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FORMATION OF SUPERCONDUCTING PAIR CORRELATIONS IN SPHERICAL EVEN-EVEN NUCLEI

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О возникновении парных корреляций сверхпроводящего типа
в сферических четно-четных ядрах

На базе специального преобразования Боголюбова для одинаковых нуклонов рассмотрено возникновение парных корреляций в основном состоянии сферических четно-четных ядер. Подтверждено, что в ядрах с заполненными подоболочками парные корреляции сверхпроводящего типа возникают при константах взаимодействия G, превышающих некоторое пороговое значение. Для такого порогового значения получены грубые оценки сверху и снизу. Показано, что в ядрах с открытой подоболочкой сверхпроводящие корреляции существуют при любых положительных значениях G. При этом пары нуклонов распределяются по всем подоболочкам, участвующим в спаривательном взаимодействии.

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Formation of Superconducting Pair Correlations
in Spherical Even-Even Nuclei

The appearance of like nucleon pair correlations in the ground state of spherical even-even nuclei is considered within the special Bogoliubov transformation. It is confirmed that in closed subshell nuclei, superconducting pair correlations appear if the coupling constant G exceeds a certain threshold value. Rough upper and lower estimates are obtained for the threshold value. It is shown that superconducting correlations exist in open subshell nuclei at any positive G. In this case, nucleon pairs are distributed over all subshells participating in the pairing interaction.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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INTRODUCTION

It was stressed in one of the very first papers [1] on the application of the idea of superconducting correlations to the atomic nuclei spectroscopy that pair correlations in nuclei can appear only if the coupling constant exceeds a certain value. It was also mentioned that the existence of such a threshold value distinguishes atomic nuclei from the infinite systems considered in the theory of superconductivity. This remark was later repeated several times [2, 3].

The necessity of a threshold was revealed by the following reasoning [1, 2]. In the simplest case when all the matrix elements of the two-body pairing interactions are replaced by the same positive constant G, the equations for the correlation function C and the chemical potential λ can be written as

$$\frac{G}{2}\sum_s \frac{1}{\sqrt{(E_s-\lambda)^2+C^2}} = 1, \tag{1}$$

$$2\sum_s v_s^2 = \mathcal{N}, \quad v_s^2 = \frac{1}{2}\left[1 - \frac{E_s-\lambda}{\sqrt{(E_s-\lambda)^2+C^2}}\right]. \tag{2}$$

Here $\mathcal{N}$ is the number of particles in the system. The summation is carried out over pairs of doubly-degenerate single-particle states in the nuclear mean field. These states are related to each other by the operation of time reversal [2]. The inequality

$$\frac{G}{2}\sum_s \frac{1}{|E_s-\lambda|} > 1 \tag{3}$$

follows from Eq. (1) for non-zero C. Inequality (3) is often considered as a relation that determines the minimal value of G, starting from which superconducting pair correlations can exist in the system. The reasoning contains a tacit assumption that λ cannot approach one of the E_s's close enough to increase considerably the sum $\sum\limits_s 1/|E_s-\lambda|$ as G decreases. The correctness of the assumption is not evident because both λ and C are calculated by solving the nonlinear system of Eqs. (1) and (2). Therefore, inequality (3) is a useful hint rather than a proof.

In this paper, we study the conditions of the formation of superconducting pair correlations between like nucleons in the ground state of spherical even-even nuclei. Since Eqs. (1) and (2) for many-level systems can only be solved numerically, we first consider the solution of equations with one and two subshells and then use the obtained results in the discussion of the many-subshell problem.

The paper contains Introduction, Sections 1–3, and Conclusions. The equations for calculating normal and abnormal single-particle densities are derived in Sec. 1. The contribution of pairing interaction to the single-particle energy is taken into account explicitly. The appearance of pair correlations in single-subshell and two-subshell systems is discussed in Sec. 2. The threshold value of G is calculated for the system with closed subshell as well. Many-subshell nuclei are discussed in Sec. 3. The main results of the paper are summed up in Conclusions.

1. MODEL HAMILTONIAN AND MAIN EQUATIONS

The Hamiltonian of the neutrons (or protons) in the nucleus with spherical symmetry is chosen [2] as

$$H = \sum_k \sum_{m_k=-j_k}^{j_k} E_k a^\dagger_{k,m_k} a_{k,m_k} - \\ - \frac{G}{4} \sum_{k,l} \sum_{m_k=-j_k}^{j_k} (-1)^{j_k-m_k} a^\dagger_{k,m_k} a^\dagger_{k,-m_k} \sum_{m_l=-j_l}^{j_l} (-1)^{j_l-m_l} a_{l,-m_l} a_{l,m_l}. \quad (4)$$

Here the indices k label single-particle states with energy E_k and angular momentum j_k; m_k is the third projection of angular momentum, $m_k = -j_k, -j_k+1, \ldots, j_k-1, j_k$; the operators $a^\dagger_{k,m_k}$ and a_{k,m_k} are fermion operators of the creation and annihilation of a particle in the state (k, m_k). We follow the tradition and call *the subshell* a set of $2j_k+1$ single-particle states with the same E_k and j_k. We consider the attractive interaction, i.e., $G > 0$.

The quasiparticle operators are introduced by the special Bogoliubov transformation with the real coefficients [2]:

$$a_{k,m_k} = u_k \alpha_{k,m_k} + (-1)^{j_k-m_k} v_k \alpha^\dagger_{k,-m_k}. \quad (5)$$

If the operators α_{k,m_k} and $\alpha^\dagger_{k,m_k}$ are the fermion annihilation and creation operators, the transformation coefficients satisfy the conditions

$$u_k^2 + v_k^2 = 1. \quad (6)$$

The quasiparticle vacuum $|\rangle$ is determined by the equations $\alpha_{k,m_k}|\rangle = 0$ for any k and m_k. If the quasiparticle operators are introduced by Eq. (5), the angular momentum of $|\rangle$ is zero and its parity is positive. This is easy to prove by applying the operators of the total angular momentum of the system of like nucleons and the parity operator on $|\rangle$. As a result, the product of neutron and proton vacuum states has zero angular momentum and positive parity, the values coincide with the angular momentum and parity of ground states of all spherical even-even nuclei. For this reason, we approximate the wave function of the ground state of a system containing an even number $\mathcal{N}$ of identical nucleons (either neutrons or protons) by an appropriate quasiparticle vacuum $|\rangle$.

The quasiparticle vacuum is connected with the state without nucleons [2]:

$$|\rangle = \prod_{k,m_k>0} \left(u_k + (-1)^{j_k-m_k} v_k a^\dagger_{k,m_k} a^\dagger_{k,-m_k}\right) |0\rangle, \tag{7}$$

where $|0\rangle$ is the state without nucleons, $a_{k,m_k}|0\rangle = 0$ for any k and m_k. If for a certain k the coefficients u_k and v_k differ simultaneously from zero ($u_k v_k \neq 0$), function (7) contains components with a different number of nucleon pairs.

The coefficients of transformation (5) can be determined from the condition of minimum of the system energy $\langle|H|\rangle$. In searching for an energy extremum, one should satisfy the constraint that the average of the nucleon number operator over quasiparticle vacuum is equal to the number of particles in the system

$$\langle|N|\rangle = \langle| \sum_{k,m_k} a^\dagger_{k,m_k} a_{k,m_k} |\rangle = \mathcal{N}.$$

Therefore, the functional to be minimized is

$$\langle|H|\rangle - \lambda \left[\langle| \sum_{k,m_k} a^\dagger_{k,m_k} a_{k,m_k} |\rangle - \mathcal{N}\right].$$

Here λ is the Lagrange multiplier usually called *the chemical potential*. One can see that the inclusion of a supplementary condition modifies the operator H into

$$H' = H - \lambda \sum_{k,m_k} a^\dagger_{k,m_k} a_{k,m_k}.$$

The average of H' over the quasiparticle vacuum is equal to

$$\langle|H'|\rangle = \sum_k (2j_k+1)(E_k-\lambda)v_k^2 - \\ - \frac{G}{2}\sum_k (2j_k+1)v_k^4 - \frac{G}{4}\left[\sum_k (2j_k+1)u_k v_k\right]^2. \tag{8}$$

The transformation coefficients u_k and v_k enter into the expression as the products v_k^2 and $u_k v_k$ only. We use the products as new variables

$$w_k = v_k^2 \quad \text{and} \quad t_k = u_k v_k. \tag{9}$$

Sometimes they are called the *normal density* and *abnormal density* because

$$w_k = \langle|a^\dagger_{k,m_k} a_{k,m_k}|\rangle \quad \text{and} \quad t_k = (-1)^{j_k-m_k}\langle|a_{k,-m_k} a_{k,m_k}|\rangle.$$

The presence of non-zero $\langle|a_{k,-m_k} a_{k,m_k}|\rangle$ is a sign of a superconducting state. It follows from Eq. (6) that the densities obey the inequalities

$$0 \leqslant w_k \leqslant 1 \quad \text{and} \quad 0 \leqslant t_k \leqslant \frac{1}{2}$$

and are connected by the relations

$$w_k^2 + t_k^2 = w_k. \tag{10}$$

The matrix element (8) is expressed via w_k and t_k as

$$\langle |H'| \rangle = \sum_k (2j_k + 1)(E_k - \lambda) w_k - \\ - \frac{G}{2} \sum_k (2j_k + 1) w_k^2 - \frac{G}{4} \left[\sum_k (2j_k + 1) t_k \right]^2. \tag{11}$$

The supplementary condition for the particle number is

$$\sum_k (2j_k + 1) w_k = \mathcal{N}. \tag{12}$$

For convenience of further calculations, we write w_k as a sum

$$w_k = \xi_k + \frac{1}{2}, \quad (-1/2 \leqslant \xi_k \leqslant 1/2)\,. \tag{13}$$

Now relations (10) are simplified

$$\xi_k^2 + t_k^2 = \frac{1}{4} \tag{14}$$

and can be satisfied by the trigonometric functions

$$\xi_k = \frac{1}{2} \cos\varphi_k, \quad t_k = \frac{1}{2} \sin\varphi_k, \quad \text{with} \quad 0 \leqslant \varphi_k \leqslant \pi.$$

Please note that $t_k > 0$ with $0 < \varphi_k < \pi$. The matrix element (8) depends on the unknown φ_k only,

$$\langle |H'| \rangle = \sum_k \big(j_k + \frac{1}{2}\big)\big(E_k - \lambda - \frac{G}{4}\big) + \sum_k \big(j_k + \frac{1}{2}\big)\big(E_k - \frac{G}{2} - \lambda\big) \cos\varphi_k \; - \\ - \frac{G}{4} \sum_k \big(j_k + \frac{1}{2}\big) \cos^2\varphi_k - \frac{G}{4} \left[\sum_k \big(j_k + \frac{1}{2}\big) \sin\varphi_k \right]^2. \tag{15}$$

For any φ_k from the interval $0 < \varphi_k < \pi$, the condition of extremum $\langle |H'| \rangle$ is

$$\frac{\partial \langle |H'| \rangle}{\partial \varphi_k} = 0. \tag{16}$$

When φ_k approaches 0 or π, the usual derivatives should be replaced by the one-sided ones. The simplest way to arrange the limiting processes is to map the entire number axis to the segment $0 \leqslant \varphi_k \leqslant \pi$ by $\varphi_k = \operatorname{arccot} x_k$ with $\infty > x_k > -\infty$. Afterwards Eq. (16) transforms into

$$\frac{\partial \langle |H'| \rangle}{\partial x_k} = \frac{\partial \langle |H'| \rangle}{\partial \varphi_k} \frac{d\varphi_k}{dx_k} = \frac{\partial \langle |H'| \rangle}{\partial \varphi_k} \left(-\frac{1}{1 + x_k^2} \right) = 0. \tag{17}$$

Three stationary points are possible for each k:

$$x_k = \infty, \quad \varphi_k = 0, \quad \xi_k = \frac{1}{2}, \quad w_k = 1, \quad t_k = 0, \tag{18}$$

$$x_k = -\infty, \quad \varphi_k = \pi, \quad \xi_k = -\frac{1}{2}, \quad w_k = 0, \quad t_k = 0, \tag{19}$$

$$x_k \text{ finite}, \quad \frac{\partial\langle|H'|\rangle}{\partial\varphi_k} = 0, \quad 0 < \varphi_k < \pi, \quad t_k > 0, \quad 0 < w_k < 1. \tag{20}$$

Stationary points (18) and (19) describe the states with normal density at subshell k strictly equal to either 1 or 0 and abnormal density equal to zero (normal solutions). Equation (20) describes the states with $t_k > 0$ and $0 < w_k < 1$ (superconducting solutions). Equation (20) can be written as

$$\big(E_k - \frac{G}{2} - \lambda\big)\sin\varphi_k - \frac{G}{2}\cos\varphi_k\sin\varphi_k + \frac{G}{2}\left[\sum_l\big(j_l + \frac{1}{2}\big)\sin\varphi_l\right]\cos\varphi_k = 0,$$

or

$$\big(E_k - \frac{G}{2} - \lambda\big)t_k - G\xi_k t_k + GD\xi_k = 0. \tag{21}$$

Here the notation

$$D = \sum_l S_l\, t_l, \quad S_l = j_l + \frac{1}{2},$$

is used. For each subshell l, the quantities S_l are equal to the number of different particle pairs that form the state (7).

Remark 1. Usually in Eq. (8), the terms proportional to v_k^4 are discarded (or absorbed into E_k by the modification of single-particle energies [2]). In this case, Eq. (21) is transformed into

$$\big(E_k - \lambda\big)t_k = -GD\xi_k.$$

We square both parts of the equation, use Eq. (14) and obtain equations analogous to Eqs. (1) and (2) with the correlation function $C = GD$.

Remark 2. Extremum conditions (18) and (19) at $\varphi_k = 0$ and $\varphi_k = \pi$ correspond to the normal solutions with $t_k = 0$. These solutions allow one to describe the system having $t_l > 0$ for a certain subshell and $t_m = 0$ for other subshells. If $t_{k'} = 0$ for a certain subshell k', then from Eqs. (21) alone it would follow that $D = 0$ and the rest of the abnormal densities would be zero.

Remark 3. The contribution of components with a different particle number to $|\rangle$ is estimated by the particle number variance

$$\mathcal{V} = \langle|N^2|\rangle - \langle|N|\rangle^2 = 2\sum_k(2j_k + 1)\, t_k^2 = 4\sum_k S_k t_k^2.$$

The particle number variance is determined by non-zero t_k only.

2. ONE AND TWO SUBSHELLS

Let us start with the simplest cases.

2.1. Single Subshell. If the system contains a single subshell with the energy E_0 and angular momentum j_0, Eqs. (21) and (12) are reduced to

$$\big(E_0 - \frac{G}{2} - \lambda\big) t_0 - G\xi_0 t_0 + GS_0 t_0 \xi_0 = 0, \tag{22}$$

$$2S_0 \left(\xi_0 + \frac{1}{2}\right) = \mathcal{N}. \tag{23}$$

If $\mathcal{N} = 2S_0$ (all single-particle states are occupied or *the subshell is closed*), the particle number equation (23) has the solution $\xi_0 = 1/2$, and therefore $t_0 = 0$. Only the normal solution is possible for any G.

If $\mathcal{N} = 2S_0 - 2P_0$, here P_0 is the number of particle pairs removed from the closed subshell. The particle number equation (23) has the solution

$$\xi_0 = 1/2 - p_0, \quad \text{with} \quad p_0 = P_0/S_0, \quad \text{and} \quad w_0 = 1 - p_0, \quad w_0 < 1,$$

and only superconducting solution exists. The abnormal density and correlation function are equal to

$$t_0 = \sqrt{p_0(1 - p_0)}\,,$$

$$C = GD = GS_0 t_0 = GS_0 \sqrt{p_0(1-p_0)} = \frac{G}{2}\sqrt{\mathcal{N}(2S_0 - \mathcal{N})}\,.$$

In the case of single open subshell, the correlation function depends linearly on G, because both ξ_0 and t_0 are independent of G. The particle number variance is also constant

$$\mathcal{V} = 4S_0 t_0^2 = 4S_0 p_0 (1 - p_0) = \frac{\mathcal{N}(2S_0 - \mathcal{N})}{S_0}.$$

The chemical potential is a linear function of G:

$$\lambda = E_0 + G\left[\left(\frac{1}{2} - p_0\right) S_0 - (1 - p_0)\right].$$

2.2. Two Subshells. For the system having two subshells, the set of equations is

$$\begin{aligned} &\big(E_1 - \frac{G}{2} - \lambda\big) t_1 - Gt_1\xi_1 + G\,(S_1 t_1 + S_2 t_2)\,\xi_1 = 0, \\ &\big(E_2 - \frac{G}{2} - \lambda\big) t_2 - Gt_2\xi_2 + G\,(S_1 t_1 + S_2 t_2)\,\xi_2 = 0, \end{aligned} \tag{24}$$

$$2\,(S_1\xi_1 + S_2\xi_2) = \mathcal{N} - S_1 - S_2. \tag{25}$$

We label subshells by the indices “1” and “2” so that $E_2 > E_1$. If $E_2 = E_1$, we face, due to definition (5), the single-subshell system with $S_0 = S_1 + S_2$. It is convenient to introduce the dimensionless chemical potential and coupling constant

$$\mu = \frac{\lambda - E_1 + G/2}{E_2 - E_1} \quad \text{and} \quad g = \frac{G}{E_2 - E_1}.$$

And Eqs. (24) can be written as

$$\begin{aligned} -\mu t_1 - g t_1 \xi_1 + g\left(S_1 t_1 + S_2 t_2\right)\xi_1 &= 0, \\ \bigl(1-\mu\bigr) t_2 - g t_2 \xi_2 + g\left(S_1 t_1 + S_2 t_2\right)\xi_2 &= 0. \end{aligned} \tag{26}$$

2.2.1. $S_1 = S_2$ ***and*** $\mathcal{N} = 2S_1$**.** Consider the system with $S_1 = S_2$. The particle number equation (25) is simplified to

$$2S_1\left(\xi_1 + \xi_2\right) = \mathcal{N} - 2S_1.$$

When $\mathcal{N} = 2S_1$, it gives $\xi_2 = -\xi_1$ and $t_2 = t_1$. Equations (26) are transformed into

$$\begin{aligned} -\mu t_1 - g t_1 \xi_1 + 2g S_1 t_1 \xi_1 &= 0, \\ \bigl(1-\mu\bigr) t_1 + g t_1 \xi_1 - 2g S_1 t_1 \xi_1 &= 0. \end{aligned} \tag{27}$$

We sum them and get the equation

$$\left(1 - 2\mu\right) t_1 = 0,$$

having two solutions: $\mu = 1/2$ and $t_1 = 0$.

The $t_1 = 0$ solution corresponds to the normal state with $\xi_1 = \pm 1/2$ and $\xi_2 = \mp 1/2$. The energy minimum is reached at $\xi_1 = 1/2$ ($w_1 = 1$) and $\xi_2 = -1/2$ ($w_2 = 0$). The solution exists for any positive G. The chemical potential μ is arbitrary.

Let us consider the $\mu = 1/2$ solution with $t_1 \neq 0$. The chemical potential is

$$\lambda = \frac{1}{2}\left(E_1 + E_2 - G\right).$$

It follows from the first equation of Eqs. (27) for $t_1 \neq 0$ that

$$\xi_1 = \frac{1}{2}\,\frac{1}{g\left(2S_1 - 1\right)}.$$

Due to Eq. (14), the real non-zero t_1 exists for $|\xi_1| < 1/2$, and therefore the superconducting pair correlations may appear if

$$g > \frac{1}{2S_1 - 1}.$$

It is convenient to introduce special notation for the critical values of the interaction constant

$$g_{\text{cr}} = \frac{1}{2S_1 - 1} \quad \text{and} \quad G_{\text{cr}} = \frac{E_2 - E_1}{2S_1 - 1}.$$

The solutions are

$$\xi_1 = \frac{1}{2}\frac{g_{\rm cr}}{g} = \frac{1}{2}\frac{G_{\rm cr}}{G},$$
$$t_1 = \sqrt{\frac{1}{4} - \xi_1^2} = \frac{1}{2}\sqrt{\frac{(g-g_{\rm cr})(g+g_{\rm cr})}{g^2}}\,.$$

For small g, $0 < g - g_{\rm cr} \ll g_{\rm cr}$, we have (the approximate equality $g + g_{\rm cr} \approx 2g$ is taken into account) $t_1 \approx \sqrt{\dfrac{g-g_{\rm cr}}{2g}} = \sqrt{\dfrac{G-G_{\rm cr}}{2G}}$, and $C = 2GS_1t_1 \approx S_1\sqrt{2G(G-G_{\rm cr})}$. Here one cannot expand the correlation function C in the Taylor series in G near $G_{\rm cr}$. As in statistical mechanics, this example demonstrates the non-analytical dependence of correlation function on coupling constant. The $G_{\rm cr}$ is the breaking point of $C(G)$

$$C(G) = \begin{cases} 0, & \text{if} \quad G \leqslant G_{\rm cr}, \\ GS_1\sqrt{1-(G_{\rm cr}/G)^2}\,, & \text{if} \quad G > G_{\rm cr}\,. \end{cases}$$

For very large G, $G \gg (E_2 - E_1)/(2S_1 - 1)$,

$$C = GS_1\sqrt{1 - \frac{(E_2-E_1)^2}{(2S_1-1)^2\,G^2}} \approx GS_1\left(1 - \frac{1}{2}\frac{(E_2-E_1)^2}{(2S_1-1)^2\,G^2} + \ldots\right).$$

The first term of the expansion in powers of $G_{\rm cr}/G$ does not depend on the difference $(E_2 - E_1)$ and coincides with the correlation function of one-subshell system having $S_0 = 2S_1$ and $p_0 = 1/2$.

The calculated critical value of the interaction constant turned out to be proportional to the ratio $1/(2S_1 - 1)$. It is not clear whether $g_{\rm cr}$ depends on the particle number or on the number of vacancies in the system.

Remark 4. Both normal ($w_1 = 1$, $w_2 = 0$, $t_2 = t_1 = 0$) and superconducting ($w_1 = 1/2 + G_{\rm cr}/(2G)$, $w_2 = 1/2 - G_{\rm cr}/(2G)$, $t_2 = t_1 > 0$) solutions are possible for $G > G_{\rm cr}$ in the considered example. The difference of their energies is easily calculated by Eq. (11) with $\lambda = 0$,

$$\langle|H|\rangle_{w_2=0} - \langle|H|\rangle_{w_2>0} = S_1\left(S_1 - \frac{1}{2}\right)G\left(1 - \frac{G_{\rm cr}}{G}\right)^2.$$

The subscripts $w_2 = 0$ and $w_2 > 0$ indicate that the Hamiltonian is averaged over the wave function of either the normal state or the superconducting one, respectively. One can see that for $G > G_{\rm cr}$, the energy of the normal state exceeds the energy of the superconducting one.

2.2.2. $S_1 \neq S_2$ ***and*** $\mathcal{N} = 2S_1$**.** Let us figure out how the value of the critical constant depends on the number of particles in the closed subshell E_1 and on the number of empty single-particle states in the subshell E_2.

For $\mathcal{N} = 2S_1$, Eq. (25) is

$$2(S_1\xi_1 + S_2\xi_2) = S_1 - S_2 \quad \text{or} \quad S_1(\xi_1 - \frac{1}{2}) + S_2(\xi_2 + \frac{1}{2}) = 0. \tag{28}$$

To simplify the calculations, we introduce new variables δ_1 and δ_2 such as

$$\xi_1 = \frac{1}{2} - \delta_1 \quad \text{and} \quad \xi_2 = -\frac{1}{2} + \delta_2.$$

It follows from Eq. (28) that the unknown δ_1 and δ_2 are connected by the equation

$$S_1\delta_1 = S_2\delta_2,$$

which can be taken into account by substitution

$$\delta_1 = S_2\delta, \quad \delta_2 = S_1\delta.$$

As $-1/2 \leqslant \xi_{1,2} \leqslant 1/2$, the variable δ should be inside the interval

$$0 \leqslant \delta \leqslant \min\left(\frac{1}{S_1}, \frac{1}{S_2}\right).$$

It follows from Eq. (14) that

$$t_1 = \sqrt{\delta_1(1-\delta_1)} = \sqrt{S_2\delta(1-S_2\delta)}, \quad \xi_1 = \frac{1}{2} - S_2\delta,$$
$$t_2 = \sqrt{\delta_2(1-\delta_2)} = \sqrt{S_1\delta(1-S_1\delta)}, \quad \xi_2 = -\frac{1}{2} + S_1\delta.$$

The unknown $\xi_{1,2}$ and $t_{1,2}$ expressed in terms of δ can be substituted into Eq. (26), the chemical potential can be excluded and the algebraic equation of the sixth degree can be obtained. The analysis of solutions of these equations is prohibitively difficult, and we narrow down the problem by looking for values of the interaction constant G at which the superconducting correlations will start to form. In other words, the unknown δ will be an infinitely small positive number.

The abnormal densities $t_{1,2} \approx \sqrt{S_{2,1}\delta}$ for small δ. Therefore, the first equation of Eqs. (26) changes into

$$-\mu\sqrt{S_2\delta} + g(S_1 - 1)\sqrt{S_2\delta}\,\xi_1 + gS_2\sqrt{S_1\delta}\,\xi_1 = 0.$$

Since we consider $\delta > 0$ ($\delta = 0$ corresponds to the normal solution), we can divide both sides of the equation by $\sqrt{S_2\delta}$. We transform the second equation of Eqs. (26) in a similar way and obtain the simplified equations

$$-\mu + g\left(S_1 - 1 + \sqrt{S_1S_2}\right)\xi_1 = 0,$$
$$1 - \mu + g\left(\sqrt{S_1S_2} + S_2 - 1\right)\xi_2 = 0.$$

The linear equation for δ follows:

$$\left[\left(S_1 - 1 + \sqrt{S_1 S_2}\right) S_2 + \left(S_2 - 1 + \sqrt{S_1 S_2}\right) S_1\right] \delta \;= \\ = \frac{1}{2}\left(\sqrt{S_1} + \sqrt{S_2}\right)^2 - 1 - \frac{1}{g}. \quad (29)$$

The coefficient for δ in the left-hand side of the equation is independent of g and is positive because $S_{1,2} \geqslant 1$. Therefore, δ is positive if the right-hand side of the equation is positive. We rewrite the right-hand side as

$$\frac{1}{2}\left(\sqrt{S_1} + \sqrt{S_2}\right)^2 - 1 - \frac{1}{g} = \frac{1}{g_{\rm cr}(S_1, S_2)} - \frac{1}{g} = \frac{g - g_{\rm cr}(S_1, S_2)}{g_{\rm cr}(S_1, S_2)\, g},$$

here

$$g_{\rm cr}(S_1, S_2) = \frac{1}{\frac{1}{2}\left(\sqrt{S_1} + \sqrt{S_2}\right)^2 - 1}. \quad (30)$$

Thus, δ will be an infinitesimal positive number if

$$0 < g - g_{\rm cr}(S_1, S_2) \ll g\; g_{\rm cr}(S_1, S_2).$$

The expression for $g_{\rm cr}(S_1, S_2)$ shows that the particle number (the size of the completely filled subshell $2S_1$) and the vacancy number of the completely empty subshell ($2S_2$) equally affect the critical value of the interaction constant. Such a somehow unexpected result can be explained by the observation that the Hamiltonian (4) has equal matrix elements for the processes of particle pair creation and destruction inside the subshell E_1 and the pair creation in the subshell E_2.

Now we calculate the correlation energy, chemical potential and particle number variance for infinitely small δ, in other words, for G satisfying the inequalities

$$0 < G - G_{\rm cr}(S_1, S_2) \ll g_{\rm cr}(S_1, S_2) G,$$

where

$$G_{\rm cr}(S_1, S_2) = (E_2 - E_1)\, g_{\rm cr}(S_1, S_2).$$

The δ is calculated from Eq. (29), afterwards δ_1 and δ_2 are determined as

$$\delta_1 = \frac{S_2}{R(S_1, S_2)}\left(\frac{1}{g_{\rm cr}(S_1, S_2)} - \frac{1}{g}\right) = \frac{S_2}{R(S_1, S_2)} \frac{g - g_{\rm cr}(S_1, S_2)}{g\; g_{\rm cr}(S_1, S_2)},$$

$$\delta_2 = \frac{S_1}{R(S_1, S_2)}\left(\frac{1}{g_{\rm cr}(S_1, S_2)} - \frac{1}{g}\right) = \frac{S_1}{R(S_1, S_2)} \frac{g - g_{\rm cr}(S_1, S_2)}{g\; g_{\rm cr}(S_1, S_2)},$$

where

$$R(S_1, S_2) = \left(S_1 - 1 + \sqrt{S_1 S_2}\right) S_2 + \left(S_2 - 1 + \sqrt{S_1 S_2}\right) S_1.$$

The correlation energy is

$$C = G\,(S_1 t_1 + S_2 t_2) \approx G\left(S_1\sqrt{\delta_1}\, + S_2\sqrt{\delta_2}\right) = \\ = G\left(\sqrt{S_1}\, + \sqrt{S_2}\right)\sqrt{\frac{S_1 S_2\,(g - g_{\rm cr}(S_1,S_2))}{R(S_1,S_2)\,g\;g_{\rm cr}(S_1,S_2)}}\,.$$

Evidently, C cannot be expanded in the Taylor series around $g_{\rm cr}$. The chemical potential is

$$\lambda = E_1 + \frac{1}{2}\left(S_1 + \sqrt{S_1 S_2}\, - 2\right)G + \\ + \frac{\left(S_1 + \sqrt{S_1 S_2}\, - 1\right)S_2}{R(S_1,S_2)}\left(1 - \frac{g}{g_{\rm cr}(S_1,S_2)}\right)(E_2 - E_1).$$

The particle number variance is

$$\mathcal{V} = 4\left(S_1 t_1^2 + S_2 t_2^2\right) = 8\frac{S_1 S_2}{R(S_1,S_2)}\left(\frac{1}{g_{\rm cr}} - \frac{1}{g}\right),$$

and therefore $\mathcal{V}$ is proportional to the difference $(g - g_{\rm cr})$ if g slightly exceeds $g_{\rm cr}$.

2.2.3. $\mathcal{N} < 2S_1$**.** Let the number of particles be $\mathcal{N} = 2S_1 - 2P_1$, that is, the P_1 pair of particles is removed from the low closed subshell. We have shown in Subsec. 2.1 that the abnormal density t_1 is positive for any G in this case. One needs to find out at what G the abnormal density t_2 will be non-zero. Two variants are possible. Either $t_2 > 0$ at any positive coupling constant or a certain critical value $\widetilde{G}$ exists such as $t_1 > 0$ and $t_2 = 0$ if $0 < G < \widetilde{G}$.

With $\mathcal{N} = 2S_1 - 2P_1$, the particle number equation (25) is

$$2S_1\xi_1 + 2S_2\xi_2 = S_1 - 2P_1 - S_2 \quad \text{or} \quad S_1\left(\xi_1 - \frac{1}{2} + p_1\right) + S_2\left(\xi_2 + \frac{1}{2}\right) = 0.$$

Here $p_1 = P_1/S_1$. We put $\xi_1 = 1/2 - p_1 - \delta_1$ and $\xi_2 = -1/2 + \delta_2$ and obtain

$$t_1 = \sqrt{(p_1 + \delta_1)\,(1 - p_1 - \delta_1)} \quad \text{and} \quad t_2 = \sqrt{\delta_2\,(1 - \delta_2)}\,.$$

New variables δ_1 and δ_2 are related to each other by $S_1\delta_1 = S_2\delta_2$, which can be satisfied if $\delta_1 = S_2\delta$ and $\delta_2 = S_1\delta$. The density $t_2 > 0$ if $\delta > 0$. The boundaries (13) of $\xi_{1,2}$ lead to the inequalities

$$0 \leqslant \delta \leqslant \min\left(\frac{1 - p_1}{S_2}, \frac{1}{S_1}\right).$$

As in the previous example, Eqs. (26) can be transformed into an algebraic equation of the sixth degree with respect to δ. We obtain the simplified equations for infinitesimal positive δ. For small δ,

$$t_1 = \sqrt{p_1(1-p_1)} + \frac{1}{2}\frac{1-2p_1}{\sqrt{p_1(1-p_1)}}S_2\delta + o(\delta),$$
$$t_2 = \sqrt{S_1\delta}\left(1 - \frac{1}{2}S_1\delta + o(\delta)\right).$$

The symbol $o(x)$ stands for the functions of x that $\dfrac{o(x)}{x} \to 0$ when $x \to 0$.

For $0 < \delta < 1$, the inequalities $0 < \delta < \sqrt{\delta} < 1$ are satisfied, and therefore the expansion of $t_{1,2}$ should be carried out for $\sqrt{\delta}$, not for δ itself. Keeping the terms with zero and first powers of $\sqrt{\delta}$, we obtain the approximate

$$t_1 = \sqrt{p_1(1-p_1)}, \qquad \xi_1 = 1/2 - p_1,$$
$$t_2 = \sqrt{S_1\delta}, \qquad \xi_2 = -1/2.$$

The approximate equations follow from the exact ones (26)

$$-\mu - g\left(\frac{1}{2} - p_1\right) + g\left(S_1 + S_2\sqrt{\frac{S_1\delta}{p_1(1-p_1)}}\right)\left(\frac{1}{2} - p_1\right) = 0,$$

$$(1-\mu)\sqrt{S_1\delta} + \frac{g}{2}\sqrt{S_1\delta} - \frac{g}{2}\left(S_1\sqrt{p_1(1-p_1)} + S_2\sqrt{S_1\delta}\right) = 0.$$

The solutions of the system of approximate equations are

$$\mu = g\left(\frac{1}{2} - p_1\right)\left(S_1 - 1 + S_2\sqrt{\frac{S_1\delta}{p_1(1-p_1)}}\right),$$

$$t_2 = \sqrt{S_1\delta} = \frac{g}{2}\,\frac{S_1\sqrt{p_1(1-p_1)}}{1 + g\left(1 + p_1(S_1-1) - (S_1+S_2)/2\right)}.$$

When calculating t_2, we ignored the term proportional to $S_1\delta$ produced in the second equation from the product $\mu\sqrt{S_1\delta}$.

The obtained solutions show that the abnormal density t_2 is the infinitely small positive number for any positive infinitely small g. The correlation function is approximately equal to

$$C \approx GS_1\sqrt{p_1(1-p_1)}\left(1 + \frac{G}{2(E_2-E_1)}S_2\right).$$

The linear on g part of t_2 is taken into account here. The chemical potential calculated with the same accuracy is

$$\lambda \approx E_1 + G\left[\left(\frac{1}{2} - p_1\right)S_1 + p_1 - 1 + \frac{G}{2(E_2-E_1)}\left(\frac{1}{2} - p_1\right)S_1S_2\right].$$

It is easy to see that the chemical potential calculated to the first order in G is equal to the chemical potential for a system consisting of a single open subshell.

2.2.4. $\mathcal{N} = 2S_1 + 2Q$**,** $0 < Q < S_2$**.** Let the number of particles be sufficient to fill the subshell E_1 completely and the subshell E_2 — partially. Equation (25) gives

$$2\left(S_1\xi_1 + S_2\xi_2\right) = S_1 - S_2 + 2Q,$$

$$S_1\left(\xi_1 - \frac{1}{2}\right) + S_2\left(\xi_2 + \frac{1}{2} - q\right) = 0, \quad q = \frac{Q}{S_2}.$$

We introduce $\varepsilon_{1,2}$ such that $\xi_1 = 1/2 - \varepsilon_1$ and $\xi_2 = -1/2 + q + \varepsilon_2$. New variables ε_1 and ε_2 are connected by the equation $S_1\varepsilon_1 = S_2\varepsilon_2$, which can be solved by substitutions $\varepsilon_1 = S_2\varepsilon$ and $\varepsilon_2 = S_1\varepsilon$.

As in the previous cases, in order to study the appearance of superconducting pair correlations, we keep the terms proportional to the zeroth and first degrees of infinitesimal $\sqrt{\varepsilon}$ and obtain

$$\begin{aligned}
\xi_1 &= \frac{1}{2} - S_2\varepsilon \approx \frac{1}{2}, & t_1 &= \sqrt{S_2\varepsilon\left(1 - S_2\varepsilon\right)} \approx \sqrt{S_2\varepsilon}\,,\\
\xi_2 &= -\frac{1}{2} + q + S_1\varepsilon \approx -\frac{1}{2} + q, & t_2 &= \sqrt{\left(q + S_1\varepsilon\right)\left(1 - q - S_1\varepsilon\right)} \approx \sqrt{q\left(1 - q\right)}\,.
\end{aligned}$$

We substitute these approximate values into Eqs. (26), divide both sides of the second equation by non-zero t_2, and determine μ and t_1 from the coupled linear equations

$$\mu \approx 1 + g\left(q - \frac{1}{2}\right)\left[S_2 - 1 + S_1\frac{t_1}{t_2}\right],$$

$$t_1 \approx \sqrt{S_2\varepsilon} = \frac{g}{2}\,\frac{S_2\sqrt{q\left(1 - q\right)}}{1 + g\left[1 + \left(S_2 - 1\right)q - \left(S_1 + S_2\right)/2\right]} \approx \frac{g}{2}S_2\sqrt{q(1 - q)}\,.$$

The obtained t_1 and t_2 are used for calculation of the correlation function and chemical potential

$$C \approx GS_2\sqrt{q\left(1 - q\right)}\left(1 + \frac{G}{2(E_2 - E_1)}S_1\right),$$

$$\lambda \approx E_2 + G\left[\left(q - \frac{1}{2}\right)S_2 - q + \frac{G}{2(E_2 - E_1)}\left(q - \frac{1}{2}\right)S_1S_2\right].$$

Please note that the correlation function and chemical potential for small g reproduce the exact solutions for the single open subshell.

The last two examples dealing with two-subshell systems having one open subshell show that both abnormal densities will be non-zero (the superconducting solutions exist for both subshells) at any small positive coupling constant. The chemical potential is found to be near the energy of the single-particle states forming the open subshell.

3. SEVERAL SUBSHELLS

Let the system have $\mathcal{M}$ subshells, $\mathcal{M} > 2$. We number the subshells so that $E_k \leqslant E_l$ if $k < l$. In the model of independent particles, as the number of particles grows, the subshells are gradually filled: from the subshells with lower single-particle energy to those with larger ones. We denote by F the number of the largest energy subshell which still has particles in it. Therefore, the total number of particles in the system is

$$\mathcal{N} = \sum_{k=1}^{F} 2S_k - 2P,$$

here P is the number of particle pairs required to fill the subshell F completely. If $P = 0$, we have the closed subshell system. If $0 < P < S_F$, the system is the open subshell system.

The average number of particles (12) can be written as

$$\sum_{k=1}^{F-1} S_k \left(\xi_k - \frac{1}{2}\right) + S_F \left(\xi_F - \frac{1}{2} + p_F\right) + \sum_{k=F+1}^{\mathcal{M}} S_k \left(\xi_k + \frac{1}{2}\right) = 0.$$

Here $p_F = P/S_F$. Instead of variables ξ_k, we introduce new unknowns δ_k:

$$\xi_k = \begin{cases} \dfrac{1}{2} - \delta_k, & 1 \leqslant k < F, \\ \dfrac{1}{2} - p_F - \delta_k, & k = F, \\ -\dfrac{1}{2} + \delta_k, & F < k \leqslant \mathcal{M}. \end{cases}$$

They are connected by

$$\sum_{k=1}^{F} S_k \delta_k = \sum_{l=F+1}^{\mathcal{M}} S_l \delta_l. \qquad (31)$$

The conditions $-1/2 < \xi_k < 1/2$, valid for any k, dictate the inequalities for δ_k:

$$0 < \delta_k < 1 \quad \text{for} \quad k \neq F, \quad \text{and} \quad -p_F < \delta_F < 1 - p_F.$$

Please note that now δ_F can be not only a positive number but also a negative one. It follows from Eq. (14) that the abnormal densities are

$$t_k = \begin{cases} \sqrt{\delta_k(1-\delta_k)}\,, & k \neq F, \\ \sqrt{(p_F + \delta_F)(1 - p_F - \delta_F)}\,, & k = F. \end{cases}$$

Equations (21) can be written as the system

$$
\begin{aligned}
\left[E_k - G\,(1-\delta_k) - \lambda\right] t_k + GD\left(\frac{1}{2} - \delta_k\right) &= 0, \qquad 1 \leqslant k < F,\\
\left[E_F - G\,(1-p_F-\delta_F) - \lambda\right] t_F + GD\left(\frac{1}{2} - p_F - \delta_F\right) &= 0,\\
\left[E_l - G\delta_l - \lambda\right] t_l - GD\left(\frac{1}{2} - \delta_l\right) &= 0, \qquad F < l \leqslant \mathcal{M}
\end{aligned}
\tag{32}
$$

that connects λ, δ_k and t_k, $k = 1, \ldots, \mathcal{M}$.

3.1. $\boldsymbol{p_F > 0}$. For the open subshell nuclei, $p_F > 0$. We are looking for the conditions under which all δ_k with $k \neq F$ will be positive infinitely small numbers. It follows from Eq. (31) that δ_F will also be an infinitesimal number of the same order as δ_k. The abnormal densities are

$$
\begin{aligned}
t_F &= \sqrt{p_F(1-p_F)} + \frac{1}{2}\frac{1-2p_F}{\sqrt{p_F(1-p_F)}}\delta_F + o(\delta_F),\\
t_k &= \sqrt{\delta_k}\,\left(1 - \frac{1}{2}\delta_k + o(\delta_k)\right), \quad k \neq F.
\end{aligned}
$$

For δ_k with $k \neq F$, the inequalities $0 < \delta_k < \sqrt{\delta_k}$ are satisfied, and therefore we consider $\sqrt{\delta_k}$ as having the first order of smallness and will keep $\sqrt{\delta_k}$ in the zeroth and first degrees. As a result, we have

$$
\begin{aligned}
t_k &\approx \sqrt{\delta_k}\,, \quad k \neq F,\\
t_F &\approx \sqrt{p_F\,(1-p_F)}\,,\\
D &\approx S_F\sqrt{p_F\,(1-p_F)} + \sum_{l \neq F} S_l\sqrt{\delta_l} \approx S_F\sqrt{p_F\,(1-p_F)}\,.
\end{aligned}
$$

The terms proportional to $S_l\sqrt{\delta_l}$ are neglected in the last expression because they are infinitely small in comparison with the finite term $S_F\sqrt{p_F\,(1-p_F)}\,$. We substitute the approximate expressions into Eq. (32) and obtain

$$
\begin{aligned}
\lambda &= E_F + \left[\left(\frac{1}{2} - p_F\right) S_F - (1-p_F)\right] G,\\
t_k &= \frac{1}{2}S_F\sqrt{p_F(1-p_F)}\,\frac{G}{E_F - E_k} + o\left(\frac{G}{E_F - E_k}\right), \quad 1 \leqslant k < F,\\
t_l &= \frac{1}{2}S_F\sqrt{p_F(1-p_F)}\,\frac{G}{E_l - E_F} + o\left(\frac{G}{E_l - E_F}\right), \quad F < l \leqslant \mathcal{M}.
\end{aligned}
$$

The correlation function and the particle number variance are

$$C \approx G\,S_F\sqrt{p_F(1-p_F)}\,\left(1+\frac{1}{2}\sum_{k=1}^{F-1}S_k\frac{G}{E_F-E_k}+\frac{1}{2}\sum_{l=F+1}^{\mathcal{M}}S_l\frac{G}{E_l-E_F}\right),$$

$$\mathcal{V} \approx S_F\,p_F(1-p_F)\left[4+\sum_{k=1}^{F-1}S_FS_k\left(\frac{G}{E_F-E_k}\right)^2+\sum_{l=F+1}^{\mathcal{M}}S_FS_l\left(\frac{G}{E_l-E_F}\right)^2\right].$$

For a small coupling constant, both the correlation function and the particle number variance are mostly determined by the abnormal density of the open subshell. The following inequalities are valid:

$$C > G\,S_F\sqrt{p_F(1-p_F)} \quad \text{and} \quad \mathcal{V} > 4S_F\,p_F(1-p_F).$$

We would like to note that the particle number variance $\mathcal{V}$ is bounded below by the positive number when $G \to 0$.

One can see that the interaction spreads the influence of non-zero t_F over all subshells in the system. The abnormal densities differ from zero at all subshells enveloped by the interaction. In the system of like nucleons with the open subshell, the superconducting solution exists at any arbitrarily small constant of attractive interaction.

3.2. $p_F = 0$. Now we consider the closed subshell system with $p_F = 0$. Let us assume for a moment that all E_k with $1 \leqslant k < F$ are equal to E_F and all E_l with $F < l \leqslant \mathcal{M}$ are equal to E_{F+1}. By this assumption, we return to the two-subshell problem with

$$\widetilde{S}_F = \sum_{k=1}^{F} S_k \quad \text{and} \quad \widetilde{S}_{F+1} = \sum_{l=F+1}^{\mathcal{M}} S_l.$$

We have shown in Subsec. 2.2.2 that in the present case, the superconducting pair correlations start to appear if the coupling constant G exceeds the threshold value (30) which is here

$$G'_{\rm cr} = \frac{E_{F+1}-E_F}{1/2\left(\sqrt{\widetilde{S}_F}+\sqrt{\widetilde{S}_{F+1}}\right)^2-1}.$$

Please note that $2\widetilde{S}_F = \mathcal{N}$. During the development of the superconducting correlations, pairs of particles begin to jump from fully occupied subshells into free subshells. The difference $(E_{F+1}-E_F)$ is the lowest energy of such transitions. Therefore, in the initial $\mathcal{M}$-subshell system, the constant $G'_{\rm cr}$ gives the lower bound for the actual critical value of the interaction constant $G_{\rm cr}$.

On the other hand,

$$G''_{\rm cr} = \frac{E_{F+1} - E_F}{1/2\left(\sqrt{S_F} + \sqrt{S_{F+1}}\right)^2 - 1}$$

is the critical constant for the system with only two interacting subshells taken into account, and the contributions of other subshells are ignored. Therefore, $G''_{\rm cr}$ gives the upper bound for $G_{\rm cr}$.

This consideration shows that in the closed subshell system, only the normal solutions are possible if the interaction constant satisfies $0 < G < G'_{\rm cr}$. All abnormal densities are equal to zero in this case. If G exceeds $G''_{\rm cr}$, the superconducting solution is possible and all abnormal densities become positive numbers. The intermediate case with $G'_{\rm cr} < G < G''_{\rm cr}$ requires additional study.

Remark 5. We have used the simplest model Hamiltonian (4) with the constant attractive interaction. The realistic Hamiltonian can be written [4] as

$$H = \sum_k \sum_{m_k=-j_k}^{j_k} E_k a^\dagger_{k,m_k} a_{k,m_k} -$$

$$- \frac{1}{4} \sum_{k,l} G_{k,l} \sum_{m_k=-j_k}^{j_k} \sum_{m_l=-j_l}^{j_l} (-1)^{j_k - m_k} a^\dagger_{k,m_k} a^\dagger_{k,-m_k} (-1)^{j_l - m_l} a_{l,-m_l} a_{l,m_l}.$$

If all matrix elements $G_{k,l}$ are positive numbers, our qualitative conclusions about the system with open subshell will survive. The expressions for λ and C will be more complicated of course.

Remark 6. We have considered the spherical nuclei. To obtain formulae for deformed nuclei, one should put $j_k = 1/2$ and $S_k = 1$ for all subshells. The formulae obtained for the closed subshell spherical nuclei are suitable for deformed nuclei. The deformed nucleus can be open subshell nucleus only if the energies E_F and E_{F+1} coincide.

CONCLUSIONS

We have considered the appearance of superconducting pair correlations in spherical even-even nucleus using the simplest model Hamiltonian. The influence of the monopole pairing interaction on the energy of single-particle states was taken into account.

It is shown that the emergence of pair correlations depends on the particle number and shell structure.

In the open subshell system, non-zero abnormal densities appear for any small positive coupling constant. The new result obtained in the present paper is that at infinitely small positive G, the abnormal densities differ from zero at each subshell participating in the pairing interaction.

In the closed subshell system, superconducting pair correlations begin to form when the coupling constant exceeds a certain critical value G_{cr}. If the coupling constant is less than G_{cr}, the normal solution is the only solution. All abnormal densities and correlation function equal to zero. The rough lower and upper bounds of G_{cr} are obtained. More accurate estimations of G_{cr} are required. Both normal and superconducting solutions are possible for G larger than G_{cr}.

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