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THERMODYNAMIC PAIRING AND ITS INFLUENCE ON NUCLEAR LEVEL DENSITY

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Abstract. *Thermodynamic properties and level densities of some selected even-even nuclei such as ^{56}Fe, ^{60}Ni, ^{98}Mo, and ^{116}Sn are studied within the Bardeen-Cooper-Schrieffer theory at finite temperature (FTBCS) taking into account pairing correlations. The theory also incorporates the particle-number projection within the Lipkin-Nogami method (FTLN). The results obtained are compare with the recent experimental data by Oslo (Norway) group. Pairing correlations are found to have significant effects on nuclear level density, especially at low and intermediate excitation energies.*

I. INTRODUCTION

Pairing correlations have important effects on the physical properties of atomic nuclei such as the binding and excitation energies, collective motions, rotations, level densities, etc. [1]. The finite-temperature Bardeen-Cooper-Schrieffer (BCS) theory [2] (FTBCS theory), a theory of superconductivity, has been widely employed to describe the pairing properties of finite systems such as atomic nuclei (see e.g. Refs. [3, 4]). The FTBCS theory predicts a collapsing of pairing gap at a given temperature T_C or the so-called critical temperature, which can be estimated as $T_C \approx 0.568\Delta(0)$ [$\Delta(0)$ is the pairing gap at zero temperature $T = 0$] [4]. Consequently, there appears a sharp phase transition from the superfluid region, where the paring gap is finite, to the normal one, where the pairing gap is zero (the so-called SN phase transition). This prediction is in very good agreement with the experimental findings in infinite systems such as metallic superconductors. However, when applying to finite small systems such as atomic nuclei or small metallic grains, the FTBCS theory fails to describe the pairing properties of these systems. One of the reason is due to the violation of the particle-number conservation within the FTBCS theory. This conservation is negligible in infinite systems but it is significant in the finite ones. A simple method to resolve the particle-number problem of the FTBCS theory is to apply the particle-number projection (PNP) proposed by Lipkin-Nogami (LN) [5]. The LN method is an approximate PNP before variation, which has been widely used in nuclear physics. The goal of this work is to apply the FTBCS theory as well as the FTBCS with Lipkin-Nogami PNP to describe the thermodynamic properties and level densities of some selected even-even nuclei (the numbers of neutrons N and protons Z are even) such as ^{56}Fe, ^{60}Ni, ^{98}Mo, and ^{116}Sn.

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II. FORMALISM

We considers a pairing Hamiltonian [6]

$$H = \sum_k \epsilon_k (a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) - G \sum_{kk'} a_k^\dagger a_{-k}^\dagger a_{-k'} a_{k'} \tag{1}$$

which describes a system of N particles with single-particle energy ϵ_k interacting via a constant monopole force G. Here $a_k^\dagger$ and a_k denote the particle creation and annihilation operators. The subscripts k are used to label the single-particle states $|k, m_k>$ in the deformed basis with the positive single-particle spin projections m_k, whereas the subscripts $-k$ denote the time-reversal states $|k, -m_k>$.

II.1. FTBCS equations

The FTBCS equations are derived based on the variational procedure to minimize the Hamiltonian $H_{\rm BCS} = H - \lambda \hat{N}$, where $\hat{N} = \sum_k \left(a_k^\dagger a_k + a_{-k}^\dagger a_{-k} \right)$ is the particle-number operator and λ is the chemical potential. At finite temperature, the minimization procedure is proceeded within the grand canonical ensemble (GCE) average [7]. The FTBCS equations for the paring gap Δ and particle number N have the form as:

$$\begin{aligned}
&\Delta = G \sum_k \tau_k; \quad N = 2 \sum_k \rho_k, \\
&\tau_k = u_k v_k (1 - 2n_k); \quad \rho_k = (1 - 2n_k) v_k^2 + n_k, \\
&u_k^2 = \frac{1}{2} \left(1 + \frac{\epsilon_k - \lambda - G v_k^2}{E_k} \right); \quad v_k^2 = 1 - u_k^2, \\
&E_k = \sqrt{(\epsilon_k - \lambda - G v_k^2)^2 + \Delta^2},
\end{aligned} \tag{2}$$

where the quasiparticle occupation number n_k is given in terms of the Fermi-Dirac distribution of free quasiparticle $n_k = \frac{1}{1+e^{\beta E_k}}$. The total (internal) energy $E_{\rm FTBCS}$ and entropy $S_{\rm FTBCS}$ of the system are then given as

$$E_{\rm FTBCS}(T) = 2 \sum_k \epsilon_k \rho_k - \frac{\Delta^2}{G} - G \sum_k v_k^4 (1 - 2n_k), \tag{3}$$

$$S_{\rm FTBCS}(T) = -2 \sum_k [n_k \ln n_k + (1 - n_k) \ln (1 - n_k)]. \tag{4}$$

II.2. FTBCS equations with Lipkin-Nogami particle-number projection (FTLN equations)

The FTLN equations are obtained by carrying out the variational calculations (within the GCE) to minimize the Hamiltonian $H_{LN} = H - \lambda_1 \hat{N} - \lambda_2 \hat{N}^2$, namely by adding a second order of the particle number operator $\hat{N}^2$ into the Hamiltonian. As the

result, the FTLN equations for the pairing gap and particle number have the form as [8]

$$\begin{aligned}
&\Delta = G\sum_k \tau_k; \quad N = 2\sum_k \rho_k,\\
&\tau_k = u_k v_k(1-2n_k); \quad \rho_k = (1-2n_k)v_k^2 + n_k,\\
&u_k^2 = \frac{1}{2}\left(1 + \frac{\epsilon'_k - \lambda - Gv_k^2}{E_k}\right); \quad v_k^2 = 1-u_k^2,\\
&E_k = \sqrt{(\epsilon'_k - \lambda - Gv_k^2)^2 + \Delta^2}; \quad n_k = \frac{1}{1+e^{\beta E_k}}\\
&\epsilon' = \epsilon_k + (4\lambda_2 - G)v_k^2; \quad \lambda = \lambda_1 + 2\lambda_2(N+1),\\
&\lambda_2 = \frac{G}{4}\frac{\sum_k(1-\rho_k)\tau_k \sum_{k'}\rho_{k'}\tau_{k'} - \sum_k(1-\rho_k^2)\rho_k^2}{\left[\sum_k(1-\rho_k)\rho_k\right]^2 - \sum_k(1-\rho_k^2)\rho_k^2}.
\end{aligned} \tag{5}$$

The FTLN total energy and entropy are then given as

$$E_{\mathrm{FTLN}}(T) = 2\sum_k \epsilon_k\rho_k - \frac{\Delta^2}{G} - G\sum_k v_k^4(1-2n_k) - \lambda_2\Delta N^2, \tag{6}$$

$$S_{\mathrm{FTLN}}(T) = -2\sum_k [n_k \ln n_k + (1-n_k)\ln(1-n_k)], \tag{7}$$

where $\Delta N^2 = \left|\left\langle \hat{N}\right\rangle^2 - \left\langle \hat{N}\right\rangle^2\right|$ is the particle-number fluctuation, whose explicit forms can be found for example in Ref. [12].

II.3. Level density

Within the GCE, the density of state is calculated as $\omega(E^*) = \frac{e^S}{(2\pi)^{3/2}D^{1/2}}$ [9], where S is the total entropy, which is the sum of the entropies for neutrons (N) and protons (Z), and

$$D = \begin{vmatrix} \frac{\partial^2\Omega}{\partial\alpha_N^2} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\alpha_N\partial\beta} \\ \frac{\partial^2\Omega}{\partial\alpha_Z\partial\alpha_N} & \frac{\partial^2\Omega}{\partial\alpha_Z^2} & \frac{\partial^2\Omega}{\partial\alpha_Z\partial\beta} \\ \frac{\partial^2\Omega}{\partial\beta\partial\alpha_N} & \frac{\partial^2\Omega}{\partial\beta\partial\alpha_Z} & \frac{\partial^2\Omega}{\partial\beta^2} \end{vmatrix}, \tag{8}$$

with $\alpha = \beta\lambda$, and Ω being the logarithm of the grand partition function

$$\Omega = \ln\left[\mathrm{tr}(e^{-\beta H})\right] = -\beta\sum_k(\epsilon_k - \lambda - E_k) + 2\sum_k \ln(1+e^{-\beta E_k}) - \beta\frac{\Delta^2}{G}. \tag{9}$$

Finally, the level density is defined as $\rho(E^*) = \frac{\omega(E^*)}{\sigma\sqrt{2\pi}}$, where $\sigma^2 = \frac{1}{2}\sum_k m_k^2 \mathrm{sech}^2\frac{1}{2}\beta E_k$ is the spin cut-off parameter. In the expressions of density of state as well as level density, E^* is the excitation energy, which is calculated by subtracting the ground-state (binding) energy from the total energy of the system

$$E^*(T) = E(T) - E_{g.s}(T=0), \tag{10}$$

where $E_{g.s}$ is the ground-state (binding) energy, which is the sum of the FTBCS or FTLN energy at $T=0$ plus the corrections due to the Wigner E_{Wigner} and deformation energies

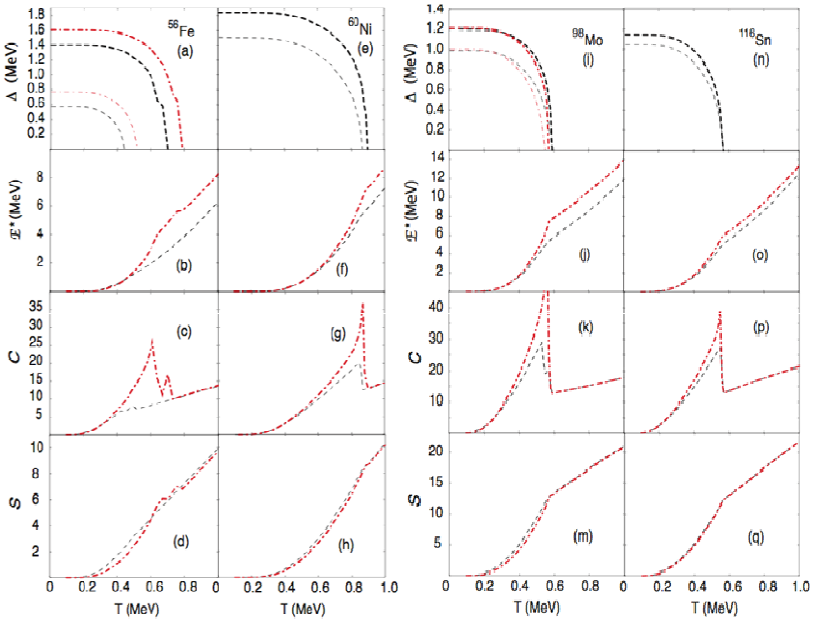

Fig. 1. Pairing gaps Δ (neutron and proton), total (neutron + proton) excitation energy E^*, total heat capacity C, and total entropy S as functions of temperature T for ^{56}Fe, ^{60}Ni, ^{98}Mo, and ^{116}Sn. In Figs 1. (a), (e), (i) and (n) the thin and thick dashed lines denote the neutron pairing gaps Δ_N, whereas the thin and thick dash dotted lines stand for the proton pairing gaps Δ_Z. Here the thin lines show the results obtained within the FTBCS, whereas the thick lines present the FTLN results. In Figs. 1 [(b) - (d)], [(f) - (h)], [(j) - (m)] and [(o) - (q)] the thin dashed and thick dash dotted lines depict the FTBCS and FTLN total (neutron + proton) results, respectively.

E_{def}

$$E_{g.s}(T=0) = E_{g.s}^{\mathrm{FTBCS(FTLN)}}(T=0) + E_{Wigner} + E_{def}. \quad (11)$$

Here, for simplicity E_{Wigner} and E_{def} are estimated from the Hartree-Fock-Bogoliubov (HFB) calculations with Skyrme BSk14 interaction [10].

III. NUMERICAL RESULTS AND DISCUSSIONS

We carried out the numerical calculations for some selected even-even nuclei, namely ^{56}Fe, ^{60}Ni, ^{98}Mo, and ^{116}Sn. The single-particle energies are calculated within the axial deformed Woods-Saxon (WS) potential including the spin-orbit and Coulomb interactions [11]. The quadrupole deformation parameters β_2 are chosen to be the same as that of Ref. [12], namely $\beta_2 = 0.24$ for ^{56}Fe and $\beta_2 = 0.17$ for ^{98}Mo, whereas β_2 for two spherical nuclei ^{60}Ni and ^{116}Sn are equal to zero. All the single-particle levels with negative energies (bound states) are taken into account. The pairing interaction parameters G are adjusted

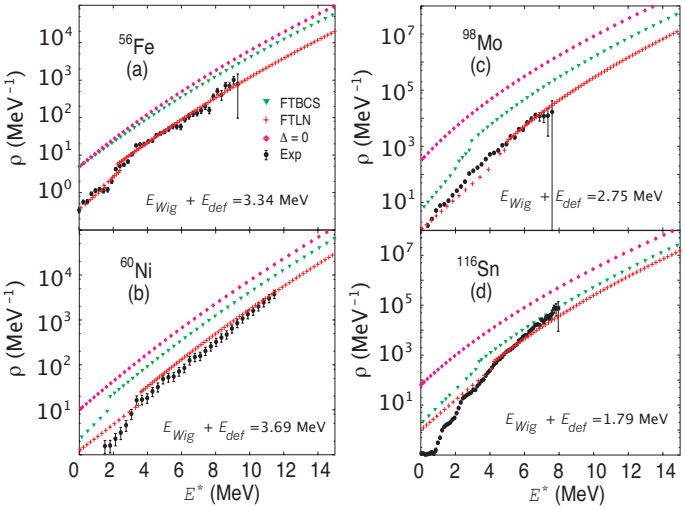

Fig. 2. Level density ρ as function of total excitation energy E^* obtained within the FTBCS (triangles), FTLN (crosses) and the case without pairing ($\Delta = 0$) (rectangles) versus the experimental data (full circles with error bars) for ^{56}Fe (a), ^{60}Ni (b), ^{98}Mo (c) and ^{116}Sn (d). The values of ground-state (binding) energy corrections $E_{Wigner} + E_{def}$ are shown in the figures..

so that the pairing gaps for neutron and proton obtained within the FTLN at $T = 0$ fits the experimental odd-even mass differences [13]. These values are $G_N = 0.312$, 0.34, 0.193 and 0.17 MeV for neutrons and $G_Z = 0.437$, 0.0, 0.314, 0.0 MeV for protons in ^{56}Fe, ^{60}Ni, ^{98}Mo, and ^{116}Sn, respectively.

Shown in Figs. 1 are the thermodynamic quantities such as pairing gaps Δ, excitation energies E^*, heat capacities C, and entropies S obtained within the FTBCS (dashed lines) and FTLN (dash dotted line) for four nuclei under consideration. The FTBCS gaps (thin lines) are seen to decrease with increasing T and vanish at a given critical temperature $T = T_C$. As the result, there appears a sharp peak in the heat capacity C at T_C, which is the signature of SN phase transition. Applying the PNP within the LN method results the FTLN pairing gaps at $T = 0$ (thick lines) which are always higher than that of the FTBCS. Consequently, the T_C values obtained within the FTLN are higher than the corresponding FTBCS ones. This feature means that the FTLN offers a pairing which is stronger and more correct than the FTBCS. The difference between the thermodynamic quantities obtained within the FTBCS and FTLN in light nuclei like ^{56}Fe is stronger than in heavy nuclei like ^{116}Sn as seen in Figs. 1. This is well-known because of the fact that the particle-number fluctuation in the light systems is usually stronger than in the heavy ones.

Shown in Fig. 2 are the level densities obtained within the FTBCS and FTLN versus the experimental data taken from Refs. [14, 15]. It is clear to see in this Fig. 2 that the level densities obtained within the FTLN fit best the experimental data for all nuclei whereas within those obtained within the FTBCS one overestimate the experimental data. The

results obtained within the non pairing case ($\Delta = 0$) are quite far from the experimental data. The ground-state energy corrections by Wigner and deformation energies, which shift up the total excitation energy E^* toward the right direction to the experimental data, are also important in present case. As the result, we can conclude that the pairing correlations together with the particle-number conservation within the Lipkin-Nogami method as well as the corrections for the ground-state energy due to the Wigner and deformation effects are all important for the description of nuclear level density.

IV. CONCLUSION

In present paper, we apply the finite-temperature BCS (FTBCS) theory as well as the FTBCS with the approximate PNP within the Lipkin-Nogami method (FTLN) to describe the thermodynamic properties as well as level densities of several selected even-even isotopes, namely ^{56}Fe, ^{60}Ni, ^{98}Mo, and ^{116}Sn. The results obtained show that the pairing correlation together with the binding energy correactions due to Wigner and deformation energies have significant effects on the nuclear level density, especially at low and intermediate excitation energies.

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