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Approach to determine nodal surfaces of some *s*-electron systems

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The paper is devoted to the study of the nodal surfaces of the wave functions for fermion systems. Using the quantum Monte Carlo method, implicit equations of nodal surfaces for some *s*-electron systems containing two–five electrons are numerically obtained. The obtained results are in agreement with the provisions of other researchers. An original method for constructing nodal surfaces is proposed, which is convenient for the implementation of quantum Monte Carlo.

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I. INTRODUCTION

The wave function describing a system of N fermions has a well-known antisymmetry property, which is expressed in the Pauli exclusion principle. The only way known to us when antisymmetry is taken into account in applications is to postulate the form of the wave function as a product or a linear combination of products of Slater determinants [1]. Different versions of the quantum Monte Carlo method (QMC) give an exact solution for systems with a sign-constant wave function in the sense that the error is determined only by statistics. An additional approximation associated with the use of Slater determinants introduces an uncontrollable error, and is very inconvenient for the implementation of Monte Carlo methods. QMC methods should basically converge to the exact solution of the Schrödinger equation (SE) if they would allow integrating over the entire domain of the wave function. However, this is not the case due to the fact that Monte Carlo methods cannot work with sign-changing functions (the sign problem) [1].

In a sense, this paper can be seen as a development of Ceperley's ideas in Ref. [2]. Due to the properties of antisymmetry, the wave function of N fermions with the same spin projection divides the entire space into $N!$ domains in each of which the wave function is of constant sign. We propose a method for constructing such domains and, using the Kurchatov version of QMC (KQMC) [3] (which is similar to what is known as Green's function Monte Carlo from Ref. [4]), on one hand, demonstrate the correspondence of the obtained results to the known provisions for ^3S He [5,6] and Li [5,7,8], on the other hand, obtain new results for such systems as Be and ^2S B. An original method to determine the nodal surface is presented, which is convenient for numerical implementation by various variations of QMC. In addition, we note that only the solution of the nonrelativistic SE is studied in the paper, therefore, relativistic effects, such as spin-orbit interactions, are not considered.

II. NODAL REGIONS

Let us consider a system of N electrons. Let N^+ electrons have a spin projection value of $+\frac{1}{2}$, and N^- has a spin projection value of $-\frac{1}{2}$, and $N = N^+ + N^-$. We number the electrons so that for $i = \overline{1, N^+}$ they have spin $+\frac{1}{2}$, and for $i = \overline{N^+ + 1, N^+ + N^-}$——$-\frac{1}{2}$, respectively. Then, there is a permutation group $G = G^+ \times G^-$ of $N^+!N^-!$ elements acting on the $3N$-dimensional phase space. An element that swaps i and j (both indices refer either to the first N^+ numbers or both to the last N^- numbers) cause a permutation of the coordinates of the ith and jth particles. Such a replacement causes a change in the sign of the wave function.

It is possible to single out the so-called nodal region (NR) in a large number of ways, i.e., domain $\Omega_1 \in \mathbb{R}^{3N}$ with the following properties:

$$\begin{aligned} &\forall\, \mathbf{r} \in \Omega_1, \quad \forall\, g \neq 1,\ g \in G\colon g(\mathbf{r}) \notin \Omega_1, \\ &\forall\, \mathbf{r} \in \mathbb{R}^{3N} \exists g \in G\colon g(\mathbf{r}) \in \overline{\Omega}_1, \end{aligned} \tag{1}$$

where $\overline{\Omega}_1$ means the closure of the domain Ω_1.

One can always choose Ω_1 in such a way that the wave function on it is of constant sign. Indeed, if Ψ on Ω_1 is not of constant sign, then,

$$\Omega_1 = \Omega_1^+ \cup \Omega_1^- \cup \Omega_1^0, \tag{2}$$

where the superscript is the sign of Ψ on this set. Let us consider any permutation from G, or any element g resulting from the product of an odd number of permutations, then,

$$\Psi(g(\mathbf{r})) = -\Psi(\mathbf{r}). \tag{3}$$

Therefore, Ψ is positive on $g(\Omega_1^-)$, and, hence, the domain $\Omega' = \Omega^+ \cup g(\Omega^-)$ is the NR on which Ψ is positive. If we consider the wave function to be analytic (in the real sense), then, the domain Ω^0 does not contain interior points and lies completely on the boundaries of the other two. Therefore, there is no need to consider it separately.

We need to highlight the following explanation. We consider the solution of the SE for the entire space $\mathbb{R}^{3N}$. There is an infinite number of NRs, defined only by symmetry. The condition that the sign of the wave function is constant means

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that Ψ must be equal to zero at the boundary of the NR. It is possible to obtain a solution of the SE with a zero boundary condition for any domain with a regular boundary. It may seem that this makes it possible to extend such a solution constructed in any NR to the entire space, acting by the elements of the group and taking into account antisymmetry. However, it is not true. SE requires continuity not only of the wave function itself, but also of its first derivative. The continuity condition for the wave function on the boundaries of the NRs will be, obviously, satisfied due to the boundary condition (Ψ is equal to zero at the boundary). However, the equality of the left and right normal derivatives at the boundary is not guaranteed (this is demonstrated by the example in Fig 1 in Ref. [2]).

Thus, only those of the total number of NRs will give the correct solution, on the boundary of which the condition of continuity of the wave function and its first derivative is satisfied. From now on, we will call such NRs right nodal regions (RNRs).

III. EXTREMAL PROPERTY OF A NODAL REGION

If it were possible to uniquely determine the NR for any system of electrons, then QMC methods would allow to solve such a problem exactly since the function is of constant sign in this domain, and a condition is set on its boundary that allows to uniquely find a solution. A huge number of works have been devoted to the permutation symmetry properties of the wave function, beginning with the works of Fermi and Dirac. However, most of them are devoted to the spin part of the wave function, which is understandable: the structure of spin and coordinate permutations is strongly related, but the study of spin permutations is certainly simpler. This has led to the fact that the coordinate structure has been studied much less fully and mainly for specific systems with a small number of electrons [9], and such knowledge is simply necessary for constructing NRs.

It is intuitively clear that the boundary of a NR must have a certain extremal property. The theorem on the extremal property of the boundary is known [1,10], but its proof is based on the variational principle and does not give an idea of the reasons for the appearance of this extremality. Below is a proof of this theorem based on the wave function continuity property. The consequences from this seem to us more useful for practical applications. In addition, we note that our proof is valid not only for the ground state of the system, but also for excited ones.

Theorem on the extremal property of a NR. The energy of the system E has an extremal property with respect to the variation of the boundary Γ of the RNR: $\frac{\delta E}{\delta \Gamma} = 0$.

Proof. Let Ψ be the correct solution of SE in the RNR Ω with the boundary Γ

$$-\Delta\Psi + E\Psi = V\Psi. \tag{4}$$

Let Ω_1 be a NR with the boundary Γ_1, which is a small distortion of Ω in a sense that for each point of the boundary Γ_1 there is a point of the boundary Γ, the distance to which is less than a small number δ. Let Ψ_1 be the solution of the equation in a new domain with a zero boundary condition, extended to the entire space by antisymmetry,

$$-\Delta\Psi_1 + E_1\Psi_1 = V\Psi_1. \tag{5}$$

Wherein, the energies from the discrete spectrum are chosen appropriately—they are close.

Then, multiplying (4) by Ψ_1 and (5) by Ψ, subtracting one from the other, and integrating over the entire space using the normalization $\int_{\mathbb{R}^{3N}} \Psi\Psi_1 dV = 1$,

$$\int_{\mathbb{R}^{3N}} \mathrm{div}(\Psi_1\nabla\Psi - \Psi\nabla\Psi_1)dV = \delta E, \tag{6}$$

where $\delta E = E - E_1$. Let us apply the Gauss theorem and note that the first term in brackets is a continuous function in $\mathbb{R}^{3N}$, and the second term is discontinuous at the incorrect boundary due to the jump of $\frac{\partial\Psi_1}{\partial\mathbf{n}}|_{\Gamma_1^i}$ (here, Γ_1^i is a common boundary element between the two images of the domains Ω_1 under the action of an element of the group),

$$\delta E = -\sum_{i=1}^{M}\int_{\Gamma_1^i}\Psi\left(\frac{\partial\Psi_1}{\partial\mathbf{n}}\bigg|_{\Gamma_1^{i+}} - \frac{\partial\Psi_1}{\partial\mathbf{n}}\bigg|_{\Gamma_1^{i-}}\right)dS, \tag{7}$$

where $\mathbf{n}$ is the normal to the surface and the sign index of Γ_1^i indicates the derivative direction at the boundary; M is the total number of boundaries between NRs.

Due to the proximity of the regions Ω_1 and Ω, as well as their boundaries, and the fact that $\Psi|_\Gamma = 0$, it could be considered that Ψ is a quantity of order δ at Γ_1, and, hence, also at Γ_1^i. It could also be considered that the difference of any derivatives of the functions Ψ_1 and Ψ is a quantity of order δ. But the derivative of the function Ψ is continuous, and when Ψ_1 and Ψ are replaced, the derivative jump in integral (7) turns into zero.

Thus, δE turns out to be a quadratic function proportional to $(\delta\Gamma)^2$. Then from (7),

$$\frac{\delta E}{\delta \Gamma} = 0. \tag{8}$$

This completes the proof.

IV. HYPOTHESES ABOUT THE CONSTRUCTION OF THE NODAL REGION

Since the NRs are uniquely determined by the SE itself [2], it would be logical to look for their structure in it. Let us write the SE for N electrons with the same spin projection in the following form:

$$\sum_{i=1}^{N}\varepsilon_i(\mathbf{r})\Psi = E\Psi, \tag{9}$$

where $\varepsilon_i(\mathbf{r}) = -\frac{1}{N}\frac{\sum_{j=1}^{N}\Delta_j\Psi}{\Psi} - V_i$, $\mathbf{r} \in \mathbb{R}^{3N}$.

This form of notation gives a partition of the entire space into $N!$ NRs naturally, but it is not yet known whether these are RNRs. The NR with number 1 is determined by the following condition: $\varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_N$. The remaining domains are obtained naturally by permutations. However, practical implementation of this condition turns out to be difficult since we are still dealing with a $3N$-dimensional space. The next assumption that we made, and which turned out to be successful, at least, for s electrons, is replacement of ε_i with V_i, that is, the total partial energy with the potential one. This seems also reasonable from the point of view of the Hohenberg-Kohn theorem [11], which makes it possible to establish a one-to-one correspondence between the potential and *the exact* Ψ. Hence, it is logical to assume that the structure of the zeros of Ψ is also determined by the potential. As follows from the SE, in the place where Ψ is equal to zero the total kinetic energy is also equal to zero. Zero kinetic energy can be observed either when the Laplacians of Ψ at the boundary, related to individual particles separately, are equal to zero, or when the sum of Laplacians of Ψ for a part of the electrons has a positive sign, and the sum of Laplacians of Ψ for the remaining electrons has a negative sign of exactly the same value. Both of these cases allow us to assume that the value of the kinetic energy at the boundary is not important from the point of view of determining the NR, and we can either assign the Nth part of the total kinetic energy at the boundary to each particle, or ignore it altogether, which will be the same from a practical point of view.

Let us designate the NR of SE solutions for s electrons the domain Ω_1 in $\mathbb{R}^{3N}$ for which the following conditions are satisfied:

$$\begin{gathered} V_1 < V_2 < \cdots < V_{N^+}, \\ V_{N^++1} < V_{N^++2} < \cdots < V_{N^++N^-}, \end{gathered} \tag{10}$$

where V_i are the partial potentials introduced by the formula,

$$V_i = \alpha \frac{2Z}{r_i} - \beta \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{1}{r_{ij}} + \frac{1-\alpha}{N} \sum_{j=1}^{N} \frac{2Z}{r_j} - \frac{1-\beta}{N} \sum_{j=1}^{N-1} \sum_{k>j}^{N} \frac{2}{r_{jk}}. \tag{11}$$

Here, α and β are any functions of particle coordinates that are symmetric in permutations $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. This is the most general form of partial potentials under the conditions $\sum_i V_i = V$ and $V_i \to V_j$ when i is replaced by j.

The statement that this is the most general form is made for the following reason. Partial potentials are considered as an element of a two-dimensional space in the basis given by the external potential, on one hand, and the interelectronic potential, on the other. Thus, the entire set of representations of potentials in the form of a sum of V_i is a two-dimensional affine plane in space with coordinates α and β, which, in the general case, are functions of all physical coordinates symmetric in permutations.

The entire space $\mathbb{R}^{3N}$ is $\bigcup_k \Omega_k$, $k = \overline{1, N^+!N^-!}$ of NRs, which are obtained from (10) by all possible permutations. The boundary of the Ω_1 domain is Γ_1 in $\mathbb{R}^{3N-1}$, which is defined by the following equalities:

$$\begin{aligned} V_i &= V_{i+1}, \quad i = \overline{1, N^+ - 1}; \\ V_i &= V_{i+1}, \quad i = \overline{N^+ + 1, N - 1}. \end{aligned} \tag{12}$$

After the introduction of partial potentials by formula (11), one needs to determine the coefficients α and β. Although any two permutation-symmetric functions α and β define a NR, it is intuitively clear that the correct NR should not be too complicated. Therefore, it is natural to assume that α and β are constants. It follows from (10) that only the first two terms in (11) play a role when specifying the NR. Divide inequalities (10) by α, then, taking into account $\gamma = \frac{\beta}{\alpha}$:

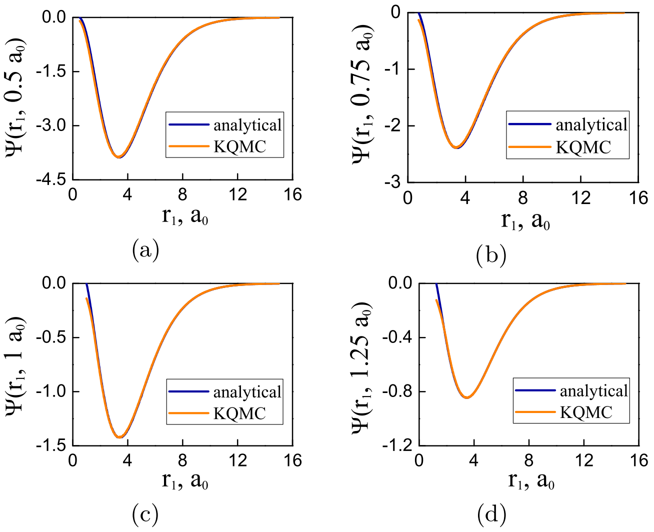


FIG. 1. Analytical solution and solution obtained by the KQMC method for $1s2s$ ^3S He without interelectronic interaction depending on $r_1 > r_2$ at (a) $r_2 = 0.5\,a_0$, (b) $r_2 = 0.75\,a_0$, (c) $r_2 = 1\,a_0$, and (d) $r_2 = 1.25\,a_0$.

$$V_i = \frac{2Z}{r_i} - \gamma \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{1}{r_{ij}}. \tag{13}$$

By varying γ, we change the boundary of the NR. The position of the boundary is very difficult to express explicitly in terms of γ, but we do not need to. According to the theorem on the extremal property of a NR, the total energy must be stationary with respect to the variation of the boundary.

Using the proposed approach, many-electron systems containing s electrons were calculated. For the calculation, we used a program that implements KQMC [3], in which the search for a solution is carried out inside one NR, and inequalities (10) act as an indication that the state vector is inside the domain. In Ref. [3] a detailed description of KQMC algorithm is provided as well as preliminary calculation approaches. Those early calculations differed from ones presented in this paper because other values for γ (and, thus, essentially another nodal structures) were used.

For two electrons that do not interact with each other in the field of an atomic nucleus, the spins of which are directed identically, the exact node $r_1 = r_2$ follows from (12), and the solution is the following Slater determinant [12]:

$$\Psi(r_1, r_2) = 4 \begin{vmatrix} R_{10}(r_1) & R_{20}(r_1) \\ R_{10}(r_2) & R_{20}(r_2) \end{vmatrix}, \tag{14}$$

where $R_{10}(r) = 2(Z)^{\frac{3}{2}} \exp(-Zr)$, $R_{20}(r) = \frac{1}{2}(\frac{Z}{2})^{\frac{3}{2}}(1 - \frac{Zr}{2}) \exp(-\frac{Zr}{2})$.

Applying the KQMC method, a solution in close proximity to the exact one was obtained (Fig. 1). When setting the

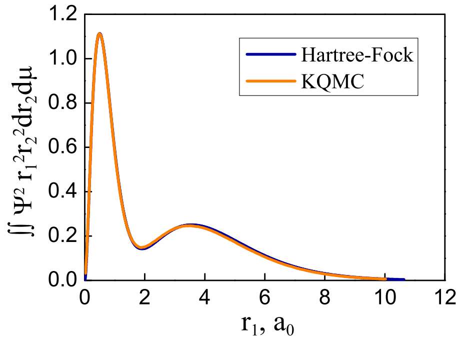


FIG. 2. Integrated square of the Hartree-Fock wave function $\int_0^\infty \int_{-1}^1 \Psi_{\mathrm{HF}}{}^2 r_1{}^2 r_2{}^2 dr_2 d\mu$ and the solution of SE by the KQMC method $\int_0^\infty \int_{-1}^1 \Psi_{\mathrm{KQMC}}{}^2 r_1{}^2 r_2{}^2 dr_2 d\mu$ for $1s2s\ {}^3S$ He (μ is the cosine of the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$).

boundary conditions, we use a method that is often used in the theory of neutron transfer, which is associated with setting the boundary condition not on the real, but on the extrapolated boundary [13].

For the simplest $1s2s\,{}^3S$ He system, from (12) the boundary value $r_1 = r_2$ is automatically obtained, which was previously obtained analytically in Refs. [5,6]. The calculation by the Hartree-Fock method gives a result that is only a few hundredths of an electronvolt less than the experimental value [14]: 59.16(4) vs 59.18(5) eV. Therefore, from the point of view of verification, we can reasonably consider the Hartree-Fock solution as quite precise.

Figure 2 shows a comparison of the results of ${}^3S$ He calculation by the Hartree-Fock method (with sufficient accuracy by our program, described and verified in Ref. [15]) and the KQMC method. In fact, we have obtained agreement of the Monte Carlo solution with the quite precise one.

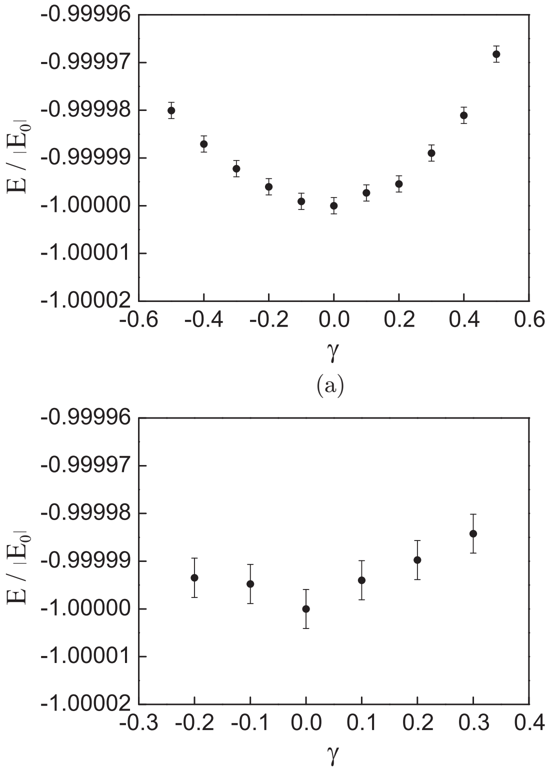
In Refs. [5,7,8], it was obtained numerically that the node $r_1 = r_2$ is also correct for Li. By varying the parameter γ with a step of 0.1, an extremum was obtained at $\gamma = 0$ on sufficient statistics [Fig. 3(a)], which leads to the value of the boundary $r_1 = r_2$ for Li. The same result was obtained for $1s^2 2s 3s\ {}^3S$ Be [Fig. 3(b)].

According to (10), the NR for Be is given by the following inequalities:

$$\frac{2Z}{r_1} - \gamma \sum_{\substack{j=1 \\ j\neq 1}}^{4} \frac{1}{r_{1j}} < \frac{2Z}{r_2} - \gamma \sum_{\substack{j=1 \\ j\neq 2}}^{4} \frac{1}{r_{2j}},$$
$$\frac{2Z}{r_3} - \gamma \sum_{\substack{j=1 \\ j\neq 3}}^{4} \frac{1}{r_{3j}} < \frac{2Z}{r_4} - \gamma \sum_{\substack{j=1 \\ j\neq 4}}^{4} \frac{1}{r_{4j}}. \tag{15}$$

By varying the parameter γ with a step of 0.1, an extremum was obtained at $\gamma = -0.2$ on sufficient statistics (Fig. 4). Based on this, the extremum is located in the range from -0.3 to -0.1, which leads to a boundary different from that specified by the equalities $r_1 = r_2,\ r_3 = r_4$.

A similar result was obtained for $1s^2 2s^2$ B$^+$, $1s^2 2s^2 3s\ {}^2S$ B, $1s^2 2s^2 3s\ {}^2S$ C$^+$ (Fig. 5).



(a)

(b)

FIG. 3. Dependence of the solution $E/|E_0|$ for (a) Li atom, (b) $1s^2 2s 3s\ {}^3S$ Be on the parameter γ, where E_0 is the total energy value at $\gamma = 0$.

In Refs. [5,16], the authors give the proof of the theorem that the ground state of the Be atom has only 2 NRs, and, accordingly, the boundary is not like Hartree-Fock ($r_1 = r_2,\ r_3 = r_4$). Our results contradict the conclusions of Refs. [5,16] from the point of view of connectivity. The proof in Refs. [5,16] is constructed as follows: a point $\mathbf{R}^* = (\mathbf{r}_1, -\mathbf{r}_1, \mathbf{r}_3, -\mathbf{r}_3)$ is taken, which goes to the point $P_{12}P_{34}\mathbf{R}^*$ (P_{ij} is a permutation operator that permutes the coordinates of the ith and jth particles) by rotating the system as a whole by 180° around the axis $\mathbf{r}_1 \times \mathbf{r}_3$. Since the ground state of Be is an S state, the wave function $\Psi(\mathbf{R})$ is

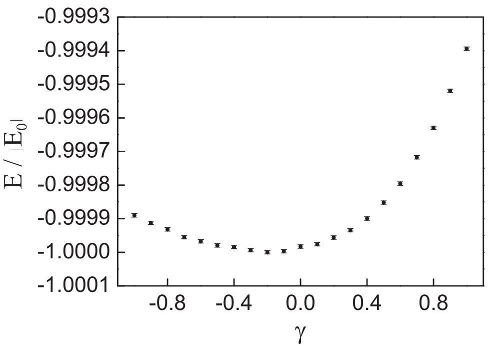


FIG. 4. Dependence of the solution $E/|E_0|$ for the Be atom on the parameter γ, where E_0 is the total energy value at $\gamma = -0.2$.

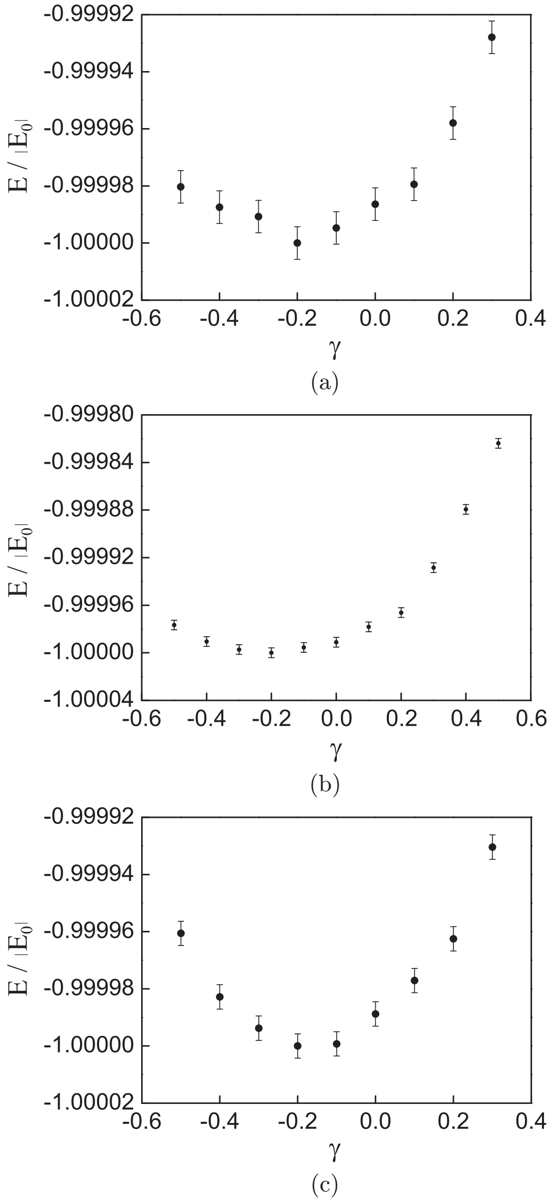


FIG. 5. Dependence of the solution $E/|E_0|$ for (a) $1s^22s^2\,\mathrm{B}^+$, (b) $1s^22s^23s\;{}^2S$ B, (c) $1s^22s^23s\;{}^2S\;\mathrm{C}^+$ on the parameter γ, where E_0 is the total energy value at $\gamma = -0.2$.

invariant under the rotations of the system as a whole around the axis $\mathbf{r}_1 \times \mathbf{r}_3$. Therefore, if one can prove that the point $\mathbf{R}^* = (\mathbf{r}_1, -\mathbf{r}_1, \mathbf{r}_3, -\mathbf{r}_3)$ does not lie on the boundary of the nodal region for the exact wave function of the Be atom [that is, one proves that $\Psi(\mathbf{R}^*) \neq 0$], this will mean that the path connecting the point $\mathbf{R}^*$ with the point $P_{12}P_{34}\mathbf{R}^*$ lies in one nodal region, and there are two of them in total. Our boundary is also not the Hartree-Fock boundary, but it satisfies $\Psi(\mathbf{R}^*) = 0$, which can be seen by substituting $\mathbf{R}^*$ into (15). In Refs. [5,16], the fulfillment of the condition $\widetilde{\Psi}(\mathbf{R}^*) \neq 0$ had been proved for the approximate wave function $\widetilde{\Psi}$, which is the first two terms of the expansion of the exact wave function Ψ in the configuration interaction basis. We are not aware of any works that provide proof of $\Psi(\mathbf{R}^*) \neq 0$ for the exact wave function of Be. Therefore, we question the correctness of the proof of the theorem in Refs. [5,16].

V. CONCLUSIONS

The paper proposes a method for constructing nodal surfaces, which is convenient for the implementation of QMC. Implicit equations of nodal surfaces for some s-electron systems containing two–five electrons are numerically obtained. In terms of single atoms, it is easy to imagine a generalization of such an approach to atoms of all elements in case we could separate the variables in the SE $\Psi = f \times g$ where the function g is responsible for the nonzero value of orbital angular momentum of the system and can be found analytically. Then, the function f can be determined by the KQMC method using the algorithm described in this article. And this will be the subject of our further research.

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