Triplet 2^3S states in four-electron Be-like ions: Bound-state properties and hyperfine-structure splitting

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(Received 2 April 2009; published 4 June 2009)

Results of variational computations of the triplet 2^3S state in beryllium atom and in some berylliumlike ions (O^{4+}, Ne^{6+}, and Mg^{8+}) are presented. In each of these systems we determine numerically the total energies of the 2^3S state and various bound-state properties. Analytical formulas are derived for the $Z^{-1}(Q^{-1})$ expansion of the total energies of the triplet 2^3S states in four-electron atomic systems. The hyperfine-structure splitting in this state is evaluated for the ^9Be atom.

In this Brief Report we consider the bound-state properties of the 2^3S state in the beryllium atom and some berylliumlike ions. This state is definitely bound (=stable) in the Be atom. The electric dipole transition (or $E1$ transition) from this state into the ground 1^1S state of the beryllium atom is strictly prohibited due to conservation of the total electron spin. In general, the 2^3S states in four-electron atoms and ions are quite similar to the triplet states in two-electron atoms and ions. This follows from the fact that two electrons in any four-electron atom or ion form a very stable $1s^2$ electron shell. The binding energy of an electron in this ($1s$) shell is much larger than that of an electron in any outer electron shell. Consequently, the two outer electrons in any Be-like system can be considered as a quasi-independent two-electron subsystem. Note that in standard notations used in atomic physics the triplet 2^3S states considered in this work can be designated as $[1s^2 2sns]^3S$ states, where $n \geq 3$.

The wave function of the triplet 2^3S state in a four-electron system can be represented as the sum of products of the spatial and spin wave functions. Below, we shall consider only one spin wave function $\chi_1 = (\alpha\beta - \beta\alpha)\alpha\alpha$, where α and β are the electron spin-up and spin-down functions [1]. The spin function χ_1 corresponds to the $S=1$ and $S_z=1$ values, where S is the total (electron) spin of the four-electron system, while S_z is its z projection.

Our main interest below is the bound-state spectrum in four-electron atomic systems. To simplify all following formulas, below we shall use only a.u. in which $\hbar=1$, $m_e = 1$, $e=1$. The nonrelativistic Hamiltonian of the four-electron atomic system takes the form (see, e.g., [2])

$$H = -(1/2)\left[\sum_{i=1}^{4}\nabla_i^2 + (1/M)\nabla_5^2\right] - \sum_{i=1}^{4}(Q/r_{i5})$$
$$+ \sum_{i=1}^{3}\sum_{j=2(>i)}^{4}(1/r_{ij}), \qquad (1)$$

where the subscripts 1, 2, 3, and 4 designate four electrons, while the subscript 5 means the positively charged nucleus. Also, in Eq. (1) Q is the nuclear charge and $\nabla_i = (\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i})$ is the gradient operator of the ith particle ($i=1,2,\dots,5$). The notation r_{ij} stands for the (ij)-relative distance coordinate between ith and jth particles, i.e., $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = r_{ji}$, where $\mathbf{r}_i$ are the Cartesian coordinates of the

ith particle. The notation M in Eq. (1) stands for the mass of the central (heavy) nucleus, i.e., $M \gg m_e = 1$. All particles (i.e., electrons and nuclei) are considered as point particles with masses m_e and M and electric charges $q=-e$ and Qe, respectively.

In this work we need to determine the accurate solutions of the Schrödinger equation $H\Psi = E\Psi$, where H is the Hamiltonian [Eq. (1)], while E is the eigenvalue (total energy) of the considered bound state, and Ψ is the corresponding wave function. In this study we consider the bound triplet 2^3S states in different four-electron atomic systems, including the Be atom and a few other similar systems. It should be mentioned that in this work the bound triplet 2^3S states in four-electron atomic systems are described by the explicitly correlated trial wave functions; we are not aware of any other studies employing such wave functions. However, in [3] the method based on Hartree-Fock configuration interaction was used for the excited states in the Be atom.

The wave function of the triplet 2^3S state in the four-electron atomic system is represented in the form

$$\Psi = \psi_{L=0}(\{r_{ij}\})(\alpha\beta - \beta\alpha)\alpha\alpha, \qquad (2)$$

where $\psi_{L=0}(\{r_{ij}\})$ is the radial part (also called spatial part) of the total wave function. All computations below are performed with the use of only one electron spin function χ_1 which corresponds to the $S=1$ and $S_z=1$ values. The two other spin functions $\chi_0 = (\alpha\beta - \beta\alpha)(\alpha\beta + \beta\alpha)$ and $\chi_{-1} = (\alpha\beta - \beta\alpha)\beta\beta$ correspond to the $S=1$, $S_z=0$ and $S=1$, $S_z=-1$ values, respectively. These three spin functions $\chi_1, \chi_0, \chi_{-1}$ form a regular triplet. To describe the experimental situations with no external magnetic field present we can use only one of these three spin functions. In this work we shall always choose $\chi_1 = (\alpha\beta - \beta\alpha)\alpha\alpha$ [see Eq. (2) above].

Now, we need to obtain the spatial part of the total wave function with the correct permutation symmetry between all identical particles 1–4 (electrons). The corresponding spatial projector is obtained in this work by calculating the explicit expression for the following spin expectation value:

$$\mathcal{P} = \mathcal{C}\langle(\alpha\beta - \beta\alpha)\alpha\alpha|\hat{\mathcal{A}}|(\alpha\beta - \beta\alpha)\alpha\alpha\rangle, \qquad (3)$$

where $\mathcal{C}$ is the normalization factor, while $\hat{\mathcal{A}}$ is the complete four-particle (or four-electron) antisymmetrizer,

TABLE I. The expectation values (in a.u.) of some properties for the bound 2^3S states of the $^\infty$Be atom and $^\infty$O^{4+}, $^\infty$Ne^{6+}, and $^\infty$Mg^{8+} ions with infinitely heavy nuclei. The notation N means the positively charged nucleus, while e designates the electron. The threshold energies of three-electron ions are taken from Refs. [6,7].

System	Be	O^{4+}	Ne^{6+}	Mg^{8+}
E	-14.43005943	-65.92092051	-105.8388513	-155.2018581
E_{tr}	14.324763177	62.228542083	102.68223148	150.136196605
$\langle r_{ee} \rangle$	4.708416	1.536522	1.159892	0.932359
$\langle r_{eN} \rangle$	2.630860	0.884010	0.670119	0.540109
$\langle r_{ee}^2 \rangle$	35.09338	3.476096	1.965085	1.263618
$\langle r_{eN}^2 \rangle$	17.13250	1.687122	0.953494	0.613169
$\langle r_{ee}^3 \rangle$	318.022	9.46608	4.00311	2.05774
$\langle r_{eN}^3 \rangle$	147.408	4.23305	1.78258	0.91427
$\langle r_{ee}^4 \rangle$	3239.8	28.904	9.1427	3.7564
$\langle r_{eN}^4 \rangle$	1451.4	12.139	3.8087	1.5578
$\langle r_{ee}^{-1} \rangle$	0.619331	1.489611	1.920863	2.351610
$\langle r_{eN}^{-1} \rangle$	2.036021	4.399377	5.580079	6.760696
$\langle r_{ee}^{-2} \rangle$	1.503650	7.421729	12.075210	17.85915
$\langle r_{eN}^{-2} \rangle$	14.27389	62.76288	99.96781	145.8098
$\langle -\frac{1}{2}\nabla_1 \rangle$	3.60761579	16.48037599	26.4597983	38.8004773
$\langle \delta_{eN} \rangle$	8.696398	77.824429	155.59634	272.92805
$\langle \delta_{ee} \rangle$	0.39902	4.30195	8.89917	16.0001
$\langle \delta_{eeN} \rangle$	37.576	3445.90	14259.9	44083.0

$$\hat{\mathcal{A}} = \hat{e} - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} - \hat{P}_{14} - \hat{P}_{24} - \hat{P}_{34} + \hat{P}_{123} + \hat{P}_{132} + \hat{P}_{124}$$
$$+ \hat{P}_{142} + \hat{P}_{134} + \hat{P}_{143} + \hat{P}_{234} + \hat{P}_{243} - \hat{P}_{1234} - \hat{P}_{1243} - \hat{P}_{1324}$$
$$- \hat{P}_{1342} - \hat{P}_{1423} - \hat{P}_{1432} + \hat{P}_{12}\hat{P}_{34} + \hat{P}_{13}\hat{P}_{24} + \hat{P}_{14}\hat{P}_{23}. \quad (4)$$

Here $\hat{e}$ is the identity permutation, while $\hat{P}_{ij}$ is the permutation of the ith and jth identical particles. Analogously, the operators $\hat{P}_{ijk}$ and $\hat{P}_{ijkl}$ are the permutations of three identical particles (i, j, and k) and four identical particles (i, j, k, and l), respectively. After some algebra one finds from Eq. (3) the explicit formula for the corresponding spatial projector

$$\mathcal{P} = \frac{1}{2\sqrt{6}}(2\hat{e} + 2\hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} - \hat{P}_{14} - \hat{P}_{24} - 2\hat{P}_{34} - 2\hat{P}_{12}\hat{P}_{34}$$
$$- \hat{P}_{123} - \hat{P}_{124} - \hat{P}_{132} - \hat{P}_{142} + \hat{P}_{134} + \hat{P}_{234} + \hat{P}_{243} + \hat{P}_{143}$$
$$+ \hat{P}_{1432} + \hat{P}_{1234} + \hat{P}_{1243} + \hat{P}_{1342}). \quad (5)$$

This projector creates the spatial part of the total (triplet) wave function with the correct permutation symmetry between all four identical particles (electrons).

The radial part $\psi_{L=0}(A;\{r_{ij}\})$ of the total wave function [Eq. (2)] is represented in the form [4,5]

$$\psi_{L=0}(A;\{r_{ij}\}) = \mathcal{P}\sum_{k=1}^{N_A} C_k \exp\left(-\sum_{ij} \alpha_{ij}^{(k)} r_{ij}^2\right), \quad (6)$$

where N_A is the number of basis functions used and C_k are the linear parameters of the variational expansion [Eq. (6)]. The notation $\alpha_{ij}^{(k)}$ stands for the nonlinear parameters of the variational expansion [Eq. (6)]. The notation $\{r_{ij}\}$ designates the set of relative coordinates which are needed for a complete description of the five-body systems (or four-electron atomic system). In fact, for all berylliumlike ions and atoms considered in this study the notation $\{r_{ij}\}$ stands for ten relative coordinates: r_{12}, r_{13}, r_{14}, r_{15}, r_{23}, r_{24}, r_{25}, r_{34}, r_{35}, and r_{45}. Note that these relative coordinates $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ are translationally and rotationally invariant. Therefore, there is no need to separate the center of mass in the original system or perform any other similar transformation. The radial basis functions in Eq. (6) are called the ten-dimensional gaussoids of the relative coordinates [5]. The summation over all possible pairs (ij), where $(ij) = (ji)$ in the exponents of Eq. (6), is taken over all possible different pairs of particles.

Analytical formulas for all matrix elements needed in bound-state computations of four-electron atomic systems are presented in our earlier work [4] (see also [5]) and are not repeated here. We use the same basis set as in [4]. For discussion of optimization of the nonlinear parameters in the radial wave functions the reader is referred to [6] (also see below). In fact, in our present computations we have used variational wave functions which contain 300 basis functions [Eq. (6)]. All nonlinear parameters in these basis wave functions have been well optimized very carefully. The final accuracy was determined from direct comparisons of our results with the analogous results obtained with the use of 400 basis functions [Eq. (6)]. Now, let us consider the bound-state properties of the triplet 2^3S state in the Be atom. Our second goal is to evaluate the hyperfine splitting in the 2^3S state of the ^{9}Be atom.

Our results for the total energies of this state and for some other bound-state properties can be found in Table I. In Table

TABLE II. The nonrelativistic energies of the $2^3 S$ states of some berylliumlike systems computed with the use of the trial wave function [Eq. (2)]. The Li$^-$ ion is unstable in the $2^3 S$ state. The nuclear masses are infinite for all atomic systems mentioned in this table.

System	E (a.u.)	System	E (a.u.)	System	E (a.u.)
Be	−14.4300594	N^{3+}	−49.5043945	Ne^{6+}	−105.838851
B$^+$	−23.7575327	O^{4+}	−65.9209205	Na^{7+}	−129.339816
C^{2+}	−35.4496814	F^{5+}	−84.6990681	Mg^{8+}	−155.201858

I we also consider the $2^3 S$ states in the O^{4+}, Ne^{6+}, and Mg^{8+} ions. The total energy of the triplet $2^3 S$ state of Be atom with the infinitely heavy nucleus ($^\infty$Be atom) is lower than −14.324 763 176 47 a.u. Infinite nuclear masses are often used in atomic calculations since the actual nuclear masses are determined experimentally and are thus subject to revision. The energy $E_{tr} = -14.324\ 763\ 176\ 47$ a.u. corresponds to the total energy of the three-electron $^\infty$Be$^+$ ion in its ground $1^2 S$ state. In other words, it represents the atomic dissociation threshold for the $^\infty$Be atom. In general, the stability of an arbitrary LS state in the $^\infty$Be atom means its stability against the dissociation $^\infty$Be$(LS) \rightarrow\ ^\infty$Be$^+(1^2 S) + e^-$. Here and below, the bound state in the Be atom is designated with the use of notation LS, where L is the angular momentum and S is the total spin of all four electrons; for the $2^3 S$ state of the Be atom $L = 0$ and $S = 1$. Note that the total energy of the ground state in the three-electron Be$^+$ ion is known to a much better accuracy than the total energy of any bound state in the four-electron Be atom. Briefly, this state in the four-electron Be-like ion (or atom) is bound if the sum of its total energy with the absolute value of the total energy of the ground $1^2 S$ state in the corresponding three-electron ion is negative. In general, such a negative sum is called the binding energy.

In addition to the triplet $2^3 S$ state in the Be atom we also consider a number of similar four-electron (or berylliumlike) ions O^{4+}, Ne^{6+}, and Mg^{8+} in their $2^3 S$ states. All nuclear masses in these computations are assumed to be infinite. In reality, the following recalculations to the finite nuclear masses are easy to perform. As follows from Table I all these ions have stable triplet $2^3 S$ states since the sum $E + E_{tr} < 0$ for each of these ions. The E_{tr} values have been taken from [6,7]. In Table I we also present some basic bound-state properties of all berylliumlike ions mentioned in this work (in the $2^3 S$ state). The physical meaning of all properties, e.g., $\langle r_{ij} \rangle$ and $\langle r_{ij}^{-1} \rangle$, uniformly follows from the notation used. Therefore, here we restrict ourselves only to a few following remarks. The notation $\langle \delta_{ij} \rangle [= \langle \delta(\mathbf{r}_{ij}) \rangle = \langle \delta(\mathbf{r}_i - \mathbf{r}_j) \rangle]$ stands for the expectation value of the two-particle delta function between particles i and j. Analogously, $\langle \delta_{ijk} \rangle$ and $\langle \delta_{ijkl} \rangle$ mean the expectation values of three- and four-particle delta functions. These delta functions are defined via two-particle delta functions as follows: $\delta_{ijk} = \delta(\mathbf{r}_i - \mathbf{r}_j) \delta(\mathbf{r}_i - \mathbf{r}_k)$ and $\delta_{ijkl} = \delta(\mathbf{r}_i - \mathbf{r}_j) \delta(\mathbf{r}_i - \mathbf{r}_k) \delta(\mathbf{r}_i - \mathbf{r}_l)$. Note also that these values are symmetric upon any permutations between particles, e.g., $\delta_{ijk} = \delta_{ikj} = \delta_{kji}$, etc.

It is clear *a priori* that for the triplet $2^3 S$ state of Be atom the expectation values of all multielectron delta functions, e.g., $\langle \delta_{eee} \rangle$, $\langle \delta_{eeeN} \rangle$ and $\langle \delta_{eeee} \rangle$, equal to zero identically. This follows from the fact that two (of three and four) electrons

always have the same spin functions (α in our case). The only delta functions which have nonzero expectation values for the $2^3 S$ state of the Be-like atomic system are δ_{eN}, δ_{ee}, and δ_{eeN}. Their expectation values can be found in Table I.

As follows from the results in Table I the triplet $2^3 S$ state in the Be atom is a weakly bound state. The binding parameter $\tau (\leq 1)$,

$$\tau = (E - E_{tr})/E = 1 - (E_{tr}/E), \qquad (7)$$

for this state is only $\tau \approx 0.0070 = 0.7\%$, i.e., it is a very small value. For many weakly bound Coulomb systems we find $\tau \leq 2\%$. Systems for which this parameter is $<1\%$ can be considered as extremely weakly bound. The structure of this state in the Be atom corresponds to a system which is very close to its dissociation threshold. Briefly, this means that the outer most electron moves far away from the nucleus. In other words, the Be atom in its triplet $2^3 S$ state can be considered as a two-particle cluster system (Be$^+ + e^-$). Such a cluster structure can also explain the instability of the triplet $2^3 S$ state in the four-electron Li$^-$ ion (the ground $1^1 S$ state in this ion is bound) (see, e.g., [4,8] and references therein). However, if the nuclear charge Q in Be-like atomic systems grows, then the corresponding binding energies increase rapidly. For instance, the triplet $2^3 S$ state in the four-electron O^{4+} ion is already quite well bound. The binding energy per electron in this state of the O^{4+} ion is ≈ 0.925 a.u. which close to the values known for a typical atomic (excited) state. As follows from Table I the bound-state properties of the O^{4+}, Ne^{6+}, and Mg^{8+} ions correspond to the properties which can be predicted for a typical atomic (excited) state.

Our analysis can be concluded with an approximate formula for the total energies of the $2^3 S$ states in four-electron atomic systems. To obtain such a formula we shall use the Q^{-1} expansion, where Q is the nuclear charge of the nuclei in four-electron atoms and ions. All nuclear masses are assumed to be equal infinity. Our total energies determined for different four-electron atoms in their $2^3 S$ states (see Table II) can be used as the test points to obtain a number of first coefficients in the $E(Q; 2^3 S)$ expansion. Note that in contrast with [9] our $E(Q; 2^3 S)$ expansion is written for the total energy rather than for ionization potential. The explicit formula is written as a Laurent expansion [10] upon Q (here and below $Q \geq 4$), i.e., it takes the form

$$E(Q; 2^3 S) = a_2 Q^2 + a_1 Q + a_0 + b_1 Q^{-1} + b_2 Q^{-2} + b_3 Q^{-3}$$
$$+ b_4 Q^{-4} + \cdots, \qquad (8)$$

where numerical values of the coefficients $a_2, a_1, a_0, b_1, b_2, b_3, \ldots$ must be determined from fitting the results of accurate numerical computations to Eq. (8). Note

TABLE III. The coefficients of the Q^{-1} expansion constructed for the total energies of the ground $2^3 S$ states in four-electron ions [Eq. (2)]. Expansions with $N=4$, 5, and 6 terms are considered.

a_2	−1.180360605	−1.180673069	−1.180475113	b_1	−0.215624003	0.170682983	−0.506676198
a_1	1.284822636	1.293709937	1.286530496	b_2		−0.592445629	1.611009814
a_0	−0.629492165	−0.719601032	−0.619163349	b_3			−2.768878074

that the principal part of the expansion [Eq. (8)] includes only integer powers of Q^{-1}. Such an expansion essentially follows from the Poincare theorem applied to the Schrödinger equation with the Hamiltonian [Eq. (1)]. As mentioned above the negatively charged Li^- ion is not bound in its $2^3 S$ state. This means that the formula [Eq. (8)] can be applied to actual systems with $Q \geq 4$. The coefficients $a_2, a_1, a_0, b_1, b_2, b_3, \ldots$ determined with our variational energies for four-electron atoms or ions can be found in Table III. The results from Tables II and III can be used in future numerical computations of the $2^3 S$ states in four-electron atoms and ions.

In contrast with the ground (singlet) state in the Be atom, the total electron spin of the triplet state in this atom is different from zero. Therefore, there is an interaction between the total electron spin $S_e = 1$ and nuclear spin I_N in those cases when $I_N \neq 0$. This is the case for the ^9Be atom, where $I_N = \frac{3}{2}$. In the first approximation, the Fermi-Segré formula [2] for the hyperfine splitting in the triplet $^3S(L=0)$ states of the ^9Be atom takes the form (in a.u.)

$$H_{HF} = \frac{8\pi\alpha^2}{3} \mu_B \mu_N g_e g_N \langle \delta(\mathbf{r}_{eN}) \rangle$$

$$\times \frac{1}{2}[F(F+1) - I_N(I_N+1) - S_e(S_e+1)], \qquad (9)$$

where $\langle \delta(\mathbf{r}_{eN}) \rangle$ is the electron-nuclear delta function for the considered triplet state, $S_e = 1$ for the triplet states, I_N is the nuclear spin, and $F = |\mathbf{F}|$, where $\mathbf{F}$ is the total angular momentum operator for the whole atom (i.e., electron shells plus nucleus). For $I_N = \frac{1}{2}$ the splitting can be observed as the doublet of states with $F = \frac{1}{2}$ and $F = \frac{3}{2}$. For $I_N \geq 1$ (the case of ^9Be atom) one can observe the triplet of states with $F = I_N - 1$, I_N, and $I_N + 1$.

The fine structure constant α, proton mass m_p, and g factors used in our present calculations were chosen from [11,12],

$$\alpha = 7.297\,352\,568 \times 10^{-3}, \quad m_p = 1836.152\,672\,61,$$

$$g_e = -2.002\,319\,304\,371\,8,$$

$$g_N(^9\text{Be}) = -1.177\,61\left(\tfrac{2}{3}\right) = -0.785\,07.$$

Also, in a.u. $\mu_B = \frac{1}{2}$, $\mu_N = \mu_B(m_e/M_p)$. Since the hyperfine splitting is traditionally expressed in *Megahertz*, the conversion factor $6.579\,683\,920\,61 \times 10^9$ MHz/a.u. has been used. Now, one can write Eq. (9) in the form

$$H_{HF} = 314.121\,190\,927 \langle \delta(\mathbf{r}_{eN}) \rangle$$

$$\times [F(F+1) - I_N(I_N+1) - S_e(S_e+1)]$$

$$= 2731.722\,897 \left[F(F+1) - \tfrac{23}{4}\right], \qquad (10)$$

where H_{HF} is in MHz, while $\langle \delta(\mathbf{r}_{eN}) \rangle \approx 8.696\,398$ (in a.u.) for the $2^3 S$ state. The hyperfine structure in the ^9Be atom includes three groups of levels with $F = \frac{1}{2}$, $\frac{3}{2}$, and $\frac{5}{2}$. The energies of these states are $-13\,658.614$, -5463.446, and 8195.169 MHz, respectively. The hyperfine-structure splittings can easily be obtained from these values. Such a hyperfine-structure splitting can be measured experimentally.

We have considered the bound-state properties and hyperfine splitting in the triplet $2^3 S$ state of the Be atom. In our present analysis we have applied the explicitly correlated wave functions written in relative five-body coordinates, r_{12}, r_{13}, r_{14}, r_{15}, r_{23}, r_{24}, r_{25}, r_{34}, r_{35}, and r_{45}. It is shown that the triplet $2^3 S$ state in the Be atom is bound (in fact, it is weakly bound). A number of bound-state properties of the triplet $2^3 S$ states in the Be atom and in analogous O^{4+}, Ne^{6+}, and Ne^{8+} ions have been determined to a relatively good accuracy. For the $2^3 S$ state in beryllium atom our variational energy is lower than the corresponding energy from [3]. All nuclei in these systems were assumed to be infinitely heavy, but by using our method it is straightforward to determine the corresponding corrections related to the finite nuclear masses [9]. We have also evaluated the hyperfine splitting in the $2^3 S$ state of the ^9Be atom [13].

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