

Energy, fine-structure, and hyperfine-structure studies of the core-excited states $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ for Be-like systems

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Variational calculations using multiconfiguration interaction wave functions are carried out on the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states for the Be I isoelectronic sequence from $Z = 3$ to 10. For each species, the upper bound, the nonrelativistic energy, the transition wavelength, the oscillator strengths, the radiative lifetime, the fine structure, the hyperfine parameters, and the coupling constants are reported. The relativistic corrections and the mass polarization are included. The upper bounds and the nonrelativistic energies obtained are much lower than the previously published values for each member of the Be I isoelectronic sequence. The calculated fine-structure results are compared with the existing theoretical and experimental data. The predicted results of the hyperfine structure in this investigation provide useful data in the experimental analysis of fine-structure transitions between the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states for berylliumlike isoelectronic sequence spectra.

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I. INTRODUCTION

In the past two decades, studies of energies, the fine structure, and the hyperfine structure for the Li-like quartet system [1–12] have been of great interest to spectroscopists because there are many strong optical transitions suitable for spectral and hyperfine-structure measurements. On the one hand, the energy spectra of the excited levels were determined by a high-resolution beam-foil technique and the hyperfine parameters and coupling constants were precisely measured by means of the atomic-beam magnetic resonance technique; on the other hand, high quality theoretical calculations have been made, which are in good agreement with experiment. The energies, the fine structure, and the hyperfine structure for the Li-like three-electron quartet system are among the most thoroughly studied both by theory and by experiment. However, for the corresponding core-excited four-electron quintet system, considerably fewer theoretical and experimental studies are available.

Bunge [13] first identified an unclassified, cascade-free, and medium-intensity line at $\lambda = 3489.7 \pm 0.2 \text{ \AA}$ and $\tau = 2.9 \pm 0.2 \text{ ns}$ in a lithium beam-foil spectra to be the core-excited Li^- transition between the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states. The predicted values $3489.5 \pm 1.1 \text{ \AA}$ and $\tau = 2.86 \pm 0.01 \text{ ns}$ agree well with the experiment. This has stimulated considerable interest on the study of the energies and the fine structure of core-excited Be-like quintet system. Theoretical and experimental progress [14–21] has been made. Calculations have been made by a variety of theoretical methods; generally speaking, the accuracy is not very high when compared with the experiment [14–16, 22–26]. Although the results of Bunge [13] agree well with the experiment of Berry *et al.* [27], the uncertainty in the theory is more than five times that in the experiment.

Theoretically speaking, the observed fine structure of

an atomic system may be affected by its hyperfine interaction. When the hyperfine interaction is considered, the total angular momentum $\mathbf{F} = \mathbf{I} + \mathbf{J}$ becomes a good quantum number, where \mathbf{I} is the nuclear spin angular momentum. The components of \mathbf{J} and \mathbf{I} are no longer rigorous, good quantum numbers. Consequently the apparent fine-structure separations in an observed spectrum may differ substantially from the real fine structure. This is clearly shown in the experimental study of lithium quartet fine structures [1,2].

In recent years, many theoretical methods, such as the Hylleraas expansion approach [28], many-body perturbation theory methods [29], the nonrelativistic multiconfiguration Hartree-Fock method [30–32], and the relativistic multiconfiguration Dirac-Fock method [33], have been used to study the hyperfine structure. Their main interest has been the hyperfine parameters and the coupling constants of low-lying states for Be-like isoelectronic sequence. To our knowledge, no calculations of the hyperfine structure have been reported for the core-excited states $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$. Since the hyperfine structure may affect the experimental analysis of the fine structure, which has been reported in the literature [1,2], it would be useful to carry out a complete hyperfine structure study on the core-excited states $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ for the Be-like system.

The purpose of this study is twofold: first, to reduce the theoretical uncertainty in the Li^- quintet transition to make a more critical comparison with experiment, and second, to investigate the effect of the hyperfine interaction on the observed fine structure to determine whether it should be considered in the experimental analysis. By constructing wave functions of sufficiently high quality, a more accurate calculation of properties such as the upper bound, the nonrelativistic energy, the transition wavelength, the oscillator strengths, the lifetime, the fine structure, the hyperfine parameters, and the cou-

pling constants can be made. The results of the fine-structure and hyperfine-structure energies of the core-excited $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states will be used to compare the observed transitions in the optical spectrum of the Be-like isoelectronic sequence. In connection with an x-ray laser, it has been proposed to use $1s2s2p^2(^5P)$ as an energy reservoir, which can be stored in a ring before undergoing photodissociation into the $1s2p^2(^4P)$ state [34]. Accurate theoretical data could be useful in this regard.

The remainder of this paper is divided into four sections. Section II describes the theory of energy, fine structure, and hyperfine structure. Section III describes how to make the choice of our basis functions and how to get nonrelativistic energies for the core-excited states $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ of the berylliumlike isoelectronic sequence Li⁻, Be I, B II, C III, N IV, O V, F VI, Ne VII. Section IV presents our main results and discussions; some comparisons are also made. Section V makes some concluding marks.

II. THEORY

A. Energy

The nonrelativistic Hamiltonian for the upper bound is given in atomic units by

$$H_0 = \sum_{i=1}^N \left[-\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right] + \sum_{\substack{i,j=1 \\ i < j}}^N \frac{1}{r_{ij}}. \quad (1)$$

The perturbation operators due to the corrections from the kinetic energy (H_k), the Darwin term (H_D), the electron-electron interaction (H_{ee}), the mass polarization (H_m), and the orbit-orbit interaction (H_{oo}) are

$$H' = H_k + H_D + H_{ee} + H_m + H_{oo}, \quad (2)$$

where

$$H_k = -\frac{1}{8c^2} \sum_{i=1}^N \mathbf{p}_i^4, \quad (3)$$

$$H_D = \frac{Z\pi}{2c^2} \sum_{i=1}^N \delta(\mathbf{r}_i), \quad (4)$$

$$H_{ee} = -\frac{\pi}{c^2} \sum_{\substack{i,j=1 \\ i < j}}^N [1 + \frac{8}{3} \mathbf{s}_i \cdot \mathbf{s}_j] \delta(\mathbf{r}_{ij}), \quad (5)$$

$$H_m = -\frac{1}{M} \sum_{\substack{i,j=1 \\ i < j}}^N \nabla_i \cdot \nabla_j, \quad (6)$$

$$H_{oo} = -\frac{1}{2c^2} \sum_{\substack{i,j=1 \\ i < j}}^N \frac{1}{r_{ij}} \left[\mathbf{p}_i \cdot \mathbf{p}_j + \frac{\mathbf{r}_{ij}(\mathbf{r}_{ij} \cdot \mathbf{p}_i) \cdot \mathbf{p}_j}{r_{ij}^2} \right], \quad (7)$$

where M is the nuclear mass, \mathbf{s}_i and \mathbf{p}_i are the spin and the linear momentum of the i th electron. The basic wave function for the four-electron system can be written as

$$\Psi_b(1, 2, 3, 4) = A \sum_i C_i \Phi_{n(i),l(i)}(1, 2, 3, 4), \quad (8)$$

where A is the antisymmetrization operator and $\Phi_{n(i),l(i)}(1, 2, 3, 4)$ is given by

$$\Phi_{n(i),l(i)}(1, 2, 3, 4) = \phi_{n(i),l(i)}(R) Y_{l(i)}^{LM}(\Omega) \chi_{SS_s}, \quad (9)$$

where

$$\phi_{n(i),l(i)}(R) = \prod_{j=1}^4 r_j^{n_j} \exp(-\alpha_j r_j). \quad (10)$$

A different set of α_j is used for each $l(i)$. The angular part is

$$Y_{l(i)}^{LM}(\Omega) = \sum_{m_j} \langle l_1 l_2 m_1 m_2 | l_{12} m_{12} \rangle \times \langle l_{12} l_3 m_{12} m_3 | l_{123} m_{123} \rangle \times \langle l_{123} l_4 m_{123} m_4 | LM \rangle \prod_{j=1}^4 Y_{l_j, m_j}(\Omega_j). \quad (11)$$

To simplify notation, this angular function is denoted as

$$l(i) = [(l_1, l_2) l_{12}, l_3] l_{123}, l_4. \quad (12)$$

In this expression, it is implied that l_{123} and l_4 couple into a wave function of the total orbital angular momentum L and the azimuthal component M . The four-electron spin wave function can also be represented in this notation as

$$\chi_{SS_s} = [(s_1, s_2) s_{12}, s_3] s_{123}, s_4. \quad (13)$$

The linear parameters C_i and the nonlinear parameters α_j are determined in the energy optimization processes.

The upper bounds of the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states are calculated using the Rayleigh-Ritz variation method

$$\delta E_b = \delta \langle H_0 \rangle = \delta \frac{\langle \Psi_b | H_0 | \Psi_b \rangle}{\langle \Psi_b | \Psi_b \rangle}. \quad (14)$$

Once the basic wave function Ψ_b and the corresponding upper bound E_b are obtained, we can implement the restricted variational method [35,36] to improve E_b . This is done by using Ψ_b as a single term to expand the total wave function as

$$\Psi_t(1, 2, 3, 4) = D_0 \Psi_b(1, 2, 3, 4) + \Psi_e(1, 2, 3, 4), \quad (15)$$

where

$$\Psi_e(1, 2, 3, 4) = A \sum_{i=1}^I D_i \psi_{n(i),l(i)}(1, 2, 3, 4). \quad (16)$$

$\Psi_e(1, 2, 3, 4)$ is a function to saturate the functional space. It takes the same form as $\Psi_b(1, 2, 3, 4)$, but the

nonlinear parameters α_j are much different from the α_j 's of $\Psi_b(1, 2, 3, 4)$. Thus another secular equation can be constructed and an energy improvement over the upper bound E_b could be obtained. In fact, one can include a very large number of linear parameters into the wave function by using a set of Ψ_e 's whose contribution can be computed individually. The total improvement to the nonrelativistic energy ΔE_{res} is the sum of the contribution from each of the Ψ_e 's. For more details we refer the reader to Refs. [35,36].

The relativistic and mass polarization corrections are given by

$$\Delta E = \langle \Psi_b | H_k + H_D | \Psi_b \rangle + \langle \Psi_b | H_{ee} + H_m + H_{oo} | \Psi_b \rangle = \Delta E_1 + \Delta E_2, \quad (17)$$

where ΔE_1 is the first-order energy from the one-particle perturbation operators and ΔE_2 is from the two-particle operators. The total energy becomes

$$E_{\text{total}} = E_b + \Delta E_{\text{res}} + \Delta E. \quad (18)$$

B. Fine structure

The fine-structure perturbation operators are given by

$$H_{\text{FS}} = H_{so} + H_{ss} + H_{soo}, \quad (19)$$

where the spin-orbit, the spin-spin, and spin-other-orbit operators are

$$H_{so} = \frac{\mathbf{Z}}{2c^2} \sum_{i=1}^N \mathbf{l}_i \cdot \mathbf{s}_i r_i^{-3}, \quad (20)$$

$$H_{ss} = \sum_{\substack{i,j=1 \\ i < j}}^N \frac{1}{c^2 r_{ij}^3} \left[\mathbf{s}_i \cdot \mathbf{s}_j - \frac{3(\mathbf{r}_{ij} \cdot \mathbf{s}_i)(\mathbf{r}_{ij} \cdot \mathbf{s}_j)}{r_{ij}^2} \right], \quad (21)$$

and

$$H_{soo} = -\frac{1}{2c^2} \sum_{\substack{i,j=1 \\ i < j}}^N \left[\frac{1}{r_{ij}^3} (\mathbf{r}_i - \mathbf{r}_j) \times \mathbf{p}_i \right] \cdot (\mathbf{s}_i + 2\mathbf{s}_j). \quad (22)$$

The \mathbf{l}_i and \mathbf{s}_i are the orbital and the spin angular momentum of the i th electron. The wave function used to calculate these perturbations in the LSJ representation is

$$\Phi_{LSJJ_z} = \sum_{M, S_z} \langle LSM S_z | JJ_z \rangle \Phi_{LSMS_z}, \quad (23)$$

where

$$\Phi_{LSMS_z} = A \sum_i C_i \phi_{n(i), l(i)}(R) Y_{l(i)}^{LM}(\Omega) \chi_{SS_z}. \quad (24)$$

The fine-structure energy levels are calculated by

$$(\Delta E_{\text{FS}})_J = \langle \Phi_{LSJJ_z} | H_{so} + H_{ss} + H_{soo} | \Phi_{LSJJ_z} \rangle. \quad (25)$$

C. Hyperfine structure

The hyperfine interaction describes the interaction between the electrons and the magnetic and electric multipole moments of the nucleus. For an N -electron system, the magnetic dipole and the electric quadrupole hyperfine-structure contribution [37,38] to the Hamiltonian in atomic units is

$$H_{\text{hfs}} = H_c + H_{\text{SD}} + H_l + H_q, \quad (26)$$

where

$$H_c = \frac{\alpha^2}{6m_p} g_I g_s \mathbf{I} \cdot \sum_{i=1}^N 8\pi \mathbf{s}_i \delta(\mathbf{r}_i) \quad (27)$$

is the Fermi contact term,

$$H_{\text{SD}} = -\frac{\alpha^2}{2m_p} \sqrt{10} g_I g_s \mathbf{I} \cdot \sum_{i=1}^N [\mathbf{C}^{(2)}(i) \times \mathbf{s}_i] r_i^{-3} \quad (28)$$

is the spin dipolar term,

$$H_l = \frac{\alpha^2}{m_p} g_I g_l \mathbf{I} \cdot \sum_{i=1}^N \mathbf{l}_i r_i^{-3} \quad (29)$$

is the orbital term,

$$H_q = -\sum_{i=1}^N \mathbf{C}^{(2)} \cdot \mathbf{Q}^{(2)} r_i^{-3} \quad (30)$$

is the electric quadrupole term, and \mathbf{I} is the nuclear spin momentum. The tensor $\mathbf{C}_i^{(2)}$ is connected to the spherical harmonics $Y_{lm}(i)$ by $C_m^{(l)} = \sqrt{\frac{4\pi}{2l+1}} Y_{lm}$. \mathbf{Q} is the nuclear electric quadrupole moment ($\langle I, M_I = I | \mathbf{Q}_0^{(2)} | I, M_I = I \rangle = \frac{Q}{2}$). g_I is the nucleus spin g factor, $g_l = (1 - \frac{m_e}{M_{\text{atom}}})$ is the orbital electron g factor, and $g_s = 2.0023193$ is the electron spin g factor. m_p is the mass of the proton.

The hyperfine interaction couples the electronic (\mathbf{J}) and the nuclear (\mathbf{I}) angular momenta to a total angular momentum $\mathbf{F} = \mathbf{I} + \mathbf{J}$. In the $|JFM_F\rangle$ representation, using $3j$, $6j$, and $9j$ coefficients, the hyperfine energy corrections [37,39] associated with the four perturbation operators are

$$\Delta E_{\text{hfs}}^{(1)} = \Delta E_c^{(1)} + \Delta E_{\text{SD}}^{(1)} + \Delta E_l^{(1)} + \Delta E_q^{(1)}, \quad (31)$$

where

$$\begin{aligned} \Delta E_c^{(1)} &= \langle IJFM_F | H_c | IJ'FM_F \rangle \\ &= \frac{1}{6} G_M g_s (-1)^{I+J+F+S+L+J'+1} \sqrt{(2J+1)(2J'+1)} \begin{pmatrix} I & 1 & I \\ -I & 0 & I \end{pmatrix}^{-1} \begin{pmatrix} S & 1 & S \\ -S & 0 & S \end{pmatrix}^{-1} \\ &\quad \times \begin{Bmatrix} I & J' & F \\ J & I & 1 \end{Bmatrix} \begin{Bmatrix} S & S & 1 \\ J' & J & L \end{Bmatrix} a_c, \end{aligned} \quad (32)$$

$$\begin{aligned}
\Delta E_{\text{SD}}^{(1)} &= \langle IJFM_F | H_{\text{SD}} | IJ'FM_F \rangle \\
&= \frac{\sqrt{30}}{4} G_M g_s (-1)^{I+J+F} \sqrt{(2J+1)(2J'+1)} \begin{pmatrix} I & 1 & I \\ -I & 0 & I \end{pmatrix}^{-1} \begin{pmatrix} S & 1 & S \\ -S & 0 & S \end{pmatrix}^{-1} \begin{pmatrix} L & 1 & L \\ -L & 0 & L \end{pmatrix}^{-1} \\
&\quad \times \left\{ \begin{matrix} I & J' & F \\ J & I & 1 \end{matrix} \right\} \left\{ \begin{matrix} S & L & J \\ S & L & J' \\ 1 & 2 & 1 \end{matrix} \right\} a_{\text{SD}}, \tag{33}
\end{aligned}$$

$$\begin{aligned}
\Delta E_l^{(1)} &= \langle IJFM_F | H_l | IJ'FM_F \rangle \\
&= G_M g_l (-1)^{I+J+F+S+L+J+1} \sqrt{(2J+1)(2J'+1)} \begin{pmatrix} I & 1 & I \\ -I & 0 & I \end{pmatrix}^{-1} \begin{pmatrix} L & 1 & L \\ -L & 0 & L \end{pmatrix}^{-1} \\
&\quad \times \left\{ \begin{matrix} I & J' & F \\ J & I & 1 \end{matrix} \right\} \left\{ \begin{matrix} L & L & 1 \\ J' & J & S \end{matrix} \right\} a_l, \tag{34}
\end{aligned}$$

$$\begin{aligned}
\Delta E_q^{(1)} &= \langle IJFM_F | H_q | IJ'FM_F \rangle \\
&= \frac{Q}{4} (-1)^{I+J+F+S+L+J+1} \sqrt{(2J+1)(2J'+1)} \begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}^{-1} \begin{pmatrix} L & 2 & L \\ -L & 0 & L \end{pmatrix}^{-1} \\
&\quad \times \left\{ \begin{matrix} I & J' & F \\ J & I & 2 \end{matrix} \right\} \left\{ \begin{matrix} L & L & 2 \\ J' & J & S \end{matrix} \right\} b_q. \tag{35}
\end{aligned}$$

In Eqs. (32)–(35), $G_M = \frac{\alpha^2 \mu_I}{m_p}$ (μ_I is the nuclear magnetic moment); a_l , a_{SD} , a_l , and b_q are the Fermi contact, the spin-dipolar, the orbital, and the electric quadrupole hyperfine parameters, which are given by [37]

$$a_c = \left\langle SLSL \left| \sum_{i=1}^N 8\pi\delta(\mathbf{r}_i) \mathbf{s}_0(i) \right| SLSL \right\rangle, \tag{36}$$

$$a_{\text{SD}} = \left\langle SLSL \left| \sum_{i=1}^N 2\mathbf{C}_0^{(2)}(i) \mathbf{s}_0(i) r_i^{-3} \right| SLSL \right\rangle, \tag{37}$$

$$a_l = \left\langle SLSL \left| \sum_{i=1}^N l_0(i) r_i^{-3} \right| SLSL \right\rangle, \tag{38}$$

and

$$b_q = \left\langle SLSL \left| \sum_{i=1}^N 2\mathbf{C}_0^{(2)}(i) r_i^{-3} \right| SLSL \right\rangle. \tag{39}$$

After the Fermi contact, the spin-dipolar, the orbital, and the electric quadrupole hyperfine parameters a_l , a_{SD} , a_l , and b_q are calculated, we can easily get the diagonal and off-diagonal hyperfine coupling constants by using the following equations [37,39]:

$$\Delta E_c^{(1)}(J, J) + \Delta E_{\text{SD}}^{(1)}(J, J) + \Delta E_l^{(1)}(J, J) = \frac{1}{2} A_J C, \tag{40}$$

$$\begin{aligned}
&\Delta E_c^{(1)}(J, J-1) + \Delta E_{\text{SD}}^{(1)}(J, J-1) + \Delta E_l^{(1)}(J, J-1) \\
&= \frac{1}{2} A_{J, J-1} [(K+1)(K-2F)(K-2I)(K-2J+1)]^{\frac{1}{2}}, \tag{41}
\end{aligned}$$

and

$$\Delta E_q^{(1)}(J, J) = B_J \frac{\frac{3}{4} C(C+1) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)}, \tag{42}$$

where $C = F(F+1) - J(J+1) - I(I+1)$ and $K = I+J+F$. These A_J , $A_{J, J-1}$, and B_J are the hyperfine coupling constants [37].

III. CHOICES OF BASIS FUNCTION AND NONRELATIVISTIC ENERGIES

In order to achieve accurate calculations for various properties of the core-excited berylliumlike system, a choice of basis function with sufficiently high quality is critical and it is our major concern. In this section we will discuss how to choose the best basis function to obtain the nonrelativistic energy beginning with the Li^- negative ions.

For the $1s2s2p^2(^5P)$ state, the parity $(-1)^{\sum_i l(i)}$ is even. There are many important angular series $[l_1 l_2 l_3 l_4]$: $[00l, l]$, $[01l, (l+1)]$, $[11l, l]$, $[02(l+1), (l+1)]$, $[11l, (l+2)]$, $[02(l+1), (l+3)]$, etc. For the $1s2p^3(^5S)$ state, the parity $(-1)^{\sum_i l(i)}$ is odd. Hence the available angular series should be $[01l, l]$, $[11l, (l+1)]$, $[02(l+1), (l+2)]$, $[12(l+1), (l+1)]$, $[12(l+1), (l+3)]$, $[22(l+1), (l+2)]$, etc. In both cases, the initial value of l is 1. To select the best basis function, our criterion is that for each l_1 , l_2 , l_3 , and l_4 angular component with more than 1.0×10^{-5} a.u. energy contribution, it is included in Ψ_b . For an angular component $[l_1 l_2 l_3 l_4]$ that contributes less than 1.0×10^{-5} a.u. but more than 1.0×10^{-7} a.u., it is included in the restricted variational calculation. For each set of orbital angular momenta l_1 , l_2 , l_3 , and l_4 , there could be several ways to couple this set into the desired total orbital angular momentum. In order to make sure that all important

TABLE I. Angular components $[l_1 l_2 l_3 l_4]$ for $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states. $[l_1 l_2 l_3 l_4]$ represents collectively the possible couplings of $l_1, l_2, l_3,$ and l_4 .

$1s2s2p^2(^5P)$					
$[00l, l]$	$[01l, (l+1)]$	$[11l, l]$	$[02(l+1), (l+1)]$	$[11l, (l+2)]$	$[02(l+1), (l+3)]$
[0011]	[0112]	[1111]	[0222]	[1113]	[0224]
[0022]	[0123]	[1122]	[0233]	[1124]	[0235]
[0033]	[0134]	[1133]	[0244]	[1135]	
[0044]	[0145]	[1144]	[0255]		
[0055]	[0156]	[1155]			
[0066]	[0167]	[1166]			
[0077]	[0178]	[1177]			
[0088]	[0189]	[1188]			
$1s2p^3(^5S)$					
$[01l, l]$	$[11l, (l+1)]$	$[02(l+1), (l+2)]$	$[12(l+1), (l+1)]$	$[12(l+1), (l+3)]$	$[22(l+1), (l+2)]$
[0111]	[1112]	[0223]	[1222]	[1224]	[2223]
[0122]	[1123]	[0234]	[1233]	[1235]	[2234]
[0133]	[1134]	[0245]	[1244]	[1246]	
[0144]	[1145]	[0256]	[1255]		
[0155]	[1156]	[0267]			
[0166]	[1167]	[0278]			
[0177]	[1178]	[0289]			
[0188]	[1189]				

combinations are included in the basis function, efforts have been made to avoid missing an important contribution for a particular coupling. In the case of Li^- , we obtain a 45 angular component 1004-term wave function for the $1s2s2p^2(^5P)$ state and a 34 angular component 825-term wave function for the $1s2p^3(^5S)$ state.

In principle, after we have obtained the wave function for the Li^- negative ions, we can exploit the same type of basis function for the core-excited berylliumlike higher- Z system. However, there are subtle changes, for example, for some angular terms, their contributions to the upper bound increase appreciably with Z , while others decrease

with Z . Hence some adjustments have been made on the choice of basis function for different Z accordingly. The basis functions that are left out in Ψ_b are again employed in the restricted variation calculation. In Table I we use $[l_1 l_2 l_3 l_4]$ to represent collectively the various orbital angular momentum couplings from $l_1, l_2, l_3,$ and l_4 , which are included in the basis functions and in the restricted variation calculation.

Once the optimized basis function is obtained, we can use it to compute the upper bound to the nonrelativistic energy for the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states. We notice that the $1s2p^3(^5S)$ state converges faster, there

TABLE II. Energies of berylliumlike $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ (in a.u.). E_b stands for upper bound; ΔE_{res} is the correction from restricted variation calculation; E_{nonrel} is nonrelativistic energies; ΔE_{rel} is the relativistic corrections and mass polarization.

Z	E_b	ΔE_{res}	E_{nonrel}	ΔE_{rel}	E_{total}
$1s2s2p^2(^5P)$					
3	-5.386 501 9	-0.000 070 9(35)	-5.386 572 8	-0.000 599 8	-5.387 172 6(35)
4	-10.423 134 8	-0.000 073 8(37)	-10.423 208 6	-0.001 972 5	-10.425 179 8(37)
5	-17.220 050 5	-0.000 081 0(41)	-17.220 131 4	-0.005 009 8	-17.225 141 3(41)
6	-25.770 617 7	-0.000 084 2(42)	-25.770 701 9	-0.010 728 5	-25.781 436 7(42)
7	-36.072 945 3	-0.000 082 3(41)	-36.073 027 6	-0.020 413 2	-36.093 440 7(41)
8	-48.126 339 7	-0.000 078 5(39)	-48.126 418 2	-0.035 616 0	-48.162 036 3(39)
9	-61.930 317 8	-0.000 078 0(39)	-61.930 395 8	-0.058 057 8	-61.988 453 6(39)
10	-77.484 732 6	-0.000 101 4(51)	-77.484 834 0	-0.089 917 5	-77.574 811 5(51)
$1s2p^3(^5S)$					
3	-5.256 052 9	-0.000 044 0(22)	-5.256 096 9	-0.000 557 2	-5.256 654 1(22)
4	-10.184 685 4	-0.000 042 4(21)	-10.184 727 8	-0.001 790 4	-10.186 518 2(21)
5	-16.876 423 9	-0.000 056 8(28)	-16.87 6480 7	-0.004 486 7	-16.880 967 5(28)
6	-25.323 439 0	-0.000 057 1(28)	-25.323 496 2	-0.009 536 2	-25.333 036 6(28)
7	-35.523 208 2	-0.000 056 9(28)	-35.523 265 1	-0.018 060 0	-35.541 324 8(28)
8	-47.474 621 8	-0.000 034 9(17)	-47.474 656 7	-0.031 400 7	-47.506 057 4(17)
9	-61.177 040 0	-0.000 037 6(18)	-61.177 077 6	-0.051 210 2	-61.228 287 8(18)
10	-76.630 168 9	-0.000 036 6(18)	-76.630 205 6	-0.079 293 2	-76.709 498 8(18)

are fewer angular coupling terms that make a significant contribution, and correlation effects between the angular components are more apparent. By contrast, the $1s2s2p^2(^5P)$ state is more difficult to compute; there are more important angular terms. The correlation and configuration-interaction effects between the various angular components are very strong. There are many components contributing significantly to the energy.

To improve the energy obtained from Ψ_b , we use the restricted variational method to compute energy contributions from each chosen angular series. By summing these contributions, the energy improvement over the upper bound E_b has been achieved. In this work, we included the orbital angular component up to $l = 9$. The energy contribution from groups with $l > 9$ is small and negligible. Thus, by summing the energies from Ψ_b and the restricted variation calculation, the total nonrelativistic energies are obtained. These values are given in Table II. In this table we have also quoted the possible error in the energy due to the missing angular components and the fact that the energy from the restricted variation calculation is not an upper bound.

IV. RESULTS AND DISCUSSION

The energies obtained in this work are substantially lower than previously published theoretical data; for example, for Li^- negative ions, the most accurate theoretical data, to our knowledge, are from Bunge [13]. His energy upper bound for the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states are $-5.386\,346$ a.u. and $-5.255\,899$ a.u., which are higher than the upper bounds obtained in this work by $0.000\,156$ a.u. and $0.000\,154$ a.u., respectively. Our extrapolated nonrelativistic energies for the two states are $-5.386\,573$ a.u. and $-5.256\,097$ a.u., which are lower than those of Bunge [13] by $94\ \mu\text{a.u.}$ and $117\ \mu\text{a.u.}$, respectively. We noted that the upper bounds obtained in this work are lower than the extrapolated results in Ref. [13] by $23\ \mu\text{a.u.}$ and $73\ \mu\text{a.u.}$

We have also used Ψ_b and the length, the velocity, and the acceleration formula to calculate oscillator strengths and the corresponding transition probabilities between the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states for this berylliumlike isoelectronic sequence. These results are presented in Table III.

Our energies for the Li^- $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states are much improved over those of Bunge [13] and our transition energy $28\,643(1)\ \text{cm}^{-1}$ is well within the quoted uncertainty of Bunge, $28\,649(9)\ \text{cm}^{-1}$; however, it lies outside of the quoted experimental uncertainty $28\,647(2)\ \text{cm}^{-1}$. The reason for this discrepancy is not clear. The higher-order relativistic and QED effects are negligibly small for this system. This discrepancy seems to suggest that our $1s2s2p^2(^5P)$ energy is too high by more than $10\ \mu\text{a.u.}$ Judging from the results from the restricted variation calculation, it is difficult to find the source of this $10\ \mu\text{a.u.}$

Our calculated radiative lifetime for the Li^- $1s2p^3(^5S)$ state, $2.91\ \text{ns}$, agrees with the $2.86 \pm 0.10\ \text{ns}$ of Bunge [13] and the $2.90 \pm 0.20\ \text{ns}$ of Berry *et al.* [40]; however, it disagrees with the later experiments of Mannervik [41], $2.3 \pm 0.1\ \text{ns}$, and Berry *et al.* [16], $2.28 \pm 0.05\ \text{ns}$. To find the reason for this discrepancy, we compare our calculated radiative lifetime with the best experimental lifetimes for the entire Be-like series. It seems that the effect from the spin-dependent interactions becomes significant for $Z \geq 8$. But, based on the close agreement between theory and experiment, it is not important for beryllium, boron, carbon, and nitrogen. This effect should be even smaller for Li^- .

In Table III we give the results of oscillator strengths from the dipole-length, -velocity, and -acceleration formula using Ψ_b . The agreement suggests that the nonrelativistic wave functions are probably quite accurate. We use the same basis function to calculate the energy contribution by including the mass polarization perturbation operator H_m in H_0 and the relativistic corrections H_k , H_D , H_{ee} , and H_{oo} with the first-order perturbation theory.

The contributions from higher-order relativistic effects

TABLE III. Transition energy and oscillator strength between $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states.

Z	$f_l/f_v/f_a$	5P lifetime (ns)		Transition energy (cm^{-1})			
		This work	Expt.	This work	Expt.	Other theor.	
						Ref. [19]	Ref. [18]
3	0.2095/ 0.2093/ 0.2277	2.9095	2.9 ± 0.2^a 2.3 ± 0.1^c	28643(1)	28647 ± 2^a	$28649(9)^b$	
4	0.1777/ 0.1773/ 0.1759	1.0265	1.1 ± 0.1^c	52376(1)	52371 ± 16^d	52416	
5	0.1408/ 0.1402/ 0.1497	0.6240	0.65 ± 0.01^d	75533(1)	75533 ± 4^e	75695	
6	0.1150/ 0.1150/ 0.1253	0.4510	0.49 ± 0.03^e	98405(1)	98419 ± 5^f	98445	99187
7	0.0970/ 0.0970/ 0.1076	0.3538	0.33 ± 0.06^e	121171(1)	121131 ± 15^f	121197	121951
8	0.0837/ 0.0837/ 0.0852	0.2917	0.21 ± 0.02^e	143966(1)	143936 ± 21^f	143947	144739
9	0.0736/ 0.0736/ 0.0703	0.2483	0.18 ± 0.02^h	166832(2)	166758 ± 28^g	166778	167616
10	0.0657/ 0.0657/ 0.0565	0.2163	0.09 ± 0.01^g	189911(2)	189879 ± 36^h	189789	190658

^aBerry *et al.* [27].

^bBunge [13].

^cMannervik [41].

^dMannervik *et al.* [14].

^eBerry *et al.* [16].

^fLivingston and Hinterlong [25].

^gHardis *et al.* [15].

^hMartinson *et al.* [24].

TABLE IV. Fine structures (cm^{-1}) for the $1s2s2p^2(^5P)$ states of the Be-like isoelectronic sequence.

Z		This work		Ref. [17]	Ref. [15]	Expt.	Ref.
		with H_{hfs}	without H_{hfs}				
3	ν_{21}	1.00	0.91				
	ν_{32}	-1.36	-1.32				
4	ν_{21}	6.16	6.15	6.65			
	ν_{32}	-2.64	-2.63	-0.52			
5	ν_{21}	22.40	22.44	22.98			
	ν_{32}	2.30	2.22	6.13			
6	ν_{21}	58.09	58.09	59.63	57	63.5(1.5)	[16]
	ν_{32}	24.53	24.53	30.21	21	21.3	[16]
7	ν_{21}	126.90	126.90	129.19	125	127(1)	[16]
	ν_{32}	78.45	78.45	86.72	73	79.5(.8)	[16]
8	ν_{21}	243.19	243.19	247.34	242	254(4)	[16]
	ν_{32}	183.91	183.90	194.95	176	188(2)	[16]
9	ν_{21}		425.22	433.19	426	419(20)	[24]
	ν_{32}		364.69	378.50	354	396(20)	[24]
10	ν_{21}	694.41	694.41	709.46	700	711(22)	[15]
	ν_{32}	649.98	648.98	665.17	633	680(7)	[15]

TABLE V. Values of the nuclear spin I , the nuclear magnetic dipole moment μ_I , and the electric quadrupole moment Q taken from Ref. [43].

Species	I^π	μ_I (nm)	Q (b)
${}^7\text{Li}^-$	3/2-	3.256427	0.0370
${}^9\text{Be I}$	3/2-	1.177492	0.0530
${}^{10}\text{B II}$	3+	1.800645	0.0847
${}^{11}\text{C III}$	3/2-	0.964000	0.03426
${}^{14}\text{N IV}$	1+	0.403761	0.0193
${}^{17}\text{O V}$	5/2+	1.893790	0.02578

TABLE VI. Hyperfine parameters of berylliumlike $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states (in a.u.).

Species	$a_c(^5P)$	$a_{\text{SD}}(^5P)$	$a_l(^5P)$	$b_q(^5P)$	$a_c(^5S)$
${}^7\text{Li}^-$	111.1622	-0.03797	0.18427	-0.07603	106.0230
${}^9\text{Be I}$	266.1643	0.16705	0.82458	0.33411	250.0465
${}^{10}\text{B II}$	525.5163	0.43720	2.16994	0.87439	487.7607
${}^{11}\text{C III}$	916.0758	0.90217	4.47131	1.80434	843.5378
${}^{14}\text{N IV}$	1464.725	1.60988	7.97872	3.21977	1340.049
${}^{17}\text{O V}$	2198.949	2.60857	12.94203	5.21714	2004.057

TABLE VII. Hyperfine coupling constants of berylliumlike $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states (in GHz).

Species	$A_3(^5P)$	$A_2(^5P)$	$A_1(^5P)$	$B_3(^5P)$	$B_2(^5P)$	$B_1(^5P)$	$A_2(^5S)$
${}^7\text{Li}^-$	2.57667	3.19949	5.74981	6.60968(-4)	-6.60968(-4)	6.60968(-5)	3.66437
${}^9\text{Be I}$	-2.24231	-2.76867	4.96801	4.16068(-3)	-4.16068(-3)	4.16068(-4)	-3.12490
${}^{10}\text{B II}$	3.39751	4.17822	7.48907	-1.74059(-2)	1.74059(-2)	-1.74059(-3)	4.66082
${}^{11}\text{C III}$	-6.35833	-7.79631	-13.8775	1.45248(-2)	-1.45248(-2)	1.45248(-3)	-8.63057
${}^{14}\text{N IV}$	6.39995	7.82996	14.0157	-1.46011(-2)	1.46011(-2)	-1.46011(-3)	8.62021
${}^{17}\text{O V}$	-18.0476	-22.0421	-39.4379	-3.16197(-2)	3.16197(-2)	-3.16197(-3)	-24.1686

are estimated by using a method described by Chung *et al.* [42]. For the core-excited $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states, it is more difficult to calculate the QED contribution. A rough estimate of the QED effect shows that the contribution is very small. They are neglected in this work.

In Table III we compared the calculated $^5P - ^5S^o$ transition energy with that of the experiment for $Z = 5-9$. For Be I and B II atoms, the experimental transition wavelength is $1909.46 \pm 0.60 \text{ \AA}$ [22]; ours is 1909.27 \AA . For B II ions, the experimental value is $1323.92 \pm 0.07 \text{ \AA}$ [14]; ours is 1323.92 \AA . Both are within the experimental uncertainty. The calculated result for Ne VII is also within the experimental uncertainty; however, for other states, we are slightly off from the experimental data (see Table III).

In this work, the fine-structure splittings are calculated with the H_{so} , H_{soo} , and H_{ss} perturbation operators by using the first-order perturbation theory on the $1s2s2p^2(^5P)$ states. We also wish to see how the hyperfine interactions may affect the "apparent" fine structure in an experiment. These results are given in Table IV. It appears that the effect coming from the hyperfine interaction is very small for these quintet states. A comparison between theoretical and experimental fine-structure data has been made. For most of our results, the fine-structure computations of this calculation are in good agreement with those of the multiconfiguration Dirac-Fock result [15,17] and with experiment. However, for the Ne ν_{32} our result is substantially lower than that of the experiment. Perhaps the neglected QED effect in our work may have contributed to this discrepancy.

The method outlined in Sec. II C is used to calculate the Fermi contact (a_c), the spin-dipolar (a_{SD}), the orbital (a_l), and the electric quadrupole (b_q) hyperfine-structure parameters and the hyperfine coupling constants A_J and B_J for the $1s2s2p^2(^5P)$ and the $1s2p^3(^5S)$ states of the different berylliumlike species. By using these parameters and coupling constants, the hyperfine-structure energies are also calculated. In this calculation, the nuclear spin I , the nuclear magnetic dipole moment μ_I , and the electric quadrupole moment Q are taken from Ref. [43]; these values are tabulated in Table V. In Table VI we give the Fermi contact (a_c), the spin-dipolar (a_{SD}), the orbital (a_l), and the electric quadrupole (b_q) hyperfine-structure parameters; in Table VII the hyperfine coupling constants A_J and B_J are presented. Un-

fortunately, to our knowledge, no calculations of the hyperfine parameters a_c, a_{SD}, a_l, b_q and the hyperfine coupling constants A_J and B_J have been reported for the core-excited $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states. Hence we cannot make any comparison with both theory and experiment.

V. SUMMARY

In this work, we have made a detailed atomic structure study on the berylliumlike $1s2s2p^2(^5P)$ and $1s2p^3(^5S)$ states for $Z = 3-10$. For each species, the results for the upper bound, the nonrelativistic energy, the transition wavelength, the oscillator strengths, the lifetime, the fine structure, the hyperfine parameters, and the hyperfine coupling constants are reported. The relativistic corrections and the mass polarization are included. The upper bounds and nonrelativistic energies obtained in this work are much lower than the previously published values for each member of the isoelectronic sequence. This leads to some improvements in the agreement with the precision experiment, for example, for the transition energies of boron and beryllium. However, we find that after we reduced the theoretical uncertainty in the Li^- transition energy, the result is slightly off from the experimental data. The lifetime is also longer than that reported in the later experiment. The reason for these discrepancies is not clear at this time.

We have studied the effect of the hyperfine interaction on the observed fine structure of 5P . Our conclusion is that this effect is very small. It is justifiable to neglect it in the fine-structure experimental analysis.

Noted added in proof. In a thesis by V. Lodwig (University of Bochum, 1989), the $\text{Li}^- 1s2s2p^2(^5P)-1s2p^3(^5S)$ transition wavelength is measured to be $3490.26(25) \text{ \AA}$ which agrees with the 3490.22 \AA obtained in this work. We are grateful to S. Mannervik (Stockholm) for bringing this result to our attention.

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