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Number-projected energy and heat capacity in the thermodynamic nuclear system.

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In order to describe thermal paired systems, an approach that combines the modified BCS method (MBCS) and the particle-number projection method (PNP) is proposed. The thermal energy and the heat capacity are numerically studied as a function of the temperature in the case of ^{162}Dy.

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1. Introduction

Recently, thermodynamic properties of hot nuclear systems have been widely investigated. Indeed, with the advent of nuclear radioactive beams, the study of these nuclei becomes an important challenge for nuclear physics. Phase transitions are the subject of peculiar interest since they are often connected to the spontaneous symmetry breaking, leading to violation of conservation laws. The evaluation of statistical properties, such as the energy and the heat capacity, as a function of the temperature, should provide information on the structure of hot nuclei.
It is well known that the symmetry violations (as the particle-number symmetry or the rotational one) in the BCS theory may imply important effects (generally so-called quantal fluctuations) on the calculation of various physical observables. At finite temperature T, statistical fluctuations are added to the quantal ones. These fluctuations arise from another symmetry violation: the unitary relation of the particle-density matrix [1]. Recently, the modified BCS method (MBCS) [1, 2] was suggested to take into account this kind of fluctuations by considering the fluctuations of the quasi-particle number which are neglected by the conventionnal finite temperature BCS approach (FTBCS)[3, 4].
The purpose of the present work is to evaluate the energy and the heat capacity as a function of the temperature for the nucleus ^{162}Dy in the framework of a microscopic model that includes the pairing effects. Since the latter play a crucial role in the description of such nuclei, they have to be taken into account rigorously. With this aim, an approach that combines the modified BCS method (MBCS) and a particle-number projection method (of projection after variation (PBCS) type) [5] is proposed. The paper is organized as follows. The formalism is presented in section 2. In section 3, the energy and heat capacity are numerically studied as a function of the temperature. Main conclusions are summarized in the same section.

2. Formalism

The intrinsic motion of N=2P paired particles is described by the Hamiltonian:

$$\hat{H} = \sum_{\nu>0} \varepsilon_\nu \left(a_\nu^\dagger a_\nu + a_{\tilde{\nu}}^\dagger a_{\tilde{\nu}} \right) - G \sum_{\nu\,\mu>0} a_\nu^\dagger a_{\tilde{\nu}}^\dagger a_{\tilde{\mu}} a_\mu , \tag{2.1}$$

where $a_\nu^\dagger$ and a_ν respectively represent the creation and an nihilation operators of the state $|\,\nu\rangle$, of energy ε_ν; and $a_{\tilde{\nu}}^\dagger$ and $a_{\tilde{\nu}}$ those of the state $|\,\tilde{\nu}\rangle$, which is the time reverse of $|\,\nu\rangle$ and has the same energy. G is the pairing strength which is assumed to be constant.
Refs.[1, 2] have shown that the quasi-particle number fluctuations are not taken into account in the FTBCS theory. The modified BCS (MBCS) approach allows one to overcome this defect, by introducing a secondary Bogoliubov transformation:

$$\begin{aligned} \bar{\alpha}_\nu^\dagger &= \sqrt{1-\eta_\nu}\,\alpha_\nu^\dagger + \sqrt{\eta_\nu}\,\alpha_{\tilde{\nu}} \\ \bar{\alpha}_{\tilde{\nu}} &= \sqrt{1-\eta_\nu}\,\alpha_{\tilde{\nu}} - \sqrt{\eta_\nu}\,\alpha_\nu^\dagger \end{aligned} \tag{2.2}$$

where $\eta_\nu = \frac{1}{1+exp(\beta E_\nu)}$, that connects between the usual quasi-particle (QP) operators $\alpha_\nu^\dagger$ and α_ν and the modified quasi-particle operators (MQP) $\bar{\alpha}_\nu^\dagger$ and $\bar{\alpha}_\nu$. By combining the Bogliubov-Valatin transformation and (2.2), one obtains:

$$\begin{aligned} a_\nu^\dagger &= \bar{u}_\nu \bar{\alpha}_\nu^\dagger + \bar{v}_\nu \bar{\alpha}_{\tilde{\nu}} \\ a_{\tilde{\nu}} &= \bar{u}_\nu \bar{\alpha}_{\tilde{\nu}} - \bar{v}_\nu \bar{\alpha}_\nu^\dagger \end{aligned} \tag{2.3}$$

where the variational parameters $\bar{u}_\nu$ and $\bar{v}_\nu$ read:

$$\begin{aligned} \bar{u}_\nu &= \sqrt{1-\eta_\nu}\, u_\nu + \sqrt{\eta_\nu}\, v_\nu \\ \bar{v}_\nu &= \sqrt{1-\eta_\nu}\, v_\nu - \sqrt{\eta_\nu}\, u_\nu \end{aligned} \tag{2.4}$$

The Hamiltonian in the MQP representation is analogous to that of the QP representation. One has just to replace the $\alpha_\nu^\dagger$ and α_ν operators by $\bar{\alpha}_\nu^\dagger$ and $\bar{\alpha}_\nu$ and the u_ν and v_ν coefficients by $\bar{u}_\nu$ and $\bar{v}_\nu$. One then obtains, after some algebra, the gap equations:

$$\bar{\Delta} = G \sum_{\nu>0} \bar{u}_\nu \bar{v}_\nu = G \sum_{\nu>0} \left[u_\nu v_\nu (1-2\eta_\nu) - \left(1-2v_\nu^2\right) \delta\eta_\nu \right] \tag{2.5}$$

$$N = 2 \sum_{\nu>0} \bar{v}_\nu^2 = 2 \sum_{\nu>0} \left[v_\nu^2 + (1-2v_\nu^2)\eta_\nu - 2u_\nu v_\nu \delta\eta_\nu \right] \tag{2.6}$$

where $\delta\eta_\nu = \sqrt{\eta_\nu(1-\eta_\nu)}$ is the QP fluctuation number.
The MBCS internal energy has then an expression similar to the BCS one:

$$E_{MBCS} = 2 \sum_{\nu>0} (\varepsilon_\nu - \frac{G}{2} \bar{v}_\nu^2) \bar{v}_\nu^2 - \frac{\bar{\Delta}^2}{G} \tag{2.7}$$

This approach allows one to establish the gap equations and the physical quantities in a simple way. However, it neglects the fluctuations of the particle number. To overcome this defect, one considers the particle-number projection method of PBCS type [5]. With this aim, one introduces the particle-number projection operator, defined by:

$$\hat{P} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \; e^{i\varphi\left(\hat{N}-2P\right)} \tag{2.8}$$

where $\hat{N}$ is the particle-number operator.
An approximate form of this operator may be obtained by a discretization of the integral based on 2(n+1) equally spaced points from 0 to π. This leads to the expression:

$$\hat{P}_n = \frac{1}{2\,(n+1)} \left\{ \sum_{k=0}^{n+1} \xi_k \, z_k^{-P} \prod_\nu \left[1 + (\sqrt{z_k} - 1)\, a_\nu^\dagger a_\nu \right] + cc \right\} \tag{2.9}$$

where

$$\xi_k = \begin{cases} \frac{1}{2} & if\ k=0\ \ or\ \ k=n+1 \\ 1 & if\ 1 \le k \le n \end{cases} , \qquad z_k = \exp\{ik\pi/(n+1)\} \tag{2.10}$$

and the notation cc means the complex conjugate with respect to z_k.
In the MQP representation, it takes the following form:

$$\begin{aligned} \hat{P}_n = \frac{1}{2\,(n+1)} \Bigg\{ \sum_{k=0}^{n+1} \xi_k \, z_k^{-P} \prod_{\nu>0} \Big[1 + (\sqrt{z_k} - 1) \left[\bar{\alpha}_\nu^\dagger \bar{\alpha}_\nu + \bar{\alpha}_{\tilde{\nu}}^\dagger \bar{\alpha}_{\tilde{\nu}} - 2 \bar{\alpha}_\nu^\dagger \bar{\alpha}_{\tilde{\nu}}^\dagger \bar{\alpha}_{\tilde{\nu}} \bar{\alpha}_\nu \right] + \\ (z_k - 1) \left[\bar{\alpha}_\nu^\dagger \bar{\alpha}_{\tilde{\nu}}^\dagger \bar{\alpha}_{\tilde{\nu}} \bar{\alpha}_\nu + \bar{v}_\nu^2 (1 - \bar{\alpha}_\nu^\dagger \bar{\alpha}_\nu - \bar{\alpha}_{\tilde{\nu}}^\dagger \bar{\alpha}_{\tilde{\nu}}) + \bar{u}_\nu \bar{v}_\nu (\bar{\alpha}_\nu^\dagger \bar{\alpha}_{\tilde{\nu}}^\dagger + \bar{\alpha}_{\tilde{\nu}} \bar{\alpha}_\nu) \right] \Big] + cc \Bigg\} . \end{aligned} \tag{2.11}$$

One obtains the formal expression of the number projected pairing energy at finite temperature T as:

$$E_{PNP} = \frac{\langle 0_T|\hat{H}\hat{P}_n|0_T\rangle}{\langle 0_T|\hat{P}_n|0_T\rangle} = E_{MBCS} + G\sum_{\nu>\mu} \bar{u}_\nu^3 \bar{v}_\nu \bar{u}_\mu \bar{v}_\mu^3 D_{\nu\mu}, \tag{2.12}$$

where $|0_T>$ is the thermal vacuum,

$$D_{\nu\mu} = 2(n+1)C_n \sum_{k=0}^{n+1} \xi_k z_k^{-P}(z_k-1)^2 \prod_{j\neq\nu\mu} \left(\bar{u}_j^2 + z_k \bar{v}_j^2\right) + cc, \tag{2.13}$$

and

$$C_n^{-1} = 2\,(n+1)\left\{\sum_{k=0}^{n+1} \xi_k z_k^{-P} \prod_{j>0} \left(\bar{u}_j^2 + z_k \bar{v}_j^2\right) + cc\right\}. \tag{2.14}$$

It then appears that the particle-number projection induces the inclusion of a corrective term in the energy expression. One notices that if one sets $z_k = 1$, the energy will thus reduce to the MBCS approach.

3. Numerical results and discussion

The previously described method is applied to the evaluation of the energy and the heat capacity in the case of ^{162}Dy neutron-rich nucleus. The single-particle energies and eigen states of the Woods-Saxon mean field explicitly dependent on the nuclear shape have been used. The equilibrium deformations are those of Möller et al. [6]. The number of oscillation shells is NMax=12. The pairing strength has been chosen such as to reproduce the even-odd mass differences [7].
In a first step, the energy versus the temperature has been studied, in both approaches: Modified BCS (MBCS) and the particle number projection method (PNP) . The obtained results are reported in figure 1 for the proton and neutron systems. One notices, in each case :

1. At low temperature (T<Tc, Tc being the critical temperature), the discrepancy between the two predictions is constant and of the order of 1.5 MeV in the proton case, and of the order of 1.3 MeV in the neutron case.

2. A monotonous increase is observed around the critical temperature for the neutron system, while it is more abrupt in the proton case.

3. When T>Tc, both curves join, since there is no more pairing in this case.

It appears that the particle-number projection effect is important at low temperature i.e. when T<Tc, and disappear at high temperature. N. Dinh Dang et al.[8] achieved to similar results by including the particle number fluctuation in the framework of the Lipkin-Nogami method in the static path approximation.
As a second step, we studied the heat capacity C which is defined as:$C = \frac{dE}{dT}$. Indeed, a clear signature of the phase transition is the discontinuity of the heat capacity C at the critical temperature T=Tc. Variations of the heat of the capacity as a function of the temperature for proton and neutron systems are given in figure 1.

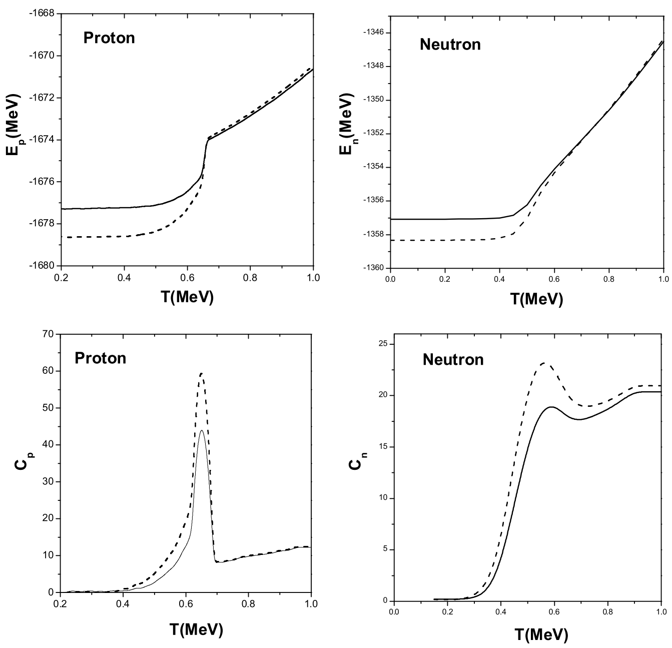

Figure 1: Variation of the energy and the heat capacity as a function of temperature for proton and neutron systems of the nucleus ^{162}Dy. The Modified BCS results are plotted as solid lines, while the particle-number projection results are represented by dashed lines.

One notes an important discrepancy between the two approaches at $T = Tc$. The quantal fluctuations are thus predominant when $T < Tc$ and decrease at high temperature. This fact has been already pointed out within the framework of more sophisticated approaches like the finite temperature Hartree-Fock Bogoliubov (FTHFB) approach (see e.g. ref [9] and references therein). On the other hand, one notices that the phase transition in the proton case is more pronounced than in the neutron one.

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