COMPETITION BETWEEN T=0 AND T=1 PAIRING IN PROTON-RICH NUCLEI

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Abstract

A cranked mean-field model with two-body T=1 and T=0 pairing interactions is presented. Approximate projection onto good particle-number is enforced via an extended Lipkin-Nogami scheme. Our calculations suggest the simultaneous presence of both T=0 and T=1 pairing modes in N=Z nuclei. The transitions between different pairing phases are discussed as a function of neutron/proton excess, T_z, and rotational frequency, \hbar\omega. The additional binding energy due to the T=0 np-pairing correlations, is suggested as a possible microscopic explanation of the Wigner energy term in even-even nuclei.
The study of pairing correlations is one of a central theme in nuclear structure physics. Although the energy gain due to pairing correlations is rather modest, these correlations strongly influence many properties of the atomic nucleus. The large body of phenomena related to pairing among like-particles can be well understood, at least qualitatively, in terms of the simple BCS model with seniority force. In light nuclei, especially those with N=Z, it is well established empirically that neutron-proton (np) short range (pairing) correlations are of importance. The mean-field formalism like the Hartree-Fock-Bogolyubov (HFB) method is in principle capable to simultaneously treat both T=0 and T=1 pairing modes. The necessary generalizations of the Bogolyubov transformation were worked out by Goswami and coworkers [1–3] and Goodman [4]. These early calculations indicated that the importance of np-pairing is restricted to the vicinity of the N=Z line, [5], and that the T=0 and T=1 pairing phases are exclusive, see also [6,7]. The formalism was further extended to describe rotating nuclei [8], suggesting a possible phase transition between the two pairing modes at high spin [9].

The recent progress in nuclear spectroscopy, related to the event of highly efficient detector arrays and development of radioactive ion beam facilities, is opening up new avenues to study the nature of nuclear interactions, in particular, np-pairing correlations at the N=Z line. Phenomena like possible phase transition between different pairing modes in rapidly rotating nuclei, the influence of np-pairing on the position of the proton drip line and the stability of drip line nuclei due to the additional binding energy emerging from np-pairing are becoming important issues in nuclear structure.

The aim of this paper is to investigate basic features of np-pairing. We present a model applicable for pairing-and-deformation self-consistent cranking calculations and introduce a method to restore approximately the particle-number symmetry. This concept is an extension of the so-called Lipkin-Nogami method for the case of a non-separable proton-neutron system. The method is independent of the kind of two-body interaction used in the calculations. Applying approximate number-projection, results in the simultaneous presence of both T=0 and T=1 pairing modes. A detailed discussion of different aspects of our model will be given in a subsequent publication.

The starting point of our calculations are the eigenstates of a deformed phenomenological single-particle potential and therefore, spherical symmetry is broken already from the beginning. The main goal is to construct a formalism which is flexible enough to account for simultaneous scattering of (i) the nucleonic pairs where both particles occupy states of different signatures and (ii) pairs where both particles occupy states of the same signature. According to Ref. [4], these two pairing modes will be further denoted as $\alpha\bar{\beta}$ and $\alpha\beta$, respectively.

The most general Bogolyubov transformation can be written as:

$$\hat{\alpha}_j^\dagger = \sum_{\alpha>0}(U_{\alpha j}a_\alpha^\dagger + V_{\alpha j}a_{\bar{\alpha}} + U_{\bar{\alpha} j}a_{\bar{\alpha}}^\dagger + V_{\bar{\alpha} j}a_{\alpha}) \quad (1)$$

where $\alpha(\bar{\alpha})$ denote single particle states (including isospin indices) of signature $r = -i(+i)$ respectively, while $j$ labels quasiparticles. Following the calculations of Ref. [8], we will further impose the so-called antilinear simplex symmetry, $\hat{S}_z^A = \hat{P}\hat{T}\hat{R}_z$ as a self-consistent symmetry (SCS), see also [10]. One should bear in mind that, due to the antilinearity of $\hat{S}_z^A$, the transformation properties of creation and destruction operators with respect to $\hat{S}_z^A$ will
depend on the phases of the single-particle states. In other words one cannot introduce any new quantum number associated with that symmetry. After applying the $\hat{S}^A_z$ symmetry the Bogolyubov transformation still remains complex but the imaginary part decouples from the real part in the sense that the different signature blocks of the density matrix, $\rho = V^* V^T$, and pairing tensor $\kappa = V^* U^T$ are either real or imaginary:

$$\rho = \begin{pmatrix} \Re(\rho_{\alpha\beta}) & 0 \\ 0 & \Re(\rho_{\alpha\beta}) \end{pmatrix} + i \begin{pmatrix} 0 & \Im(\rho_{\alpha\beta}) \\ \Im(\rho_{\alpha\beta}) & 0 \end{pmatrix}$$

(2)

$$\kappa = \begin{pmatrix} 0 & \Re(\kappa_{\alpha\beta}) \\ \Re(\kappa_{\alpha\beta}) & 0 \end{pmatrix} + i \begin{pmatrix} 0 & \Im(\kappa_{\alpha\beta}) \\ \Im(\kappa_{\alpha\beta}) & 0 \end{pmatrix}$$

(3)

Furthermore, the complex structure of the single particle potential, $h$, and the pairing potential, $\Delta$, and consequently the HFB equations are fully determined by the complex structure of the $\rho$ and $\kappa$ matrices, respectively.

In this work we restrict the two-body $np$-pairing interaction to a simple extension of the standard seniority pairing interaction. It is separable in the particle-particle channel, $\overline{v}_{\alpha\beta\gamma\delta} \propto g_{\alpha\beta} g_{\gamma\delta}^*$, with $g_{\alpha\beta}$ proportional (up to a phase factor) to the overlap $\langle \alpha_\tau | \beta_\tau \rangle$ between single-particle wave functions. Apart from weak modifications due to the isovector components of the nuclear-mean field, like the static Coulomb potential, the interaction is dominated by $a\alpha$ and $a\bar{\alpha}$ types of pairing.

In order to relate the structure of the $a\alpha$ and $a\bar{\alpha}$ pairing modes to the isospin quantum numbers, let us briefly consider a nucleus with isospin- and time-reversal symmetry. By decomposing the pairing potential into the different isospin components $(T,T_z)$ one finds that the $T=1$ and $T=0$ components of the $np$-pairing depend on the combinations of the same elements of the pairing tensor but with opposite sign $[^4]$. Consequently, with the pairing tensor of the form of (3), the $T=0$ component of $a\alpha$ pairing is ruled out due to the $\hat{S}^A_z$ symmetry. Similar analysis shows that $T=1$ component of the $a\alpha$ pairing also vanishes. Therefore, in our model the $a\alpha$ pairing is equivalent to $T=1$ and $a\bar{\alpha}$ to $T=0$. This simple analysis also reveals the important role played by symmetries in the theoretical description of $np$-pairing, see also $[^3]$.

The average gap parameters are equal to (we adopt the convention where $\tau = 1$ for neutrons and $\tau = -1$ for protons)

$$\Delta_{\alpha_\tau,\beta_\tau}^{T=1} = -\delta_{\alpha_\tau,\beta_\tau} \Delta_{\alpha_\tau,\beta_\tau}^{T=1} \quad \text{where} \quad \Delta_{\alpha_\tau,\beta_\tau}^{T=1} = G_{\alpha_\tau,\beta_\tau}^{T=1} \sum_{\alpha_\tau > 0} K_{\alpha_\tau,\beta_\tau},$$

(4)

for $T=1$ $pp$- ($nn$-) pairing,

$$\Delta_{\alpha_\tau,\beta_{-\tau}}^{T=1} = -\langle \alpha_\tau | \beta_{-\tau} \rangle \Delta_{\alpha_\tau,\beta_{-\tau}}^{T=1} \quad \text{where} \quad \Delta_{\alpha_\tau,\beta_{-\tau}}^{T=1} = \frac{1}{2} G_{\alpha_\tau,\beta_{-\tau}}^{T=1} \sum_{\alpha_\tau,\beta_{-\tau} > 0} \langle \alpha_\tau | \beta_{-\tau} \rangle \left\{ K_{\alpha_\tau,\beta_{-\tau}} + K_{\beta_{-\tau},\alpha_\tau} \right\}$$

(5)

for $T=1$ ($a\alpha$) $np$-pairing and

$$\Delta_{\alpha_\tau,\beta_{-\tau}}^{T=0} = i \tau \langle \alpha_\tau | \beta_{-\tau} \rangle \Im(\Delta_{\alpha_\tau,\beta_{-\tau}}^{T=0}) \quad \text{and} \quad \Delta_{\alpha_\tau,\beta_{-\tau}}^{T=0} = -i \tau \langle \alpha_\tau | \beta_{-\tau} \rangle \Im(\Delta_{\alpha_\tau,\beta_{-\tau}}^{T=0})$$

where

$$\Delta_{\alpha_\tau,\beta_{-\tau}}^{T=0} = \frac{i}{2} G_{\alpha_\tau,\beta_{-\tau}}^{T=0} \sum_{\alpha_\tau,\beta_{-\tau} > 0} \langle \alpha_\tau | \beta_{-\tau} \rangle \left\{ \Im(K_{\alpha_\tau,\beta_{-\tau}}) - \Im(K_{\alpha_\tau,\beta_{-\tau}}) \right\}$$

(6)
for $T=0$ ($\alpha\alpha$) $np$-pairing. The strengths of the interaction are denoted by $G^{T=\tau}_{\tau\tau'}$.

To prevent a sudden collapse of the static pairing correlations, e.g. induced by fast nuclear rotation we introduce an approximate particle-number projection using the Lipkin-Nogami (LN) method \cite{nogami}. This method is equivalent to a restricted HFB-type variation, $\delta \langle HFB | \mathcal{H}^\omega | HFB \rangle = 0$, for the Routhian:

$$
\mathcal{H}^\omega = \hat{H}^\omega - \sum_{\tau} \lambda^{(1)}_{\tau} \Delta \hat{N}_\tau - \sum_{\tau\tau'} \lambda_{\tau\tau'}^{(2)} \Delta \hat{N}_\tau \Delta \hat{N}_{\tau'}. \tag{7}
$$

In the LN method the parameters $\lambda^{(1)}_{\tau}$ are standard Lagrange-type multipliers whereas the parameters $\lambda^{(2)}_{\tau\tau'}$ are kept constant during the variational procedure and eventually adjusted self-consistently using three additional subsidiary conditions.

$$
\langle \mathcal{H}^\omega (\Delta \hat{N}_\tau, \Delta \hat{N}_{\tau'}) \rangle = 0. \tag{8}
$$

where $\Delta \hat{N}_\tau \equiv \hat{N}_\tau - N$ and the symbol $\langle \cdots \rangle$ stands for the average over the $|HFB\rangle$ state. The LN theory is technically similar to the HFB theory but for the Routhian \cite{lipkin}. The resulting LN equations take the form of HFB equations with a single-particle field and pairing field renormalized as follows:

$$
h^L_{\tau\tau'}^{LN} \rightarrow h^{(2)}_{\tau\tau'} \rho_{\tau\tau'} \quad \text{and} \quad \Delta^{LN}_{\tau\tau'} \rightarrow \Delta^{(2)}_{\tau\tau'} K_{\tau\tau'}. \tag{9}
$$

An open question in mean-field calculations with $np$-pairing is related to the strength of the interaction. Whereas the strength of the $pp$- and $nn$- seniority pairing force is well established by a fit to the odd-even mass differences, very little is known about the strength of the $np$-pairing force. Based on isospin-symmetry arguments, it seems well justified to assume that at the $N\sim Z$ line $G^{T=1}_{pp(nn)} \sim G^{T=1}_{np}$. Therefore, our results will be presented either as a function of or at a given value of the parameter $x^{T=0}$ that scales the strength of $T=0$ $np$-pairing with respect to the average strength calculated for $nn$- and $pp$- pairing correlations i.e. $x^{T=0} = G^{T=0}_{np}/G^{T=1}_{np}$ while $G^{T=1}_{np} = (G^{T=1}_{nn} + G^{T=1}_{pp})/2$.

Fig. 1 shows the pairing gaps at zero frequency for a self-conjugate, $N=Z$, nucleus calculated with (BCSLN) and without (BCS) approximate number projection as a function of $x^{T=0}$. In this case we also disregard the Coulomb interaction and, therefore, $\Delta^{T=1}_{pp} = \Delta^{T=1}_{nn} = \Delta_0$ and $G^{T=1}_{pp} = G^{T=1}_{nn} = G^{T=1}_{np}$. The BCS version of our model has been discussed in the literature \cite{lipkin} and the solutions can be characterized as follows: (i) For $x^{T=0} < 1$ ($G^{T=0}_{np} < G^{T=1}_{np}$) the $T=1$ pairing is energetically favoured over the $T=0$ pairing. The pairing energy depends only on $\Delta^2 \equiv 2\Delta^2_0 + (\Delta^{T=1}_{np})^2$ and no energy is gained by activating the $T=1 np$-pairing. (ii) The solution at $x^{T=0} = 1$ ($G^{T=0}_{np} = G^{T=1}_{np}$) is highly degenerate. The HFB energy depends only on $\Delta^2 \equiv 2\Delta^2_0 + (\Delta^{T=1}_{np})^2 + |\Delta^{T=0}_{np}|^2$. Also in this limit, no energy is gained due to $np$-pairing. (iii) The solution at $x^{T=0} > 1$ ($G^{T=0}_{np} > G^{T=1}_{np}$) corresponds to a pure $T=0$ $np$-pairing phase.

As shown in Fig. 1, the results from the number-projected calculations are quite different. The critical value of the strength necessary to activate $T=0$ $np$-pairing is larger, $x^{T=0}_{\text{crit}} \approx 1.1$. The LN-method introduces different modifications of the pairing potential for the $T=1$ $pp$- and $T=1$ $np$-pairing field. It causes that at $x^{T=0} < x^{T=0}_{\text{crit}}$ and under the assumption of $G^{T=1}_{np} = G^{T=1}_{\tau\tau'}$ the pairing gap for the $T=1 np$-pairing, $\Delta^{T=1}_{np}$, becomes zero. It implies that the LN method has an isovector component, that requires further investigation. However,
at $x^{T=0} > x^{T=0}_{crit}$ the T=0 np-pairing correlations coexists with the T=1, $|T_z|=1$ pairing. The exclusiveness of T=0 and T=1 pairing phases in N=Z nuclei is a generic feature of the BCS method and is smeared out in the number-projected calculations.

For N≠Z both BCS and BCSLN models provide solutions which are qualitatively similar to the T_z=0, BCSLN case i.e. the T=0 np-pairing correlations coexist with the T=1 pp- and nn-pairing correlations. It is worth stressing that the value of $x^{T=0}_{crit}$ is strongly T_z dependent i.e. increases quite rapidly with neutron/proton excess or, alternatively, np-correlations are restricted to small $|T_z|$. In consequence, our calculations suggest a critical value of $|T_z^{crit}|$ beyond which, i.e., for $|T_z| > |T_z^{crit}|$, there is no collective solution to np-pairing, see Fig. 2.

The additional binding arising from T=0, np-correlations as well as the narrow region where it is active, is shown in Fig. 2. Early calculations of nuclear masses based on a macroscopic-microscopic approach have shown particularly strong deviations from the experimental data in the vicinity of the N∼Z line [12]. Most probably, only part of these deviations can be attributed to np-pairing while part of it can be accounted for by the self-consistent mean-field. One can assume that the single-particle mean field is properly taken into account by the extended Thomas-Fermi model which is a semi-classical approximation to the Hartree-Fock method [13]. In this model there is a systematic binding energy offset by ~ 2 MeV at the N=Z line that one might associate to the lack of np-pairing correlations. Based on this assumption and the results of [13] we can estimate the strength of the T=0 pairing force $G^{T=0} \approx 1.2G^{T=1}$ as shown in Fig. 2. The shell-model estimate of Ref. [14] yields $G^{T=0} \approx 1.3G^{T=1}$. Modern versions of macroscopic-microscopic mass calculations [13] cure the difficulties arising around the N∼Z line by introducing an extra term to the liquid drop formula - the so called Wigner energy [16]. Hence, a possible microscopic origin of the Wigner term in even-even nuclei are the T=0 np-pairing correlations.

A third way to generate a phase transition from T=1 to T=0 pairing is by rotation [8,9]. The results of cranking calculation for $^{46,48}$Cr are shown in Fig. 3. These are qualitative calculations at constant deformation and as such should not directly be compared to the experimental data. The calculations are performed with and without the T=0 force. At $\hbar \omega = 0$, the strength of the T=0 force is undercritical and T=0 pairing is not active. At a certain critical frequency, $\hbar \omega^{crit}$, there is a sudden onset of T=0 pairing, see also [14]. The latter effect can be viewed as either a phase transition or band crossing. The coherent action of centrifugal and Coriolis forces tend to align the angular momentum of the quasi-particles along the rotational axis. It weakens the T=1 pairing correlations and simultaneously, increases the number of pairs of nucleons with parallel coupled angular momenta, thus enforcing the T=0, αα, np-pairing correlations. In the T=0 phase, angular momentum is built by smoothly aligning np-pairs along the rotational axis, without involving any pair breaking mechanism. This situation is totally different from the well known response of the T=1 pairing to nuclear rotation, where pairs are broken to generate angular momentum. With increasing frequency, the T=0 pairing correlations tends to saturate. Note that the T=0 phase coexists with T=1 pp- and nn-pairing phases although the onset of T=0 np-correlations suppresses the T=1 phase. However, our calculations show that the T=0 np-pairing and T=1 np-pairing phases are always exclusive at $\hbar \omega \neq 0$, independently on their relative strengths.

The influence of the T=0 np-pairing correlations on the dynamical moment of inertia is conspicuous. Nuclear rotation in the presence of T=0 pairing correlations resembles classical
rigid body like rotation even though $T=1$ $pp$- and $nn$-pairing correlations are present. Note also that the moments of inertia at large frequency in the presence of $T=0$ pairing exceed by far the value obtained for a system without pairing, see Fig. 3. Even though the situations discussed above were visualized for $^{46,48}\text{Cr}$ only, these classes of solutions appear to be generic for all even-even nuclei with $N\sim Z$, i.e. do not depend qualitatively on $A$.

Our results can be summarized as follow: The previously suggested exclusiveness of the $T=0$ and $T=1$ pairing phases does not find support in our calculations. The sudden phase transition between the $T=0$ and $T=1$ pairing modes is a generic feature of the BCS approximation for $N=Z$ nuclei. This phase transition becomes smeared out in number-projected LN calculations. There, the $T=0$ $np$-pairing correlations coexist with $T=1$ $nn$- and $pp$-pairing correlations over a broad range of the strength $G_{np}^{T=0}$ as well as rotational frequency $\hbar \omega$, when $x_{T=0} > x_{crit}$. However, pairing correlations of $\alpha\alpha$ and $\alpha\tilde\alpha$ type counteract. For $N \neq Z$, the $T=0$ $np$-pairing correlations and $T=1$ $nn$- and $pp$-pairing correlations do coexist in both BCS and number-projected LN calculations. The $T=0$ $np$-pairing correlations are confined to a narrow region along the $N=Z$ line. The additional binding arising from these correlations may be viewed as a microscopic origin of the Wigner term in even-even nuclei. Even in the cases where $np$-pairing correlations are not present in the ground state one can generate $T=0$ $np$-pairing correlations at large rotational frequencies. An onset of $\alpha\alpha$ $np$-pairing quite dramatically influences the mechanism of building angular momenta. The $T=0$ $np$-pairs can easily be decoupled from the deformed core by the Coriolis force and consequently nuclear rotation resembles rigid-body like rotation though $pp$- and $nn$-pairing correlations are present. In both BCS and number-projected calculations, the $T=0$ and $T=1$ phases of $np$-pairing are exclusive at $\hbar \omega \neq 0$. We believe that this exclusiveness is an artifact related to our schematic interaction and/or the assumed self-consistent symmetries.

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**Figure captions**

**Fig. 1** Average pairing gaps for a self-conjugate nucleus, $N=Z$, as a function of $x_{T=0} = G_{np}^{T=0}/G_{np}^{T=1}$. Left (right) panel shows the results of calculations without (with) particle number projection.

**Fig. 2** Calculated additional binding energy, $E(x_{T=0}) - E(x_{T=0} = 1)$, arising from the presence of $T=0$ pairing for a number of Cr-isotopes in the vicinity of the $T_z=0$ line. Different
curves denote results for: \( x^{T=0} = 1.1 (\bullet), 1.2 (\triangle), 1.3 \) (solid triangles) and 1.4 \((\star)\). The solid line without symbols denotes the Wigner energy term due to [12] and the dotted line \((\ast)\) marks the result of the ETFSI-model [13].

**Fig. 3** The calculated dynamical moments of inertia for \(^{46}\text{Cr}\) and \(^{48}\text{Cr}\). Open circles correspond to the case of pure \(T=1, T_z = \pm 1\) pairing and the sharp peak in \(J^{(2)}\) is due to the breaking of the \(f_{7/2}\) pairs. The curve marked by solid dots indicate calculations with undercritical \(T=0\) \(np\)-pairing strength at \(\hbar \omega = 0\). The sudden rise of the moment of inertia corresponds to the critical frequency, where the \(T=0\) pairing correlations switch on. Note the entirely different behaviour of the moment of inertia for the two cases. The dotted line \((\ast)\) denotes the calculations without pairing.
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