Microscopic structure of fundamental excitations in $N=Z$ nuclei

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Excitation energies of the $T=1$ states in even-even as well as $T=0$ and $T=1$ states in odd-odd $N=Z$ nuclei are calculated within the mean-field approach. It is shown that the underlying structure of these states can be determined in a consistent manner only when both isoscalar and isovector pairing collectivity as well as isospin projection, treated within the iso-cranking approximation, are taken into account. In particular, in odd-odd $N=Z$ nuclei, the interplay between quasiparticle excitations (relevant for the case of $T=0$ states) and iso-rotations (relevant for the case of $T=1$ states) explains the near-degeneracy of these fundamental excitations.

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It is well known that pairing properties of finite Fermi systems are number-parity dependent. This is particularly well documented in atomic nuclei which exhibit phenomena like odd-even mass staggering or odd-even staggering of the moments of inertia. These phenomena origin from simple phase-space quenching due to the odd (quasi)particle known as the blocking effect. Within the standard BCS theory of superconductivity the blocking effect can be naturally accounted for by assuming the ground state of the odd system to be a one-quasiparticle (qp) or two-quasiparticle (2qp) in odd-odd (o–o) nuclei] excitation on top of the even-even vacuum, $\alpha^\dagger|\text{vac}\rangle$. In fact, the simplicity and consistency of the BCS treatment of even and odd nuclei was of paramount importance to establish the theory of superconductivity in atomic nuclei.

The classical BCS theory requires to be extended only in the closest vicinity of the $N=Z$ line. In these nuclei, apart from the isovector pairing mode, also isoscalar neutron-proton Cooper pairs coupled to non-zero angular momentum can be formed. However, the empirical fingerprints of this pairing phase are not very clear. The problem is rather complex, because it requires a detailed understanding of both pairing phenomena and the nuclear symmetry energy. An invaluable source of information allowing to disentangle these effects, are the isobaric excitations in $N=Z$ nuclei as already discussed in [3–6]. Unfortunately, most of these studies were either purely phenomenological or based on, in our opinion, inconsistent models. In this letter, we argue that the proper understanding of the isobaric excitations can be obtained only on a microscopic level. It requires that both isoscalar and isovector pairing as well as isospin projection (at least approximate) are taken into account. Moreover, within such a model, the standard BCS scheme of elementary excitations does not apply any longer. We provide the necessary extensions of the BCS theory which allow for a simultaneous description of (i) the mass-excess in $N=Z$ nuclei, (ii) isospin $T=1$ excitations in even-even (e–e) $N=Z$ nuclei [theory of $T=2$ states in e–e nuclei was given in our previous letter [7]], and (iii) $T=0$ and $T=1$ states in o–o nuclei.

![FIG. 1. The single-particle routhians (upper panel) versus iso-cranking frequency for the equidistant level model. Solid (dashed) lines depict downsloping, $|+\rangle$, and upsloping, $|−\rangle$, sp states carrying iso-alignments of $±1/2$, respectively. At each level crossing (indicated by arrows) the configuration changes, and hence excitation energy and iso-alignment (lower panel).](image-url)
shown in Fig. 8 the reoccupation process which takes place at each level crossing \([\omega_c^{(n)}]\) conserves the iso-signature symmetry. In other words, cranking the lowest sp configuration (vacuum) gives only states of even isospin. Hence, states of odd isospin are obtained by promoting one particle from the \(|-\rangle\) state to the lowest \(|+\rangle\) state as depicted in Fig. 1. The lowest odd-T branch of the iso-rotational band is obtained by cranking this particle-hole (p-h) excited state. The excitation energy and initial alignment of this p-h state are \(\delta e\) and \(T_e=1\), respectively. The p-h excitation modifies the iso-rotational spectrum in the following manner: First of all it blocks the level crossing at \(\hbar \omega = \delta e\). The allowed crossings appear at frequencies \(\hbar \omega_c^{(n)} = 2n\delta e\ [n=1,2,3,...]\). At each level crossing the isospin changes by \(\Delta T_e=2\) giving rise to an odd-T iso-rotational band. The total excitation energy of the band follows

\[
\Delta E = \frac{1}{2} \delta e + \frac{1}{2} \delta e T_x^2
\]

dependence. The formula (1) is similar to the one obtained previously for the states of even isospin. Indeed, the moment of inertia (MoI) of the even-T iso-rotational band [built on the vacuum] comes out identical to the MoI of the odd-T band [built on the lowest p-h excitation]. However, the odd-T band is shifted in energy by \(\delta e/2\) due to the required p-h excitation. Although the sp model is oversimplified, it reveals the nature of odd- and even-T states in e-e nuclei: Due to iso-signature symmetry, odd-T states are based on an excited p-h configuration and cannot be reached by iso-cranking the vacuum configuration to an odd-T \(x\) value. For a realistic model including pairing correlations, this corresponds to the lowest two-quasiparticle (2qp) state.

We now proceed to investigate how the excitation scheme is modified in the presence of pairing correlations. Our hamiltonian is based on the deformed single particle potential of Woods-Saxon (WS) type \(\beta\). The two-body correlations contain both isovector and isoscalar seniority-type pairing:

\[
\hat{H}^w = \hat{h}_{WS} + G_{T=1} \hat{P}_1^+ \hat{P}_1 + G_{T=2} \hat{P}_1^+ \hat{P}_0 - \hbar \omega \hat{I}_x
\]

where \(\hat{P}_1^+\) and \(\hat{P}_0^+\) create isovector and isoscalar pairs, respectively. The Hamiltonian \(\beta\) is solved using the Lipkin-Nogami method. The model is very similar to the one described in detail in Ref. \(\beta\). However, different to Ref. \(\beta\) we now employ the most general Bogolyubov transformation. It allows us to fully explore the isoscalar pairing channel without any symmetry induced restrictions i.e. to include simultaneously \(a\alpha\) and \(\alpha\alpha\) isoscalar pairs. It is important to stress that the model is identical the one used in Ref. \(\beta\) to compute \(T=2\) excitations in e-e nuclei. Like before, we set the deformation to \(\beta_2 = 0.05\). In the applications to e-e nuclei we use the same values of \(x^{T=0} = G_{T=0}/G_{T=1}\) and cut-off parameters, while for the o-o (\(N=Z=A/2\)) cases the cut-off parameters and \(x^{T=0}\) values deduced for the e-e \(N=Z=A/2-1\) neighbour were used consequently. Excitation energies as discussed in this work are not affected by the kind of \(T=0\) pairing used in the calculations (\(\alpha\alpha\), \(\alpha\alpha\) or mixed phases). In the following we restrict the calculations to (\(\alpha\alpha\) pairing in the \(T=0\) channel, which in the presence of standard cranking corresponds to states of low angular momentum \(\beta\).

In our previous letter we have shown that the cranked ground state configuration \(|vac\rangle\) with \(T_e=\sqrt{6}\) \([T_e=\sqrt{T+1}]\) yields surprisingly accurate predictions for \(\Delta E_{T=2}\). However, as mentioned above we cannot repeat this procedure for the \(T=1\) states and determine the frequency \(\hbar \omega\) for the \(|vac\rangle\) so that \(T_e=\sqrt{2}\). This would violate the iso-signature symmetry. The proper trial wave function corresponds to the lowest elementary excitation, i.e. to \(2qp, \alpha\alpha\alpha\alpha\alpha\) excitation. Hence, we do proceed as follow: (i) At each iteration step we perform the standard Hartree-Fock-Bogolyubov (HFB) transformation

\[
\begin{pmatrix}
U^{(k)}
\end{pmatrix} \rightarrow \begin{pmatrix}
V^{(k)*}
\end{pmatrix}
\]

for the two lowest quasiparticle states \(k=1,2\). Moreover (ii) we impose a certain, very small, spatial cranking frequency \(\hbar \omega \sim 0.01\) MeV to remove the degeneracies in the qp spectrum. This does not influence the excitation energy, \(\Delta E_{T=1}\), and is further justified because the \(T=1\) state have, in general, \(I \neq 0\). Finally, (iii) since at the iso-frequency zero the alignment \(|2qp|I_x|2qp\rangle_{\omega=0}=0\), we determine the cranking frequency \(\hbar \omega\) so that our solution satisfies the condition of \(T_e=1\).

The results of our calculations are shown in Fig. 2. The agreement between the data is more than satisfactory given the simplicity of our model. Moreover, because all parameters follow exactly those used for the calculations of the \(T=2\) states \(\beta\) we have a consistent scheme that
accounts simultaneously for the mass excess (the Wigner energy), the $T=1$, and $T=2$ states in $e-e$ $N=Z$ nuclei.

Isoscalar pairing plays a crucial and, interestingly, different role regarding the nature of these states. Although the $T=2$ states are predicted to be purely isovector paired, isoscalar correlations are vital in restoring the correct inertia parameter \[ 2 \] and, hence, the excitation energy. In contrast, the $T=1$ states are calculated to have only isoscalar pairing, see Fig. 3b. Already the 2qp excitation results in strongly reduced isovector pairing. With increasing iso-cranking frequency the iso-alignment of the system increases smoothly, and the weak isovector pairing becomes quenched, see Fig. 3. Apparently, by decreasing isovector pairing the systems gains alignment and, in turn, also energy. This process counterbalance the energy loss due to the disappearance of the isovector pairing. Once the nucleus reaches the alignment corresponding to $T_x=1$ it becomes trapped. This accounts for the cranking condition of $T_x=1$, since the 2qp configuration decouples from the core and becomes fully aligned. There is no collective rotation of the core. This state does not change until very high iso-frequencies where isoscalar pairing is destroyed and either the sp state is reached or isovector pairing sets in again. For example, for $^{44}$Ti depicted in Fig. 3, the nucleus is trapped at $\hbar \omega \sim 1.5$ MeV and stays there until $\hbar \omega \sim 5.8$ MeV. An interesting consequence emerges from the pairing properties of this state. Due to isospin symmetry, the $o-o$ $T_z=\pm 1$ states are also expected to have a predominantly isoscalar pairing field. Therefore, transfer reactions from odd-odd $T_z=\pm 1$ to the $T_x=0,T=1$ state and vice versa may be sensitive to isoscalar pairing correlations.

Let us finally turn to the spectrum of $o-o$ $N=Z$ nuclei. There, the ground state is determined by the competition between the $T=1$ and $T=0$ states, respectively. Though the lowest $T=0$ and $T=1$ states are nearly degenerate, the $T=0$ states are favored in lighter nuclei (below $f_{7/2}$ sub-shell) whereas the $T=1$ states become the ground state in heavier nuclei. There are two exceptions from this rule, namely $^{34}$Cl and $^{38}$Cu. Several authors already pointed out that the structure of the ground state of $o-o$ $N=Z$ nuclei reflects the delicate balance between the symmetry energy and pairing correlations, and that the energy difference may constitute a sensitive probe for the role of isovector and isoscalar pairing correlations. The works of dealt mainly with data analysis and did not attempt to provide a microscopic explanation. The considerations of Ref. 3 are based on the mean-field model with isovector pairing only and the ad hoc assumption that the symmetry energy corresponds to $E_{sym} \sim T(T+1)$ although it is known that microscopic mean-field models yield $E_{sym} \sim (N-Z)^2 \sim T^2$.

To better understand the situation in $N=Z$ $o-o$ nuclei let us come back for a while to the extreme sp picture. In this model two valence nucleons can form either an isovector, $T=1$, pair $(|+\rangle|+\rangle)$ giving rise to iso-aligned ground state configuration or an isoscalar pair $(|\rangle|\rangle)$ forming a $T=0$ p-h excitation. The energy of both states is completely degenerate. Again, pairing correlations will modify this simple picture.

Within the standard mean-field theory for pairing correlations (HFB) the ground states of $o-o$ $N \neq Z$ nuclei are described as 2qp excitation of the $e-e$ vacuum, $a^+ a^+ |vac\rangle$. These ground states are all minimal isospin states $T = |T_z| = |N-Z|/2$. Hence, for reason of consistency, all states of minimal isospin in $o-o$ nuclei, including the $T=0$ states in $N=Z$ nuclei, have to be treated as 2qp states. Therefore, we calculate the $T=0$ ground state of the $o-o$ $N=Z$ nuclei by blocking the lowest 2qp states self-consistently, similarly to the case of $e-e$ $T=1$ states. However, no iso-cranking is necessary, since $T=0$.

In contrast, due to the isospin symmetry, the $T=1$ state of the $o-o$ $N=Z$ nucleus can be regarded as a linear combination of the isobaric analogue states i.e. the $(N+1,Z-1)$ and $(N-1,Z+1)$ $e-e$ neighbours. Hence, it represents the vacuum of an $e-e$ nucleus, however excited in isospace. Since in this case we project on good $T_z=0$, the $e-e$ vacuum need to be iso-cranked to yield the correct value of $T_x=\sqrt{2}$. The difference between the theoretical approach to calculate $T=0$ and $T=1$ states in $o-o$ nuclei is shown schematically in the inset of Fig. 3, which elucidates the role played by blocking and iso-cranking, respectively. The difference in structure between these states is easy to understand qualitatively. Indeed, since no blocking but only iso-cranking is applied for $T=1$
states, isovector pairing is not reduced at all. However, isoscalar pairing is suppressed due to the isospin anti-pairing effect [7]. In contrast, the \(T=0\) state experience strongly reduced pairing correlations due to the blocking effect. Note, that both isoscalar and isovector correlations are reduced as compared to the e–e neighbour. Hence, the \(T=0\) and \(T=1\) states in o–o and e–e \(N=Z\) nuclei are of different nature, since they are based on two different fundamental excitations. It is therefore straightforward to understand the basic differences in the excitation energy pattern of e–e and o–o nuclei. In e–e nuclei, we need to consider both quasi-particle excitations and isospin cranking for the \(T=1\) excitation. Both are costly in energy and hence the excitation energy is rather high. In o–o nuclei, we simply deal with the competition between iso-cranking (\(T=1\)) and 2qp excitation (\(T=0\)). Energytically, to first approximation, these effects are very similar.

To get a quantitative estimate on the energy difference of the \(T=0\) and \(T=1\) states \(\Delta E = \Delta E_{T=1} - \Delta E_{T=0}\) in o–o nuclei, we performed a set of calculations following the rules sketched above. The results are presented in Fig. 4. As mentioned above, to first order these two basically different states are almost degenerate in experiment (●). Similar result are indeed obtained in our calculations (○). This result is particularly interesting because it was claimed previously, that this degeneracy is a proof of lacking \(T=0\) pairing correlations [6]. Evidently, these claims were based upon a poor understanding of the underlying structure of the elementary excitations allowed in the presence of proton-neutron pairing correlations.

![Graph showing \(\Delta E\) vs. \(A\)](image)

FIG. 4. Empirical (●) and calculated (○) excitation energies, \(\Delta E = \Delta E_{T=1} - \Delta E_{T=0}\), of the lowest \(T=0\) and \(T=1\) states in o–o \(N=Z\) nuclei. The insert indicates schematically the two different excitation modes of the \(T=0\) and \(T=1\) states in our calculations, see text for more details.

Note, that in our calculations we obtain not only the near-degeneracy but also an inversion of the sign of \(\Delta E\) which, in agreement with experiment, takes place somewhere around the \(f_{5/2}\) sub-shell. The inversion reflects basically the different mass dependence of the symmetry energy and the pairing correlations. Since the value of \(\Delta E_{T=1}\) is governed by the symmetry energy, it will decrease with mass as \(\sim 1/A\). On the other hand, the value of \(\Delta E_{T=0}\) is governed by pairing properties, i.e. depends on the size of the effective pairing gap including both \(T=0\) and \(T=1\) pairing correlations. Apparently, the pairing correlations do not fall off with mass as rapidly as \(1/A\) giving rise to the inversion.

In summary, we have presented a consistent microscopic explanation of the pairing phenomena in o–o and e–e \(N=Z\) nuclei based on the mean-field approximation. Our model includes, in a self-consistent manner, both isoscalar and isovector pairing correlations, and takes into account projection onto good particle-number (within the so called Lipkin-Nogami approximation [4], and isospin [within isospin cranking formalism [7]]. In e–e \(N=Z\) nuclei the \(T=1\) excitation is described as an iso-cranked 2qp configuration. According to the model, with increasing iso-frequency, the valence pair decouples from the fully isoscalar-paired core and aligns along the x-axis in isospace forming a trap at iso-alignment \(T_x = 1\). In o–o \(N=Z\) nuclei the \(T=1\) excitation is described by means of the iso-cranked o–o ‘false vacuum’ with \(T_x = \sqrt{2}\). Hence, this state represents a mixture of e–e neighbours (\(Z–1, N+1\) and \(Z+1, N–1\)) in accordance with isospin symmetry. The \(T=0\) excitations in o–o \(N=Z\) nuclei, on the other hand, are treated as 2qp excitations on top of the o–o ‘false vacuum’ similar to the standard self-consistent BCS treatment of all o–o \(N \neq Z\) nuclei. The model simultaneously account for the Wigner energy the excitation energies of the \(T=1\) and \(T=2\) states in e–e nuclei, the near-degeneracy as well as inversion of \(T=0\) and \(T=1\) states in o–o \(N=Z\) nuclei.

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