Particle-number conservation in thermodynamic systems within the Richardson model

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Abstract. To describe thermal pairing systems, an approach that combines the modified BCS method and the Lipkin-Nogami particle-number projection method is proposed. The expressions of the thermal pairing gap and internal energy are derived. The latter are numerically studied as a function of the temperature within the Richardson model.

1. Introduction
In finite systems, such as atomic nuclei, it is well known that the symmetry violations (as the particle-number symmetry or the rotation one) in the BCS theory may imply important effects (generally so-called quantal fluctuations) on the calculation of various physical observables [1] such as the energy [2, 3, 4, 5, 6], the charge square radius and the quadrupole and hexadecapole moments [7, 8], or the moment of inertia [9].

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 [11]. Recently, the modified BCS method (MBCS) [10, 11, 12, 13, 14, 15] was suggested to take into account this kind of fluctuations by considering the fluctuations of the quasi-particle number which are neglected by the conventional finite temperature BCS approach (FTBCS) [16, 17, 18, 19, 20, 21]. The evaluation of the pairing gap as a function of the temperature within this approach has shown that this quantity decreases monotonously with increasing T. As a consequence, the sharp superfluid-normal phase transition observed using the BCS approach is washed out [10, 11, 12]. It has been shown in ref. [12] that the thermodynamic approach overcomes only the quasiparticle-number fluctuations but does not resolve the problem of the particle-number symmetry violation in the BCS approach. The aim of the present paper is to propose an approach that combines the MBCS method and the Lipkin-Nogami particle-number projection method [22, 23]. The paper is organized as follows. The formalism is presented in section 2, after a brief recall of the MBCS method. The thermal pairing gap and the internal energy are then deduced. They are numerically studied as a function of the temperature within the Richardson model [24], which also provides exact solutions, in section 3. Main conclusions are summarized in section 4.
2. Formalism

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

\[ \hat{H} = \sum_{\nu>0} \varepsilon_\nu \left( a_\nu^\dagger a_\nu + a_\nu^\dagger \tilde{a}_\nu \right) - G \sum_{\nu \mu>0} a_\nu^\dagger a_\mu^\dagger a_\mu a_\nu, \]  

(1)

where \( a_\nu^\dagger \) and \( a_\nu \) respectively represent the creation and annihilation operators of the state \( | \nu \rangle \), of energy \( \varepsilon_\nu \); and \( a_\nu^\dagger \) and \( a_\nu \) 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.

Let us recall that in the case of the BCS approach, the use of the canonical Bogoliubov transformation from the particle operators \( a_\nu^\dagger \) and \( a_\nu \) to the quasiparticle ones \( \alpha_\nu^\dagger \) and \( \alpha_\nu \) [1]:

\[ a_\nu^\dagger = u_\nu \alpha_\nu^\dagger + v_\nu \alpha_\nu \]
\[ a_\nu = u_\nu \alpha_\nu - v_\nu \alpha_\nu^\dagger \]

(2)

allows one to obtain the gap equations in the form [17]:

\[ \Delta = G \sum_{\nu>0} u_\nu v_\nu (1 - 2\eta_\nu) \]
\[ N = 2 \sum_{\nu>0} \left[ v_\nu^2 + (1 - 2v_\nu^2)\eta_\nu \right] \]

(3)

(4)

where \( \eta_\nu \) is the quasi-particle occupation number given by the Fermi-Dirac distribution:

\[ \eta_\nu = \frac{1}{1 + \exp(\beta E_\nu)} \]

(5)

and \( E_\nu \) is the quasiparticle energy given by:

\[ E_\nu = \sqrt{(\varepsilon_\nu - \lambda - Gv_\nu^2)^2 + \Delta^2} \]

(6)

The internal energy of the system then reads:

\[ E_{FTBCS} = 2 \sum_{\nu>0} \varepsilon_\nu - 2G \sum_{\mu>0} (v_\mu^2 + (1 - 2v_\mu^2)\eta_\mu) \left[ v_\nu^2 + (1 - 2v_\nu^2)\eta_\nu \right] - \frac{\Delta^2}{G} \]

(7)

Ref.[11, 12] 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:

\[ \tilde{\alpha}_\nu^\dagger = \sqrt{1 - \eta_\nu} \alpha_\nu^\dagger + \sqrt{\eta_\nu} \alpha_\nu \]
\[ \tilde{\alpha}_\nu = \sqrt{1 - \eta_\nu} \alpha_\nu - \sqrt{\eta_\nu} \alpha_\nu^\dagger \]

(8)

that connects between the usual quasi-particle (QP) operators \( \alpha_\nu^\dagger \) and \( \alpha_\nu \) and the modified quasi-particle operators (MQP) \( \tilde{\alpha}_\nu^\dagger \) and \( \tilde{\alpha}_\nu \). By combining the two transformations (2) and (8), one obtains:

\[ a_\nu^\dagger = \tilde{u}_\nu \alpha_\nu^\dagger + \tilde{v}_\nu \tilde{\alpha}_\nu \]
\[ a_\nu = \tilde{u}_\nu \tilde{\alpha}_\nu - \tilde{v}_\nu \alpha_\nu^\dagger \]

(9)

where the variational parameters \( \tilde{u}_\nu \) and \( \tilde{v}_\nu \) read:

\[ \tilde{u}_\nu = \sqrt{1 - \eta_\nu} u_\nu + \sqrt{\eta_\nu} v_\nu \]
\[ \tilde{v}_\nu = \sqrt{1 - \eta_\nu} v_\nu - \sqrt{\eta_\nu} u_\nu \]

(10)
The Hamiltonian in the MQP representation is analogous to that of the QP representation. One has just to replace the \( \alpha^\dagger_\nu \) and \( \alpha_\nu \) operators by \( \bar{\alpha}^\dagger_\nu \) and \( \bar{\alpha}_\nu \) and the \( u_\nu \) and \( v_\nu \) coefficients by \( \bar{u}_\nu \) and \( \bar{v}_\nu \). One then obtains, after some algebra, the gap equations:

\[
\bar{\Delta} = G \sum_{\nu > 0} \bar{u}_\nu \bar{v}_\nu = G \sum_{\nu > 0} [u_\nu v_\nu + (1 - 2v^2_\nu) \delta \eta_\nu] \quad (11)
\]

\[
N = 2 \sum_{\nu > 0} \bar{v}^2_\nu = 2 \sum_{\nu > 0} \left[ u^2_\nu - 2(1 - 2u_\nu v_\nu) \delta \eta_\nu \right] \quad (12)
\]

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:

\[
E_{\text{MBCS}} = 2 \sum_{\nu > 0} (\varepsilon_\nu - \frac{G}{2} \bar{v}^2_\nu) \bar{v}^2_\nu - \frac{\Delta^2}{G} \quad (13)
\]

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. In order to take them into account, one has to perform the same calculation by starting from the Lipkin-Nogami Hamiltonian \([22, 23]\) instead of the usual BCS auxiliary Hamiltonian, that is:

\[
\hat{H}' = \hat{H} - \lambda \hat{N} - \lambda^2 \hat{N}^2 \quad (14)
\]

and to express it in the MQP representation. One notes that \( \lambda \) is a Lagrange multiplier and \( \lambda^2 \) is kept constant, \( \hat{N} \) is the particle number operator defined by:

\[
\hat{N} = \sum_{\nu > 0} \left( a_\nu^\dagger a_\nu + a_\nu^\dagger \bar{a}_\nu \right). \quad (15)
\]

The \( \bar{u}_\nu \) and \( \bar{v}_\nu \) parameters are then chosen such as to minimize the expectation value of the Hamiltonian \( \hat{H}' \):

\[
\frac{\partial}{\partial \bar{v}_\nu} \langle \psi | \hat{H}' | \psi \rangle = 0, \quad \forall \nu. \quad (16)
\]

Thus, \( \bar{u}_\nu \) and \( \bar{v}_\nu \) are given by:

\[
\begin{align*}
\bar{u}^2_\nu & = \frac{1}{2} \left\{ 1 \pm \frac{\varepsilon_\nu - \lambda + (4\lambda_2 - G) \bar{v}^2_\nu}{\sqrt{(\varepsilon_\nu - \lambda - G \bar{v}^2_\nu + 4\lambda_2 \bar{v}^2_\nu)^2 + \Delta^2}} \right\} \quad (17)
\end{align*}
\]

with:

\[
\lambda_2 = \frac{G}{4} \sum_{\nu > 0} \bar{u}_\nu^3 \bar{v}_\nu + \sum_{\nu > 0} \bar{u}_\nu \bar{v}^3_\nu - \sum_{\nu > 0} \bar{u}^4_\nu \bar{v}^4_\nu \quad (18)
\]

It appears that the fact to take into account the particle-number fluctuations induce a renormalization of the single particle energy by a \( (4\lambda_2 \bar{v}^2_\nu) \) term.

Let us introduce the occupation number:

\[
\bar{\eta}_\nu = \frac{1}{1 + \exp(\beta \bar{E}_\nu)} \quad (19)
\]

where \( \bar{E}_\nu \) is given by:

\[
\bar{E}_\nu = \sqrt{(\varepsilon_\nu - \lambda - G \bar{v}^2_\nu + 4\lambda_2 \bar{v}^2_\nu)^2 + \Delta^2} \quad (20)
\]
The calculations are thus formally the same as in the usual Lipkin-Nogami method. One just has to replace $u_\nu$ and $v_\nu$ and the quasi-particle operators by the modified ones. One deduces then the Modified Lipkin-Nogami internal energy:

\[
E_{LN} = 2 \sum_{\nu>0} (\epsilon_\nu - G\bar{v}_\nu^2 + 4\lambda_2\bar{v}_\nu^2)\bar{v}_\nu^2 - \frac{\Delta^2}{G} - 4\lambda_2 \sum_{\nu>0} \bar{u}_\nu^2\bar{v}_\nu^2 \tag{21}
\]

The last term of equation (21) represents the correction to the energy, that is due to the particle-number fluctuations. One notes that when $T=0$ MeV, equations (17) and (18) reduce to those of the usual Lipkin-Nogami method.

3. Numerical results - Discussion
In order to test the previously described approach, we performed numerical calculations using the Richardson model \[24\], which provides exact solutions. We considered a system of $N=10$ particles, with a total degeneracy of pairs $\Omega=10$ and a pairing-strength $G=0.4$. In a first step, we have evaluated the thermal pairing gap as a function of the temperature when $0 \leq T \leq 2MeV$. In figure 1, we reported the results obtained using the conventional FTBCS theory, the MBCS method and the Modified Lipkin-Nogami approach. The figure shows that the pairing gap collapses at a critical temperature $T_c = 0.4MeV$ in the FTBCS theory. This result is a signature of the phase transition from the superfluid state to a normal one. However, the MBCS and Modified Lipkin-Nogami methods predict a monotonous decrease of the pairing gap as a function of the temperature. N. Dinh Dang et al. \[10\] achieved to similar results by taking into account the particle-number fluctuations using the Lipkin Nogami method in the static path approximation.
Moreover, one notes that the pairing gap in the case of the Modified Lipkin-Nogami method is greater than the predictions of the two other approaches. At $T = 0 MeV$ the discrepancy is of about $0.5 MeV$, and it decreases with increasing temperatures. This discrepancy is attributed to the particle-number fluctuations effect. Indeed, it was shown in ref.[10] that this effect is important at low temperature i.e. when $T < T_c$. Moreover, their effect vanishes at high temperature while the statistical fluctuations become important. As a consequence, the predictions of the Modified Lipkin-Nogami method converge to the MBCS results when $T > T_c$.

As a second step, the excitation energy given by:

$$E^* = E(T) - E(0)$$

has been evaluated as a function of the temperature. The obtained results are reported in figure 2. The latter shows the behavior of this quantity in the case of the FTBCS, MBCS and the Modified Lipkin-Nogami methods. The predictions of these models are also compared to the exact ones. One notes that the exact results are better reproduced when the Modified Lipkin-Nogami method is used. One deduces then that the effect of the particle-number fluctuations is non-negligible. Moreover, one observes an important discrepancy of the order of 1 MeV between the Modified Lipkin-Nogami method and the exact results at high temperature. This effect could be attributed to the fact that the Lipkin-Nogami method remains an approximate projection method.

4. Conclusion
In the present work, we have performed an analysis of the pairing gap and the excitation energy in the case of thermodynamic systems by combining the Lipkin-Nogami method and the MBCS approach. The evaluation of these quantities as a function of the temperature when
$0 \text{MeV} \leq T \leq 2 \text{MeV}$ has shown a cancelation of the sharp superfluid-normal phase transition that was observed with the usual FTBCS method. On the other hand, the results confirm that the particle-number fluctuations are important at low temperature, and their effects are non-negligible. Finally, the excitation energy is better reproduced when the modified Lipkin-Nogami method is used instead of the MBCS one.

References

[1] Ring P and Schuck P 1980 The Nuclear Many-Body Problem (Berlin: SPRINGER)
[2] Fellah M, Hammann T F and Medjadi D E 1973 Phys. Rev. C 8 1585
[3] Oudih M R, Fellah M and Allal N H 2003 Int. J. Mod. Phys. E 12 109
[4] Oudih M R, Fellah M, Allal N H and Benhamouda N 2006 Int. J. Mod. Phys. E 15 643
[5] Allal N H, Fellah M, Oudih M R and Benhamouda N 2006 Eur. Phys. J. A 27 301
[6] Oudih M R, Fellah M, Allal N H and Benhamouda N 2007 Phys. Rev. C 76 047307
[7] Benhamouda N, Oudih M R, Allal N H and Fellah M 2001 Nucl. Phys. A 690 219
[8] Benhamouda N, Allal N H, Fellah M and Oudih M R 2005 Int. J. Mod. Phys. E 14 197
[9] Allal N H and Fellah M 1991 Phys. Rev. C 43 2648
[10] Dinh Dang N 1990 Z. Phys. A 335 253
[11] Dinh Dang N and Arima A 2003 Phys. Rev. C 68 014318
[12] Dinh Dang N 2006 Nucl. Phys. A 784 147
[13] Ponomarev V Yu and Vdovin A I 2005 Phys. Rev. C 72 034309
[14] Dinh Dang N and Arima A 2006 Phys. Rev. C 74 059801
[15] Ponomarev V Yu and Vdovin A I 2006 Phys. Rev. C 74 059802
[16] Sano M and Yamazaki S 1963 Prog. Theor. Phys. 29 397
[17] Moretto L G 1972 Nucl. Phys. A 185 145
[18] Goodman A 1981 Nucl. Phys. A 352 30
[19] Alasia F, Civitarese O and Reboiro M 1987 Phys. Rev. C 35 812
[20] Esebbag C and Egido J L 1993 Nucl. Phys. A 552 205
[21] Sandulescu N, Civitarese O and Liotta R J 2000 Phys. Rev. C 61 044317
[22] Lipkin H J 1960 Ann. Phys. 12 425
[23] Nogami Y 1964 Phys. Rev. B 313 134
[24] Richardson R W and Sherman N 1964 Nucl. Phys. 52 253
[25] Dinh Dang N, Ring P and Rossignoli R 1993 Phys. Rev. C 47 47