EPJ Web of Conferences **38**, 04004 (2012)
DOI: 10.1051/epjconf/20123804004

Pairing and thermodynamics properties of finite-systems with fixed number of particles

D. Gambacurta[1,a] and D. Lacroix[1]

GANIL, CEA/DSM and CNRS/IN2P3, Boîte Postale 55027, 14076 Caen Cedex, France

Abstract. A canonical description of the thermodynamical pairing properties of small systems is achieved by using the Variation After Projection approach at finite temperature. The minimization of the free energy is made by a direct evaluation of the energy and full diagonalization of the entropy. We use the Richardson - pairing model whose exact solution allows to study the reliability of different approaches. We show that the Projection After Variation approach, that is usually performed at zero temperature with rather good success, provides a quite poor description at finite temperature. On the contrary, the Variation After Projection applied at finite temperature provides a perfect reproduction of the exact canonical properties of odd or even systems from very low to high temperature.

1 Introduction

The study of hot nuclei properties and the search for possible phase transitions, as for example the shape, pairing and liquid-gas one, have been extensively investigated in recent decades to understand the temperature dependence of nuclei and nuclear matter properties. It is well known that, in infinite Fermi systems, a sharp phase transition from the superfluid phase to the normal-fluid one occurs at finite temperature. This phase transition is characterized by the fact that the pairing gap goes abruptly to zero. In small systems, like nuclei, thermal/quantal phase transitions are smoothed or washed out by finite size effects.

In the last years many studies have underlined the importance of finite size effect on pairing correlations and the necessity to develop theories beyond the Bardeen-Cooper-Schrieffer (BCS) or the Hartree-Fock-Bogoliubov (HFB) ones in order to preserve the number of particles.

Quantal fluctuations beyond the mean-field approximation can be incorporated by using projection techniques. In the pairing case, improvement beyond the BCS and/or HFB, is obtained by considering a state with good particle number $|\Psi_N\rangle = P_N|\Phi_0\rangle$, where P_N is the projector on N particles while $|\Phi_0\rangle$ denotes a quasi-particle (BCS or HFB) state. The explicitly breaking of the symmetry, the $U(1)$ one in the present case, allows to grasp the physics of pairing while its restoration is required to describe the onset of pairing in very small systems.

In the study of the thermodynamics properties of finite systems statistical fluctuations should also be described in a proper way. The use of the BCS or HFB framework at finite temperature amounts to give a Grand-canonical description of the system. A natural extension of these approaches able to provide a canonical description of finite system at thermal equilibrium has been proposed already some times ago [1] by considering a many-body projected statistical density operator $\hat{D}_N$, preserving the good particle number.

However, due to the complexity of this approach, approximations or alternative theories have been proposed, by using the static-path-approximation [2], by introducing the Modified BCS theory [3] or within the thermofield method [4]. Other extensions have been proposed by adding quantum fluctuation associated to RPA modes described on top of a BCS plus Lipkin-Nogami projection approach [5] or in the static path approximation [6].

Even in very schematic models [7], unless an exact treatment is made either by direct diagonalization [8] or by quantum Monte-Carlo techniques [9], a canonical finite temperature method based on mean-field theory and valid at arbitrary low or high temperature remains problematic and appears as a challenge in this field [10].

While the results presented in Ref. [1] were very promising, this method has never been applied due to its complexity. Here, we apply it for the first time (see also [11]) to the Richardson hamiltonian at thermal equilibrium and show that this approach provides a proper description of both thermal and quantal fluctuations from very low to high temperature.

2 Description of the method and applications to the Richardson Model

The finite temperature BCS (FT-BCS) is equivalent to the Grand-Canonical description of the thermodynamics pairing properties of the system. The FT-BCS equations are obtained by minimizing the Helmholtz free energy F

$$\delta F = \delta(\mathrm{Tr}[\hat{H}\hat{D}] - TS - \mu\mathrm{Tr}[\hat{N}\hat{D}]) = 0, \qquad (1)$$

where $\hat{D}$ is the BCS density operator

$$\hat{D} = \frac{1}{Z}\exp(-\beta\hat{h}), \qquad (2)$$

$\beta = 1/(k_B T)$, $\hat{h}$ is the quasi-particle effective BCS hamiltonian and S denotes the associated entropy,

$$S = -k_B\mathrm{Tr}(\hat{D}\ln\hat{D}). \qquad (3)$$

[a] e-mail: gambacurta@ganil.fr

The Lagrange parameter μ is used to impose the proper average number of particles. In this way, the FT-BCS equations can be obtained, which are formally equivalent to the zero temperature BCS ones except that the gap depends now on the temperature through

$$\Delta_i = \sum_j \frac{\Delta_j G_{ij}}{2E_j}(1-2f_j), \tag{4}$$

where G_{ij} are the pairing matrix elements and

$$f_j = (1+e^{\beta E_j})^{-1} \tag{5}$$

are the quasi-particle occupation numbers. In order to remove the particle number fluctuations present in FT-BCS, we introduce, as described in Ref. [1], the projected density operator $\hat{D}_N$

$$\hat{D}_N = \frac{1}{\mathcal{Z}}\hat{P}_N \exp(-\beta\hat{h})\hat{P}_N, \tag{6}$$

where P_N is the projector on N particles

$$P_N = \frac{1}{2\pi}\int_0^{2\pi} e^{i\phi(\hat{N}-N)}d\phi \tag{7}$$

and

$$\mathcal{Z} = \mathrm{Tr}(\hat{P}_N \exp(-\beta\hat{h}). \tag{8}$$

The canonical description of a quantum finite system is obtained by minimizing the Helmholtz free energy F

$$\delta F = \delta(\mathrm{Tr}[\hat{H}\hat{D}_N] - TS) = 0, \tag{9}$$

where S denotes the entropy associated to the projected density, i.e.

$$S = -k_B \mathrm{Tr}(\hat{D}_N \ln \hat{D}_N). \tag{10}$$

As mentioned above, because of its complexity, this method was applied only to the case of the two-level degenerate system. In order to test more deeply the applicability and potentialities of this method, we apply it to the Richardson model [7]. The pairing Hamiltonian of the system is given by

$$\hat{H} = \sum_{i,\sigma=\pm} \varepsilon_i \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma} - G\sum_{i,j}\hat{c}^\dagger_{i,+}\hat{c}^\dagger_{i,-}\hat{c}_{i,-}\hat{c}_{i,+}. \tag{11}$$

The results discussed below are obtained for a system of $\Omega = 10$ doubly-folded equidistant levels whose energies are

$$\varepsilon_i = \left(i - \frac{1}{2}(\Omega+1)\right)\Delta\varepsilon, \qquad i = 1,\ldots.,\Omega \tag{12}$$

and a pairing strength $G = 0.4\Delta\varepsilon$. In the following, the total energy, pairing gap and the temperature are given in units of $\Delta\varepsilon$. The hamiltonian $\hat{h}$ is written as a sum of quasi-particle excitations

$$\hat{h} = \sum_k E_k \hat{\alpha}^\dagger_k \hat{\alpha}_k, \tag{13}$$

where the E_k quasi-particle energies, while the quasi-particle creation operators write

$$\hat{\alpha}^\dagger_k = u_k\hat{c}^\dagger_{k,+} - v_k c_{k,-}, \quad \hat{\alpha}^\dagger_{\bar{k}} = u_k\hat{c}^\dagger_{k,-} + v_k c_{k,+}. \tag{14}$$

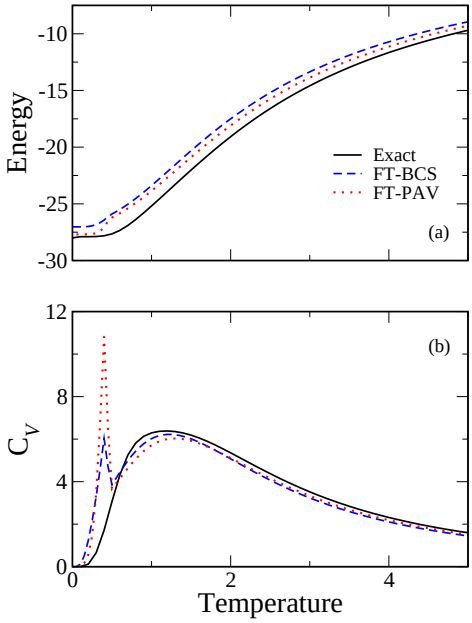

Fig. 1. The energy (panel (a)) and heat capacity (panel (b)) obtained with the FT-BCS (dashed line), PAV (filled circles) and exact solution (solid line) for a system of $N = 10$ particles as a function of the temperature.

At this point, two levels of complexity exist in the application of projection techniques. The projection can be made either before (Variation After Projection [VAP]) or after (Projection After Variation [PAV]) variation [12]. The latter is much less demanding since it only requires to solve finite temperature BCS (FT-BCS) equations and make projection without minimizing Eq. (9). As an illustration, the temperature dependence of the energy $\langle E\rangle$ and the associated heat capacity defined through $C_V = \partial\langle E\rangle/\partial T$ obtained with FT-BCS (dashed line) and FT-PAV (dotted line) are compared to the exact result (solid line) in figure 1 for $N = 10$ particles. The exact solution is obtained following Ref. [8].

In addition to the systematic overestimation of the energy, the FT-BCS theory applied to finite systems suffers from the sharp superfluid to normal phase transition as the temperature increases. In contrast, the exact solution display a much smoother behaviour. It is clearly seen in this figure that, except in the very small temperature case, the FT-BCS+PAV does even a worse job and does not cure the threshold effect.

In the VAP case, the variational principle (9) is minimized by varying both the components (u_k, v_k) and the energy E_k consistently [1]. Such a minimization is rather complex, since the mean-field hamiltonian $\hat{h}$ and the operator $\hat{P}_N \exp(-\beta\hat{h})\hat{P}_N$ do not commute and therefore cannot be diagonalized simultaneously. In practice, the variational principle is minimized by writing first the energy in terms of the one- and two-body density of the projected density, both of them written as a non-trivial function of the u_k, v_k and E_k (see Eq. (36) in Ref. [1]). The minimization is car-

ried out via a sequential quadratic programming method by using the v_k and E_k as variational parameters. To compute the free energy without approximation, at each iteration of the minimization, the entropy is calculated by

$$S = -k_B \sum_i D_i^N log D_i^N \tag{15}$$

where D_i^N are the eigenvalues of the statistical operator $\exp(-\beta\hat{h})/Z$ in the Fock space composed by all the many-body configurations with N particles. Each configuration is characterized by η pairs and I unpaired particles, with $2\eta + I = N$. Moreover, since states with a different number of unpaired particles cannot be connected by the operator $\exp(-\beta\hat{h})$, the problem is reduced to the diagonalization of block matrices for each allowed seniority I. The required computational cost is thus given essentially by two operations, i.e. the calculation of the matrix elements of the statistical operators and the diagonalization itself. For the latter, a standard QR algorithm is used. The calculation of the matrix elements is done by using the bit representation of the many-body states (see for example Ref. [13]). Each configuration is identified by an integer word whose bits correspond to the single particle levels and have value 1 or 0 depending on whether the level is occupied or empty. In such a way all the matrix elements can be obtained by using very simple logical operations which allow to perform calculations much faster.

In figure 2, the result obtained in FT-VAP is compared to the exact solution for a system of $N = 10$ particles at various temperature. In FT-VAP, the gap is given by Eq. (42) of Ref. [1] while in the exact case it is computed through

$$\Delta = \sqrt{-G(E - E_0)} \tag{16}$$

where E is the total exact energy and E_0 is given by

$$E_0 = \sum_i \left(\varepsilon_i - \frac{G}{2} n_i\right) n_i \tag{17}$$

containing both the single-particle and the self-energy terms, n_i being the occupation numbers. In this figure, we see that, except for the small systematic difference observed for the gap, the FT-VAP approach provides a perfect description of the thermodynamics of a system with fixed particle number in any range of temperature. None of the limitations [14, 15] appearing in other mean-field based theories are seen. In particular, the entropy, that is an approximation in FT-VAP, perfectly matches the exact one. The same quality of agreement is found also at higher temperature (up to $T = 10\Delta\varepsilon$).

We further investigated the applicability of FT-VAP for odd number of particles. Taking advantage of the fact that the FT-BCS density mixes up odd and even parities as soon as a non-zero temperature is applied, we used the same technique as in the even case. The only difference is that now the projector entering in the density (Eq. (6)) corresponds to an odd number of particles. In top panel of figure 3, the pairing gap obtained in FT-VAP for $N = 10$ and $N = 11$ particles is compared to the exact case. In bottom panel of this figure we show the spin susceptibility that, in the small magnetic field limit, identifies with the fluctuation of the magnetization $\hat{M} = -\mu_B \sum_{\sigma,i} \sigma \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma}$ [9], i.e.

$$\chi(T) = -\frac{1}{T}\left(\langle \hat{M}^2 \rangle - \langle \hat{M} \rangle^2\right). \tag{18}$$

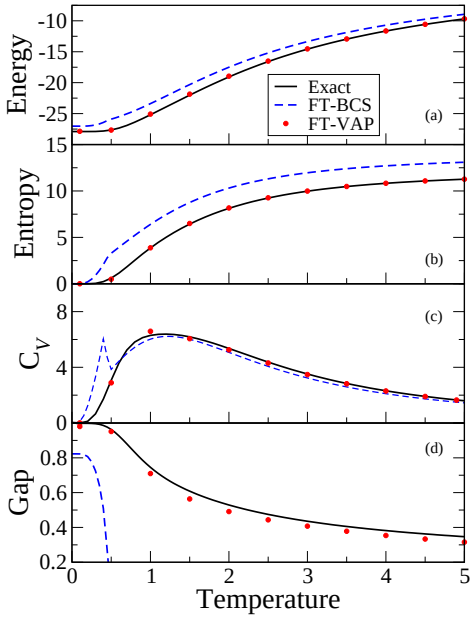

Fig. 2. The energy $\langle H \rangle$ (panel (a)), the entropy (panel (b)), the heat capacity (panel (c)) and the average gap (panel (d)) obtained with the FT-VAP (filled circles) are compared to the exact (solid line) and FT-BCS case (dashed line) for a system of $N = 10$ particles.

In small systems, large differences are observed in the thermodynamics of odd and even systems [10]. This is clearly seen especially at low temperature for the gap. The spin susceptibility further underlines the differences. The FT-VAP perfectly grasps the thermodynamics of odd systems and one cannot distinguish its result from the exact solution.

Due to the necessity to make use of explicit diagonalization for the entropy, calculations for larger systems are not easily affordable. Approximated methods to evaluate the projected entropy are thus necessary for the study of larger systems. In this regard, an attempt was made in [16] where an approximated way to calculate the entropy, based on the Peierls inequality, was used. However, although the critical temperature shifts up with respect to the Grand-Canonical case, this method still suffers of a sharp phase transition that is washed out when the projected entropy is exactly evaluated. The investigation and the development of new methods to evaluate the entropy in an approximated way allowing at the same time to describe properly both low and high temperature properties are needed. Work in this direction is in progress. Here we just propose a simple and direct approach that can be used for larger systems in the low-temperature region. As mentioned above the most time requiring operation in the free energy minimization, consists in the calculation of the eigenvalues of the statistical density operator needed to evaluate the entropy. In order to do that all the many-body configurations with N particles characterized by η pairs and seniority I such as $2\eta + I = N$ have to be considered. However, if we are

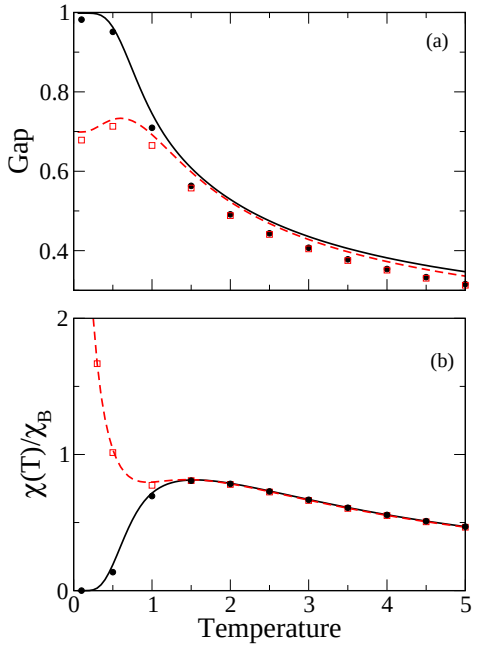

Fig. 3. Mean gap (panel (a)) and spin susceptibility (panel (b)) as a function of the temperature for $N = 10$ (filled circles) and $N = 11$ (open squares) particles as a function of T obtained with the FT-VAP. The corresponding exact result for the even and odd systems are presented respectively with solid and dashed lines. In this figure, the spin susceptibility is normalized by the bulk high temperature value $\chi_B = 2\mu_B^2/\Delta\varepsilon$.

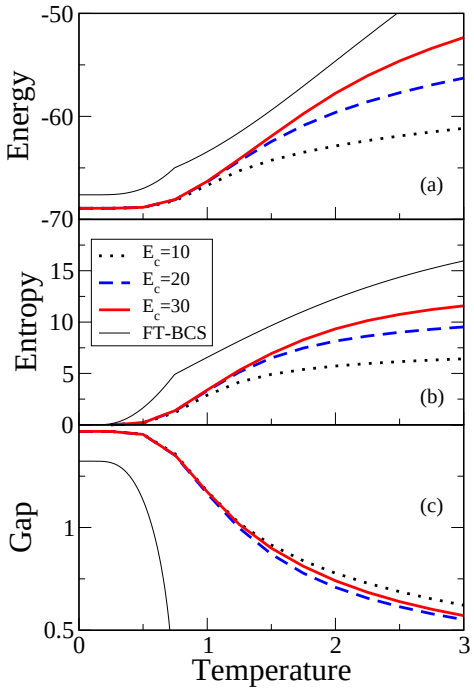

Fig. 4. From top to bottom, the energy $\langle H \rangle$ (panel (a)), the entropy (panel (b)) and the average gap (panel (c)) obtained with the FT-VAP for different cutoff E_c (in units of the level spacing $\Delta\varepsilon$) for a system of $\Omega = N = 16$ particles. See the text for more details. The FT-BCS results (thin lines) are shown for comparison. No exact solution can be obtained in this case by direct diagonalization.

interested to the low temperature behaviour, high energy configurations are expected to be less important. Therefore, in the evaluation of the entropy, we consider only the many-body configurations whose energy is less than an energy cutoff E_c. We thus increase E_c to study the reliability of the obtained solution. In figure 4, we can see how this procedure allows to properly describe the low temperature properties of a system of $N = \Omega = 16$ for which the exact solution can not be obtained with the standard technique [8]. By increasing the energy cutoff E_c we can also easily understand up to which temperature the solution is reliable.

3 Conclusions and outlook

In this work, the variation after projection approach at finite temperature has been applied to describe the pairing properties of a superconducting system within a canonical description. The minimization of the free energy is made with no approximation on the entropy. The FT-VAP provides a perfect reproduction of the exact result in the Richardson Hamiltonian case both in the low and high temperature limit and does not have the limitation of other mean-field based approaches. Due to the necessity to make use of explicit diagonalization for the entropy, the present approach is still restricted to rather small number of particles. However, a simple and direct method for the study of the low temperature properties of larger systems has been also proposed here.

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