accuracy of the results was maintained in the intermediate field regions and also in the very strong field regions, which are known to be difficult for achieving high accuracy. The flexibility of the B splines is demonstrated here by the uniformly accurate results in the transition from spherical symmetry to Landau symmetry as the field strength of the magnetic field is increased. The energy levels of all the low-lying states with various ranges of magnetic field strength have been compared with published values. They are in good agreement with the most updated values and compare favorably with all other published results.

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I. INTRODUCTION

Strong magnetic fields have been of interest for some time in solid-state physics, astrophysics, surface physics, and plasma physics. In particular, the discovery of extremely high fields in white dwarf stars and neutron stars has renewed interest in the investigation of the energy levels of the hydrogen atom in very strong magnetic fields. The problem of a hydrogen atom in a uniform magnetic field of arbitrary strength is made difficult by the nonseparability of the Schrödinger equation for an electron under the combined effects of the nuclear Coulombic electric field and the external uniform magnetic field and from the fact that as the strength of the magnetic field increases the symmetry of the problem changes from spherical (Coulomb symmetry as $B\rightarrow0$) to cylindrical (Landau symmetry as $B\rightarrow\infty$). This problem has been considered in numerous theoretical and experimental works. Details and references on these research may be found in the articles by Brandi [1], Garstang [2], Simola and Virtamo [3], Avron, Herbst, and Simon [4], Aldrich and Greene [5], Starace and Webster [6], Lindgren and Virtamo [7], Pavlov-Verevkin and Zhilinskii [8], Doman [9], Wunner, Ruder, and Herold [10], Clark [11,12], Wadehra [13], Ruder *et al.* [14,15], Avron [16], Cohen and Hermann [17], Friedrich [18], Chen [19–21], Le Guillou and Zinn-Justin [22], Rösner *et al.* [23,24], Forster *et al.* [25], Delande and Gay [26,27], Galas [28], Grozdanov and Tayior [29], Rech, Gallas, and Gallas [30], Liu and Starace [31], Ivanov [32], Handy *et al.* [33], Johnson, Blundell, and Sapirstein [34], Shertzer [35], Baye and Vincke [36], Fonte *et al.* [37], O'Mahony and Mota-Furtado [38], Chen and Goldman [39–41], and Xi *et al.* [42]. Methods for the solutions of such equations with nonseparable variables used include expansion of the wave functions, group theoretical method [26,27], second-order perturbation [29], variational method [23–25,29,37], finite-difference approximation [33], finite-element method [35], finite basis expansion [39–41], R-matrix method [38], Lagrange basis [36], and B splines basis [42], etc. Some of these works achieved partial success in the treatment of special aspects of the problem, such as in low fields, very high fields, or intermediate fields etc. In 1984, Rösner *et al.* [24] calculated the energy levels with high accuracy for some low-lying states of the problem. They expanded the wave functions either in terms of spherical harmonics (for weak and moderate fields) or in terms of Landau states (for strong and very strong fields). The results of their numerical calculation in the case of weak and very strong fields were accurate. But in the transition region they could not obtain accurate results. Ivanov [32] supplemented these works in the intermediate field and obtained somewhat better results by using a finite-difference method. Chen and Goldman [39–41] used a finite basis expansion with a basis set composed of products of Slater- and Landau-type functions, in the variational method for both the relativistic and nonrelativistic calculations. They obtained very accurate results. Xi *et al.* [42] expanded the wave functions by using the B splines as the basis set in the spherical coordinate system. They could handle accurately the problem in the transition region for which most of the other methods had difficulties in achieving high accuracy. But they could not achieve the same degree of accuracy for the very strong fields ($\gamma\geqslant100$).

In this paper, we report a calculation by using B splines in the cylindrical coordinate system with the variational method. It is shown here that the highly localized piecewise polynomials of the B splines with carefully adjusted knot sequences can efficiently handle the problem of a hydrogen atom in the magnetic fields of arbitrary strength. As we are also interested in the behavior of a hydrogen atom in very

high magnetic field strength, the cylindrical coordinate system is adopted.

The aim of the present work is to calculate with a high degree of accuracy energy levels of low-lying states in the presence of a uniform magnetic field of arbitrary strength B over the whole range of $0 \leq B \leq 2.35 \times 10^{11}$ T. Section II serves to describe the variational method and the numerical treatment used. In Sec. III, we compare our results with other theoretical calculations. Discussions and conclusions are given in the final section.

II. METHOD AND NUMERICAL TREATMENT

The nonrelativistic Hamiltonian of a hydrogen atom in a uniform magnetic field B, which is assumed to be in the z direction, may be written in the cylindrical coordinate system as

$$H = -\nabla^2 - \frac{2}{r} + \gamma(L_z - 1) + \frac{\gamma^2}{4}\rho^2, \tag{1}$$

with

$$r = \sqrt{\rho^2 + z^2} \quad \text{and} \quad \rho^2 = x^2 + y^2,$$

where the magnetic field strength B is expressed in units of $B_0 = 2\alpha^2 m_e^2 c^2/(e\hbar) \approx 4.70 \times 10^5$ T and $\gamma = 2B/B_0$. In this work only the spin-down state is considered and the Rydberg atomic units (energies in units of 1 Ry $= \alpha^2 m_e c^2/2$, and lengths in units of Bohr radius $a_B = \hbar/\alpha m_e c$) are used. The energies of the corresponding spin-up state are obtained by adding a constant 2γ to that of the spin-down state.

First of all, the ϕ dependence of the eigenfunctions of Eq. (1) may be factored out,

$$\psi(\rho, z, \phi) = \psi(\rho, z) e^{im\phi} \ .$$

Only the states with $m = 0$ are considered in this work. The wave functions are then expressed as sums of products of B splines in the ρ and z variables as

$$\psi(\rho, z) = \sum_{ij} \alpha_{ij} B_i(\rho) B_j(z) \ .$$

The Schrödinger equation for the Hamiltonian may then be written as a generalized eigenvalue problem in a matrix form for the coefficients α's:

$$H\alpha = ES\alpha \, . \tag{2}$$

Equation (2) is solved iteratively by using the variational method based on the Galerkin method.

The advantage of the numerical treatment by using the B splines lies in the flexibility and simplicity. The B splines are piecewise polynomials and are completely determined by the given order k, which is a non-negative integer, and the knot sequence τ consisting of a nondecreasing sequence of points $\tau = \{t_i\}$, $t_1 \leq t_2 \leq \cdots \leq t_{n-1} \leq t_n$. To be precise, the kth-order B splines are defined by the kth-order divided difference of truncated polynomials,

$$B_{i,k,\tau}(x) = (t_{i+k} - t_i)[t_i, \ldots, t_{i+1}](t - x)_+^{k-1},$$

where $(t-x)_+^{k-1}$ is the truncated polynomial of degree $k-1$,

$$(t-x)_+^{k-1} = \begin{cases} (t-x)^{k-1} & \text{for } t > x, \\ 0 & \text{for } t < x. \end{cases}$$

Further details of the B splines may be found in the excellent book by de Boor [43]. A completely equivalent definition for the B splines, which is more convenient for the purpose of numerical calculation, is through the following recursive formula:

$$B_{i,k,\tau}(x) = \frac{x - t_i}{t_{i+k+1} - t_i} B_{i,k-1,\tau}(x) + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} B_{i+1,k-1,\tau}(x),$$

with

$$B_{i,1,\tau}(x) = \begin{cases} 1 & \text{for } t_i \leq x \leq t_{i+1}, \\ 0 & \text{otherwise.} \end{cases}$$

From this definition, it can readily be seen that the B splines have finite support. Among the whole B splines basis set for a knot sequence τ with order k only the functions $B_{i-k+1,k,\tau}$, $B_{i-k+2,k,\tau}$, $\ldots$, $B_{i,k,\tau}$ are nonzero in the region $t_i \leq x \leq t_{i+1}$. Hence, the nonzero matrix elements constructed by the B splines are sparse. Another advantage of the B splines is their flexibility. By adjusting the values in the knot sequence, the B splines may be modified to accommodate for various needs arising from the specific physical situations. The regions with rapidly changing wave functions may be easily handled by a corresponding increase of the density of the knot sequence there. For example, as the magnetic field strength is increased, the range of the wave function expands in the ρ axis but shrinks in the z axis. This situation may be easily tackled by adjusting the knot sequences for the $\{\rho_i\}$ and $\{z_j\}$ accordingly. The order and number of the B splines have been kept at 7 and 56, respectively, for all calculations in this work.

III. RESULTS

We have calculated the energy levels of the low-lying ($m = 0$) states from $1s$ up to $4f$ of a hydrogen atom in uniform magnetic fields by using B splines. The strength of the fields covers a range from $\gamma = 0$ to $\gamma = 100\,000$ for the ground state and up to $\gamma = 2000$ for the $2s$ and $2p$ states. The results are tabulated in Tables I–III and compared with those published in the literature.

Our results of the energies in the ground state are listed in the last column of Table I. The precision of the calculation is high and stable. An accuracy of up to ten digits for the energies in the region $0 \leq \gamma \leq 200$ and up to eight digits for $\gamma > 200$ has been maintained. Given in the first column are the lower and upper bounds of the energies obtained by Fonte *et al.* [37] and by Liu and Starace [31]. Fonte *et al.* used a variational method employing semiparabolic coordinates and a harmonic-oscillator basis. They gave error estimates for both the eigenvalues and the eigenfunctions. They have difficulties in strong magnetic fields. Liu and Starace proposed an adiabatic approximation in the cylindrical coordinate system employing a single configuration wave func-

TABLE I. Ground-state energies (in units of Rydberg atomic units) for a hydrogen atom in a uniform magnetic field of arbitrary strength. a: Lower (upper bound): F denotes Fonte *et al.* [37] variational. L denotes Liu and Starace [31] cylindrical adiabatic approximation. b: Chen and Goldman [41]: basis expansion and variation method. c: Rösner *et al.* [23,24]: numerical multiconfiguration Hartree-Fock method. d: Ivanov [32]: finite-difference method. e: Xi *et al.* [42]: B splines basis expansion in spherical coordinate system. f: Present work. Numbers in parentheses represent the upper bound of the energy values.

γ	a	b	c	d	e	f
0					1.00000000	1.0000000000
0.0002			1.000200		1.00019998	1.0001999800
0.002			1.001988		1.00199800	1.1001998000
0.02			1.019800		1.01980009	1.0198000878
0.2			1.180763		1.18076313	1.1807631235
1	$1.662337793(5)^F$	1.66233779346	1.662338		1.66233778	1.6623377850
2	$2.044427815(20)^F$	2.04442781532	2.044428		2.0444277	2.0444278053
3	$2.32906598(614)^F$	2.3290659786	2.329066		2.3290659	2.3290659662
4			2.561596		2.5615958	2.5615960169
5	$2.5364(818)^L$				2.7607954	2.7607977148
6			2.936492		2.9364918	2.9364919568
7					3.0945431	3.0945432264
8					3.2387697	3.2387699647
9					3.3718149	3.3718152944
10	$4.430791(1825)^F$		3.495594		3.4955939	3.4955942951
12					3.7207760	3.7207765486
14			3.922425	3.9224234	3.9224247	3.9224250960
15					4.0161278	4.0161281686
16					4.1057577	4.1057580851
18					4.2743561	4.2743563664
20		4.430797030	4.430797	4.430797	4.4307967	4.4307969687
22					4.5770037	4.5770038684
24					4.7144561	4.7144562474
25	$4.5864(8174)^L$				4.7802730	4.7802731438
26					4.8443185	4.8443186382
28					4.9675262	4.9675263316
30			5.084843	5.084834	5.0848431	5.0848431942
32					5.1969021	5.1969021186
34					5.3042341	5.3042340504
36					5.4072893	5.4072892877
38					5.5064535	5.5064534192
40			5.602058(60)	5.602054	5.6020596	5.6020594559
100	$7.4720(6054)^L$		7.5781(805)	7.57958	7.57961	7.5796079443
200	$9.2924(4774)^L$	9.454290216	9.4531(50)	9.45423	9.45432	9.4542886885
400			11.7023(39)	11.70324	11.7036	11.70329920
1000			15.3241(53)	15.32473	15.329	15.32483814
2000	$8.5508(6204)^L$	18.6095300	18.60896(986)	18.60931	18.63	18.60951488
5000		23.746816				23.7467269
10000						28.2816839
50000						41.1594818
100000						47.7829865

tion. They provided both upper and lower bounds for the binding energies of the ground state of a hydrogen atom in strong magnetic fields. Our values basically fall within most of the error bounds of both works. Listed in the second column are the available results of Chen and Goldman [41], which are considered one of the most updated values. In the region of low to intermediate field strength, our results agree with their calculations for the first 7–9 digits. In very strong magnetic fields the agreement is reduced to 5–7 digits. The results of Rösner *et al.* [24] and Ivanov [32] are displayed in the third and fourth columns, respectively. Rösner *et al.* used a numerical multiconfiguration Hartree-Fock method to obtain energies in the weak and in the very strong field strength with an accuracy of seven digits. The precision of their results in the region of $\gamma \geqslant 40$ is less accurate. Ivanov used a finite-difference method to improve the results of Rösner *et al.* in the transition region. The precision of Ivanov's results was 7–8 digits. Our results are in good agreement with the results of Ivanov, but maintain a higher degree of accuracy. Finally, listed in the fifth column are the results of Xi

TABLE II. Energies of $2p$ ($m=0$) state (in units of Rydberg atomic units) for a hydrogen atom in a uniform magnetic field of arbitrary strength. a: Ivanov [32]: finite-difference method. b: Rösner *et al.* [23,24]: numerical multiconfiguration Hartree-Fock method. c: Xi *et al.* [42]: *B* splines basis expansion in spherical coordinate system. d: Present work.

γ	a	b	c	d
0			0.25000000	0.25000000
0.0002		0.2501999	0.25019988	0.25019988
0.001		0.2509970	0.25099700	0.25099700
0.002		0.2519880	0.25198800	0.25198800
0.01	0.25970082	0.2597008	0.25970083	0.25970083
0.02	0.26881293	0.2688129	0.26881293	0.26881293
0.04	0.28538742	0.2853874	0.28538742	0.28538741
0.06	0.30003254	0.3000325	0.30003254	0.30003253
0.1	0.3248202	0.3248202	0.32482016	0.32482015
0.14	0.3452365	0.3452365	0.34523645	0.34523644
0.2	0.3703681	0.3703681	0.37036808	0.37036807
0.3	0.40300823	0.4030083	0.40300827	0.40300828
0.4	0.42853095	0.4285310	0.42853099	0.42853100
0.6	0.4673572	0.4673569	0.46735693	0.46735693
1.0	0.5200137	0.5200132	0.52001323	0.52001323
1.4	0.5562670	0.5562670	0.5562670	0.55626701
2	0.5954217	0.5954219	0.5954217	0.59542194
3	0.6400803	0.6400802	0.6400801	0.64008036
4	0.671394	0.6713901(4)	0.6713909	0.67139145
6	0.714324	0.714320(31)	0.7143217	0.71432364
10	0.765308	0.7652975(3036)	0.7652994	0.76529969
14		0.7963735(76)	0.796374	0.79637498
20		0.8267545(72)	0.826753	0.82675546
40		0.8774672(83)	0.877467	0.87746760
60		0.9018597(604)	0.90186	0.90185996
100		0.9272354(7)	0.92723	0.92723438
140		0.9409211(3)	0.94092	0.94092118
200		0.9530640(1)	0.95305	0.95306399
400		0.9707261	0.9706	0.97072608
1000		0.9849900	0.984	0.98498997
2000		0.9911896	0.99	0.99118929

et al. [24] by using the *B* splines in the spherical coordinate. They achieved high accuracy in the region $\gamma<100$. Our results are in good agreement with theirs in this region. The degree of accuracy of their results is decreased as the magnetic field strength is increased, as the rate of convergence in their calculation for high magnetic fields is relatively slow. When $\gamma=2000$ they gave results with four digits only. In contrast, our results maintained a higher degree of accuracy in the region of very high magnetic field strength ($\gamma\geqslant 100$). We can summarize the above comparison in Table I as follows: In the region $0\leqslant\gamma<100$, our results are in good agreement with the results of Rösner *et al.*, Ivanov, and Xi *et al.* In the very strong magnetic fields ($100\leqslant\gamma\leqslant 2000$), the accuracy of the results of Rösner *et al.*, Ivanov, and Xi *et al.* are poor. The high degree of accuracy of our results has been maintained in this region and are in agreement with the results of Chen and Goldman for the first six digits. We have also calculated the energies with high accuracy for high magnetic field strength ($\gamma\geqslant 2000$). The result for $\gamma=5000$ agrees with that of Chen and Goldman up to five digits. We presented also the results in the region of very intense magnetic fields $\gamma\geqslant 100\,000$ where to our knowledge up to now no results have been published for the ground state.

In Table II, we list the energies of the low-lying excited $2p$ ($m=0$) states. The results of Ivanov, Rösner *et al.*, and Xi *et al.* are also listed in the table. Our results are in good agreement with those of other calculations in the region of $\gamma\leqslant 3$. The precision of the results is up to 6–8 digits of accuracy. In the region of $4\leqslant\gamma\leqslant 200$, the results of Rösner *et al.* are less accurate, and the accuracy of the results of Xi *et al.* decreases in this region. In contrast, we can easily obtain good results with a precision up to eight digits. In the region of very strong magnetic fields ($200<\gamma\leqslant 2000$), our results are in agreement with the result of Rösner *et al.* up to a precision of seven digits. The accuracy of the results of Xi *et al.* is very low in this region.

The energies of the $2s$ state are given in Table III, together with the results of Ivanov and of Rösner *et al.* We have maintained an accuracy of eight digits for all the energies. In the region of $\gamma\leqslant 1$, the published results of Rösner *et al.* have been maintained to an accuracy of seven digits and are in agreement with our results. In the region of

TABLE III. Energies of the $2s$ state (in units of Rydberg atomic units) for a hydrogen atom in a uniform magnetic field of arbitrary strength. a: Ivanov [32]: finite-difference method. b: Rösner *et al.* [23,24]: numerical multiconfiguration Hartree-Fock method. c: Present work.

γ	a	b	c
0			0.25000000
0.0002		0.2501997	0.25019971
0.001		0.2509930	0.25099300
0.002		0.2519720	0.25197200
0.01		0.2593031	0.25930312
0.02		0.2672484	0.26724835
0.04		0.2794796	0.27947964
0.06		0.2877269	0.28772692
0.1		0.2961783	0.29617830
0.14		0.2985628	0.29856275
0.2		0.2979734	0.29797334
0.3		0.2967346	0.29673460
0.4		0.2983327	0.29833268
0.6		0.3055311	0.30553113
1.0		0.3209379	0.32093795
1.4	0.3334499	0.3334492	0.33344962
2	0.347883	0.3478880	0.34788939
3	0.365144	0.365131(87)	0.36515383
4	0.377681	0.37762(85)	0.37769290
6	0.395508	0.39530(63)	0.39551564
10	0.417894	0.41777(98)	0.41790363
14	0.432454	0.43237(53)	0.43247238
20	0.4476701	0.44761(73)	0.44768422
40		0.476352(425)	0.47639850
60		0.492573(627)	0.49260765
100		0.512339(77)	0.51236192
140		0.524938(68)	0.52495663
200		0.537921(45)	0.53793620
400		0.562050(65)	0.56205587
1000		0.5917099(180)	0.59171424
2000		0.6124793(844)	0.61248116

$\gamma>3$, Rösner *et al.* gave only bounds with an accuracy of 4–5 digits. Our results as well as those of Ivanov have been maintained to an accuracy of 5–6 digits, which falls within the bounds.

In order to test the applicability of the B splines for higher excited states, we also calculated the energy levels of $3s$, $3p$, $3d$, and $4f$ states for $m=0$ in the field region of $0\leqslant\gamma\leqslant 10$. The results are tabulated in Table IV and Table V. Also included in the tables are the published results of Ivanov and of Rösner *et al.* for comparison. In the neighborhood of $0.2\leqslant\gamma\leqslant 0.3$ no results have been given by Rösner *et al.* Our results are also in agreement with the results of Ivanov and of Rösner *et al.* for an accuracy of 4–7 digits. The situation in the cases of $3s$, $3p$, $3d$, and $4f$ are similar to the cases of $2s$ and $2p$ states.

From the above comparison, it is demonstrated that our method is a powerful tool in handling the problem of a hydrogen atom in a magnetic field of arbitrary strength.

IV. DISCUSSION AND CONCLUSIONS

The problem of a hydrogen atom in an external magnetic field of arbitrary strength has been solved by various methods. For example, Rösner *et al.* calculated the energies of many low-lying states of the problem. They expanded the wave function either in terms of spherical harmonics (for weak and moderate fields) or in terms of Landau states (for strong and very strong fields), the r- and z-dependent expansion functions are determined with the use of an adopted version of the multiconfigurational Hartree-Fock code of Froese Fischer [44]. An accuracy of seven digits has been obtained in the region of weak and strong field strength for most of the low-lying states. Our results are in good agreement with theirs. But they could not obtain satisfactory results in the transition region between the Coulomb and Landau symmetries. A slightly improved result in the region of intermediate strength has been presented by Ivanov using a finite-difference method. In the basis expansion method, Chen and Goldman employed a basis set that combines together Slater-type and Landau-type functions. This basis set contains correct behavior at both the Coulomb limit ($B=0$) and the Landau limit ($B\rightarrow\infty$). The transition from Coulomb symmetry to Landau symmetry was smoothly achieved by varying two nonlinear parameters λ and β, which characterize the Coulomb and Landau orbitals, respectively. They have obtained accurate energies for the ground and low excited states of the problem for both relativistic and nonrelativistic calculations. The variational parameters λ and β play an important role for the efficiency of the method, and the incorporation of Landau-type functions in the basis set allowed them to achieve highly accurate results for the very strong magnetic fields. Suitable choices of the variational parameters as the field strength is varied allow them to achieve accurate results in the whole range of fields strength. Our results are in good agreement with the results of Chen and Goldman in the whole region for the ground state. Xi *et al.* also used the B splines as the basis set for expanding the wave function, but they employed the spherical coordinate system. They also obtained accurate results in the region $\gamma<100$. Our results are in very good agreement with their results in this region. But they were unable to achieve high accuracy in the very strong-magnetic field ($\gamma\geqslant 100$), because in the strong-magnetic-field region Landau symmetry dominates. This symmetry cannot be properly handled in the spherical coordinate system. On the other hand, their progress in this region was also hampered by the rapid increase of the size of the basis set.

In this paper, we have presented results of a successful application of the B splines basis in cylindrical coordinates for the calculation of energies of low-lying $1s$, $2s$, $2p$, $3s$,$3p$, $3d$, and $4f$ states of a hydrogen atom in magnetic fields of arbitrary strength. An accuracy of 8–10 digits has been maintained for all the energies in various states with arbitrary magnetic field strength. They compare favorably with the most updated published results. The high accuracy of the energies over the whole region including the region with very strong magnetic fields is achieved by carefully adjusting the knot sequences only. The B splines can easily handle the atom in the transition region where both

TABLE IV. Energies of $3s$, $3p$ $(m=0)$ states (in units of Rydberg atomic units) for a hydrogen atom in a uniform magnetic field of arbitrary strength. a: Ivanov [32]: finite-difference method. b: Rösner *et al.* [23,24]: numerical multiconfiguration Hartree-Fock method. c: Present work.

		$3s$			$3p$	
γ	a	b	c	a	b	c
0			0.11111111			0.11111111
0.0002		0.1113095	0.11130956		0.1113104	0.11131039
0.001		0.1120720	0.11207198		0.1120931	0.11209312
0.002		0.1129547	0.11295474		0.1130392	0.11306976
0.01		0.1173387	0.11733863		0.1193757	0.11937573
0.02		0.1172685	0.11726841		0.1247571	0.12475712
0.04		0.1065539(50)	0.10656056		0.1308128	0.13081275
0.06		0.09343459	0.09345169		0.1344065	0.13440650
0.1	0.08713344	0.08713337	0.08713731		0.1397834	0.13978337
0.14	0.0862250	0.08622455(551)	0.08622492		0.1442643	0.14426424
0.2	0.0830400		0.08303934		0.1498509	0.14985090
0.3	0.075656		0.07568542		0.1570134	0.15701336
0.4	0.072072	0.0694(720)	0.07207151	0.162446	0.1624457	0.16244568
0.6	0.070700	0.07022(84)	0.07076951	0.1703662	0.1703659	0.17036638
1.0	0.071458	0.07128(53)	0.07146367	0.1804491	0.180441(63)	0.18044898
1.4	0.0724765	0.07238(53)	0.07248119	0.1869843	0.186979(93)	0.18698412
2	0.073710	0.073658(753)	0.07372298		0.1937062(144)	0.19370916
3	0.075195	0.075172(231)	0.07521137		0.2010007(54)	0.20100238
4	0.07626	0.076249(91)	0.07627660		0.2059002(34)	0.20590129
6	0.07775	0.077741(69)	0.07775927		0.2123613(32)	0.21236194
10		0.079554(72)	0.07956546		0.2196909(18)	0.21969114

TABLE V. Energies of $3d$, $4f$ $(m=0)$ states (in units of Rydberg atomic units) for a hydrogen atom in a uniform magnetic field of arbitrary strength. a: Ivanov [32]: finite-difference method. b: Rösner *et al.* [23,24]: numerical multiconfiguration Hartree-Fock method. c: Present work.

		$3d$			$4f$	
γ	a	b	c	a	b	c
0			0.11111111			0.06250000
0.0002		0.1113107	0.11310689		0.06269893	0.06269693
0.001		0.1121008	0.11210076		0.06347332	0.06347319
0.002		0.1130698	0.11306976		0.06439456	0.06439344
0.01		0.1200958	0.12009583		0.07001254	0.07001241
0.02		0.1272339	0.12723386		0.07380055	0.07380038
0.04		0.1373908	0.13739075		0.07607329	0.07606243
0.06		0.1438266	0.14382657		0.07613841	0.07613813
0.1		0.1498760	0.14987603	0.07648	0.07647957	0.07647923
0.14		0.1501991	0.15019906	0.077508	0.07738(67)	0.07750556
0.2		0.1451139	0.14511383	0.079192	0.07913(27)	0.07918930
0.3	0.1353427	0.1353427	0.13534274	0.081562	0.081535(97)	0.08155964
0.4	0.130985	0.1284(315)	0.13097442	0.083387	0.083385(421)	0.08339919
0.6	0.129795	0.1287(301)	0.12979562	0.086083	0.086074(92)	0.08608101
1.0	0.1324671	0.13202(63)	0.13246604		0.0894514(93)	0.08945428
1.4	0.1352546	0.13499(537)	0.13525446		0.0916065(113)	0.09160822
2	0.138574	0.13841(65)	0.13857978		0.0937956(84)	0.09379658
3	0.142547	0.14245(60)	0.14255444		0.0961373(89)	0.09613790
4	0.145400	0.14533(45)	0.14540915		0.0976912(31)	0.09769242
6	0.1493976	0.149356(431)	0.14940534		0.09972083(145)	0.09972097
10	0.154311	0.154286(333)	0.15431648		0.1019939(42)	0.01019938

Slater- and Landau-type functions alone cannot achieve high accuracy. An advantage of the method is the fact that the Hamiltonian matrix constructed from the B splines basis is sparse and the evaluation of the matrix elements is straightforward. An efficient diagonalization package utilizing the sparseness of the matrix elements was developed. The convergence of the diagonalization procedure is fast, stable, and the demand on the memory space of the computer is reasonable. In contrast to the results of Xi *et al.*, we have demonstrated the applicability of the B splines for a hydrogen atom even in the region with very strong magnetic fields.

Our results show that B splines can be successfully applied in accurate calculation of the nonrelativistic problem of a hydrogen atom in a uniform magnetic field of arbitrary strength. The accuracy of these results warrants the relevance of further studies on the additional corrections such as the relativistic effect, the finite-nuclear-size correction, and the effects of finite nuclear mass. Further application of the B splines to these effects as well as $m \neq 0$ excited states will be presented in a future work.

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