Microscopic, nonharmonic description of rotations and pairing vibrations in deformed *pf*-shell nuclei

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Angular-momentum- and particle-number-projected self-consistent Hartree-Bogoliubov wave functions are used within the generator-coordinate method for the description of excited states in ^{48}Ti and ^{56}Fe. Bands based on the ground state and first pairing-vibrational state respectively are studied. In the ground band of ^{56}Fe an antipairing effect occurs parallel with an increase of correlations in the excited band, so that for higher J the ground band becomes less paired than the excited one.

[NUCLEAR STRUCTURE ^{48}Ti, ^{56}Fe; calculated rotational spectra. Hartree-Bogoliubov, generator-coordinate method, J projection.]

The existence of collective modes based on fields which create or annihilate two particles has been first suggested by Bohr and Mottelson.[1] A number of theoretical approaches have been suggested to describe those pairing vibrations in the framework of the random-phase approximation (RPA), by the boson expansion method, and by the generator-coordinate method (GCM) (Ref. 2–7). However, there have been only a few attempts to investigate pairing vibrations in deformed nuclei. In all these cases the (harmonic) RPA with schematic interactions were used.[8,9] An alternative, nonharmonic treatment with arbitrary forces is presented in this note. It is a generalization of the GCM method which has been applied for the calculation of pairing-vibrational 0^+ states in spherical nuclei.[2,6,7]

A family of paired wave functions $\phi(\Delta)$ is introduced which depends on a parameter Δ, describing the amount of pairing correlations in the wave function but not necessarily equal to the energy gap. The broken symmetries are restored by projecting[10] $\phi(\Delta)$ on good angular momentum J and good proton and neutron numbers with the projection operators P_J, Q_P, and Q_N, respectively.[10] This yields the state $\phi_J^{(P,N)}(\Delta)=P_J Q_P Q_N \phi(\Delta)$, which must be normalized. The trial wave function for the system in the rotational state J is assumed to be the linear superposition[11]

$$\Psi_J^{(P,N)}=\int f_J^{(P,N)}(\Delta)\phi_J^{(P,N)}(\Delta)\,d\Delta\,. \tag{1}$$

The amplitudes $f_J^{(P,N)}(\Delta)$ are determined by solving the corresponding Hill-Wheeler equations[11] for each J value separately. For each J the lowest eigenvalue of Eq. (1) should correspond to the yrast level of the nucleus and the first excited 0^+ state to its pairing-vibrational state, in analogy to the spherical description of Refs. 2, 6, and 7. However, since a deformed nucleus is considered there will also be, for $J^\pi > 0^+$, excited states not belonging to the ground-state rotational band. In the present description these states appear either as rotational J^π states based on the 0^+ pairing-vibrational one or as pairing-vibrational J^π states based on the corresponding member of the ground-state rotational band.

In the present calculations self-consistent wave functions and realistic interactions are used. The $\phi(\Delta)$ are assumed axially symmetric and are obtained by solving the Hartree-Bogoliubov equations of the modified Hamiltonian[12] $H'=H-\lambda V_P$, where V_P is the pairing part of the two-body interaction contained in H and λ is a Lagrange multiplier used to fulfil the subsidiary condition that the pairing energy Δ assumes a variable value,[12] with

$$\Delta=\frac{1}{2}\sum_{iklmn} V_{iklmn}\langle c_i^\dagger c_k^\dagger\rangle\langle c_n c_m\rangle\,. \tag{2}$$

A harmonic-oscillator basis with oscillator length $b=2.09$ fm is used, which included the $1s$, $1p$, $2s$-$1d$, and $2p$-$1f$ shells. In order to make the total calculation free from adjustable parameters, an effective interaction has been derived from the realistic Hamada-Johnston potential in the following way: The Bethe-Goldstone equation was solved by Barrett, Hewitt, and McCarthy[13] with a harmonic-oscillator Pauli operator which forbids intermediate states with one particle in the $1s$-, $1p$-, and $2s$-$1d$ shells and states with two particles in the $2p$-$1f$ shell. The starting energies were determined by the Bethe-Brandow-Petschek theorem using single-particle energies obtained by a preceding Brueckner calculation with pure harmonic-oscillator wave functions as single-particle states. The spectrum of the intermediate oscillator states was shifted downwards by a constant $C=42$ MeV

which roughly yields good binding energy. The Coulomb force has been included.

For the solution of the Hill-Wheeler equations

$$\sum_k \{\langle \phi_J^{(P,N)}(\Delta_k)|H|\,\phi_J^{(P,N)}(\Delta_i)\rangle - E\langle \phi_J^{(P,N)}(\Delta_k)\phi_J^{(P,N)}(\Delta_i)\rangle\} f_J^{(P,N)}(\Delta_k) = 0 \text{ for all } i, \tag{3}$$

three discrete generator points were used, viz., the Hartree-Fock solution, the Hartree-Bogoliubov solution, and a solution with a pairing energy Δ [see Eq. (2)] of twice the Hartree-Bogoliubov value. With this choice of the generator points Δ_k the pairing-vibrational 0^+ state is numerically reliable within 0.1 MeV. The formal expressions of the overlaps occurring in Eq. (3) and details of its solution can be found in Refs. 14 and 15.

The method described above was applied to ^{48}Ti and ^{56}Fe. In Fig. 1 the calculated and experimental[16-19] spectra are compared. The odd spins and the states with $J \geq 6$ have been omitted because of the lack of experimental information. The ground band is not well described since the formalism in its present state is not able to reproduce shape-vibrational-like spectra as they appear approximately in ^{48}Ti and ^{56}Fe. This shall be achieved in the future by introducing additional appropriate generator coordinates.[15] In addition, the force is free from adjustable parameters. However, the excitation energies of the second 0^+ and 2^+ states are in reasonably good agreement with experiment; they deviate by less than 1 MeV from the experimental data. For the correspondence between the measured and calculated pairing-vibrational 0^+ states, which is indicated by the dashed lines in Fig. 1, we followed for ^{48}Ti a suggestion of Sörensen[3] and in ^{56}Fe the second excited 0^+ state was chosen because the first one is supposed to originate from a coupling of two-quadrupole phonons rather than being a pairing-vibrational state. These assignments are also supported by the experimental cross sections for two-nucleon transfer reactions as discussed later on.

The pairing energies Δ_J, which are defined in correspondence to Eq. (2) but in addition with projection on good angular momentum and proton and neutron number, are plotted in Fig. 2. One may notice the antipairing effect in the ground-state rotational bands, which is well known in *sd*-shell nuclei[12] and in the rare-earth region.[20] The behavior of the excited bands based on the first excited pairing-vibrational 0^+ state may be different however. In model calculations[21] it has been shown that the pairing-vibrational state is strongly paired (superfluid) when the ground state shows

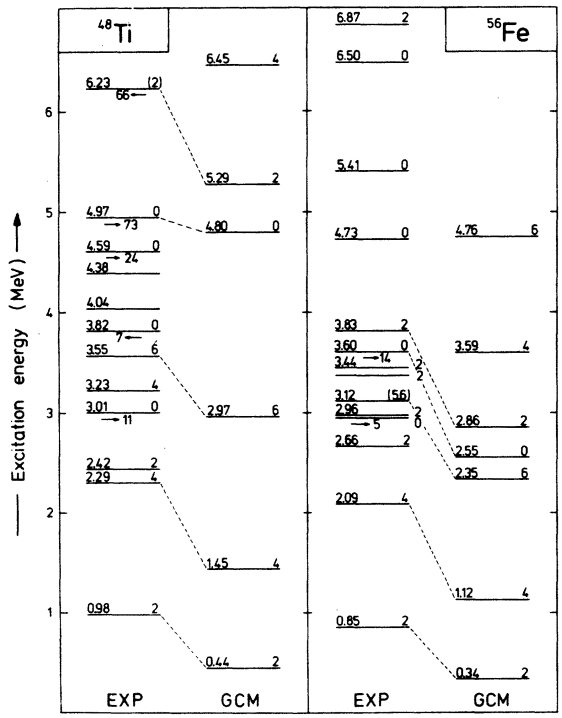

FIG. 1. The excitation spectra are plotted for ^{48}Ti and ^{56}Fe, calculated with the generator coordinate method (GCM) and compared with experimental data (EXP). For some experimental levels the (p,t) and (t,p) intensities are given for the reactions leading to this level from the ground state of $N+2$ or $N-2$ (arrow pointing left or right, respectively). Transition strengths to excited states are quoted relative to the ground state which is normalized to 100.

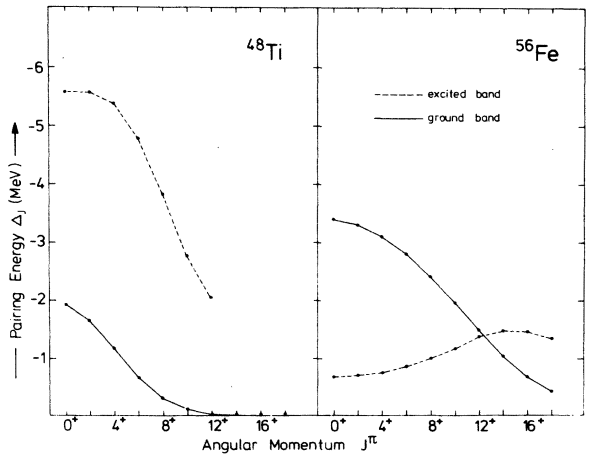

FIG. 2. The pairing energies Δ_J for the rotational bands based on the ground state (solid line) and on the pairing vibrational state (dashed line) are plotted against the angular momentum.

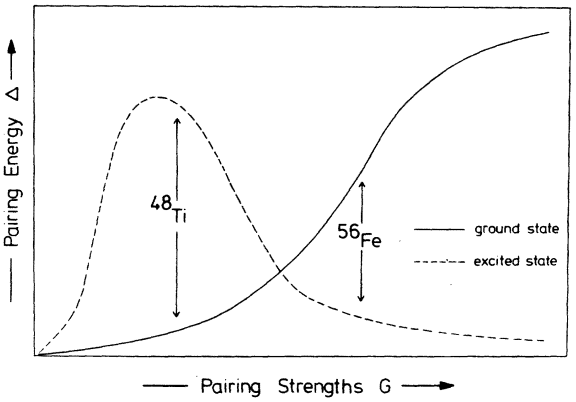

FIG. 3. Schematic picture for the dependence of the pairing energy of the 0^+ ground state (solid line) and of the 0^+ pairing vibrational state (dashed line) against the pairing force strengths. The positions of ^{48}Ti and ^{56}Fe as calculated from the present GCM, are indicated.

small pairing (normal) and vice versa. Keeping also in mind that for vanishing pairing force strengths G both the ground state and the two-quasiparticle excited state have vanishing pairing energies, one knows that the dependence of the pairing energies on the force strength G looks qualitatively like that sketched in Fig. 3. If one realizes that with increasing J the Coriolis force tends to reduce the effect of the pairing force, the behavior of the pairing correlations in Fig. 2 is easily explained as follows: The situation which corresponds to the 0^+ states of ^{56}Fe and ^{48}Ti is indicated in the schematic Fig. 3. The change of the pairing energies with increasing J in Fig. 2 correspond to that with decreasing G in Fig. 3. For ^{56}Fe the point where the two curves in Fig. 3 cross corresponds to $J \approx 12$ in Fig. 2, where the excited band becomes more strongly paired than the ground band. From Fig. 3 one also understands that the pairing in the excited band of ^{48}Ti remains larger than in the ground band.

The moments of inertia change in accordance with the pairing correlations and are in qualitative agreement with the experimental data, if the correspondence is taken as indicated in Fig. 1. For the 2^+-0^+ splitting of the excited band in ^{48}Ti is larger than for the ground band, whereas it is just the other way around in ^{56}Fe.

From model calculations[5,6] one expects that the two-particle transfer cross section to a superconducting pairing-vibrational state is about equally as large as that to the normal ground state, whereas it is very much smaller in cases when the excited state is normal and the ground state is superfluid. This is borne out in the present calculation by relating the calculated pairing energies Δ_J (Fig. 2) to the experimental (p, t) and (t, p) cross sections (see Fig. 1). It confirms strongly our assignments of the 0^+ (4.97 MeV) and the 2^+ (6.23 MeV) states in ^{48}Ti as pairing vibrations. In ^{56}Fe the 0^+ state at 3.60 MeV is populated only weakly, which is in agreement with the small pairing energy Δ_J for this state (see Fig. 2). In the present calculations both proton-proton and neutron-neutron pairing were allowed, but it appears that only the neutrons are paired. The calculated states are therefore neutron-pairing-vibrational states and the proton-pairing-vibrational states should occur at higher energies. This corresponds to the fact that in the $(^3\text{He}, n)$ experiment[17] the 0^+ state at 3.60 MeV in ^{56}Fe is not observed, but only 0^+ states above 5 MeV.

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