

E4-2011-91

V. A. Kuz'min, T. V. Tetereva¹

INFLUENCE OF MONOPOLE PAIRING POTENTIAL
ON THE ENERGIES OF THE SINGLE-NUCLEON STATES
IN THE PROBLEM OF THE PAIRING CORRELATIONS
OF SUPERCONDUCTIVE TYPE

Submitted to «Ядерная физика»

¹Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, 119991 Russia

Кузьмин В. А., Тетерева Т. В.

E4-2011-91

Учет связи монопольного спаривания с энергиями
однуклонных состояний в задаче о парных корреляциях
сверхпроводящего типа

Корреляционная функция, химический потенциал, коэффициенты специального преобразования Боголюбова и одноквазичастичные энергии вычислены с учетом влияния потенциала монопольного спаривания на энергии одночастичных состояний нуклонов в среднем поле ядра.

Работа выполнена в Лаборатории теоретической физики им. Н. Н. Боголюбова ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 2011

Kuz'min V. A., Teterova T. V.

E4-2011-91

Influence of Monopole Pairing Potential on the Energies
of the Single-Nucleon States in the Problem of the Pairing Correlations
of Superconductive Type

The correlation function, chemical potential, coefficients of Bogoliubov's special transformation and one-quasiparticle energies have been calculated with taking into account the influence of monopole pairing on the energy of single-particle states in nuclear mean field.

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

Preprint of the Joint Institute for Nuclear Research. Dubna, 2011

1. INTRODUCTION

The idea that the superconducting pairing correlations exist inside the atomic nuclei was formulated more than fifty years ago [1]. As in the microscopic theory of superconductivity [2], it was assumed that a weak attractive interaction acts between the nucleons moving inside the nuclear mean field. This interaction can glue two nucleons into a pair having zero angular momentum. Those pairs behave like bosons and may form a condensate revealing the superfluid properties. The theoretical description of the system of fermions with an attractive interaction is based on the method of the canonical transformation [3,4] in which the quasiparticle creation and annihilation operators are introduced as the linear combinations of the nucleon creation and annihilation operators. The state having no quasiparticles (the quasiparticle vacuum) is considered as the approximate ground state of the system, consisting of even number of nucleons of the same kind (either protons or neutrons) [5].

The accuracy of the canonical transformation method had been studied in many papers. The main attention had been paid to the problem that the quasiparticle vacuum state being a condensate of the nucleon's pairs is not the eigenstate of the particle number operator. The ways of projecting the wave functions obtained by canonical transformation method on the states with definite number of particles were designed and their accuracy was studied (for example and future references, see the papers [5–7]).

The analysis of the accuracy of the canonical transformation method overlooks quite often one more approximation, namely, that the influence of an interaction resulting in the pairing correlations of superconducting type on the energies of single-particle states was not accounted for. In other words, in order to simplify the calculations and in order to get the solutions in explicit form, the terms similar to $G \sum_s v_s^4$ were neglected in the expression for the energy of the quasiparticle vacuum state (see Eq. (3) below). Sometimes this approximation was considered as the using of the approximate equations of the canonical transformation method. Sometimes it was interpreted as the renormalization of the energy of single-particle state [5]. The neglecting of the terms similar to Gv_s^4 can be physically justified if one uses as a mean field potential the phenomenological shell potential with parameters fitted to reproduce the experimental

values of single-particle energy. In that case fitting procedure accounts implicitly for the pairing potential. If the mean field potential is calculated in the framework of the Hartree–Fock or the Hartree–Fock–Bogoliubov approximations and obtained single-particle energies are to be compared to the experimental ones, the account of the influence of pairing interaction on the energy of single-particle state becomes advisable.

As far as we know, in the literature there are no estimations of the accuracy of this approximation and of the influence of the coupling between the pairing interaction and the single-particle energies on the correlation function, the chemical potential and the energy of quasiparticle states.

In the present paper the problem of the nuclear pairing correlations of superconducting type is solved without this approximation. We consider the simplest model of deformed nucleus with constant pairing to avoid unnecessary technical complications. The extension of the presented considerations to the cases of spherical symmetry and/or of more realistic pairing potentials is quite straightforward.

The basic formulae of the model and the solution of the equations are described in the next section. Also it is shown how the exact equations and their solutions may be reduced to well-known approximate ones. The third section contains the results of numerical calculations and discussion. The main results are summarised in the last section.

2. THE EQUATIONS

We consider the neutron subsystem of a deformed nucleus. The Hamiltonian of the model for describing the superconducting correlations is [5]

$$H - \lambda \hat{N} = \sum_s \sum_{\sigma=\pm 1} (E_s - \lambda) a_{s,\sigma}^\dagger a_{s,\sigma} - G \sum_{s,s'} a_{s,+}^\dagger a_{s,-}^\dagger a_{s',-} a_{s',+}. \quad (1)$$

Here $a_{s,\sigma}^\dagger$ and $a_{s,\sigma}$ are nucleon creation and annihilation operators; indices s and σ list the single-particle states with explicit indication of the sign of the projection of angular momentum, $\sigma = \pm 1$; E_s is the single particle energy; G is the constant of the pairing interaction; \hat{N} is the particle number operator, and λ is the chemical potential. The quasiparticle operators are introduced by the Bogoliubov–Valatin special transformation

$$a_{s,\sigma} = u_s \alpha_{s,\sigma} + \sigma v_s \alpha_{s,-\sigma}^\dagger. \quad (2)$$

The Hamiltonian (1) reduces to

$$\begin{aligned}
H - \lambda \hat{N} = & 2 \sum_s (E_s - \lambda) v_s^2 - G \sum_s v_s^4 - G \left[\sum_s u_s v_s \right]^2 + \\
& + \sum_s \{ (E_s - \lambda - G v_s^2) (u_s^2 - v_s^2) + 2C u_s v_s \} \{ \alpha_{s,+}^\dagger \alpha_{s,+} + \alpha_{s,-}^\dagger \alpha_{s,-} \} + \\
& + \sum_s \{ 2(E_s - \lambda - G v_s^2) u_s v_s - C(u_s^2 - v_s^2) \} \{ \alpha_{s,-} \alpha_{s,+} + \alpha_{s,+}^\dagger \alpha_{s,-}^\dagger \} + \\
& + \dots \quad (3)
\end{aligned}$$

Here the standard definition of the correlation function is used [5],

$$C = G \sum_{s'} u_{s'} v_{s'}. \quad (4)$$

The ellipsis denotes the terms containing the normal product of four creation and annihilation quasiparticles operators. These terms disappear after averaging over the quasiparticle vacuum Φ_0 , $\alpha_s \Phi_0 = 0$.

Either the condition of minimum of the ground-state energy $(\Phi_0, (H - \lambda \hat{N}) \Phi_0)$ or the principle of compensation of dangerous diagrams, $(\Phi_0, \alpha_{s,\sigma} \alpha_{s',\sigma'} (H - \lambda \hat{N}) \Phi_0) = 0$, together with the requirement that the transformation (2) should keep the fermion commutation rules, leads to the system of equations

$$\begin{aligned}
2(E_s - \lambda - G v_s^2) u_s v_s - C(u_s^2 - v_s^2) &= 0, \\
u_s^2 + v_s^2 &= 1.
\end{aligned} \quad (5)$$

The usual equations of the theory of superconducting correlations [5] can be obtained by discarding the term $G v_s^2$ inside the first brackets of the first equation.

Chemical potential λ is chosen so that the average number of particles in a state Φ_0 equals the number of particles in the system,

$$(\Phi_0, \hat{N} \Phi_0) = \left(\Phi_0, \sum_{s,\sigma} a_{s,\sigma}^\dagger a_{s,\sigma} \Phi_0 \right) = 2 \sum_s v_s^2 = N. \quad (6)$$

It is convenient to pass from the u_s and v_s coefficients of the transformation (2) to the combinations

$$\begin{aligned}
t_s &\equiv u_s v_s = (\Phi_0, a_{s,+} a_{s,-} \Phi_0), \\
w_s &\equiv v_s^2 = (\Phi_0, a_{s,\sigma}^\dagger a_{s,\sigma} \Phi_0),
\end{aligned}$$

those are usually named the abnormal and the normal densities, respectively. With variables t_s and w_s equations (5) take the form

$$\begin{aligned} 2(C - Gt_s)w_s + 2(E_s - \lambda)t_s - C &= 0, \\ w_s^2 - w_s + t_s^2 &= 0. \end{aligned} \quad (7)$$

We eliminate the unknown w_s from Eqs. (7) by the standard method [8]. Let us consider the equations as the pair of equations with respect to w_s . The equations will have the common root w_s , if the determinant composed of the coefficients of the system and named *resultant* equals zero,

$$\begin{vmatrix} C - Gt_s & (E_s - \lambda)t_s - C/2 & 0 \\ 0 & C - Gt_s & (E_s - \lambda)t_s - C/2 \\ 1 & -1 & t_s^2 \end{vmatrix} = 0. \quad (8)$$

An algebraic quartic equation with respect to t_s is obtained by expanding the determinant,

$$G^2t_s^4 - 2GCt_s^3 + ((E_s - \lambda)^2 + C^2 - G(E_s - \lambda))t_s^2 + \frac{1}{2}GCt_s - \frac{1}{4}C^2 = 0. \quad (9)$$

The roots of a quartic equation can be expressed through the radicals composed of the coefficients of the equation. However, the expressions obtained are too cumbersome for using them. Therefore, we solved this equation numerically. From the solutions one must select the real root satisfying the inequalities

$$0 < t_s \leq \frac{1}{2}, \quad (10)$$

which follow immediately from the conditions $t_s \equiv u_s v_s$ and $u_s^2 + v_s^2 = 1$. Taking this root t_s , we obtain from the first of Eqs. (7)

$$w_s = \frac{C/2 - (E_s - \lambda)t_s}{C - Gt_s}. \quad (11)$$

If one forgets for a short time that the C is proportional to the G , and puts $G = 0$, Eq. (9) goes into

$$((E_s - \lambda)^2 + C^2) t_s^2 - \frac{1}{4}C^2 = 0,$$

and the well-known approximate solution

$$t_s = \frac{C}{2\sqrt{(E_s - \lambda)^2 + C^2}} \quad \text{and} \quad w_s = \frac{1}{2} - \frac{1}{2} \frac{E_s - \lambda}{\sqrt{(E_s - \lambda)^2 + C^2}}. \quad (12)$$

emerges [5].

The values of t_s and w_s calculated according to Eqs. (9)–(11) depend on the parameters C and λ . The t_s and w_s are substituted into Eqs. (4) and (6). And the system of two equations with respect to C and λ is obtained:

$$\begin{aligned} G \sum_s t_s - C &= 0, \\ 2 \sum_s w_s - N &= 0. \end{aligned} \quad (13)$$

These equations are solved numerically by the iterations.

3. NUMERICAL RESULTS

The calculations are carried out for neutrons of the nucleus ^{166}Er with $N = 98$. The single-particle energies E_s were calculated with the deformed Saxon–Woods potential for $A = 165$ [9].

The calculations were carried out by the following way. For initial values C and λ the coefficients of Eq. (9) were evaluated for each s . For each s all four roots were determined and the tests showed that only one root t_s satisfies the inequalities (10). The corresponding w_s was found from Eq. (11). New values of C and λ were obtained by solving Eq. (13).

The table shows the correlation function, the chemical potential obtained by solving the exact Eqs. (9), (11) and (13). These results are marked by the letter «a» in the table and below. The label «b» indicates the solutions of Eqs. (13), when t_s and w_s were calculated according to the usual approximate formulae (12). It is seen that for all considered values of G the exact equations lead to the smaller values of the correlation function and the chemical potential. In the model of the independent particles, the energy of last occupied level $E_F = -6.218$ MeV and

Correlation functions, chemical potentials, the difference of the ground-state energies and the dispersion of the particle number in Φ_0 state for the neutrons of ^{166}Er nucleus calculated for different values of pairing constant

G , MeV	C , MeV		λ , MeV		$E_{\text{gr}}^{\text{a}} - E_{\text{gr}}^{\text{b}}$, MeV	$E_{\text{gr}}^{\text{a}} - E_{\text{gr}}^{\text{b}'}$, MeV	ΔN	
	a	b	a	b			a	b
0.108	0.439	0.515	-5.771	-5.712	-5.217	-0.010	1.53	1.78
0.122	0.838	0.893	-5.743	-5.674	-5.803	-0.009	2.33	2.46
0.136	1.254	1.306	-5.703	-5.624	-6.370	-0.009	2.89	2.99

the energy of first vacant state $E_{F+1} = -5.250$ MeV. Thus, in both cases, the chemical potentials are between the levels which would be the last occupied and the first vacant ones in the absence of an interaction.

As G increases, the values of C and λ grow and the small, in size of several tens of KeV, decrease of the correlation function and of the chemical potential in the case (a) compared with the case (b) may be masked by the process of fixing of the constant G by fitting to the experimental values of the pairing energy [5,9].

The energy of ground-state (quasiparticle vacuum) equals the average value of the Hamiltonian over Φ_0 and is given in the first line of Eq. (3). The table shows the difference between the ground-state energies calculated by

$$E_{\text{gr}}^{\text{a}} = (\Phi_0, H\Phi_0)_{\text{a}} = 2 \sum_s E_s w_s(\text{a}) - G \sum_s w_s^2(\text{a}) - G \left[\sum_s t_s(\text{a}) \right]^2,$$

$$E_{\text{gr}}^{\text{b}} = (\Phi_0, H\Phi_0)_{\text{b}} = 2 \sum_s E_s w_s(\text{b}) - G \left[\sum_s t_s(\text{b}) \right]^2.$$

A noticeable difference in the energies of the ground states is explained by the fact that the renormalization of single-particle energies $E_s - Gv_s^2 \rightarrow E_s$ discards the term $G \sum_s v_s^4$ in E_{gr}^{b} . Equation (3) shows that renormalization of the single-particle energies removes the contribution of this term to ground-state energy even for the trivial solution in which $u_s v_s = 0$ for any s . The authors of several papers (see, for example, [10,11]) neglect the $G \sum_s v_s^4$ term in the calculations of the u_s and v_s coefficients, of the correlation function and the chemical potential, but restore its in computation of the ground-state energy, arriving at

$$E_{\text{gr}}^{\text{b}'} = (\Phi_0, H\Phi_0)_{\text{b}} - G \sum_s w_s^2(\text{b}) =$$

$$= 2 \sum_s E_s w_s(\text{b}) - G \left[\sum_s t_s(\text{b}) \right]^2 - G \sum_s w_s^2(\text{b}).$$

The table shows that the difference between E_{gr}^{a} and $E_{\text{gr}}^{\text{b}'}$ is in ten KeV range, so the accounting of this term allows one to get almost exact value of ground-state energy using the solution of approximate equations.

The dispersions of the particle number in Φ_0 state

$$\Delta N = \sqrt{(\Phi_0, \hat{N}^2 \Phi_0) - (\Phi_0, \hat{N} \Phi_0)^2} = 2 \sqrt{\sum_s t_s^2}$$

are shown in two last columns of the table. The particle number dispersion calculated with the solution of exact equations is slightly less than the dispersion

obtained with the solution of approximate equations. For all the considered values of coupling constant G , the ratios of the particle number dispersions are close to the ratios of the correlation functions

$$\frac{\Delta N_a}{\Delta N_b} \approx \frac{C_a}{C_b}.$$

The energies of one-quasiparticle states, abnormal densities t_s and v_s coefficients are displayed on the figures. The points presenting the values calculated with the same G are connected by the fragments of straight line. The second row of Eq. (3) gives the Hamiltonian of the independent quasiparticle model, and the coefficient at the operator $\alpha_{s,\sigma}^\dagger \alpha_{s,\sigma}$ is the energy of the quasiparticle state $\alpha_{\sigma,s}^\dagger \Phi_0$. It is

$$\xi_s = (E_s - \lambda_a - Gw_s)(1 - 2w_s) + 2C_a t_s$$

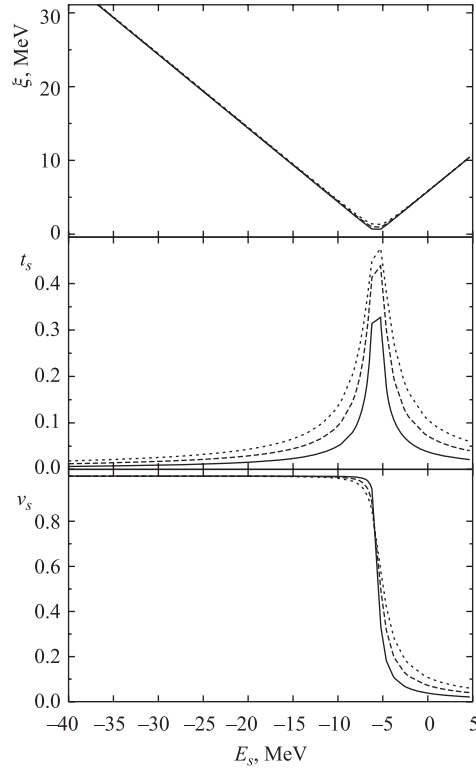


Fig. 1. The properties of the single-quasiparticle states calculated with the solutions of the exact equations. The results obtained for G equal to 0.108, 0.122 and 0.136 are presented by solid, dashed and short-dashed lines, respectively

for the case (a). The dependence of ξ_s on E_s is shown in the upper part of Fig. 1. The largest difference between the ξ_s values calculated with the different G is observed near to the chemical potential, at the small $|E_s - \lambda_a|$. It is interesting to compare ξ_s to the corresponding one-quasiparticle energy calculated in case (b),

$$\varepsilon_s = \sqrt{(E_s - \lambda_b)^2 + C_b^2}.$$

The ratios ξ_s/ε_s are shown in the upper part of Fig. 2. The ξ_s are larger than ε_s almost everywhere except the small region around λ where exact quasiparticle energies are smaller than the approximate ones.

The t_s values calculated in the case (a) are shown in the middle panel of Fig. 1 and their ratios to $t_s(b)$ — in Fig. 2. The t_s depends on the coupling constant G , and t_s calculated by solving exact equations is less than the t_s obtained by approximate formulae. It is interesting to note that the solutions of

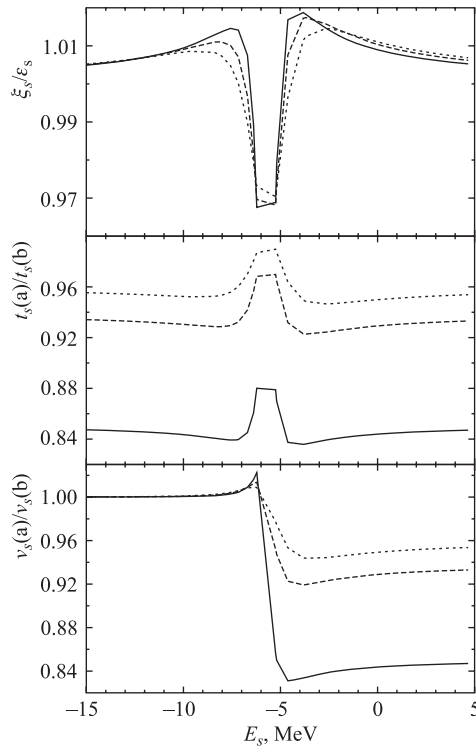


Fig. 2. The ratios of single-quasiparticle energies, abnormal densities and v_s coefficients calculated with the solutions of the exact and approximate equations. For the legend see Fig. 1

exact equations grow faster in the region of Fermi surface than the solutions of approximate equations (the ratios $t_s(a)/t_s(b)$ have a peak near $\lambda_{a,b}$).

The v_s coefficients calculated with solution of the exact equations are shown in the lower part of Fig. 1 and their ratios to v_s obtained with solution of approximate equations — in Fig. 2. In the (a) case v_s varies with E_s more steeply near the Fermi surface than v_s calculated from the approximate equations. It agrees with general rule: when C decreased the dependence of v_s on E_s near λ became sharper, transforming into a step at the $C = 0$. The differences in the behaviour of v_s are smoothed out as the coupling constant G increases.

4. CONCLUSIONS

We have calculated the correlation function, the chemical potential, coefficients of a Bogoliubov–Valatin transformation and energy single-quasiparticle states for the nuclear problem of pairing correlations of superconducting type, keeping the term $G \sum_s v_s^4$ usually neglected, i.e., using the exact equations.

Comparison with results of calculations based on the traditional method of renormalization of single-particle energies has shown that the correlation function and the chemical potential in the exact calculations are slightly less than the values obtained with the solutions of approximate equations. But this discrepancy can be easily compensated by a small increase of the constant of monopole pairing. And so, it is not crucial probably.

It has been shown that the traditional solution of model equations, based on the method of renormalization of the single energy, yields significantly larger energy of the quasiparticle vacuum compared to the one obtained by the exact solution of the model. This follows from the fact that the renormalization procedure discards the part of the attractive pairing interaction contribution to the energy of the ground state. The account of the term $G \sum_s v_s^4$ allows one to reproduce the ground-state energy quite well using the solution of the approximate equations.

The authors are thankful to A. V. Sushkov for numerous discussions and help in calculations.

REFERENCES

1. A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev. **110**, 936 (1958).
2. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **106**, 162 (1957); Phys. Rev. **108**, 1175 (1975).
3. N. N. Bogoliubov, Nuovo Cim. **7**, 794 (1958).
4. J. C. Valatin, Nuovo Cim. **7**, 843 (1958).

5. V.G. Soloviev, *Teoriya slozhnyh yader* (Nauka, M., 1971), in Russian; *Theory of Complex Nuclei* (Pergamon Press, Oxford, New York, Sydney, Paris, 1976), in English.
6. N.K. Kuzmenko and V.M. Mikhajlov, *EChAYa* **20**, 830 (1989), in Russian; *Sov. J. Part. Nucl.* **20**, 357 (1989), in English.
7. N. Sandulescu and G.F. Bertsch, *Phys. Rev. C* **78**, 064318 (2008).
8. B.L. van der Waerden, *Modern Algebra*, vol. 1 (Ungar, 1949).
9. V.G. Soloviev, *Teoriya atomnogo yadra. Yadernye modeli* (Energoizdat, M., 1981), in Russian;
10. A. Pavlikovsky, W. Rybarska, *JETP* **43**, 543 (1962), in Russian.
11. S. Pilat, K. Pomorski, and A. Staszczak, *Z. Phys. A* **332**, 259 (1989).

Received on September 6, 2011.

Редактор *Е. И. Кравченко*

Подписано в печать 01.11.2011.

Формат 60 × 90/16. Бумага офсетная. Печать офсетная.

Усл. печ. л. 0,81. Уч.-изд. л. 1,1. Тираж 310 экз. Заказ № 57476.

Издательский отдел Объединенного института ядерных исследований
141980, г. Дубна, Московская обл., ул. Жолио-Кюри, 6.

E-mail: publish@jinr.ru

www.jinr.ru/publish/