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On the Validity of the Mean Field Approach for the Description of Pairing Collapse in Finite Nuclei*

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Abstract:

The transition from the superfluid to the normal phase in nuclei with increasing temperature and angular velocity is investigated within various approximations and in an exactly soluble model. It is found that the simple mean field theory always predicts a sharp phase transition, as for infinite systems. In theories taking into account fluctuations this sharp collapse is dramatically changed. In some cases no phase transition is observed.

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Pairing correlations in nuclei are due to the fact that the short range character of the effective particle-particle force favors pairs of identical nucleons coupled to angular momentum zero. This can be described in a very elegant way by the BCS-approach[1]) originally invented for infinite systems in the theory of superconductivity, and applied to finite nuclei by Bohr, Mottelson and Pines[2]), and also Belyaev[3]). In analogy to the superconductor in which one observes a phase transition to a normal conductor for a sufficiently high magnetic field and for increasing temperature, it has been predicted that for nuclear superfluidity an overall pairing collapse at higher angular momenta[4]) should take place together with the breaking of individual pairs by the Coriolis force[5]), and also by higher temperatures[6]), in which the increasing excitation energy allows the population of unpaired configurations. So far these phase transitions in nuclei have not been experimentally observed, but calculations in simple models[7,8]) and in realistic nuclei[9,10]) have shown, that indeed within the cranked Hartree-Fock-Bogoliubov (HFB) formalism a sharp transition to a normal fluid phase occurs at higher angular velocities. Similarly one has found a pairing collapse with increasing temperature in model[11])- and in realistic calculations[12-14]). In all these studies simple-minded mean field theory (BCS or HFB) has been applied. Based on such calculations one would be led to believe that in rare earth nuclei neutron pairing vanishes for spins larger than 30 $\hbar$ and that proton pairing vanishes for spins larger than 50 $\hbar$. The pairing collapse with temperature should occur at roughly T = 0.5 MeV for nuclei in this region.

Mean field theories are classical approximations, which provide an accurate description in the limit of large particle numbers and sufficiently large interaction strength. The crucial quantity however, is not the total

particle number, which is always large in heavy nuclei, but the number of valence particles participating in the collective process of pairing. This number is not very large even for heavy nuclei,as can be seen from the fact that the experimental gap Δ is only increased by a factor 5 as compared to an average pairing matrix element between two single nucleons. Another indication is that in BCS theory pairs are scattered around the Fermi surface in an energy interval of about $\Delta \approx 1$ MeV. Assuming an average level distance of 200-300 keV we see that only 3-5 pairs of nucleons participate in pairing for nuclei in the rare earth region. The collectivity of pairing correlations is therefore much lower than the collectivity of shape correlations. There BE2-values of several hundred Weisskopf units are observed and the quadrupole matrix element is increased by a factor 15-20. At least all the nucleons in the valence shell are influenced by deformation.

It is well-known that the mean field approximation breaks down in the region of a phase transition, where fluctuations become important. The simple BCS or HFB approach therefore is expected to fail at high angular velocities and at temperatures where the pairing correlations become small.

In this letter we therefore investigate the validity of the mean field approach in the two cases:

i) at zero temperature and with increasing angular velocity

ii) at zero angular velocity and with increasing temperature.

The first case corresponds to a study of the yrast line of heavy deformed nuclei up to very high spins. This region has been subjected to considerable investigation in the last fifteen years both experimentally and theoretically. However, from the level scheme alone it seems to be very difficult to gain information on changes of the pairing correlations at high spins[10]). Only at

spin zero, where the quasiparticle energies are larger than the gap parameter Δ, has one a real gap in the excitation spectrum which causes the decrease of the moment of inertia by a factor 2-3 as compared to the rigid body value. At higher angular momenta they can become much smaller than the gap parameter Δ, they may even vanish, and one then finds gapless superconductivity[15,16]), in which Δ undergoes only slight changes. If one assumes that in this case the quasiparticle energies in the rotating frame are statistically distributed around the Fermi surface one finds the rigid body value for the moment of inertia[17]). It is therefore rather easy to understand why one observes in many cases experimental momenta of inertia close to the rigid body values[18]).

A direct measurement of pair transfer matrix elements, which certainly contain the necessary information, can in principle be performed using two-particle transfer following Coulomb excitation[19]). However, so far it has been restricted to spin values smaller than 20 $\hbar$.

At the moment one has therefore to rely on theoretical studies. In this case one has to go beyond the mean field approach, i.e. beyond cranked HFB, and has to take into account fluctuations. There are of course many types of fluctuations as can be seen from a study of the Cranked Random Phase Approximation (CRPA)[20]). In our case the important correlations are connected with the pairing degree of freedom. In particular the orientation of the BCS function in gauge space is fixed, a fact which is connected with the violation of particle number. Number projection takes these fluctuations into account, because it is a superposition of all orientations together with their proper weights. Of course pairing correlations have to be determined selfconsistently. We have to carry out a variation after projection on particle number. The trial wave functions used in this procedure are clearly

more general than the BCS or HFB functions. In particular they include in principle also the possibility for a pairing collapse. In some simple models they even contain the exact solutions, whereas BCS becomes exact only for particle number $N \to \infty$.

In Fig.1 we show the results of a theoretical investigation of the nucleus ^{168}Yb. The configuration space and the residual interaction of Baranger and Kumar[21]) was used and the unprojected (selfconsistent cranking SCC) as well as the particle number projected (PNP) energy surface in the rotating frame was minimized by general HFB-functions. The Munich code was used and details of the calculation are given in ref.[10]). The gap parameters Δ_p and Δ_n shown in the figure are obtained in both cases from the pairing energy:

$$\Delta_\tau = G_\tau \cdot \sqrt{\langle P^+_\tau P_\tau \rangle} \qquad (1)$$

where G_τ is the pairing force strength of protons (τ=p) and neutrons (τ=n) and P^+ creates a Cooper pair coupled to angular momentum zero. The exchange term containing the contraction $\langle a^+ a \rangle$ which leads to the Gv^4-term in the simple BCS theory is as usual neglected in both cases. The Δ defined in this way would therefore vanish for wavefunctions having no pairing correlations.

The value Δ defined in eq.(1) measures the energy gained by the pairing interaction. It is larger than the change of the total energy. Namely in order to gain pairing energy we have to scatter nucleons to states around the Fermi surface, and have to pay for this accordingly in a change of the single particle energy going in the opposite direction. Nevertheless the definition (1) seems to us to be the proper measure of pairing correlations.

The nucleus ^{168}Yb has a particularly low neutron level density at the Fermi surface. Therefore the gap parameter for neutrons is rather low at spin zero and vanishes quickly in the unprojected SCC theory. At I = 20 ħ we find a sharp neutron pairing collapse. This is connected with a smooth alignment of a $\nu i_{13/2}$ pair, because the interaction between g- and s-band is rather large and therefore no backbending is observed.

In the number projected calculation the neutron gap does not vanish. It is reduced in the region of alignment, which corresponds to a transition to a blocked two-quasiparticle state. However for all higher angular momenta it falls very slowly. In the region between 20 ħ and 30 ħ, where constant moments of inertia close to the rigid body value have been observed[18]) it is about 500 keV and even at the highest spins it still remains roughly 300 keV. A similar result has already been observed by the Juelich group[22]) in the spin region below 30 ħ for a variation after number projection in a restricted space and in a number of neighboring nuclei by our group[10]).

It turns out that the level density at the Fermi surface and the pp-force in realistic calculations do not seem to be large enough that fluctuations can be neglected. In this sense the nuclear system is too small to produce a superfluid-normal phase transition. Up to now we have used only monopole pairing. Finite range forces as simulated by quadrupole pairing also allow pairing correlations in aligned configurations and the resulting pairing is then even less reduced with increasing angular velocity[23]). Additional correlations coming from fluctuations of other type are expected to increase the pairing energy, i.e. to prevent a pairing collapse even more.

These studies have been carried out using realistic force parameters. They seem to indicate, that the Mottelson-Valatin effect does not exist in real nuclei at least in all those which have been investigated so far.

It is certainly interesting to study what happens to the predicted pairing collapse induced by temperature in calculations based on the mean field approach[12-14]), on including additional fluctuations. At finite temperatures we have two kinds of fluctuations, quantal fluctuations, which are already important at T = 0, and thermal fluctuations. Again one would like to start with the quantum fluctuations of the orientation in gauge space, i.e. to use number projected temperature dependent mean field theory. So far, however, such a method has not been developed. We therefore investigate in the following first only the thermal fluctuations in the realistic case. Finally we discuss an exactly soluble model, which includes as well quantal as thermal fluctuations.

Treating the pairing gap as a collective coordinate on can derive a classical Hamiltonian function in the framework of adiabatic time-dependent Hartree-Fock theory:

$$H(p_\Delta,\Delta) = \frac{1}{2B(\Delta)}\, p_\Delta^2 + V(\Delta) \tag{2}$$

The potential $V(\Delta)$ is given by the temperature dependent mean field energy and the mass parameter $B(\Delta)$ is for separable forces equal to the cranking mass[24]):

$$B(\Delta) = \frac{1}{4}\sum_{k>0} E_k^{-3}(1 - 2v_k^2)^2(1 - 2f_k) \tag{3}$$

where v_k^2 are BCS occupation numbers, E_k are quasiparticle energies and f_k are occupation factors of the Fermi-Dirac distribution at temperature T.

Using the Hamiltonian function (2) we can calculate the probability $p(\Delta)$ that the nucleus has the gap Δ.

$$p(\Delta) \propto \sqrt{B(\Delta)}\, \exp(-F(\Delta)/T) \tag{4}$$

where $F(\Delta)$ is the free energy obtained from $V(\Delta)$.

Neglecting the Δ-dependence of the mass, one then ends up with a method used by Moretto[25]) and Goodman[26]) for model cases. We take the Δ-dependence of the mass-parameter into account and apply this method to a realistic case, namely again to the nucleus ^{168}Yb. In Fig.2 we show the mean field value for the gap and the average gap:

$$\bar{\Delta} = \int_0^\infty p(\Delta)\Delta d\Delta \tag{5}$$

We see, that, as expected, the sharp pairing collapse at T = 0.5 MeV is considerably smeared out by classical thermal fluctuations. We also find, however, that neglecting the Δ-dependence of the mass over-emphasizes this effect somewhat. In fact large pairing correlations decrease the mass-parameter, which makes it less probable for the system to stay in regions of large pairing.

In order to study the influence of correlations in an exactly soluble model we use a single j shell, which is filled by N particles interacting via a monopole pairing force:

$$H = -G\, P^+P \tag{6}$$

This Hamiltonian is diagonal in the seniority scheme[24]). The eigenvalue are expressed as

$$E(N,v) = -G(N - v)(2j - v + N + 3) \tag{7}$$

where v is the seniority. Since the number of states with seniority v is given by the recurrence relation

$$\left[\sum_I (2I + 1)\right]_v = \left[\sum_I (2I + 1)\right]_{v-1} \frac{(2j + 4 - v)(2j + 3 - 2v)}{v(2j + 5 - 2v)} \tag{8}$$

we can easily evaluate the temperature dependent pairing correlation energy E(T) In the exact calculation the pairing gap is then expressed as

$$\Delta(T) = \sqrt{-GE(T)} \tag{9}$$

It is compared with the gap parameter $\Delta(T)$ in the temperature dependent BCS approximation for various particle numbers N and different j-values in Fig.3. Taking into account, that the units in this figure are (j+1/2)G we see that, as expected, the effective pairing matrix element (9) increases with j, i.e. with the level density at the Fermi surface, and also with the particle number. We find in all cases that in the mean field theory a sharp pairing collapse occurs at roughly $T_c = 0.2\ (j+1/2)\ G$. As the pairing parameter Δ at the ground state, this critical temperature is increased for higher level density and for stronger pairing force. This collapse is smeared out in the exact calculation. However we observe that the mean field theory provides a rather good approximation for large particle numbers and high j-values, i.e. for high level densities.

Summarizing our results we find: A theoretical treatment of the pairing collapse going beyond the mean field theory shows the superfluid-normal phase

transition can be smeared out considerably in finite nuclei. For the case of pairing collapse driven by the angular velocity at zero temperature a realistic calculation is possible and shows that the Mottelson-Valatin effect hardly exists in realistic nuclei. For the phase transition driven by temperature, classical calculations of the thermal fluctuations and exactly soluble models indicate that perhaps considerable pairing correlations may be expected at much higher temperatures than predicted by temperature dependent HFB theory.

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Figure Captions:

Fig.1 Gap parameters Δ as defined in eq.(1) for the nucleus ^{168}Yb as a function of the angular momentum I at zero temperature: full lines correspond to neutrons, dashed lines to protons. Selfconsistent cranking (SCC) is compared which exact number projection before the variation (PNP).

Fig.2 The gap parameter for the nucleus ^{168}Yb as a function of the temperature at zero angular momentum. Δ is the gap parameter calculated in mean field theory (HFB). $\bar{\Delta}$ are average gap parameters as defined in eq.(5). In the full line the Δ-dependent mass is taken into account, in the dashed line this mass is set constant as in refs. [25]) and [26]).

Fig.3 Pairing collapse in the single-j model of eq.(6) as a function of the temperature (in units of $(j+\frac{1}{2})G$). Different combinations of the level size j and the particle number N are shown. The lower curves are calculated intemperature dependent BCS approximation, the upper curves are exact results (eq.9). We also indicate the exact gap for infinite temperature.

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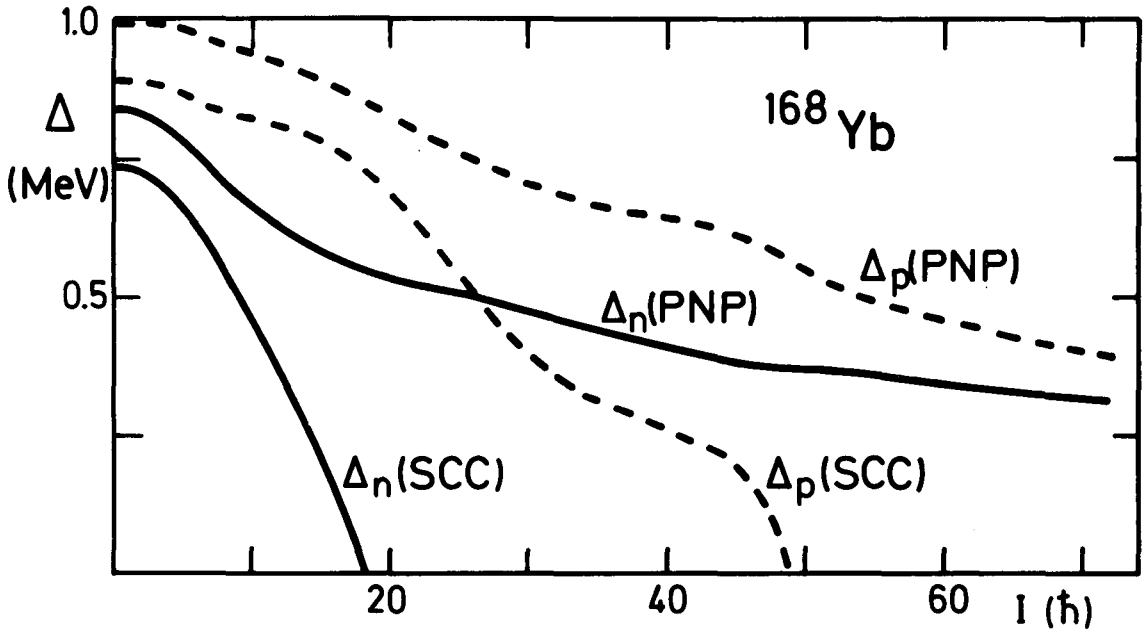

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Fig. 1

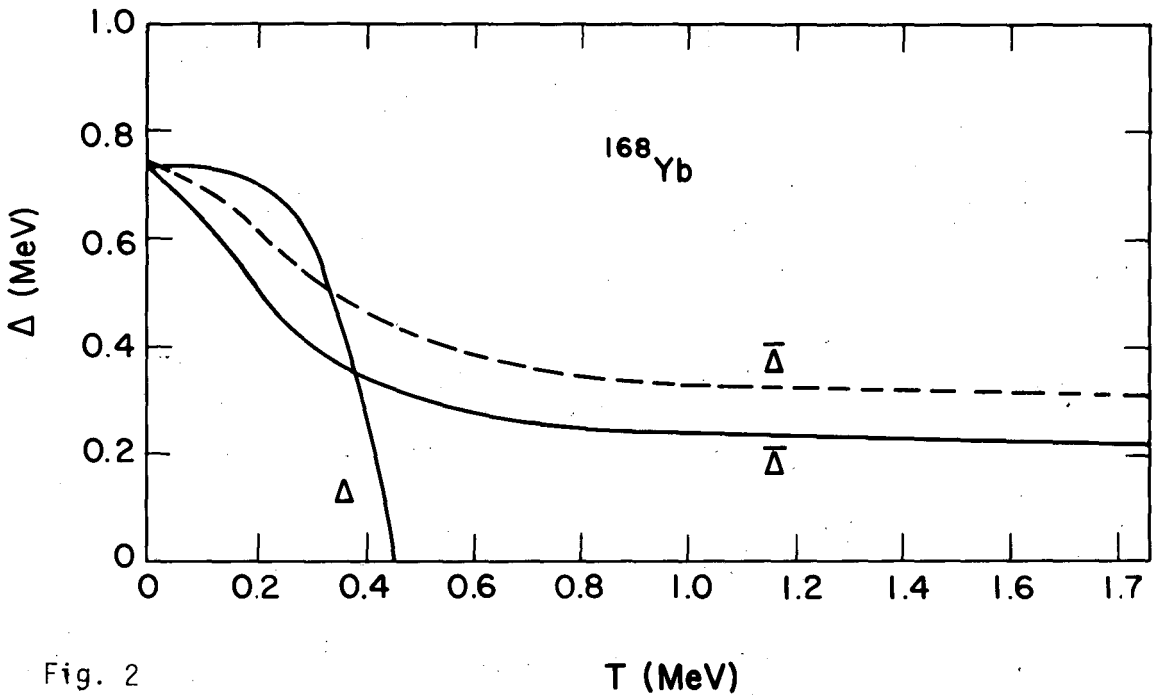

Fig. 2

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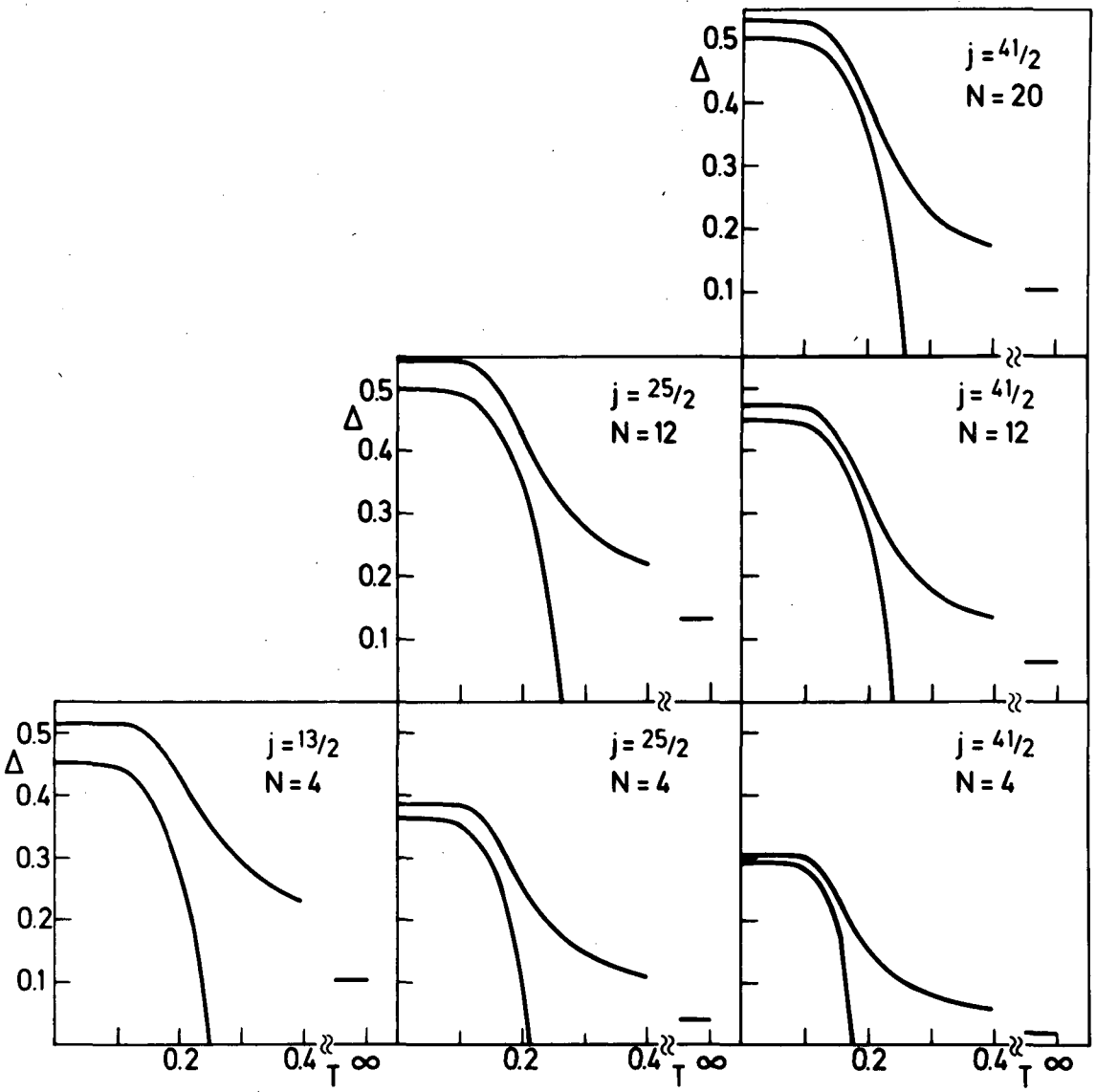

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Fig. 3

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