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SOLVING THE SCHRÖDINGER AND DIRAC EQUATIONS FOR A HYDROGEN ATOM IN THE UNIVERSE'S STRONGEST MAGNETIC FIELDS WITH THE FREE COMPLEMENT METHOD

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ABSTRACT

The free complement method for solving the Schrödinger and Dirac equations has been applied to the hydrogen atom in extremely strong magnetic fields. For very strong fields such as those observed on the surfaces of white dwarf and neutron stars, we calculate the highly accurate non-relativistic and relativistic energies of the hydrogen atom. We extended the calculations up to field strengths that exceed the strongest magnetic field ($\sim 10^{15}$ G) ever observed in the universe on a magnetar surface. These are the first reported accurate quantum mechanical calculations ever to include such strong fields. Certain excited state bands in extremely strong fields showed perfect diamagnetism with an infinite number of degenerate states with the same energies as for a hydrogen atom in the absence of a field. Our method of solving the Schrödinger and Dirac equations provides an accurate theoretical methodology for studying phenomena that occur under strong magnetic fields.

Key words: ISM: atoms – magnetic fields – relativistic processes – stars: magnetars – stars: neutron – white dwarfs

1. INTRODUCTION

Since Zeeman (1897) first observed the splitting of an atomic spectral line under a magnetic field in 1896, atoms and molecules in magnetic fields have been extensively studied both theoretically and experimentally. Several new sciences have been born from such research (Ruder et al. 1994). For astronomy, magnetic fields play an important role in various situations in space, for example, white dwarf, neutron star, interstellar space, the Sun, and even on the Earth. Interstellar magnetic fields were already discovered by Jansky (1932) who first detected the radio emission from the Milky Way. In this region, the dominant species should be hydrogen and the Zeeman splitting related to the hyperfine structure of a neutral hydrogen atom has been studied extensively with radio spectroscopy (Bolton & Wild 1957; Smith 1968). Magnetic fields may even have a crucial role in star evolution. Chemical and material sciences based on the quantum mechanical principle in strong magnetic fields would be very important for understanding material compositions in interstellar regions and binary systems. In compact objects, very strong magnetic fields have been observed on the surfaces of white dwarfs (10^6–10^9 G) and neutron stars ($\sim 10^{13}$ G; Ruder et al. 1994; Schmidt et al. 1996; Lai 2001; Mori & Ho 2007). Recently, even stronger fields ($\sim 10^{15}$ G) were observed on the surface of a magnetar, an object that was predicted by a theoretical simulation by Duncan & Thompson (1992) and experimentally observed by Kouveliotou et al. (1998). These are the strongest magnetic fields ever observed in the universe.

In such a strong magnetic field, unknown interesting chemistry and phenomena may be found in the studies of atoms and molecules because spin–magnetic interactions are common in the interstellar space and may even become dominant over the ordinary Coulomb forces. New concepts may be derived from the super-strong interactions between spin and magnetic field. The present study is a first step for us in this direction. Since humans cannot generate such strong magnetic fields beyond 10^7 G in the laboratory on the Earth yet, we have to rely on observations in space and highly reliable theoretical studies of quantum molecular science. In other words, for the science of the super-strong magnetic fields, only "space" is a real experimental field: it is very interesting for quantum molecular science to demonstrate the relativistic and quantum electrodynamic (QED) effects interacting with the super-strong magnetic fields. Such strong fields exist only in space. Combining the theoretical considerations with the real observations in astronomy would open an important interdisciplinary field of astronomy and molecular science. However, in spite of their importance, there are almost no accurate quantum mechanical studies for the atomic and molecular systems under super strong magnetic fields over neutron star class.

As a first step of such studies, in the present paper we solve the Schrödinger equation (SE) and the relativistic Dirac equation (DE) very accurately for the hydrogen atom in extremely strong magnetic fields. In spite of its apparent simplicity, we have never known its exact solutions. Many theoretical studies have been reported for the hydrogen atom (Ruder et al. 1994; Chen & Goldman 1992; Kravchenko et al. 1996; Stubbins et al. 2004; Thirumalai & Heyl 2009) and for the hydrogen molecular ion (Vincke & Baye 2006), but several obstacles prevented the solutions since the strong vector potential of the magnetic field competes with the scalar Coulomb potential (Ruder et al. 1994). Chen & Goldman (Chen & Goldman 1992) first provided accurate solutions of both the SE and DE using the variational approach. Stubbins et al. (Stubbins et al. 2004) introduced parabolic coordinates in the SE to represent a highly distorted wave function in strong fields. This approach provided accurate and stable solutions for the very strong fields found in neutron stars (5×10^3 atomic units (a.u.) = $\sim 10^{13}$ G, where 1 a.u. $\approx 2.35 \times 10^9$ G).

We introduce a free complement (FC) method that provides a fast converging series to the exact wave function of the SE and DE in an analytical expansion form (Nakatsuji 2000, 2004, 2005; Nakatsuji et al. 2007; Nakashima & Nakatsuji 2007, 2008). We increase the magnetic field strength to $\sim 5 \times 10^5$ a.u. ($\sim 10^{15}$ G), corresponding to the universe's strongest level (Duncan & Thompson 1992; Kouveliotou et al. 1998), and finally up to $\sim 5 \times 10^9$ a.u. ($\sim 10^{19}$ G) for the SE and $\sim 5 \times 10^6$ a.u. ($\sim 10^{16}$ G) for the DE. To our knowledge,

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accurate quantum mechanical calculations of the hydrogen atom in magnetic fields beyond 5×10^3 a.u. have not been previously performed. This should also be the first time very accurate calculations are performed considering the relativistic effects: we found that the relativistic corrections and the effect of nuclear magnetic moment are significant in super strong magnetic fields. These data would be helpful, for example, when we want to investigate the magnetic field strength of a star by comparing the real observations to the theoretical values.

In the present paper, our aim is twofold: to show the accuracy and reliability of our theory and to provide physical considerations which are important for space physics and chemistry in strong magnetic fields. Highly accurate calculations of atoms in their ground and excited states are useful not only for understanding spectroscopic observations in astronomy (Ruder et al. 1994; Schmidt et al. 1996; Lai 2001; Mori & Ho 2007; Duncan & Thompson 1992; Kouveliotou et al. 1998), but also for condensed-matter physics (Praddaude 1972) and chaos studies (Delande & Gay 1986).

2. THEORY AND FORMULA

2.1. Hamiltonian in Magnetic Fields

The electronic Hamiltonian of the SE of the hydrogen atom in a magnetic field can be written in atomic units as

$$H = \frac{1}{2}\mathbf{p}^2 + \frac{1}{2}\mathbf{A}^2 + \mathbf{A}\cdot\mathbf{p} + \frac{1}{2}\sigma\cdot rot\mathbf{A} - \frac{1}{r}, \tag{1}$$

where $\mathbf{p}$ and $\mathbf{A}$ are the momentum operator and vector potential, respectively, and σ is the Pauli spin matrix. For a uniform magnetic field $\mathbf{B}$, $\mathbf{A} = \mathbf{B}/2 \times \mathbf{r}$ with the Coulomb gauge. We fix the direction of the magnetic field to the z-axis, $\mathbf{B} = (0, 0, B)$, without losing generality. The last term represents the scalar Coulomb potential, where r is the nucleus–electron distance.

The Dirac Hamiltonian of the system under consideration is given by

$$H = \begin{pmatrix} \left[-\frac{1}{r} + c^2\right] I_{(2)} & c\left[\sigma\cdot(\mathbf{p}+\mathbf{A})\right] \\ c\left[\sigma\cdot(\mathbf{p}+\mathbf{A})\right] & \left[-\frac{1}{r} - c^2\right] I_{(2)} \end{pmatrix}, \tag{2}$$

where $I_{(2)}$ is a two-dimensional unit matrix and c is the speed of light or the inverse of the fine structure constant in atomic units: $c = 137.0359987652$ is used in this work (Kinoshita & Nio 2003; Karshenboim & Ivanov 2003). We furthermore examine the effect of the nuclear magnetic moment $\boldsymbol{\mu}$ mainly derived from nuclear spin, although it should be much smaller than the very strong external field. The additional vector potential is represented by $\mathbf{A}_\mu = 1/c^2 \cdot (\boldsymbol{\mu} \times \mathbf{r})/r^3$, where the point-charge nucleus model is employed.

2.2. Free Complement Wave Function and Variation Method

The FC method (originally referred to as the free iterative complement interaction method; Nakatsuji 2000, 2004; Nakatsuji 2005; Nakatsuji & Nakashima 2005) has been developed by the present authors to solve the SE and the DE of atoms and molecules very accurately (Nakatsuji et al. 2007; Nakashima & Nakatsuji 2007, 2008). One of the authors proposed a recurrence formula which is guaranteed to converge to the exact solution of the SE (Nakatsuji 2000, 2004). This series explicitly includes the Hamiltonian of the system,

$$\psi^{(n+1)} = [1 + C^{(n)} g(H - E^{(n)})]\psi^{(n)}, \tag{3}$$

where n is iteration number, $C^{(n)}$ is a variational parameter, g is a scaling function which is necessary to scale the Coulomb singularity in the Hamiltonian (Nakatsuji 2004), and $E^{(n)}$ is the expectation energy of $\psi^{(n)}$. To accelerate convergence, we may expand the right-hand side of Equation (3) and collect the independent functions $\{\phi_i^{(n)}\}$ with the independent coefficients $\{c_i^{(n)}\}$ and we get the FC wave function defined by

$$\psi = \sum_{i=1}^{M_n} c_i^{(n)} \phi_i^{(n)}. \tag{4}$$

Here, we call the iteration number "order n" and the number of independent functions "dimension M_n". The unknown coefficients $\{c_i^{(n)}\}$ are determined by applying the variational principle. This method is also applicable to the relativistic case without significant modifications except for an introduction of the inverse variational method (Nakatsuji 2005; Hill & Krauthauser 1994).

In the FC method, the wave function appropriate to the given system is automatically generated by its Hamiltonian given by Equations (1) or (2) (Nakatsuji 2000, 2004, 2005; Nakatsuji et al. 2007; Nakashima & Nakatsuji 2007, 2008). This brings a remarkable advantage that the FC method is easily applicable to the systems under an extreme environment. The non-relativistic wave function of the SE obtained by the FC method is

$$\psi = \sum_j \sum_i c_{i,j} \xi^{a_i} \eta^{b_i} \exp(-\kappa_j \xi - \lambda_j \eta - \omega_j \xi\eta) \cdot (\xi\eta)^{\frac{|m|}{2}} \exp(im\varphi) \pm (\xi \leftrightarrow \eta), \tag{5}$$

where a_i and b_i are nonnegative integers and κ_j, λ_j, and ω_j are the exponential parameters. We use parabolic coordinates, $\xi = r + z$, $\eta = r - z$, $\varphi = \tan^{-1}(y/x)$, appropriate for atoms in a very strong magnetic field. This wave function was generated from the starting initial function ψ_0, which is the Slater orbital with the Landau exponent (Landau & Lifschitz 1977) ($a_i = b_i = 0$ in Equation (5)), using the g function of $g = r = (\xi + \eta)/2$, which is necessary to scale the Coulomb singularity in the Hamiltonian (Nakatsuji 2004). For calculations of higher excited states, we used several sets of exponents. The quantum number m denotes the angular momentum around the z-axis. The last term of Equation (5) represents the parity in exchanging ξ and η. The coefficients $c_{i,j}$ are determined by the variational principle.

For the relativistic case, the FC wave function for the DE is represented by the four spinor wave functions $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)^T$ with

$$\psi_k = \sum_i c_i^{(k)} \xi^{a_i^{(k)}} \eta^{b_i^{(k)}} / (\xi + \eta)^{d_i^{(k)} + \delta} \cdot \exp(-\kappa\xi - \lambda\eta - \omega\xi\eta) \cdot (\xi\eta)^{\frac{|m_k|}{2}} \exp(im_k\varphi) \pm (-1)^k (\xi \leftrightarrow \eta), \tag{6}$$

where $k = 1, \ldots, 4$. $a_i^{(k)}$, $b_i^{(k)}$, and $d_i^{(k)}$ represent nonnegative integers satisfying the inequality $a_i^{(k)} + b_i^{(k)} - d_i^{(k)} \geqslant 0$. This wave function was generated from ψ_0, for which $a_i^{(k)} = b_i^{(k)} = 0$ and $d_i^{(k)} = 0$ for $k = 1, 2$ and $d_i^{(k)} = 1$ for $k = 3, 4$, and the g function, $g = 1 + r = 1 + (\xi + \eta)/2$. $m_k = J_z + (-1)^k \cdot 1/2$, where J_z represents the quantum number of the total angular momentum in the z-direction. δ is a noninteger value that describes a weak singularity at the nucleus–electron coalescence region.

Table 1
Nonrelativistic Energies of the Ground State of a Hydrogen Atom in Different Magnetic Fields

B (a.u.)	κ	λ	Energy (a.u.)	Ref. (1)
1	1.15	1.15	**−0.831168896733158035610298234503559705611004577717002209388184300295699656934350847856146741513327534829336**52976	−0.8311688967331580356102
5×10^2	7	3.5	**−6.257087674680561894010102367681545211777205209640199**2672	−6.2570876746805618940
5×10^3	20	5	**−11.873418282681209744546572815086010150477203**7798	−11.873418282681209744
5×10^4	35	6	**−20.580180557741971432410795124707830**767	
5×10^5	76	8.5	**−32.915252164723518976446267**2277	
5×10^6	126	11	**−49.2425605275670870**14413	
5×10^7	207	14	**−69.80569222088335**336	
5×10^8	311	19	**−94.7753875986**76842	
5×10^9	394	22	**−124.277796**777099	

Reference. (1) Stubbins et al. 2004.

An important feature of the relativistic FC method is that the balancing among different spinors is automatically taken care of in the generation step of the wave function (Nakatsuji 2005). The coefficients $c_i^{(k)}$ are determined by the inverse Hamiltonian variation method (Hill & Krauthauser 1994) that avoids the variational collapse problem in relativistic calculations. A noninteger power of δ makes analytical integrations difficult to evaluate in the case when κ and λ are different. We cannot neglect a weak singularity, which is an essential feature of the relativistic wave function, and therefore, we introduced a variation method on the scaled DE, $g^{(\delta)}(H - E)\psi = 0$ (Nakatsuji 2004), where $g^{(\delta)} = (\xi + \eta)^{-\delta}$. Then, the resultant integrals are almost the same as in the SE case and can be analytically evaluated. A similar idea was used by Sundholm & Pyykkö to avoid a similar integration difficulty (Sundholm et al. 1987). This method is also applicable to other systems that involve similar difficulties in solving the DE.

3. RESUTS AND DISCUSSION

3.1. Schrödinger Non-relativistic Case

First, we deal with the ground state ($m = 0$, beta spin, and gerade parity) of a hydrogen atom in the magnetic field of $B = 1$ (a.u.) with the FC wave function of Equation (5). κ and λ are set equal and roughly optimized, and $\omega = B/4$ since the Landau orbital is used for every calculation described in this paper. At the FC order $n = 100$ with the number of complement functions $M_n = 5151$, we obtain the energy **−0.831168896733158035610298234503559705611004577717002209388184300295699656934350847856146741513327534829336**529768079476 a.u., whose precision exceeds 100 digits. The number of significant digits was judged from the energy convergence behavior upon increasing the order of the FC calculations. To our knowledge, this is the highest number of significant digits calculated by the variation method to date. Throughout this paper, bold face is used to indicate figures expected to be correct.

Table 1 shows the energies of the ground state in different magnetic fields up to $B = 5 \times 10^9$ (a.u.) with the roughly optimized κ and λ; $\kappa \neq \lambda$ due to the highly distorted wave function (Stubbins et al. 2004). The calculations, except for $B = 1$ (a.u.), were performed at $n = 70$ and $M_n = 5040$. With $B = 5 \times 10^3$ (a.u.), the calculated energy has a precision exceeding 45 digits. We achieve a precision of 25–26 digits for $B = 5 \times 10^5$ (a.u.) (the universe's strongest field level) and 10–11 digits for $B = 5 \times 10^9$ (a.u.). For $B > 1$ (a.u.), the magnetic–spin interaction eclipses the Coulomb interaction. The stabilization energies by the magnetic field from zero-field solution were 11.37 a.u. (309.48 eV) for $B = 5 \times 10^3$ (a.u.) and 69.31 a.u. (1885.90 eV) for $B = 5 \times 10^7$ (a.u.), already reaching KeV order.

We calculated the expectation values of length of the ground state using the most accurate wave functions. For $B = 1$, 5×10^5, and 5×10^9 (a.u.), the expectation value $\langle r \rangle$ was 1.19196, 7.00223×10^{-2}, and 3.38197×10^{-2}, respectively, and the expectation value $\langle z^2 \rangle$ was 7.44660×10^{-1}, 9.36398×10^{-3} and 2.23840×10^{-3}, respectively. The electron approaches closer to the nucleus with increasing B, but not so much on the z-axis even in ultra-strong fields. On the other hand, the expectation value $\langle (x^2 + y^2)/2 \rangle$ was 5.35833×10^{-1}, $1.999950378 \times 10^{-6}$, and $1.999999988951 \times 10^{-10}$ for $B = 1$, 5×10^5, and 5×10^9 (a.u.), respectively. This quantity drastically decreases with increasing B and approaches the value, $1/B$, corresponding to the expectation value of the pure Landau orbital (Landau & Lifschitz 1977). The remaining difference from the value $1/B$ indicates that the Coulomb potential still affects the shape of the wave function even in very strong magnetic fields. The ratio $\langle z^2 \rangle^{1/2} / \langle (x^2 + y^2)/2 \rangle^{1/2}$, which represents the extent of distortion in the z-direction, was 1.17887, 6.84259×10^1, and 3.34544×10^3 for $B = 1$, 5×10^5, and 5×10^9 (a.u.), respectively. As B increases, the shape of the wave function becomes highly distorted and spindling along the z-axis.

3.2. Energy Spectral Curves of the Ground and Excited States Against the Strength of Magnetic Field

Understanding the behavior of the ground and excited state energy levels as a function of magnetic field strength would enable us to identify the magnitude of the magnetic field strength of a star under investigation for which one has the observed spectra of the hydrogen atom on the star. Alternatively, one may also predict the existence of hydrogen on a given star. We therefore calculated the energy spectra of the ground and many excited states of the hydrogen atom as a function of the applied magnetic field.

We calculated the FC wave functions of the hydrogen atom in their ground and excited states in the order $n = 15$. To describe several states, we included five different exponents in ψ_0 for every different symmetry. Figure 1 shows the plots of the energies of the 186 states in $B = 0.01$ to 10^6 (a.u.) on a logarithmic scale with $m = 0$ to -30 of both parities (only beta spin state). In Figure 1(a), a small plot for $B < 0.5$ (a.u.) includes higher-excited states with alpha spin solutions and describes complicated state-repulsions due to the competitions between the magnetic vector potential and the Coulomb potential from the nucleus. This certainly may produce a quantum chaotic

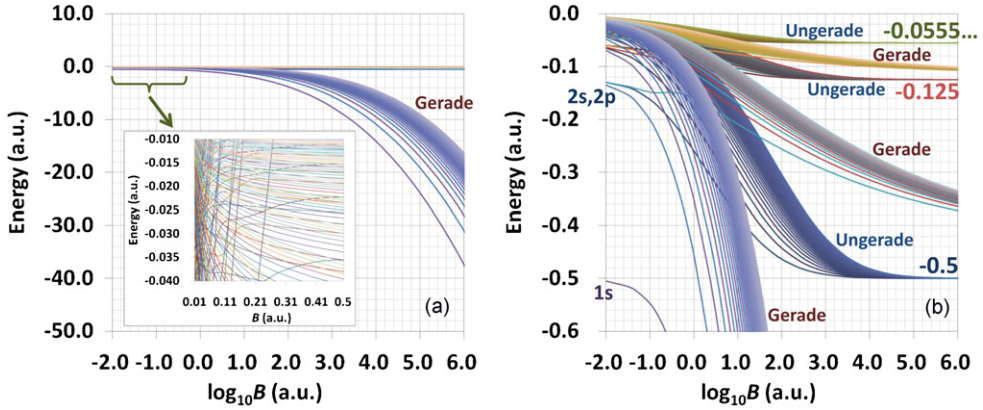

Figure 1. (a) Energy spectra curves for many excited states as a function of B. (b) Enlarged view of the energy region from −0.6 to 0.0 a.u.

phenomenon (Delande & Gay 1986). For $B > 1$ (a.u.), however, the chaotic behaviors disappear for the lower-level excited states, and some sets of the state curves begin to create band structure for $B > 100$ (a.u.). The lowest energy band consists of the lowest states on each m with gerade parity. The third and fifth lowest bands are also composed of gerade states. Similarly, the second, fourth, and sixth bands consist of ungerade states. The energies of the most stable band become drastically lower with increasing B, but the other bands are not so much stabilized by the strong magnetic field. Surprisingly, as B increases, the ungerade bands converge to −0.5, −0.125, and −0.0555 a.u., the energy eigenvalues of the free hydrogen atom, with perfect diamagnetism arising from an infinite number of degenerate states composed of $m = 0, -1, -2, \ldots$. Moreover, the energy curves starting from $2p$, $3p$, ... states in the zero field make up the lowest ungerade band converging to −0.5 a.u. This is equivalent to the 1 s state energy in the zero field.

These phenomena can be explained using the adiabatic approximation that separates the z-directional motion from the high-speed rotations on the x, y plane in a very strong magnetic field. In this treatment, the wave function on the x, y plane is exactly represented by the Landau orbital (Landau & Lifschitz 1977) and the motion along the z-axis is solved in the mean field potential after integration over the x, y plane. Since the Landau orbital approaches the Dirac-δ function as B becomes very strong, the mean field potential approaches $-1/|z|$ but the value at $z = 0$ is not infinite. This finite value is proportional to $\sqrt{B}$. The one-dimensional SE with potential $-1/|z|$ is the same as the radial SE of the free hydrogen atom. The ungerade solutions are not affected by the potential at $z = 0$ because their wave functions are always zero at $z = 0$. In contrast, the gerade solutions are largely affected by the potential around $z = 0$. The component states of the most stable band always have a non-zero wave function at $z = 0$ and become very low as B increases. Thus, the gerade solutions behave more intricately than the ungerade ones. For the ungerade states, the same energies as those of the free hydrogen atom are derived from the mean field potential on the z-direction and their infinite degeneracy comes from the degenerate Landau levels of $m = 0, -1, -2, \ldots$ on the x,y plane (Landau & Lifschitz 1977). If electron correlations exist as in hydrogen clusters or solids, this macro degeneracy may be removed and some interesting phenomena may appear.

3.3. Dirac Relativistic Case

Let us solve the DE of the present system. We performed the calculations for the ground state ($J_z = -1/2$) and the first excited state ($J_z = -3/2$) in magnetic fields up to $B = 5 \times 10^6$ (a.u.). As far as we know, as in the non-relativistic SE case, no solutions of the DE of the hydrogen atom in a field exceeding $B = 5 \times 10^3$ (a.u.) have been reported. The same exponents κ, λ, and ω were used as in the non-relativistic case, except for $B = 1$ (a.u.) where $\kappa = \lambda = 1$. $\delta = 1 - \sqrt{l^2 - (1/c)^2}$ was used with $l = -1$ and $l = -2$ for $J_z = -1/2$ and $J_z = -3/2$ states, respectively. In the $B = 1$ (a.u.) case, the calculations were performed with the ordinary energy variation method on $n = 15$ ($M_n = 1326$) for $J_z = -1/2$ and on $n = 15$ ($M_n = 1411$) for $J_z = -3/2$. For the other fields, the energy variation for the scaled DE was done on $n = 11$ ($M_n = 1405$) for $J_z = -1/2$ and on $n = 11$ ($M_n = 1495$) for $J_z = -3/2$. For these states, the wave functions have odd parities for the first and fourth components and even parities for the second and third components.

Table 2 shows the calculated energies of the DE in different magnetic fields from $B = 1$ to 5×10^6 (a.u.) The values are precise to about 20–21 digits and 13 digits for the cases of $B = 1$ and 5×10^3 (a.u.), respectively. These seem to represent the highest precision reported to date. Even for $B = 5 \times 10^6$ (a.u.), the accuracy retains eight digits. The excitation energy to $J_z = -3/2$ becomes larger as B grows, since the ground state is greatly stabilized by the strong magnetic field. The value $\Delta E_{\rm rel}$ shown in Table 2 is the energy difference between the relativistic and the non-relativistic energies. For $B = 1$ (a.u.) only, $\Delta E_{\rm rel}$ was negative. However, as B increases, the relativistic effect mainly influences the kinetic part because of the high-speed rotation on the x, y plane and $\Delta E_{\rm rel}$ changes to be positive and larger. For $B = 5 \times 10^6$ (a.u.), the relativistic correction reached 10^{-2} a.u. order (10 mH order) even for the lightest hydrogen atom.

3.4. Effect of the Nuclear Magnetic Moment in the Relativistic Level

Finally, we examined the effect of the nuclear magnetic moment and its interaction with external fields. The calculations were performed with the energy variation on the regular Hamiltonian with $\mathbf{A}_\mu$, as the integration does not diverge for $\mathbf{A}_\mu$ proportional to $1/r^2$. Table 2 shows the absolute energy $E_{+\mu}$ and the hyperfine splitting $\Delta E_\mu = E_{-\mu} - E_{+\mu}$. $E_{-\mu}$ is the energy for $\boldsymbol{\mu} = (0, 0, -\mu)$ and $E_{+\mu}$ is the one for $\boldsymbol{\mu} = (0, 0, +\mu)$, where the proton magnetic moment μ in a.u. is calculated from NIST 2006 data[2] by dividing $\mu_p = 1.410606662 \times 10^{-26}$ (J/T) by $1.854801830 \times 10^{-23}$ (J/T). Figure 2 illustrates the energy diagrams of the ground state with the total energies for

[2] NIST 2006, see http://physics.nist.gov/cuu/Constants/.

Table 2
Relativistic Energies Without and With $\mathbf{A}_\mu$ and Hyperfine Splitting of the Ground ($J_z = -1/2$) and First Excited ($J_z = -3/2$) States in Different Magnetic Fields

B (a.u.)	J_z	Energy (a.u.) Without $\mathbf{A}_\mu$	Energy (a.u.) With $\mathbf{A}_\mu$: $E_{+\mu}$	$\Delta E_{\rm rel}$ (a.u.)	ΔE_μ (a.u.)	Ref. (1)
1	$-1/2$	**−0.831173225931949858604**898	**−0.83117328917637**599	-4.32919×10^{-6}	$1.2648878243 \times 10^{-7}$	−0.831173226
	$-3/2$	**−0.4565972367504565531**701	**−0.4565972405190042903**5	-1.78326×10^{-7}	$7.53709524950 \times 10^{-9}$	−0.45659724
5×10^2	$-1/2$	**−6.25703258758415**206	**−6.25703499760**355	5.50870×10^{-5}	$4.82001558 \times 10^{-6}$	−6.2570326
	$-3/2$	**−4.53121620696889**230	**−4.53121655876**5117	3.01738×10^{-5}	$7.03592119 \times 10^{-7}$	
5×10^3	$-1/2$	**−11.87308840114**975	**−11.873099906**426	3.29881×10^{-4}	2.3010220×10^{-5}	−11.87308
	$-3/2$	**−9.0412182349**798	**−9.041220036**253	1.80428×10^{-4}	3.602538×10^{-6}	
5×10^4	$-1/2$	**−20.57885494676**216	**−20.57890691**136	1.32561×10^{-3}	1.0392480×10^{-4}	
	$-3/2$	**−16.34774466727**414	**−16.34775317**894	7.83333×10^{-4}	1.702330×10^{-5}	
5×10^5	$-1/2$	**−32.911133514**717	**−32.91135**488	4.118650×10^{-3}	4.4274×10^{-4}	
	$-3/2$	**−27.066308151**761	**−27.066345**642	2.633807×10^{-3}	7.4831×10^{-5}	
5×10^6	$-1/2$	**−49.231972**282	**−49.2328**679	1.058824×10^{-2}	1.7948×10^{-3}	
	$-3/2$	**−41.62849**255	**−41.6286**432	7.238773×10^{-3}	3.109×10^{-4}	

Reference. (1) Chen & Goldman 1992.

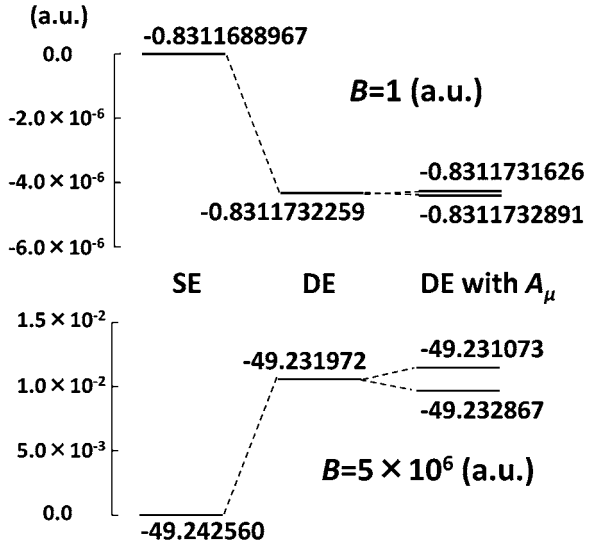

Figure 2. Energy diagrams and splitting in the SE and DE without and with $\mathbf{A}_\mu$.

$B = 1$ and 5×10^6 (a.u.) from the SE, DE, and DE with $\mathbf{A}_\mu$ ($\boldsymbol{\mu} = (0, 0, \pm\mu)$). As B increases, ΔE_μ becomes larger and reaches 1.8×10^{-3} a.u. in $B = 5 \times 10^6$ (a.u.). ΔE_μ is only 1–1.5 orders of magnitude smaller than the relativistic effect $|\Delta E_{\rm rel}|$ in every case and its amplitude becomes relatively higher with increasing B. For direct comparison with accurate experimental observations, therefore, this effect is not negligible in very strong fields. As shown in Figure 2, we can discuss not only the relative splitting but also the very accurate absolute energies from the DE including spin, angular momentum, and spin–orbit interactions with an external strong magnetic field and nuclear magnetic moment.

4. CONCLUSIONS

In this paper, the SE and the DE of the hydrogen atom in extremely strong magnetic fields, which even exceed the strongest field observed in the universe, were solved quite accurately with the FC method developed in our laboratory. We have provided the estimate of the accuracy of the relativistic corrections in super strong magnetic fields. This observation should be very valuable and physically important for space chemistry in an extreme environment, where relativity can be very important. Hyperfine splitting due to the nuclear magnetic moment was also evaluated very accurately at the relativistic level.

We have demonstrated the exotic behaviors of the energy of the excited states against the strength of the magnetic fields. In an ultra-strong magnetic field, the macro degenerate bands of ungerade symmetry converged to the field-free energy levels of the hydrogen atom. This phenomenon may result from the symmetry coupled with the ultra-strong magnetic field. These would help us to understand unusual spectroscopic phenomena on the surface of a star or the interstellar region in strong magnetic fields. We believe that these numerical observations are highly original. Since the chaotic behavior in a magnetic field may prevent simple theoretical expectations, we may have to rely on the quantum mechanical simulations.

In strong magnetic fields, the finite mass corrections and the QED corrections to the vacuum polarization on the ultra-magnetized vacuum are important (Herold et al. 1981; Vincke & Baye 1988; van Adelsberg & Lai 2006). We did not introduce any of these corrections here, but they will be evaluated in a future study using the highly accurate zeroth-order wave functions obtained here at both the Schrödinger and Dirac equation levels. The very highly accurate numerical results we provide in this paper should become very important when one has to compare theory and experimental observation to fine details in the future when experimental accuracy is much improved.

The present work may advance our ability to study the nature of substances on space objects or in interstellar regions under very strong magnetic fields (Ruder et al. 1994; Schmidt et al. 1996; Lai 2001; Mori & Ho 2007; Duncan & Thompson 1992; Kouveliotou et al. 1998). Our global purpose is to make our methodology based on the quantum mechanical principle a more reliable theoretical tool to predict and explain real phenomena in space. The present paper is a step toward this purpose on astronomical topics and we could provide very accurate fundamental data to address it. We believe that combining the theoretical quantum mechanical studies in molecular science with the observations in astronomy should provide a powerful method for understanding space. We hope this study has also introduced an accurate predictive science to several fields related to strong magnetic fields.

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