

Bound-state energies of lithium in magnetic fields using Hylleraas basis functionsYin Tang,¹ Liming Wang,² Xuanyu Song,¹ Xiaofeng Wang,¹ Z.-C. Yan,^{2,3,*} and Haoxue Qiao^{1,†}¹*Department of Physics, Wuhan University, Wuhan 430072, China*²*Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3*³*State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China and Center for Cold Atom Physics, Chinese Academy of Sciences, Wuhan 430071, China*

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The variational method in Hylleraas coordinates is applied to calculate the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states of the lithium atom in magnetic fields with field strength up to 2×10^9 G. The computational method is based on multiple basis sets that are optimized for all nonlinear parameters for a given field strength. The oscillator strengths are also investigated for some transitions in magnetic fields.

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I. INTRODUCTION

Astrophysicists have been adopting spectral characteristics to measure abundances of cosmic light elements that can be used to diagnose the primordial abundances produced in the standard theory of Big Bang nucleosynthesis (BBN). The spectral data of light elements from theoretical calculations in a field-free space, such as hydrogen, helium, lithium, etc., cannot be used to analyze the spectral data of experimental observations in the universe, because of the existence of strong magnetic fields on the surfaces of white dwarf (10^6 – 10^9 G) and neutron stars (10^{11} – 10^{13} G) [1]. A large number of theoretical calculations of spectral data in strong magnetic fields are needed for astrophysical observations. Recently, a novel chemical bonding mechanism has been found in investigating the behavior and properties of diatomics in a strong magnetic field [2], which may further stimulate the study of light elements under extreme conditions.

In the past three decades, many detailed theoretical data have been successfully applied to the studies on the observed spectra of white dwarf stars [3–13]. The atomic hydrogen in an arbitrary magnetic field has been investigated in detail by Rösner *et al.* [3] and the results are in agreement with the observed data [4]. For two-electron atoms in magnetic fields, theoretical calculations have also been performed and the results are also in agreement with astronomical data [12–14]. The next simple atom is the three-electron atomic lithium that has an open and a closed shell and can be considered as a prototype for other alkali-metal atoms. However, astrophysicists have been plagued with the lithium problem that the predicted primordial ${}^7\text{Li}$ abundance is four times that measured in the atmospheres of galactic halo stars [15]. Theoretical calculation of lithium in strong magnetic fields has received more and more attention. It should be pointed out that, in the past several years, significant progress has been made on precision calculations of low-lying states of lithium under the field-free condition [16–20].

Early theoretical studies on lithium in a magnetic field include the Hartree-Fock (HF) approach [21] without considering the electron-electron correlations. Later, some research groups [22–25] applied the same method to calculate different states of lithium in strong magnetic fields. In [26] an approach called the modified freezing full-core method was used, where the electron-electron correlation effect was partially taken into account by the two-electron core. Although this method is computationally simple and effective for computing some properties of lithium in magnetic fields, it is less precise. Then Guan and Li [27] improved this method by introducing the full-core-plus-correlation (FCPC) method, where the inner core is described by a single predetermined wave function and the correlation between the inner core and the outer electron is described by a configuration-interaction wave function. Wang and Qiao [28] also studied the problem of lithium in magnetic fields using the FCPC method in cylindrical coordinates, where the range of magnetic field strength is extended up to $\beta = 50$ (β denotes the magnetic field strength in two atomic units, i.e., $\beta = B/B_0$, where $B_0 = 4.7011 \times 10^5$ T. Al-Hujaj and Schmelcher [29] also extended their method from two-electron systems to lithium in magnetic fields and calculated the total energies and one-electron ionization energies for the ground and several excited states of symmetries ${}^2 0^+$, ${}^2 (-1)^+$, ${}^4 (-1)^+$, ${}^4 (-1)^-$, ${}^2 (-2)^+$, ${}^4 (-2)^+$, and ${}^4 (-3)^+$.

In 1995, Yan and Drake [30] obtained the high-precision variational energy eigenvalues for the $1s^2 2s^2 S$, $1s^2 2p^2 P$, and $1s^2 3d^2 D$ states of lithium using multiple basis sets in Hylleraas coordinates without a magnetic field. These calculations have then been improved constantly [16,17]. It is evident that the variational method in Hylleraas coordinates is so far the most accurate one for solving three-electron bound-state eigenvalue problems. In the present work, we use the Hylleraas basis sets to calculate variationally the energy eigenvalues of lithium in the presence of a magnetic field. The energy levels of the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states are obtained and compared with other methods [27–29]. The dipole oscillator strengths are also computed.

This paper is organized as follows. In Sec. II, we present the lithium Hamiltonian for the case of infinite nuclear mass and the dipole oscillator strength in the length gauge. The structure of the Hylleraas variational basis set is also presented. In Sec. III the results of our calculations are displayed. A summary is given in Sec. IV.

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II. THEORY AND METHOD

A. Wave function of lithium

In the limit of infinite nuclear mass, the nonrelativistic Hamiltonian of lithium in a magnetic field pointing in the z direction can be written as (atomic units are used throughout)

$$H = \sum_{i=1}^3 \left(-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{i>j}^3 \frac{1}{r_{ij}} + \sum_{i=1}^3 \left[\frac{1}{3} \beta^2 r_i^2 - \frac{2}{3} \sqrt{\frac{\pi}{5}} \beta^2 r_i^2 Y_{20}(\theta_i, \phi_i) \right] + \beta (L_z + 2S_z), \quad (1)$$

where $Z = 3$ denotes the number of nuclear charges, $Y_{20}(\theta_i, \phi_i)$ is the spherical harmonics, and L_z and S_z represent the z components of the total orbital angular momentum L and the total spin angular momentum S , respectively. It is clear that $(H, L_z, S^2, S_z, \hat{\Pi}, \hat{\Pi}_z)$ mutually commute so that they can share common eigenvectors, where $\hat{\Pi}$ is the parity operator for the $(x, y, z) \rightarrow (-x, -y, -z)$ operation, and $\hat{\Pi}_z$ is the z parity operator for the $(x, y, z) \rightarrow (x, y, -z)$ operation.

Upper bounds to energies of lithium in magnetic fields are calculated using the Rayleigh-Ritz variational method. In our calculations, the trial wave function is a linear combination of the following Hylleraas basis functions:

$$\Psi = A[\phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)], \quad (2)$$

where

$$\phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} \exp(-\omega_1 r_1 - \omega_2 r_2 - \omega_3 r_3) \times \mathcal{Y}_{(l_1 l_2) l_{12}, l_3}^{L M_L}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \chi_1, \quad (3)$$

$$\mathcal{Y}_{(l_1 l_2) l_{12}, l_3}^{L M_L}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = r_1^{l_1} r_2^{l_2} r_3^{l_3} \sum_{m_1 m_2 m_3} \langle l_1 m_1; l_2 m_2 | l_{12} m_{12}; l_{12} m_{12} \rangle \times \langle l_{12} m_{12}; l_3 m_3 | l_{12} l_3; L M_L \rangle \times Y_{l_1 m_1}(\hat{\mathbf{r}}_1) Y_{l_2 m_2}(\hat{\mathbf{r}}_2) Y_{l_3 m_3}(\hat{\mathbf{r}}_3) \quad (4)$$

is the vector-coupled product of spherical harmonics for the three electrons to form a state of total angular momentum L and the z component M_L , which is also an eigenstate of $\hat{\Pi}$ and $\hat{\Pi}_z$ with the corresponding eigenvalues $\Pi = (-1)^{l_1+l_2+l_3}$ and $\Pi_z = (-1)^{l_1+l_2+l_3+M_L} = \Pi(-1)^{M_L}$, respectively; this is because $\hat{\Pi} Y_{lm}(\hat{\mathbf{r}}) = (-1)^l Y_{lm}(\hat{\mathbf{r}})$ and $\hat{\Pi}_z Y_{lm}(\hat{\mathbf{r}}) = (-1)^{l-m} Y_{lm}(\hat{\mathbf{r}})$. In magnetic fields a lithium

energy eigenvalue may be designated by the notation $1s^2 n l_{M_L}^{\Pi}$, where $1s^2 n l^{2S+1} L^{\Pi}$ is the corresponding zero field energy term. Notice that Π_z is known when both Π and M_L are given. It should be pointed out that due to the existence of $Y_{20}(\theta_i, \phi_i)$ in the Hamiltonian, one has $[H, L^2] \neq 0$; thus L is no longer a good quantum number when $\beta \neq 0$. In Eq. (3), ω_1 , ω_2 , and ω_3 are nonlinear variational parameters that are optimized by Newton's method [30] for a given strength of the magnetic field. According to the above, a basis set should contain $[(l_1, l_2) l_{12}, l_3] L$ with all possible L . A basis set is generated by including all non-negative integer powers of r_i and r_{ij} in the radial part such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega, \quad (5)$$

where Ω is an integer. In our calculations, the basis set is divided into sectors with different L and each such sector has its own nonlinear parameters ω_1 , ω_2 and ω_3 , as well as its own size-controlling parameter Ω . Meanwhile, to avoid a near linear dependence and numerical instability, we drop terms with $j_1 > j_2$ for $l_1 = l_2$ and $\omega_1 \approx \omega_2$ and drop terms with $j_1 = j_2$ for $j_{23} > j_{31}$ [30]. Convergence in energy is studied by increasing Ω progressively. Also in Eq. (3) χ_1 is the common eigenstate of (S^2, S_z) with the corresponding eigenvalues $S = 1/2$ and $M_S = -1/2$:

$$\chi_1 = \alpha(1)\beta(2)\beta(3) - \beta(1)\alpha(2)\beta(3). \quad (6)$$

Finally

$$A = (1) - (12) - (13) - (23) + (123) + (132) \quad (7)$$

is the three-electron antisymmetrizer.

B. Dipole transition in magnetic field

The dipole transition matrix element between initial state $|i\rangle$ and final state $|f\rangle$ is

$$P_{fi}^{\sigma} = \langle f | \sum_{n=1}^3 r_n C_{\sigma}^{(1)}(\hat{\mathbf{r}}_n) | i \rangle, \quad (8)$$

where $C_{\sigma}^{(1)}(\hat{\mathbf{r}}_n) = \sqrt{4\pi/3} Y_{1\sigma}(\hat{\mathbf{r}}_n)$. In the length gauge the corresponding oscillator strength is

$$f_{fi}^{(\sigma)} = 2(E_f - E_i) \left| \langle f | \sum_{n=1}^3 r_n C_{\sigma}^{(1)}(\hat{\mathbf{r}}_n) | i \rangle \right|^2. \quad (9)$$

TABLE I. Energy convergence of the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states at $\beta = 0.009$, as the size of the basis set N is enlarged. All energies are given in atomic units.

N	$E(1s^2 2s_0)$	N	$E(1s^2 2p_{-1})$	N	$E(1s^2 3d_{-2})$
105	-7.484 983 92	112	-7.424 492 30	107	-7.329 624 88
258	-7.486 545 47	286	-7.426 908 97	268	-7.357 459 07
562	-7.486 564 32	646	-7.427 243 28	596	-7.358 477 16
1124	-7.486 565 93	1208	-7.427 264 10	1088	-7.358 499 21
2093	-7.486 566 21	2176	-7.427 265 29	1920	-7.358 501 24
2578	-7.486 566 51	2721	-7.427 265 38	2184	-7.358 501 68
Extrap.	-7.486 566 8(3)		-7.427 265 6(3)		-7.358 501 8(2)
Ref. [27]	-7.486 301 8		-7.426 897 7		-7.358 242 1

TABLE II. Energy convergence with respect to the total angular momentum L for the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states at $\beta = 0.009$ and $\beta = 0.27$. N_L is the number of terms for given L , and ΔE_L is the corresponding contribution to the energy.

L	$1s^2 2s_0$		$1s^2 2p_{-1}$		$1s^2 3d_{-2}$	
	N_L	$-\Delta E_L$	N_L	$-\Delta E_L$	N_L	$-\Delta E_L$
		$\beta = 0.009$		$\beta = 0.009$		$\beta = 0.009$
		$\beta = 0.27$		$\beta = 0.27$		$\beta = 0.27$
0	1670	7.477 545 49	6.273 076 63	1 2337	7.409 217 06	6.950 376 56
2	768	0.000 021 02	0.898 123 95	3 240	0.000 048 31	0.148 924 74
4	100	1.244×10^{-10}	0.071 191 77	5 120	2.9447×10^{-9}	0.006 803 56
6	18	1.9362×10^{-15}	0.006 841 51	7 18	5.99×10^{-13}	0.000 390 01
8	18	6.25068×10^{-20}	0.000 719 08	9 6	1.7×10^{-17}	0.000 003 58
10	4	2.96×10^{-24}	0.000 061 94			
$\beta(M_L + 2M_S)$		0.009	0.27		0.018	0.54
Total	2578	7.486 566 51	7.520 014 91	2721	7.427 265 38	7.646 491 58

TABLE III. Comparison of the energies for the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states in the field regime $\beta \leq 0.5$.

β	$1s^2 2s_0$		$1s^2 2p_{-1}$		$1s^2 3d_{-2}$	
	Present	Others	Present	Others	Present	Others
0.0000	-7.478 060 323	-7.477 795 7 ^a -7.477 766 ^b -7.476 336 0 ^c	-7.410 156 524	-7.409 790 7 ^a -7.407 126 ^b -7.408 803 7 ^c	-7.335 523 537	-7.335 263 8 ^a -7.332 617 ^b -7.334 763 6 ^c
0.0005	-7.478 558 8(1)	-7.478 032 ^b	-7.411 153 9(2)	-7.408 174 ^b	-7.336 500 7(2)	-7.334 097 ^b
0.0009	-7.478 955 5(2)	-7.478 690 7 ^a -7.477 230 3 ^c	-7.411 947 5(1)	-7.411 581 6 ^a -7.410 594 6 ^c	-7.338 189 4(1)	-7.337 920 0 ^a -7.337 419 7 ^c
0.0045	-7.482 436 7(2)	-7.482 171 9 ^a -7.480 677 0 ^c	-7.418 932 1(2)	-7.418 565 6 ^a -7.417 576 7 ^c	-7.348 185 6(1)	-7.347 695 1 ^a -7.347 191 2 ^c
0.005	-7.482 907 6(1)	-7.482 888	-7.419 879 5(1)	-7.416 994 ^b	-7.348 823 7(1)	-7.346 296 ^b
0.009	-7.486 566 8(3)	-7.486 301 8 ^a	-7.427 265 6(2)	-7.426 897 7 ^a	-7.358 501 7(1)	-7.358 242 1 ^a
0.01	-7.487 451 9(2)	-7.490 983 ^b -7.485 639 8 ^c	-7.429 059 0(1)	-7.427 571 7 ^c	-7.360 448 1(2)	-7.359 815 6 ^c
0.015	-7.491 669 8(1)	-7.491 432 6 ^a	-7.437 723 9(1)	-7.437 353 3 ^a	-7.370 339 1(1)	-7.370 157 9
0.02	-7.495 655 0(1)	-7.495 390 1 ^a -7.493 900 0 ^c	-7.445 913 9(2)	-7.445 539 8 ^a -7.444 479 0 ^c	-7.379 006 0(1)	-7.378 755 4 ^a -7.378 232 7 ^c
0.025	-7.499 335 5(1)	-7.502 724 ^b	-7.453 671 9(2)	-7.451 086 ^b	-7.386 700 0(1)	-7.383 648 ^b
0.027	-7.500 732 9(1)	-7.500 467 8 ^a	-7.456 663 8(2)	-7.456 283 9 ^a	-7.389 588 9(2)	-7.389 355 9 ^a
0.04	-7.508 846 7(3)	-7.508 581 0 ^a	-7.474 761 7(2)	-7.474 368 4 ^a	-7.406 261 4(1)	-7.406 010 2 ^a
0.05	-7.514 047 8(4)	-7.513 781 7 ^a -7.517 154 ^b -7.512 210 2 ^c	-7.487 339 6(3)	-7.486 934 3 ^a -7.484 773 ^b -7.485 838 2 ^c	-7.417 236 9(2)	-7.416 978 0 ^a -7.414 207 ^b -7.416 424 4 ^c
0.063	-7.519 633 (1)	-7.519 371 8 ^a	-7.502 305 4(4)	-7.501 882 9 ^a	-7.429 822 8(2)	-7.429 562 6 ^a
0.09	-7.527 736 (2)	-7.527 504 9 ^a	-7.529 578 3(2)	-7.529 117 5 ^a	-7.451 761 9(1)	-7.451 505 4 ^a
0.1	-7.529 807 (1)	-7.533 495 ^b -7.527 837 6 ^c	-7.538 654 8(4)	-7.536 032 ^b -7.536 692 5 ^c	-7.458 823 8(1)	-7.455 585 ^b -7.457 783 3 ^c
0.12	-7.532 562 (2)	-7.532 294 9 ^a	-7.555 491 7(1)	-7.554 985 1 ^a	-7.471 637 6(5)	-7.471 386 9 ^a
0.15	-7.534 029 (1)	-7.533 767 8 ^a	-7.578 049 9(1)	-7.577 498 9 ^a	-7.488 222 9(1)	
0.2	-7.531 188 7(2)	-7.530 963 2 ^a	-7.610 130 7(2)	-7.609 509 5 ^a	-7.510 607 6(2)	-7.510 411 1 ^a
0.23	-7.527 185 (1)	-7.526 979 1 ^a	-7.626 759 9(1)	-7.626 102 5 ^a	-7.521 571 8(3)	
0.25	-7.523 918 (6)	-7.523 594 6 ^a -7.528 055 ^b -7.521 612 7 ^c	-7.636 927 4(3)	-7.636 248 3 ^a -7.634 547 ^b -7.634 124 5 ^c	-7.528 018 7(1)	-7.524 481 ^b -7.5263 592 ^c
0.27	-7.520 016 (1)	-7.519 726 2 ^a	-7.646 491 6(1)	-7.645 730 ^a	-7.533 850 (1)	-7.533 749 6 ^a
0.3	-7.513 400 (2)	-7.513 158 0 ^a	-7.659 533 (3)	-7.658 809 ^a	-7.541 506 (3)	-7.541 488 4 ^a
0.35	-7.500 958 (7)	-7.500 583 6 ^a	-7.678 598 (3)	-7.677 857 ^a	-7.551 717 (2)	
0.45	-7.471 460 (2)	-7.471 052 7 ^a	-7.707 760 (1)	-7.707 054 ^a		
0.5	-7.454 284 (1)	-7.458 550 ^b -7.452 904 6 ^c	-7.718 357 (4)	-7.716 679 ^b -7.715 194 4 ^c	-7.566 400 (1)	-7.562 892 ^b -7.564 296 9 ^c

^aReference [27].

^bReference [29].

^cReference [28].

The final state $|f\rangle$ and the initial state $|i\rangle$ must obey the selection rule $\sigma = M_{L_f} - M_{L_i}$. In this work, we investigate the absorption strengths for the $1s^2 2s_0 - 1s^2 2p_{-1}$ and $1s^2 2p_{-1} - 1s^2 3d_{-2}$ transitions in lithium as a function of the magnetic field strength.

III. RESULTS AND DISCUSSION

In our calculations, the nonrelativistic energies of lithium under field-free conditions are $-7.478\,060\,32$ for the $1s^2 2s^2 S$ state, $-7.410\,156\,52$ for the $1s^2 2p^2 P$ state, and $-7.335\,523\,53$ for the $1s^2 3d^2 D$ state. Comparing to the results in [26–29], our calculations have significantly improved their values. However, the most accurate results are those obtained by Wang *et al.* [20] using large-scale Hylleraas basis sets. Such a large-scale calculation seems to be difficult to apply to the case when the magnetic field is present, because more extra angular configurations are needed as the total angular momentum L is not conserved. Nevertheless, Table I shows a convergence study for the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states with $\beta = 0.009$, as the size of the basis set is enlarged progressively, along with the extrapolated values with the uncertainties attached in the brackets. The extrapolation is estimated based on the pattern of successive differences between two adjacent calculations. One can see that a convergence of about seven significant digits has been reached with the size of the basis set up to ~ 2500 . Comparing to [27], our results are more accurate than theirs by at least three orders of magnitude. Table II further lists the convergence study of these energies against the total angular momentum L for the cases of $\beta = 0.009$ and 0.27 . For the weak magnetic field of $\beta = 0.009$, the main contribution comes from the configurations $L = 0$ for the $1s^2 2s_0$ state, $L = 1$ for the $1s^2 2p_{-1}$ state, and $L = 2$ for the $1s^2 3d_{-2}$ state, respectively. As L increases the corresponding contributions decrease rapidly. In the stronger magnetic field of $\beta = 0.27$ more angular configurations are required in order to achieve a full convergence; this is because the system becomes more deviated from the spherical symmetry of the field-free situation. In all our calculations, we only consider the angular momentum configurations of parity $(-1)^L$; the contributions from the configurations of parity $(-1)^{L+1}$ are negligibly small; see [27] for a discussion.

Table III presents a more comprehensive listing for the energies of the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states, together with a comparison with some recent results [27–29]. It can be seen that our calculations have significantly improved the previous results in this field regime. It is seen, however, that the energies of $1s^2 2s_0$ from [29] appear abnormally low compared to the results of [27,28] and to this work. It should be pointed out that, as β increases beyond 0.5, the cylindrical symmetry becomes more and more dominant, causing slower convergence in energy. It is thus preferable to use cylindrical coordinates in the basis set [31], instead of Hylleraas ones. A similar situation appears in the calculation of helium energy levels in magnetic fields using Hylleraas coordinates [31,32].

After we have obtained the wave functions of the lithium in magnetic fields, we can study the dipole oscillator strength between states permitted by the selection rules. In Fig. 1, we plot the dipole oscillator strengths for the $1s^2 2s_0 - 1s^2 2p_{-1}$ and

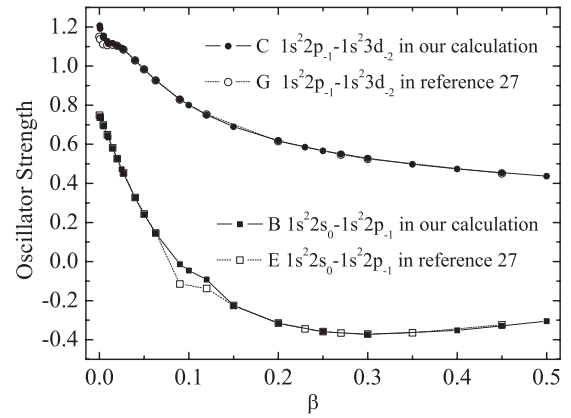


FIG. 1. Oscillator strengths for the $1s^2 2s_0 - 1s^2 2p_{-1}$ (curves E and B) and $1s^2 2p_{-1} - 1s^2 3d_{-2}$ (curves G and C) transitions of lithium as a function of the magnetic field strength.

$1s^2 2p_{-1} - 1s^2 3d_{-2}$ transitions as a function of β . As a comparison, we also plot the corresponding oscillator strengths in Ref. [27]. Our data also show that in the regime of $\beta \leq 0.09$ the $1s^2 2s_0 - 1s^2 2p_{-1}$ oscillator strength decreases monotonically with increasing β . As β is near 0.09, the oscillator strength is close to zero; this is because the corresponding energy values of the $1s^2 2s_0$ state and the $1s^2 2p_{-1}$ state are near degenerate. In the regime of $0.09 \leq \beta \leq 0.12$, our calculated values are higher than the results in Ref. [27]. For the $1s^2 2p_{-1} - 1s^2 3d_{-2}$ oscillator strength, our results are in good agreement with Ref. [27]. Figure 2 shows the difference in oscillator strength between our present calculations and those from [27], against the magnetic field strength.

IV. SUMMARY

By using the Hylleraas coordinates in variational basis sets, we have calculated the energy levels of the $1s^2 2s_0$, $1s^2 2p_{-1}$, and $1s^2 3d_{-2}$ states of lithium in magnetic fields. Our results have greatly improved the previous calculations for these states in the regime of $\beta \leq 0.5$. It should be

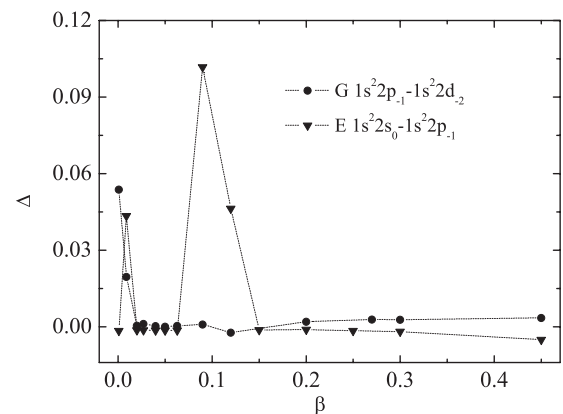


FIG. 2. Δ denotes the difference in oscillator strength between our calculations and those from Ref. [27], as a function of the magnetic field strength.

mentioned that our approach can similarly be applied to other low-lying excited states of lithium. It has been suggested, however, that for larger value of β , cylindrical coordinates are preferred due to the switch over from spherical-dominated symmetry to cylindrical-dominated symmetry. We have also investigated the dipole oscillator strengths and compared with the results of [27], where some improvement has been obtained.

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