Neutron-Proton pairing effect on the thermodynamical quantities of even-even proton-rich nuclei

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Abstract. Expressions of the thermodynamical quantities, i.e. the energy $E$, the entropy $S$ and the heat capacity $C$ are established by including the isovector neutron-proton (np) pairing effect. They are deduced using temperature-dependent gap equations. $E$, $S$ and $C$ are numerically studied as a function of the temperature for some even-even proton-rich nuclei. The single-particle energies used are those of a Woods-Saxon deformed mean field. It is shown that the isovector pairing effect on $E$, $S$ and $C$ is non-negligible, not only in the $0 \leq T \leq T_{cnp}$ region ($T_{cnp}$ being the critical temperature beyond which the np pairing vanishes), but also in the $T_{cnp} \leq T \leq T_{cn}$ region ($T_{cn}$ being the neutron-system critical temperature).

1. Introduction

The experimental study of proton-rich nuclei became possible since they may be produced at radioactive nuclear beam facilities. Since in this kind of nuclei protons and neutrons Fermi levels are close to each other, it is expected that the neutron-proton (np) pairing correlations are non-negligible [1]. They have been studied in many papers at zero temperature (see e.g. [1]-[5]).

In hottest nuclei, the pairing correlations play an important role in the phase transition. They have been studied extensively in the pairing between like-particles case using for instance the finite temperature BCS (FTBCS) model [6]-[8], but for the np pairing, only a limited number of studies have been performed (see e.g. [9]-[10]). The purpose of the present work is to study the thermal effects of the np pairing correlations, in the isovector case, on some thermodynamical quantities i.e. the energy, the entropy and the heat capacity. The formalism is explicited in next section. In section 3, the model is numerically applied to $N = Z$ even-even nuclei using the single-particle energies of a deformed Woods-Saxon mean field. Main conclusions are summarized in last section.
2. Formalism

Let us start with the isovector pairing Hamiltonian, describing a system of $N$ neutrons and $Z$ protons \cite{11}--\cite{13}:

$$
\mathcal{H} = \sum_{\nu>0,t} \varepsilon_{\nu t} (a_{\nu t}^{+} a_{\nu t} + a_{\nu t}^{+} a_{\nu t}^{+}) + H_{nn} + H_{pp} + H_{np}
$$

(1)

where $t$ corresponds to the isotopic spin component ($t = n, p$), $a_{\nu t}^{+}$ and $a_{\nu t}$ respectively represent the creation and annihilation operators of the particle in the state $|\nu t\rangle$, of energy $\varepsilon_{\nu t}$ (which is assumed to be independent from the temperature); $|\nu t\rangle$ is the time-reverse of $|\nu t\rangle$ which has the same energy and $H_{tt'}$ ($t, t' = n, p$) corresponds to the pairing interaction given by:

$$
H_{tt'} = -G_{tt'} \sum_{\nu, \mu > 0} P_{\nu \mu t}^{+} P_{\mu \nu t'}^t
$$

(2)

with: $P_{\nu \mu t}^{+} = a_{\nu t}^{+} a_{\mu t}^{+}$, $P_{\nu \mu p}^{+} = (a_{\nu p}^{+} a_{\mu p}^{+} + a_{\nu p}^{+} a_{\mu p}^{+})$ and $G_{tt'}$ refers to the pairing-strength which is assumed to be constant.

Let us define the auxiliary Hamiltonian:

$$
H = \mathcal{H} - \sum_{t=n,p} \lambda_t N_t
$$

(3)

where $\lambda_t$ are Lagrange parameters and the $N_t$ are the particle-number operators:

$$
N_t = \sum_{\nu>0} (a_{\nu t}^{+} a_{\nu t} + a_{\nu t}^{+} a_{\nu t}) \quad t = n, p
$$

(4)

The diagonalization of the Hamiltonian $H$ using the Feynman path-integral technique is exposed in detail in ref. \cite{11} and will not be recalled here. Its diagonal form is given by \cite{11}--\cite{13}:

$$
H = \sum_{\nu>0, t} \tilde{\varepsilon}_{\nu t} + \sum_{\nu>0, t=1,2} E_{\nu \tau} \left( \alpha_{\nu \tau}^{+} \alpha_{\nu \tau} - \alpha_{\nu \tau} \alpha_{\nu \tau}^{+} \right)
$$

(5)

where we set $\tilde{\varepsilon}_{\nu t} = \varepsilon_{\nu t} - \lambda_t - (G_{tt} + G_{np})/2$, $t = n, p$, $\alpha_{\nu \tau}^{+}$ is the creation operator of a quasiparticle of $\tau$ ($\tau = 1, 2$) type, given by the generalized Bogoliubov-Valatin transformation:

$$
\alpha_{\nu \tau}^{+} = \sum_{\nu>0} \left( u_{\nu \tau t} a_{\nu t}^{+} + v_{\nu \tau t} a_{\nu t} \right) \quad \text{with} \quad \tau = 1, 2 \text{and} t = n, p
$$

(6)

The quasiparticle energies $E_{\nu \tau}$ are given by:

$$
E_{\nu \tau} = \sqrt{\frac{1}{2} \left( E_{\nu n}^2 + E_{\nu p}^2 + 2\Delta_{np}^2 + (-1)^{\tau+1} R_{\nu} \right)}
$$

(7)

with the notations:

$$
R_{\nu} = \sqrt{\left( E_{\nu n}^2 - E_{\nu p}^2 \right)^2 + 4\Delta_{np}^2 \left( (\varepsilon_{\nu n} - \varepsilon_{\nu p})^2 + (\Delta_{nn} + \Delta_{pp})^2 \right)}
$$

$$
E_{\nu t} = \sqrt{\tilde{\varepsilon}_{\nu t}^2 + \Delta_{tt}^2} \quad t = n, p
$$

$\Delta_{tt'}$ ($t, t' = n, p$) represent the gap parameters and are solutions of the generalized gap equations:

$$
\frac{4\Delta_{nn}}{G_{nn}} = \sum_{\nu \tau} \frac{1}{E_{\nu \tau}} \tanh \frac{1}{2} \beta E_{\nu \tau}
$$

$$
\left\{ \Delta_{nn} + \frac{(-1)^{\tau+1}}{R_{\nu}} \left[ (E_{\nu n}^2 - E_{\nu p}^2) \Delta_{nn} + 2\Delta_{np}^2 (\Delta_{nn} + \Delta_{pp}) \right] \right\}
$$

(8)

(9)
\[
\frac{4\Delta_{pp}}{G_{pp}} = \sum_{\nu\tau} \frac{1}{E_{\nu\tau}} \tanh \frac{1}{2} \beta E_{\nu\tau}
\times \left\{ \Delta_{pp} + \frac{(-1)^{\tau+1}}{R_{\nu}} \left[ \left( E_{\nu\tau}^2 - E_{\nu\tau}^2 \right) \Delta_{pp} + 2\Delta_{np}^2 \left( \Delta_{nn} + \Delta_{pp} \right) \right] \right\}
\]

\[\frac{2}{G_{np}} = \sum_{\nu\tau} \frac{1}{E_{\nu\tau}} \tanh \frac{1}{2} \beta E_{\nu\tau}
\times \left\{ 1 + \frac{(-1)^{\tau+1}}{R_{\nu}} \left[ E_{\nu\tau}^2 + E_{\nu\tau}^2 + 2 \left( \Delta_{nn} \Delta_{pp} - \tilde{\epsilon}_{\nu\tau} \tilde{\epsilon}_{\nu\tau} \right) \right] \right\}
\]

\[
\left\langle N_t \right\rangle = \sum_{\nu} \left\{ 1 + \sum_{\tau} \frac{\partial E_{\nu\tau}}{\partial \lambda_t} \tanh \frac{1}{2} \beta E_{\nu\tau} \right\}
\]

with

\[
\frac{\partial E_{\nu\tau}}{\partial \lambda_{n(p)}} = \frac{1}{2E_{\nu\tau}} \left[ -\tilde{\epsilon}_{\nu\tau(n(p)} \right.
+ (-1)^{\tau+1} \tilde{\epsilon}_{\nu\tau(n(p)} \left( E_{\nu\tau(n(p)}^2 - E_{\nu\tau(n(p)}^2 \right) + 2\Delta_{np}^2 \left( \tilde{\epsilon}_{\nu\tau(n(p)} - \tilde{\epsilon}_{\nu\tau(n(p)} \right) \right]
\]

\(\beta\) being the inverse of the temperature.

The partition function of the system is then given, after some algebra, by:

\[ Z = e^\Omega \]

with

\[
\Omega = -\beta \left[ \frac{\Delta_{nn}^2}{G_{nn}} + \frac{\Delta_{pp}^2}{G_{pp}} + \frac{\Delta_{np}^2}{G_{np}} \right] - \beta \sum_{\nu} (\tilde{\epsilon}_{\nu\tau} + \tilde{\epsilon}_{\nu\tau})
+ \sum_{\nu} \ln \left[ 4^2 \cosh^2 \frac{\beta E_{\nu\tau1}}{2} \cosh^2 \frac{\beta E_{\nu\tau2}}{2} \right]
\]

Starting from the grand potential \(\Omega\) defined in (16), one may easily deduce the thermodynamical quantities. Indeed, the energy of the system \(E\) is obtained by deriving expression (16) with respect to the temperature:

\[ E = -\left( \frac{\partial \Omega}{\partial \beta} \right)_{\alpha_t=cte} \quad \alpha_t = \lambda_t, \beta \quad t = n, p \]

that is:

\[ E = -\frac{\Delta_{nn}^2}{G_{nn}} - \frac{\Delta_{pp}^2}{G_{pp}} - \frac{\Delta_{np}^2}{G_{np}} + \sum_{\nu} (\tilde{\epsilon}_{\nu\tau} + \tilde{\epsilon}_{\nu\tau}) - \sum_{\nu\tau} \tanh \frac{\beta E_{\nu\tau}}{2} \left( \tilde{\epsilon}_{\nu\tau} \tilde{\epsilon}_{\nu\tau} \right) \]

where

\[
h_{\gamma} = \epsilon_{\nu\tau} \tilde{\epsilon}_{\nu\tau} + \epsilon_{\nu\tau} \tilde{\epsilon}_{\nu\tau} + \frac{(-1)^{\tau+1}}{R_{\nu}} \times \left[ 2\Delta_{np}^2 \left( \epsilon_{\nu\tau} - \epsilon_{\nu\tau} \right) \left( \tilde{\epsilon}_{\nu\tau} - \tilde{\epsilon}_{\nu\tau} \right) + \left( \epsilon_{\nu\tau} \tilde{\epsilon}_{\nu\tau} - \epsilon_{\nu\tau} \tilde{\epsilon}_{\nu\tau} \right) \left( E_{\nu\tau}^2 - E_{\nu\tau}^2 \right) \right]
\]
In the same way, using the usual definition of the entropy $S$:

$$S = \Omega + \beta E - \alpha_n N_n - \alpha_p N_p$$  \hspace{1cm} (19)

one has:

$$S = \sum_{\nu \tau} \left\{ \ln \left( 4 \cosh^2 \frac{\beta E_{\nu \tau}}{2} \right) - \beta E_{\nu \tau} \tanh \frac{\beta E_{\nu \tau}}{2} \right\}$$  \hspace{1cm} (20)

Finally, the heat capacity which is proportional to $\frac{\partial S}{\partial \beta}$ may be written:

$$C = -\beta \frac{\partial S}{\partial \beta} = \frac{1}{2} \sum_{\nu \tau} \frac{E_{\nu \tau}}{\cosh^2 \frac{\beta E_{\nu \tau}}{2}} \left( \beta^2 \frac{E_{\nu \tau}}{\cosh^2 \frac{\beta E_{\nu \tau}}{2}} + \beta \frac{\partial E_{\nu \tau}}{\partial \beta} \right)$$  \hspace{1cm} (21)

It is worth noticing that at the limit when $\Delta_{np}$ goes to zero, expressions (18), (20) and (21) reduces to their homologues of the conventional finite temperature BCS (FTBCS) method.

3. Numerical results - Discussion

We considered even-even nuclei such as $N = Z$ and of which “experimental” values of the pairing gap parameters at zero temperature are known. These values are deduced from the even-odd mass differences as defined in ref. [14] using the experimental mass values of the Möller table [15]. The pairing-strength values have been directly deduced from the experimental values of the pairing gap parameters at zero temperature. We used the single-particle energies of a Woods-Saxon mean field with the parameters defined in ref. [16].

In the present work, we chosen four nuclei, i.e. $^{40}$Ca, $^{56}$Ni, $^{68}$Se and $^{76}$Sr as an example. The variations of the various pairing gap parameters $\Delta_{\nu \nu}$, the energy of the system $E$, the entropy $S$ as well as the heat capacity $C$ as a function of the temperature are shown in figs. 1 to 4 and discussed in what follows. We reported in same figures the same quantities evaluated using the conventional FTBCS theory.

3.1. Gap parameters

From figs 1 to 4, one may notice that the $\Delta_{np}$ behavior is similar to that of $\Delta_{nn}$ and $\Delta_{pp}$ of the FTBCS method [7]; whereas the overall trend of the gap parameters $\Delta_{nn}$ and $\Delta_{pp}$ is different from that of the FTBCS method. Indeed, when $T = T_{cnp}$ (i.e. when $\Delta_{np}$ vanishes), the $\Delta_{nn}$ and $\Delta_{pp}$ values, which were constant, present a sudden increasing. This fact has been already underlined in refs [11]-[13]. One can also notice that the critical temperature values of the neutron and proton systems $T_{cn}$ and $T_{cp}$ are clearly greater than in the conventional FTBCS case. Finally, the phase transition when $\Delta_{np} = 0$ is very sharp.

3.2. Energy of the system

Figs 1 to 4 show that the energy $E$ is quasi-constant when $T < T_{cnp}$ (i.e. when the isovector pairing effect exists) and suddenly grows when $T = T_{cnp}$, that is when $\Delta_{np}$ vanishes. The sharp transition of $E$ is due to the sharp transition of $\Delta_{np}$. The np pairing effect then leads to a diminution of the energy, besides the discrepancy which is due to the shift in the $T_{cn}$ and $T_{cp}$ values. Moreover, one notices that the increase of energy is more important at $T = T_{cnp}$ than at the critical temperatures of the neutron and proton systems.
3.3. Entropy
The isovector pairing effect on the entropy differs from one nucleus to another (see figs 1 to 4): in the $0 \leq T \leq T_{cnp}$ region, the difference between the two models only appears if the $T_{cnp}$ value is sufficiently important, as in the $^{76}$Sr case. For the $^{40}$Ca, $^{56}$Ni and $^{68}$Se nuclei, in the interval where the np pairing exists, the entropy is still zero and there is no difference between the present model predictions and the conventional FTBCS ones.

For all studied nuclei, the discrepancy that appears between the np and FTBCS predictions in the $T_{cnp} \leq T \leq T_{cn}$ interval is due to the shift in the $T_{cn}$ and $T_{cp}$ values which has previously been mentioned.

3.4. Heat capacity
Variations of the heat capacity $C$ as a function of the temperature are given in figs. 1 to 4 in the isovector pairing case, as well as in the pairing between like-particles one. As in the entropy case, the behavior of $C$ differs from one nucleus to another. Indeed, for the nucleus $^{76}$Sr, one observes three peaks which correspond to the three critical temperatures (even if those that correspond to $T_{cnp}$ and $T_{cp}$ are somewhat small). For nuclei $^{40}$Ca, $^{56}$Ni and $^{68}$Se, the isovector pairing effect on the heat capacity is not visible since $C$ is still zero in both models when $T$ reaches its critical value $T_{cnp}$.

Here again, the shift between the $T_{cn}$ and $T_{cp}$ values of the FTBCS model and the present one explain the discrepancy between the two graphs when $T > T_{cnp}$. Obviously, when $T > T_{cn}$, the two models lead to the same predictions, since there is no more pairing in this region.

4. Conclusion
Expressions of the main nuclear thermodynamical quantities i.e. the energy $E$, the entropy $S$ and the heat capacity $C$ including the isovector np pairing correlations have been derived from recently established generalized equations. They have been numerically studied as a function of the temperature $T$ within the framework of a deformed Woods-Saxon mean-field for $N = Z$ nuclei. The obtained results have been compared to those obtained using the conventional FTBCS method.

It has been shown that the isovector np pairing effect on $E$, $S$ and $C$ is non-negligible. Moreover, the behavior of these quantities as a function of the temperature may be explained by the behavior of the various gap parameters. Indeed, $\Delta_{np}$ behaves like $\Delta_{nn}$ and $\Delta_{pp}$ in the conventional FTBCS model; whereas the overall trend of the gap parameters $\Delta_{nn}$ and $\Delta_{pp}$ of the present model is different from that of the FTBCS method. It has also been noticed that the critical value of temperature $T_{cnp}$ beyond which $\Delta_{np} = 0$ is smaller than $T_{cp}$ and $T_{cn}$ and that the critical values of the temperature $T_{cp}$ and $T_{cn}$ in the present model are greater than those of the FTBCS model. As a consequence, in the region $T > T_{cnp}$, although $\Delta_{np} = 0$, the np pairing effect leads to a discrepancy between the present model and the FTBCS previsions for all studied thermodynamical quantities.

In the interval where $\Delta_{np} \neq 0$, the np pairing effect on the energy is a lowering of about 1%, on average, for all considered nuclei; whereas its effect on the entropy and the heat capacity depends on the $T_{cnp}$ value.

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Figure 1. Variations of the various gap parameters, the energy $E$, the entropy $S$, and the heat capacity $C$ of the system as a function of the temperature $T$ for the nucleus $^{40}\text{Ca}$. Solid lines refer to the isovector pairing and dashed lines to the pairing between like-particles.

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Figure 2. Same as Fig. 1 for the nucleus $^{56}\text{Ni}$.
Figure 3. Same as Fig. 1 for the nucleus $^{68}$Se.
Figure 4. Same as Fig. 1 for the nucleus $^{76}\text{Sr}$. 