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Neutron-proton pairing in the BCS approach

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We investigate the BCS treatment of neutron-proton pairing involving time-reversed orbits. We conclude that an isospin-symmetric Hamiltonian, treated with the help of the generalized Bogolyubov transformation, fails to describe the ground state pairing properties correctly. In order for the np isovector pairs to coexist with the like-particle pairs, one has to break the isospin symmetry of the Hamiltonian by artificially increasing the strength of the np pairing interaction above its isospin-symmetric value. We briefly discuss the prescription how to choose the coupling constant of this auxiliary isospin-breaking pairing force. [S0556-2813(97)03710-2]

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I. INTRODUCTION

Pairing correlations are an essential feature of nuclear structure [1]. In proton-rich nuclei with $N \approx Z$ the neutron and proton Fermi levels are close to each other and therefore the neutron-proton (np) pairing correlations can be expected to play a significant role in their structure and decay (for a review of the early work on np pairing theory see Ref. [2]). In contrast, in the heavier nuclei with large neutron excess the neutron-proton pairing correlations can be usually neglected.

There has been a recent revival of interest in the theoretical description of pairing involving both neutrons and protons [3–6]. This renaissance stems from the advent of experiments with radioactive beams, as well as from the application of neutron-proton pairing concepts in the description of alpha decay [7] and double-beta decay [8,9]. However, the theoretical treatment is not without a controversy. While intuition and arguments of isospin symmetry suggest that the neutron-proton pairing correlations should be as important as the like-particle pairing correlations in the $N \simeq Z$ nuclei, the balance between these pairing modes is delicate and the standard approximations often fail.

In order to elucidate what is going on we examine the treatment of neutron-proton pairing in the generalized Bogolyubov transformation approach, in particular the role of isospin symmetry. The problem at hand is the determination of the ground state of an even-even system with the Hamiltonian

$$H = \sum_{jmt} \epsilon_{jt} a^\dagger_{jmt} a_{jmt} - \frac{1}{4} \sum_{jmj'm'} \sum_{tt'} G_{tt'} a^\dagger_{jmt} a^\dagger_{\overline{jmt'}} a_{\overline{j'm't'}} a_{j'm't}, \qquad (1)$$

where (jmt) represents the angular momentum, its projection, and the isospin projection of the single-particle (s.p.) state created (annihilated) by the operator $a^\dagger_{jmt}$ (a_{jmt}), and as usual $a_{\overline{jmt}} = (-1)^{j-m} a_{j-mt}$. The three coupling constants $G_{tt'}$ (we assume that $G_{tt'} = G_{t't}$) characterize the monopole pairing interaction. The interaction couples only states in time-reversed orbits, but allows an arbitrary combination of the isospin projection indices. Obviously, when isospin symmetry is imposed, the s.p. energies become independent of the isospin label t, and $G_{nn} = G_{pp} = G_{pn} = G_{np} \equiv G$. The interaction then describes the isovector $T=1$ pairing. However, as will be seen below, it is advantageous to keep the general form of the Hamiltonian (1).

One can find the exact ground state of Eq. (1) in the simple case of a one- or two-level system. However, in the general case of a multilevel system the dimension increases exponentially and therefore the standard procedure is to use the generalized Bogolyubov transformation approach in the form [10] where the quasiparticle operators are related to the particle operators by

$$\begin{pmatrix} c^\dagger_{j1} \\ c^\dagger_{j2} \\ c_{\overline{j1}} \\ c_{\overline{j2}} \end{pmatrix} = \begin{pmatrix} u_{11j} & u_{12j} & v_{11j} & v_{12j} \\ u_{21j} & u_{22j} & v_{21j} & v_{22j} \\ -v_{11j} & -v^*_{12j} & u_{11j} & u^*_{12j} \\ -v^*_{21j} & -v_{22j} & u^*_{21j} & u_{22j} \end{pmatrix} \begin{pmatrix} a^\dagger_{jp} \\ a^\dagger_{jn} \\ a_{\overline{jp}} \\ a_{\overline{jn}} \end{pmatrix}. \qquad (2)$$

Here j denotes the full set of quantum numbers of a s.p. orbit, and the indices ''1'' and ''2'' are the quasiparticle analogs of p or n, i.e., of the corresponding isospin projections. The transformation amplitudes $u_{ik,j}$ and $v_{ik,j}$ with $i \neq k$ describe the neutron-proton pairing. They are, in general, complex. We refer to [5] and [10] for the unitarity conditions which $u_{ik,j}$ and $v_{ik,j}$ have to obey, as well as for the relation between the amplitudes and the gap parameters Δ_p, Δ_n, and Δ_{np}.

To find the ground state we minimize the quantity H_0, the expectation value of the Hamiltonian in the quasiparticle vacuum, while simultaneously obeying the unitarity conditions and the usual conservation (on average) of the number of neutrons and protons. (This procedure is equivalent to demanding that the ''dangerous graph'' term H_{20}, which creates or annihilates a pair of quasiparticles, vanish.) We use the Newton-Raphson method [11] and check, by comparing to the ''standard BCS'' solution for $G_{np}=0$, that the ground state energy is lower than in the state without the neutron-proton pairing. The procedure allows us to find at

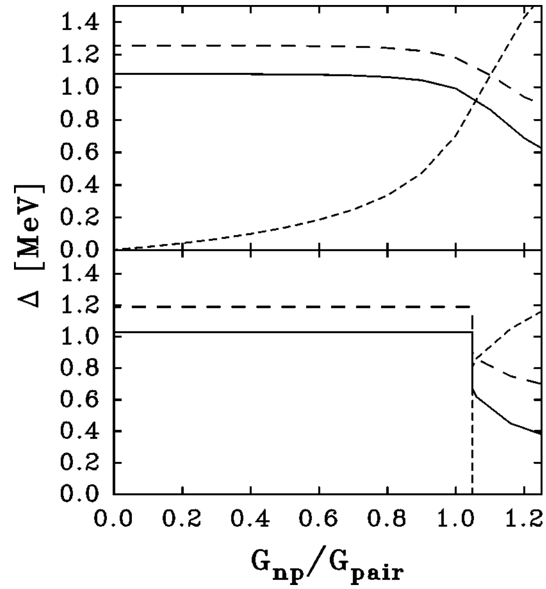

FIG. 1. The pairing gaps for the one-level case with $\Omega=11$, $N=6$, and $Z=4$. $G_{\mathrm{pair}}=0.242$ MeV was used and the results are plotted as a function of the ratio G_{np}/G_{pair}. In both panels of the figure long-dashed lines, solid lines, and short-dashed lines represent the neutron-neutron (Δ_{nn}), proton-proton (Δ_{pp}), and proton-neutron (Δ_{pn}) pairing gaps, respectively. The upper panel is for the exact solution with gaps determined as described in the text. The lower panel is for the BCS solution.

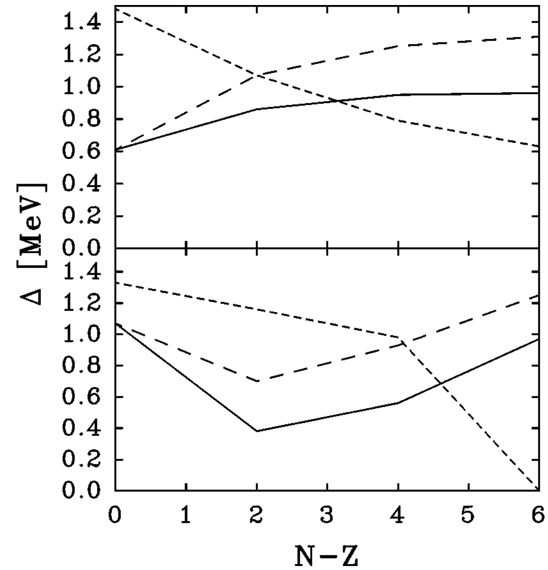

FIG. 2. The pairing gaps for the one-level case with $\Omega=11$, as function of the neutron excess $N-Z$. Short-dashed lines, long-dashed lines, and solid lines correspond to values of Δ_{pn}, Δ_{nn}, and Δ_{pp}, respectively. Both panels are for $Z=4$ while the neutron number is varied; $G_{\mathrm{pair}}=16/(N+Z+56)$ MeV. The exact solutions for $G_{np}/G_{\mathrm{pair}}=1.1$ are in the upper panel. The BCS solutions for $G_{np}/G_{\mathrm{pair}}=1.25$ are in the lower panel.

the same time the gain in the ground state binding energy associated with the neutron-proton pairing.

II. ISOSPIN-SYMMETRIC HAMILTONIAN

The Hamiltonian (1) with $\epsilon_{jp}=\epsilon_{jn}$ and $G_{nn}=G_{pp}=G_{np}$ describes the isovector pairing, in which all three kinds of pairs (nn, pp, and np with $T=1$) are treated equally on the interaction level. One expects then that in an even-even nucleus with $N=Z$ the corresponding gap parameters should be the same for all three possible pairs.

In fact, in the exactly solvable manifestation of this Hamiltonian, in which there is only one s.p. state of degeneracy 2Ω, this is indeed the case. Defining the pair creation operator as

$$S_{t_z}^{\dagger}=\sum_{j,m>0}[a_{jm}^{\dagger}a_{j\overline{m}}^{\dagger}]_{t_z}^{T=1}, \quad (3)$$

where t_z is the corresponding isospin projection, the quantity related to the pairing gap Δ_{t_z} is the ground state expectation value $\mathcal{N}_{t_z}=\langle S_{t_z}^{\dagger}S_{t_z}\rangle$. (We calculate the ''gap'' Δ_{t_z} from the expression $\mathcal{N}_{t_z}=\Delta_{t_z}^2/G_{t_z}^2$ valid up to the terms $1/\Omega$. This relation, however, fails for full shells.) As shown in [3], based on the earlier work on this SO(5) model, one can obtain analytic expressions for $\mathcal{N}_{t_z}$. Indeed, when $N=Z$ and both are even, all three values of $\mathcal{N}_{t_z}$ are equal, and when $N-Z$ increases, $\mathcal{N}_0$, and therefore also Δ_{np}, sharply decreases, while the other two $\mathcal{N}_{t_z=\pm 1}$ remain the same or increase with $N-Z$. We expect that this behavior is ''generic,'' i.e., survives even in the case of more than one single-particle level.

Indeed, the generalization of the one-level model to the case of two nondegenerate levels [12] supports this conjecture. Such a generalization is straightforward if we restrict ourselves only to the states with seniority zero. It is then easy to construct the corresponding Hamiltonian matrix which has very manageable dimensions even for large Ω. For completeness we give the expressions for the corresponding matrix elements, applicable to both the one- and two-level models for seniority-zero states in the Appendix. (The results shown in Figs. 1 and 2 below are, for simplicity, for the one-level case.)

Unlike the exact solutions described above, the generalized Bogolyubov transformation approach gives very different results in the isospin-symmetric case. It has been known for some time [13] that in the one-level case the approach leads to no np pairing when $N>Z$. The relationship between the occurrence of np pairing and the conservation of average values of the total isospin (T^2) and its projection T_z, in a multilevel BCS approach was studied by Ginocchio and Weneser [14]. These authors have reported the finding of a class of BCS solutions with the same ground state energy and different values of T_z and the fact that the solution corresponding to the maximum isospin projection ($T=T_z$) has no proton-neutron pairing. Our calculations show that these results are generally valid when the dependence of np pairing correlations upon the neutron (or proton) excess and the relaxation of the isospin symmetry are explicitly considered. We find, in fact, that the ground states of even-even nuclei with $N>Z$ have vanishing Δ_{np} when isospin-symmetric Hamiltonian is used. For $N=Z$ nuclei there is still no mixing. But in that case there are two *degenerate* minima of the energy: one with nonvanishing $\Delta_n=\Delta_p$ and $\Delta_{np}=0$, and the other one with $\Delta_n=\Delta_p=0$ and $\Delta_{np}\neq 0$. (This conclusion was also reached in [4] for the one-level model, and in [6] in the more general case.)

We see, therefore, that the generalized Bogolyubov transformation fails to describe correctly the treatment of isovector-pairing correlations. However, since we expect, as stated above, that the effect of np pairing decreases fast with increasing $N-Z$, the standard BCS theory is still applicable for most heavier nuclei where $N-Z$ is relatively large.

III. BREAKING THE ISOSPIN SYMMETRY

Let us consider now what happens when the requirement of isospin symmetry is relaxed; i.e., in the Hamiltonian (1) one allows different coupling constants $G_{nn}\neq G_{pp}\neq G_{np}$, and possibly different single-particle energies for neutrons and protons. It was shown already 30 years ago [10] that such a Hamiltonian, treated using the generalized Bogolyubov transformation (2), results in nonvanishing Δ_{np} in nuclei with $N\simeq Z$.

The Hamiltonian which breaks isospin symmetry leads, naturally, to eigenstates that do not have a definite value of isospin. Since the quasiparticle vacuum mixes states with different particle number, and therefore also with different isospin, even for an isospin-conserving Hamiltonian, it is perhaps worthwhile to explore effects associated with such a more general situation.

It is straightforward to treat the Hamiltonian (1) exactly in the one- or two-level model; the corresponding Hamiltonian matrix can be calculated using the formulas in [15] (see also the Appendix). The corresponding eigenstates are no longer characterized by isospin T. Instead, all isospin values between $T_z\equiv T_{\min}=(N-Z)/2$ and $T_{\max}=(N+Z)/2$ contribute to the wave function. The ground state energy $E_{\text{g.s.}}$ of a one-level system with $G_{np}\neq G_{\text{pair}}\equiv G_{nn}=G_{pp}$ decreases monotonically with increasing G_{np}. However, the binding energy gain between a system with no neutron-proton interaction (and therefore $\Delta_{np}=0$) and the system with pure isovector interaction (and $\Delta_{np}\neq 0$) is only of the order $1/\Omega$,

$$\Delta E=E_{\text{g.s.}}(G_{np}/G_{\text{pair}}=1)-E_{\text{g.s.}}(G_{np}=0)=-G_{\text{pair}}Z/2, \tag{4}$$

compared to the leading term $-G_{\text{pair}}\Omega(N+Z)/2$. Moreover, the exact wave function of the ground state corresponding to the isovector-pairing Hamiltonian with $G_{np}/G_{\text{pair}}=1$ can be obtained from the ground state of the isospin-violating Hamiltonian with *any* $G_{np}/G_{\text{pair}}\neq 1$ by simply projecting onto a state with isospin $T=T_{\min}$. This is an exact statement which follows from the uniqueness of the zero-seniority state with given (N,Z,T).

In Fig. 1 we show the exact and BCS gap parameters for the one-level system as a function of the ratio G_{np}/G_{pair}. The degeneracy Ω and the pairing strength G_{pair} are chosen in such a way that they resemble the situation in finite nuclei discussed later on. One can see that the two methods give qualitatively similar results. They agree with each other quite well, with the exception of the narrow region near the ''critical point'' of the BCS method (for the plotted case this point is at $G_{np}/G_{\text{pair}}=1.05$). As usual, the BCS method is characterized by the sharp phase transition while the exact method goes more smoothly through the ''critical point,'' as it must for a finite system. Nevertheless, the basic similarity is apparent.

It is now clear that the failure of the BCS method to describe the neutron-proton pairing in the isospin-symmetric case is not a fundamental one. It is related to the abrupt phase transition inherent in the BCS. The isospin-symmetric value $G_{np}=G_{\text{pair}}$ is less than the critical value needed for the phase transition from the pure like-particle pairing to the situation where both like-particle and neutron-proton pairs coexist. Since, as stated earlier, the quasiparticle vacuum breaks isospin anyway, it should not matter much that the isospin violation is also imposed on the Hamiltonian level. We have to choose, however, the proper value of the coupling constant G_{np}.

The natural way to fix the ratio G_{np}/G_{pair} is in nuclei with $N\simeq Z$ where one can use the arguments of isospin symmetry to estimate the gap Δ_{np}. This is easy to do for the pairing Hamiltonian (1). But a similar procedure can be also done when working with a ''realistic'' Hamiltonian with nonconstant pairing matrix elements. Such Hamiltonians are essentially always isospin symmetric. To break the symmetry, and allow the coexistence of the like-particle and neutron-proton pairs, we propose to add to the realistic Hamiltonian the interaction term

$$H_{\text{aux}}=\frac{1}{4}\sum_{jmj'm'} G_{np}a^{\dagger}_{jmn}a^{\dagger}_{\overline{jm}p}a_{\overline{j'm'}p}a_{j'm'n}, \tag{5}$$

containing an adjustable parameter G_{np}. This parameter is then fixed in such a way that in nuclei with $N\simeq Z$ the corresponding gaps have values following from isospin symmetry. Once determined, the value of G_{np} should be kept fixed for calculation of other nuclei for which the same single-particle level scheme is applicable. While our prescription is unique for the pure pairing Hamiltonian (1), it is not obviously unique for the realistic Hamiltonian. But as long as the isospin breaking is relatively mild, its actual form should not matter much.

What happens when neutrons are added to the symmetric $N=Z$ even-even nucleus? We show in Fig. 2 again the comparison between the exact and BCS gaps in the degenerate case, now as a function of $N-Z$. There are again basic similarities between the two situations, but the quantity Δ_{np} decreases more rapidly with $N-Z$ in the BCS case than in the exact case. We believe that this feature is related to the approximation involved in relating the gap Δ_{t_z} to the ground state expectation value $\mathcal{N}_{t_z}$ in the exact case. What is clearly visible in both cases, and intuitively obvious, is the tendency of the Δ_{np} to decrease with increasing $N-Z$. This tendency have been noted many times before; see e.g., [3,5]. In particular Ref. [5] has shown that in the BCS approach for real nuclei, and with the ratio G_{np}/G_{pair} fixed so that at $N\simeq Z$ the gap Δ_{np} has reasonable value, the effect of neutron-proton pairing disappears at $N-Z\geqslant 6$. It is important to keep in mind that the decrease of Δ_{np} with increasing $N-Z$ occurs even though the protons and neutrons occupy the same shell.

IV. CONCLUSIONS

We have shown that treating pairing properties of a system of interacting protons and neutrons with the help of the generalized Bogolyubov transformation requires special care. The corresponding system of equations allows, in principle, three different solutions. There is the trivial ''normal'' solution with no pairing whatsoever. But there are also two competing solutions with pairing correlations present. One, in which there are no neutron-proton pairs, corresponds to a product state with the neutron-neutron and proton-proton pairs not communicating with each other. The other solution corresponds to a system in which like-particle and neutron-proton isovector pairs coexist. When the generalized Bogolyubov transformation is used, there is a sharp phase transition between these two paired regimes, with the critical pairing strength $G_{np}/G_{\rm pair}$ somewhat larger than unity.

Thus, if one wants to describe the neutron-proton pairing using the quasiparticle transformation method, one has to break isospin symmetry at the Hamiltonian level. We propose to fix the unknown degree of isospin breaking in such a way that the gap Δ_{np} in $N \simeq Z$ nuclei is reasonable, i.e., comparable to the gaps Δ_{nn} and Δ_{pp}. With this assignment all traces of the isovector neutron-proton pairing disappear for $N-Z \geqslant 6$ in real nuclei.

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APPENDIX

For the exact diagonalization in the space of pairs with zero seniority we use the basis $|\mathcal{N},T,T_z\rangle$, where $\mathcal{N}$ is the total number of pairs, T is the isospin, and T_z its projection. The necessary matrix elements of the pair creation and annihilation operators are

$$\langle \mathcal{N}+1,T+1,T_z+t_z|S^\dagger_{t_z}|\mathcal{N},T,T_z\rangle = \frac{\langle TT_z 1 t_z|T+1,T_z+t_z\rangle}{\sqrt{2T+3}} \times[(T+1)(2\Omega-\mathcal{N}-T)(T+\mathcal{N}+3)/2]^{1/2}, \quad (A1)$$

$$\langle \mathcal{N}+1,T-1,T_z+t_z|S^\dagger_{t_z}|\mathcal{N},T,T_z\rangle = \frac{\langle TT_z 1 t_z|T-1,T_z+t_z\rangle}{\sqrt{2T-1}} \times[T(2\Omega+1-\mathcal{N}+T)(\mathcal{N}-T+2)/2]^{1/2}, \quad (A2)$$

$$\langle \mathcal{N}-1,T+1,T_z-t_z|S_{t_z}|\mathcal{N},T,T_z\rangle = \frac{\langle TT_z 1 -t_z|T+1,T_z-t_z\rangle}{\sqrt{2T+3}} \times[(T+1)(2\Omega+3-\mathcal{N}+T)(\mathcal{N}-T)/2]^{1/2}, \quad (A3)$$

$$\langle \mathcal{N}-1,T-1,T_z-t_z|S_{t_z}|\mathcal{N},T,T_z\rangle = \frac{\langle TT_z 1 -t_z|T-1,T_z-t_z\rangle}{\sqrt{2T-1}} \times[T(2\Omega+2-\mathcal{N}-T)(\mathcal{N}+T+1)/2]^{1/2}. \quad (A4)$$

For the case of two levels the basis is $|\mathcal{N}_1,\mathcal{N}_2,T_1,T_2,T_{1z},T_{2z}\rangle$ with the obvious constraint $\mathcal{N}_1+\mathcal{N}_2=\mathcal{N}$ (total number of pairs) and a similar one for T_z. The Hamiltonian matrix is easily constructed from the expressions above, with terms diagonal in $\mathcal{N}_1,\mathcal{N}_2$ and terms where $\mathcal{N}_1 \to \mathcal{N}_1 \pm 1$, and $\mathcal{N}_2 \to \mathcal{N}_2 \mp 1$. In addition there is a diagonal shift of $2\epsilon\mathcal{N}_2$, where ϵ is the splitting of the single-particle states.

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