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Pairing correlations at high spin and finite temperature: a modified BCS approach

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Abstract. The modified BCS approach for rotating nuclei is extended in order to include thermal excitations. The formalism is developed in order to take into account both high-spin- and temperature-dependent effects. The method seems to be appropriate for the microscopic description of the pairing correlations at excitation energies above the yrast line.

1. Introduction

Heavy-ion reactions are a very rich source of information concerning the behaviour of the nucleus at high spin and high excitation energy (Lieder and Ryde 1978). In particular, they enable us to study the de-excitation process of fast rotating, highly excited nuclei (Wakai and Faessler 1978, Liotta and Sorensen 1978). Recently, both experimental (Newton *et al* 1981, Collins *et al* 1982) and theoretical results (Egido and Ring 1982, Fedotkin *et al* 1983, Faessler *et al* 1983, Civitarese *et al* 1983) on the de-excitation of giant resonances built on high-spin states above the yrast line have been reported. These processes, like backbending, are strongly correlated with the nuclear shapes and their stability. From the theoretical point of view, the best results have been obtained with the Strutinsky model (Brack *et al* 1972).

While the classical liquid-drop model (Cohen *et al* 1974) is able to describe average nuclear properties in terms of deformations, the most significant quantum-mechanical corrections arise from the shell structure and from the short-range (pairing) correlations (Ansari *et al* 1980).

In dealing with high-spin states, the short-range effects are usually neglected by the argument that the pair correlations would break down at relatively moderate values of the angular momentum, I, because of the Coriolis force. However, in a recent article (Markum *et al* 1982a) it was shown that, especially for large deformations, pairing can persist up to $I \simeq 60\hbar$. This result indicates that, in dealing with fast rotating systems, one should not neglect *a priori* the effect of the pairing interaction. The same conclusion might also be valid for the case of high-spin states above the yrast line (finite temperatures), where it has been argued that the pairing effect would vanish due to the strong antipairing thermal effects (Egido and Ring 1982).

Two well known models exist which allow us to study pairing forces at high-spin states. The most adequate model is given by the cranked Hartree–Fock–Bogoliubov theory

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(Ansari *et al* 1980, Goodman 1974), which requires the calculation of matrix elements and diagonalisation of high-dimensional matrices in a self-consistent manner. Alternatively, pairing effects can be taken into account by solving the BCS equations in the modified approach which accounts for the breaking of the time-reversal symmetry (Marshalek 1977, Markum *et al* 1982b).

The influence of the thermal excitations on the pairing correlations has been studied long ago (Huizenga and Moretto 1972), and its inclusion within the cranked Hartree–Fock–Bogoliubov theory has recently been reported for the case of an exactly solvable model (Goodman 1981). However, the difficulties posed by the temperature-dependent cranked Hartree–Fock–Bogoliubov method in realistic calculations are still present and the need for a suitable formalism evidences itself, especially in view of the importance of the inclusion of thermal degrees of freedom.

The aim of this paper is to discuss the extension of the modified BCS approach (Markum *et al* 1982b) for the case of finite temperatures. This motivation appears to be justified in order to account simultaneously for the high-spin and thermal effects in the presence of the pairing correlations. Here we show that both degrees of freedom can be properly included in a microscopic fashion, which, like in the case of high-spin states (Markum *et al* 1982a, b) might also enable us to perform numerical estimates of the pairing correlations.

2. Theory

We want to outline in some detail the derivation of the BCS equations for a rotating system ($T=0$ case) in order to illustrate the differences with respect to the situation at high angular momentum and finite temperature ($T\neq 0$ case).

2.1. $T=0$ case

Here we follow the method discussed by Marshalek (1977) with the modifications presented by Markum *et al* (1982b). Our starting point is the definition of the Hamiltonian which describes the structure of the yrast line. For a rotating deformed nucleus, with pairing correlations, we thus write the model Hamiltonian as

$$H=H_{\rm sp}+H_{\rm rot}+H_{\rm pairing} \tag{1}$$

where $H_{\rm sp}$ is the single-particle term, $H_{\rm rot}$ is the cranking term and $H_{\rm pairing}$ is the pairing interaction. They are defined by

$$H_{\rm sp}=\sum_i e_i a_i^+ a_i \qquad H_{\rm rot}=-\omega \hat{J}_x \qquad H_{\rm pairing}=-G\sum_{i,j>0} a_i^+ a_{\bar{i}}^+ a_{\bar{j}} a_j . \tag{2}$$

In equations (2), e_i are the single-particle energies which usually correspond to a deformed Woods–Saxon potential, a_i^+ (a_i) are the creation (annihilation) operators for the single-particle states $|i\rangle$, $|\bar{i}\rangle$ are the time-reversed orbits, ω is the rotational frequency, $\hat{J}_x$ is the x component of the angular momentum operator and G is the pairing constant. Because we are interested in the exact treatment of the Coriolis interaction, we diagonalise the Hamiltonian $H^{(1)}=H_{\rm sp}+H_{\rm rot}$ thus:

$$H^{(1)}=\sum_{i>0}(E_i b_i^+ b_i + E_{\bar{i}} b_{\bar{i}}^+ b_{\bar{i}}). \tag{3}$$

In this new basis, the orbitals $|i\rangle$ and $|\hat{i}\rangle$ are not related by a time-reversal operation because the inclusion of the cranking term breaks this symmetry. In terms of the model single-particle states one has

$$b_i^+ = \sum_{j>0} A_{ji} a_j^+ \qquad b_{\hat{i}}^+ = \sum_{j>0} \hat{A}_{ji} a_{\hat{j}}^+ . \tag{4}$$

Due to the breaking of the time-reversal symmetry $\hat{A}_{ji} \neq A_{ji}^*$. More generally, equations (4) can be written in terms of the single-particle states which are eigenstates of the rotation operator $\exp(-i\pi \hat{J}_x)$ (Ansari *et al* 1980, Marshalek 1977, Goodman 1974).

As has already been pointed out (Marshalek 1977), the form (equation (2)) for the pairing Hamiltonian remains invariant only under transformation to another time-reversal-symmetric basis. But, in the present case, we must consistently write H_{pairing} in terms of the operators b_i^+, $b_{\hat{i}}^+$. We thus obtain

$$H_{\text{pairing}} = -G \sum_{ijmn>0} F_{ij}^* F_{n\hat{m}} b_i^+ b_{\hat{j}}^+ b_{\hat{m}} b_n \tag{5}$$

with

$$F_{i\hat{j}} = \sum_{l>0} A_{li} \hat{A}_{lj}. \tag{6}$$

If we neglect the off-diagonal part of the $F_{i\hat{j}}$ factors (which can be treated perturbatively (Marshalek 1977, Markum *et al* 1982a)) the pairing Hamiltonian reads

$$H_{\text{pairing}} = -G \sum_{ij>0} F_{i\hat{i}}^* F_{j\hat{j}} b_i^+ b_{\hat{i}}^+ b_{\hat{j}} b_j. \tag{7}$$

The BCS transformation to the quasiparticle basis $(\alpha_i^+, \alpha_{\hat{i}}^+)$ can readily be performed on the single-particle Hamiltonian $H^{(1)}$ (equation (3)) and on the new pairing term (equation (7)). The well known variational procedure, with the constraint of the 'on the average' particle number conservation, leads to the gap parameter

$$\Delta = G \sum_{i>0} F_{i\hat{i}} u_i v_i \tag{8}$$

and to the gap equation

$$1 = \tfrac{1}{2} G \sum_{i>0} \frac{F_{i\hat{i}}^2}{[(\bar{E}_i - \lambda)^2 + \Delta^2 F_{i\hat{i}}^2]^{1/2}} \tag{9}$$

with $\bar{E}_i = \frac{1}{2}(E_i + E_{\hat{i}})$. Consequently, the quasiparticle energies are defined by

$$\varepsilon_i = [(\bar{E}_i - \lambda)^2 + \Delta^2 F_{i\hat{i}}^2]^{1/2} + \bar{E}_i' \qquad \varepsilon_{\hat{i}} = [(\bar{E}_i - \lambda)^2 + \Delta^2 F_{i\hat{i}}^2]^{1/2} - \bar{E}_i' \tag{10}$$

with $\bar{E}_i' = \frac{1}{2}(E_i - E_{\hat{i}})$. In equations (8)–(10) u_i and v_i are the BCS occupation numbers and λ is the usual Lagrange multiplier associated with the particle number conservation. Therefore, we can write the quasiparticle Hamiltonian as

$$H_{\text{qp}} = \sum_{i>0} (\varepsilon_i \alpha_i^+ \alpha_i + \varepsilon_{\hat{i}} \alpha_{\hat{i}}^+ \alpha_{\hat{i}}). \tag{11}$$

As is evident from equations (8)–(11), the usual BCS results are re-obtained in the limit $\omega = 0$, for which $E_i = E_{\hat{i}}$ and $F_{i\hat{i}} = 1$, while for $\omega \neq 0$ the same equations display the well known Coriolis antipairing behaviour and they also lead to gapless superconductivity (namely, ε_i and $\varepsilon_{\hat{i}}$ can be negative or zero for $\Delta \neq 0$) (Marshalek 1977).

2.2. $T \neq 0$ case

The temperature-dependent effects are accounted for by the definition of the density operator in the grand canonical ensemble (Goodman 1981, 1982):

$$\hat{\rho} = \exp[-\beta(H-\lambda N)]/Z, \tag{12}$$

H being the Hamiltonian (1). Z is the partition function

$$Z = \mathrm{Tr}(\exp[-\beta(H-\lambda N)]) \tag{13}$$

where $\beta = 1/T$ (we define the temperature T in MeV). The expectation value of any given operator $\hat{O}$ is thus defined by the quantum-statistical average over the ensemble

$$\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho} O). \tag{14}$$

The temperature-dependent BCS equations can be obtained by adopting for the Hamiltonian $H' = H - \lambda N$ the corresponding expression in the (b^+, b) basis and by performing the usual transformation to the quasiparticle basis:

$$b_i^+ = u_i \alpha_i^+ + v_i \alpha_{\bar{i}}. \tag{15}$$

The next step consists of the normal ordering of the resulting contributions, in terms of α_i^+ and α_i, with the proper inclusion of the thermal expectation values, which means that Wick's theorem for finite temperatures (Fetter and Walecka 1971) is applied to define the normal ordering of $H' = H - \lambda N$ in the quasiparticle basis. After some algebra, we obtain, for the one-quasiparticle term (H'_{11}) and for the two-quasiparticle term (H'_{20}),

$$\begin{aligned} H'_{11} = \sum_{i>0} \{ & [u_i^2 E_i - v_{\bar{i}}^2 E_{\bar{i}} - \lambda(u_i^2 - v_{\bar{i}}^2) + 2F_{i\bar{i}} u_i v_{\bar{i}} \Delta] \alpha_i^+ \alpha_i \\ & + [u_{\bar{i}}^2 E_{\bar{i}} - v_i^2 E_i - \lambda(u_{\bar{i}}^2 - v_i^2) + 2F_{i\bar{i}} u_i v_i \Delta] \alpha_{\bar{i}}^+ \alpha_{\bar{i}} \} \\ H'_{20} = \sum_{i>0} & [2u_i v_i (\bar{E}_i - \lambda) - \Delta F_{i\bar{i}}(u_{\bar{i}}^2 - v_{\bar{i}}^2)](\alpha_i^+ \alpha_{\bar{i}}^+ + \alpha_{\bar{i}} \alpha_i) \end{aligned} \tag{17}$$

respectively.

The terms with four-quasiparticle operators and Hartree corrections are not given here because they do not contribute to H'_{11} or to H'_{20}. The gap parameter Δ is defined by the equation

$$\Delta = G \sum_{i>0} F_{i\bar{i}} u_i v_i (1 - f_i - f_{\bar{i}}) \tag{18}$$

where f_i and $f_{\bar{i}}$ are the thermal occupation probabilities given formally by

$$f_i = \langle \alpha_i^+ \alpha_i \rangle \qquad f_{\bar{i}} = \langle \alpha_{\bar{i}}^+ \alpha_{\bar{i}} \rangle, \tag{19}$$

being the expectation values (19) defined in the form of equation (14).

The usual procedure for solving the BCS equations can now be applied, thus requiring that H'_{11} be linear in the $\alpha_i^+ \alpha_i$ and $\alpha_{\bar{i}}^+ \alpha_{\bar{i}}$ terms, with the condition $H'_{20} = 0$. With the definitions for H'_{11} and H'_{20} (cf equations (17)), one obtains the system of equations

$$\begin{aligned} \varepsilon_i &= u_i^2 E_i - v_{\bar{i}}^2 E_{\bar{i}} - \lambda(u_i^2 - v_{\bar{i}}^2) + 2F_{i\bar{i}} u_i v_{\bar{i}} \Delta \\ \varepsilon_{\bar{i}} &= u_{\bar{i}}^2 E_{\bar{i}} - v_i^2 E_i - \lambda(u_{\bar{i}}^2 - v_i^2) + 2F_{i\bar{i}} u_i v_i \Delta \\ 0 &= 2u_i v_i (\bar{E} - \lambda) - \Delta F_{i\bar{i}}(u_{\bar{i}}^2 - v_{\bar{i}}^2). \end{aligned} \tag{20}$$

The system of equations (20) is similar to the corresponding one for the $T = 0$ case. The

functional dependence on T is here represented only by the gap parameter Δ of equation (18). Thus the solutions are of the same form as for the $T=0$ case, namely the quasiparticle energies ε_i and $\varepsilon_{\bar{i}}$ are given by equations (10). Finally, with the Hamiltonian $H'=H-\lambda N$, written in the form (11), the expectation values f_i and $f_{\bar{i}}$ read

$$f_i=(1+\exp(\varepsilon_i/T))^{-1} \qquad f_{\bar{i}}=(1+\exp(\varepsilon_{\bar{i}}/T))^{-1}. \tag{21}$$

Because of the functional dependence of Δ with f_i and $f_{\bar{i}}$, the gap equation is given by

$$1=\tfrac{1}{2}G\sum_{i>0}\frac{F_{i\bar{i}}^2(1-f_i-f_{\bar{i}})}{[(\bar{E}_i-\lambda)^2+\Delta^2F_{i\bar{i}}^2]^{1/2}}. \tag{22}$$

The influence of the off-diagonal terms in H_{pairing} of equation (5) can be evaluated like in the $T=0$ case, adopting the renormalisation procedure which has been proposed by Markum *et al* (1982b), namely replacing $F_{i\bar{i}}$ by the renormalised values

$$F_{i\bar{i}}^{\text{renorm}}=F_{i\bar{i}}\left(1+\sum_{\substack{j,k>0\\ j\neq k}}F_{j\bar{k}}^2\Big/\sum_{j,k>0}F_{j\bar{k}}^2\right)^{1/2}. \tag{23}$$

Alternatively, one can also take the limit for small ω values and by considering the cranking term, $-\omega\hat{J}_x$, as a perturbation, one has to leading order in ω (Marshalek 1977)

$$F_{i\bar{i}}^2=1-4\omega^2\sum_{j\neq i}\frac{|\langle j|\hat{J}_x|i\rangle|^2}{(e_j-e_i)}. \tag{24}$$

Therefore, both limits $\omega=0$ and $T=0$ can be taken on the gap equation (22), thus leading to the usual BCS equations with $\varepsilon_i=\varepsilon_{\bar{i}}$, $F_{i\bar{i}}=1$ and $f_i=f_{\bar{i}}=0$.

The application of the procedure discussed above to the description of high-spin states above the yrast line requires the adoption of the ω and T values which are consistent with the desired values of the total angular momentum and of the excitation energy above the yrast line. With these values one can thus first diagonalise the single-particle terms of (1), and with the solutions the F factors of equation (6) can readily be obtained. Next, the temperature-dependent BCS equations can be solved, and with them the quasiparticle energies and the gap parameter are determined for the given values of T and ω. In the same manner, the quasiparticle factors u_i, v_i and f_i are determined and with them the expectation values of the physical observables, like the angular momentum I, the number of particles N, etc, can be evaluated.

3. Conclusion

We have shown how to describe pairing correlations at finite temperatures and high-spin states within a modified BCS approach. The method is based on the same considerations which lead to the description of the pairing force within a time-reversal-invariant theory for $I\neq 0$, with the extension in the present case to finite temperatures. The main advantage of the present formalism is that the simplicity of the BCS description is recovered also for the $T\neq 0$ situation. Therefore the method seems to be a suitable one for the description of high-spin states above the yrast line, at least within the degree of approximation posed by the BCS theory.

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