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Systematic Study of the Thermal Pairing Re-entrance in the ^{72}Ti Nucleus

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ABSTRACT

Finite-temperature Hartree-Fock-Bogoliubov calculations are performed in $^{72}T_i$ by using Skyrme interactions, to predict the finite-temperature pairing re-entrance phenomenon for the system of neutrons. It is also shown that pairing re-entrance modifies the neutron single-particle energies around the Fermi level, as well as the occupation numbers and quasiparticle levels. It is also shown that neutron resonant states are expected to contribute substantially to pairing correlations and the two predicted critical temperatures are $T_{c1} = 0.1 - 0.2\,MeV$ and $T_{c2} = 0.7 - 0.9\,MeV$. On the other hand, our results for the ground-state energies, proton and neutron separation energies are in very good agreement with experiment where available.

Keywords: Nuclear density functional theory, Pairing correlation, Nuclear forces

1. Introduction

The magic nuclei near the drip line are weakly bound and the pairing correlations are quenched at zero temperature $T = 0\,MeV$, but when these nuclei are thermally excited, this can provide a significant variation in the rearrangement of the particles over the single-particle states. As it is shown, that both resonant and non-resonant continuum phase space are active in creating the pairing field [1,2], the pairing correlations can take place in this doubly magic nuclei at finite temperature, this phenomenon is known as the "pairing re-entrance" [1]. At finite temperature, pairing re-entrance in the equilibrium state was predicted for the first time in the neutron channel of extremely neutron-rich nuclei [1], $^{176-180}Sn$. The persistence of pairing correlations has been studied [3-5]. The effect of the resonant continuum upon pairing correlations was studied by the framework of BCS approximation, both for zero [6] and finite temperature [7] and by the framework of HFB theory [8] where the quasiparticle energy spectrum of the HFB equations

contains discrete bound states,resonances, and resonance continuum states and that the non-resonant continuum has been shown to be very effective, especially for coordinate-space HFB calculations in large boxes that involve huge amounts of discretized quasiparticle continuum states [9]. In this study, we investigate the finite-temperature Hartree-Fock-Bogoliubov (FT-HFB) theory by using Skyrme forces, to study the pairing properties of the magic nuclei far from the stability, where the Fermi level is closer to the last occupied level and the continuum coupling effect is very important. It is shown that the finite temperature pairing re-entrance in the equilibrium state may occur in a nucleus, $^{72}T_i$, presently synthesized at nuclear facilities.

2. Theoretical calculation

Subsequently, we briefly present the basic theoretical background of the finite temperature - HFB and we restrict ourselves to give the main equations. In this case, the radial FT-HFB equations read [10]:

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$$\begin{pmatrix} h_T(r)-\lambda & \Delta_T(r) \\ \Delta_T(r) & -h_T(r)+\lambda \end{pmatrix}\begin{pmatrix} U_i(r) \\ V_i(r) \end{pmatrix} = E_i \begin{pmatrix} U_i(r) \\ V_i(r) \end{pmatrix} \quad (1)$$

where E_i is a positive quasiparticle energy eigenvalue, $U_i(r)$ and $V_i(r)$ are the components of the radial FT-HFB wave function and λ is the Fermi energy, which is introduced to fix the average particle number. The quantity $h_T(r)$ denotes the thermal averaged mean field Hamiltonian and $\Delta_T(r)$ is the thermal averaged pairing field. For the zero-range Skyrme forces, the FT-HFB formalism can be written directly by introducing particle and pairing densities [11]:

$$\rho(r) = \frac{1}{4\pi}\sum_i (2j_i+1)\left[V_i^*(r)V_i(r)(1-f_i)+U_i^*(r)U_i(r)f_i \right] \quad (2)$$

$$J(r) = \frac{1}{4\pi}\sum_i (2j_i+1)\left[j_i(j_i+1)-l_i(l_i+1)-\frac{3}{4} \right]\left\{ V_i^2(1-f_i)+U_i^2 f_i \right\} \quad (3)$$

$$\tau(r) = \frac{1}{4\pi}\sum_i \left\{ \left[\left(\frac{dV_i}{dr}-\frac{V_i}{r}\right)^2 + \frac{l_i(l_i+1)}{r^2}V_i^2 \right](1-f_i) + \left[\left(\frac{dU_i}{dr}-\frac{U_i}{r}\right)^2 + \frac{l_i(l_i+1)}{r^2}U_i^2 \right]f_i \right\} \quad (4)$$

where $f_i = \left[1+\exp(E_i/k_\beta T)\right]^{-1}$ is the thermal occupation probability of quasiparticle states, k_β is the Boltzmann constant and T is the temperature. The thermal average pairing field is calculated with a density dependent contact force of the following form [12]:

$$V(r-r') = V_0\left[1-\eta\left(\frac{\rho(r)}{\rho_0}\right) \right]\delta(r-r') \quad (5)$$

where $\rho(r)$ is the density and V_0 is the strength of the force. With this force, the thermal averaged pairing field is local and is given by[11]:

$$\Delta_T(r) = V_{eff}(\rho(r))\frac{1}{4\pi}\sum\left(2j_i+1\right)U_i^*(r)V_i(r)(1-2f_i) \quad (6)$$

$$\equiv V_{eff}(\rho(r))\kappa_T(r)$$

where $\kappa_T(r)$ is the thermal averaged pairing tensor given by[11]:

$$\kappa_T(r) = \frac{1}{4\pi}\sum g_{i,q}U_{i,q}^*(r)V_i(r)(1-2f_i) \quad (7)$$

where $g_i = 2j_i+1$ is the degeneracy of the state i with angular momentum $j_i = l_i + s_i$ and the summation is going over the whole quasiparticle spectrum, including the existing unbound states inside the cut-off. The thermal average pairing gap is obtained from the thermal average pairing field $\Delta_T(r)$ and the thermal pairing tensor $\kappa_T(r)$ solutions of the finite-temperature HFB model, and is defined as [1]:

$$\Delta = \frac{\int d^3r \Delta_T(r)\kappa_T(r)}{\int d^3r \kappa_T(r)} \quad (8)$$

In practice, the self-consistent FTHFB equations (1) are solved by iterations, fixing at each interaction the canonical potential λ and the pairing field $\Delta_T(r)$, until the convergence of the single particle energies and of the pairing gap.

3. Calculations and results

In this study, the FT-HFB calculations are performed in coordinate representation using Dirichlet boundary conditions, which serve to the discretization of the continuum states entering into pairing correlations. We have found that the semi-magic nuclei $^{72}T_i$, with 22 protons and 50 neutrons, manifest the re-entrance phenomenon for the neutron channel only by the SIII, SLY4 and SLY5 forces.
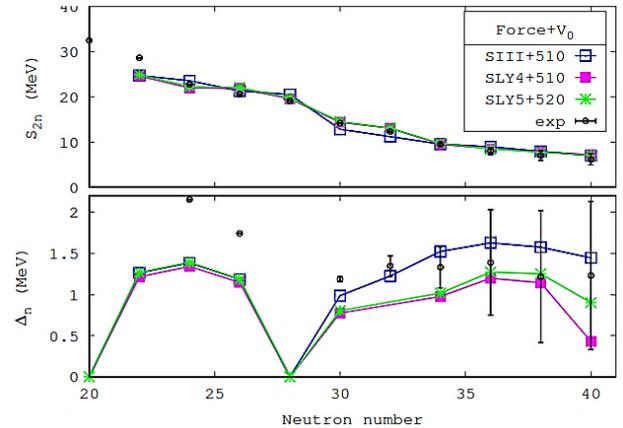
Fig.1 Two-neutron separation energy (upper panel) and neutron pairing gaps (lower panel) versus the number of neutrons for Z=22 isotopes obtained within the FTHB model at zero temperature, for SLY4-5 and SIII Skyrme forces. The experimental data are deduced from AME2012 mass table [14]

The value of the pairing strength V_0 (in $MeV.fm^3$) has been fixed for each Skyrme interactions such as to reproduce the experimental two-neutron separation energies S_{2n} and the proton pairing gaps Δ_n for Z=22 determined from the three-point formula [13]. The comparison between the model predictions for S_{2n} and Δ_n, and the experimental data are shown in Fig. 1.

The pairing re-entrance phenomenon is predicted for SLY5, SLY4, and SIII Skyrme forces FIG 2 with critical

temperatures $T_{c1} = 0.1 - 0.2\ MeV$ and $T_{c2} = 0.7 - 0.9\ MeV$ .These critical temperatures correspond to the low- and high-temperature boundaries of the pairing re-entrance domain. Out of this domain, matter is predicted to be in its normal phase where pairing is quenched.
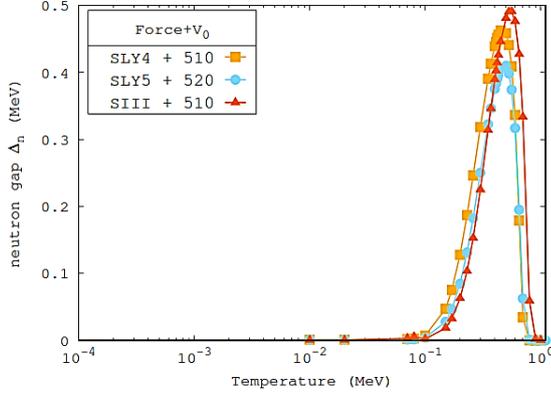
Fig.2 *Temperature-average neutron pairing gap versus temperature for $^{72}T_i$ nuclei based on SLY4-5 and SIII Skyrme interactions*

The structure of the single-particle states around the Fermi energy provides a good understanding of the theoretical results for pairing re-entrance. As nuclei get closer to the drip-lines, the coupling to the continuum becomes more and more important, and continuum resonant states may play an important role if they are located at low energy [1,5,9,18]. For pairing re-entrance, it is important that these resonant states are sufficiently high (above 2 MeV) such that the ground-state is unpaired, but at the same time, it shall be sufficiently low (below 4 MeV) to be populated by low-temperature thermal excitation [1,5]. If the energy of the resonance state matches these two conditions, the re-entrance phenomenon can occur at finite-temperature. The quenching mechanism is indeed the same in the re-entrance case as well as in the ordinary paired nuclei: the single particle thermal excitation breaks the Cooper pairs, since the cost in kinetic energy of having particles well above the Fermi energy is not anymore compensated by the gain in forming Cooper pairs. Since the quenching mechanism is the same for ordinary paired nuclei and for pairing re-entrance, the critical temperature T_{c2} is also limited to values around about 1 MeV.

In order to understand the behavior of the nuclear structure of $^{72}T_i$ in the region of re-entrance, results obtained from FT-HFB with SLY4 force were analyzed. As shown in Fig. 3, at $T = 0$, all the states are fully occupied and thus they do not contribute to superfluidity, as it is known that the pairing correlations arise essentially from gas states. At $T = 0.3\ MeV$ the levels start to be unoccupied and thus we can use them to build pairing correlations. It has also been noticed that not only the occupations probabilities are modified by the temperature, but also the canonical energies e_{lj}, which are

almost constant up to $T = 0.5\ MeV$ and change by about $300\ KeV$ at $T = 1\ MeV$. Although the change in occupation and energy shift are strongly correlated, one can conclude that the main effect on pairing re-entrance comes from the formation of holes in this shell.
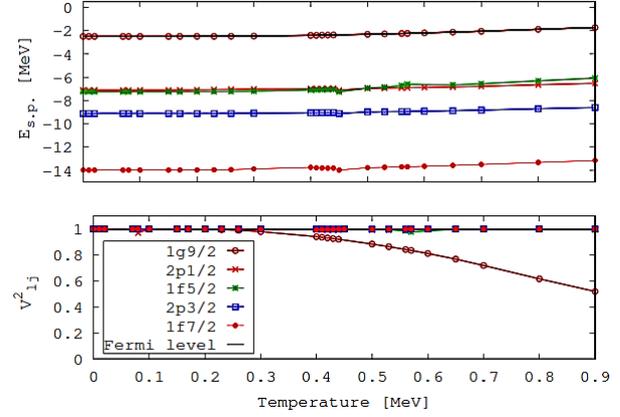
Fig.3 *Evolution of canonical neutron states (upper panel) and their occupation probability (lower panel) as a function of the temperature for ^{72}Ti*
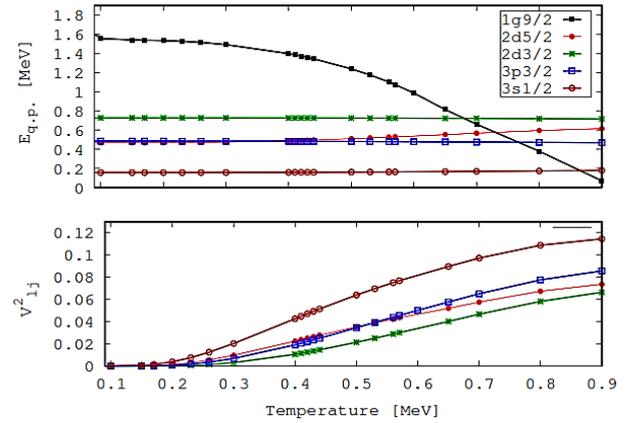
Fig.4 *Temperature evolution of the neutron quasi-particle energies corresponding to the states around the Fermi energy:1g9/2(hole), and 2d5/2, 2d3/2, 3p3/2 and 3s1/2(particles) and their occupation probability (lower panel) as a function of the temperature for $^{72}T_i$*

In fact, the quasi-particle states 2d3/2, 3p3/2 and 3s1/2 in Fig.4 (top panel) are slowly increasing as function of the temperature compared to the state 2d5/2. In contrast, the quasi-particle state 1g7/2 (hole) is a decreasing function. Assuming that the quasi-particle energy is related to the s.p. energies by the following relation $E_{qp} = \sqrt{(e_{s.p.} - \mu)^2 + \Delta^2}$, and knowing that the chemical potential $\mu(T)$ is a decreasing function of the temperature, it can be understood that for constant $e_{s.p.}$ and Δ, the quasi-particle energy decrease for hole states and increase for particle states around the Fermi level. The effect of the

temperature on changing the occupation numbers is shown in Fig.4 (lower panel) that shows the increasing occupation number of the particle states as function of temperature.

4. Conclusion

Based on the FT-HFB approach, it is found that the finite temperature pairing re-entrance phenomenon in the thermal equilibrium state could occur in the ^{72}Ti nuclei and could play a non-negligible role. The presence of the temperature modifies the occupation probabilities of the last major shell creating holes, thus allowing the formation of pairing correlations between these states. The domain of temperature where this phenomenon could occur, as well as the size of the neutron pairing gap, yet depends on the detailed s.p. level structure which varies from one interaction to another. Our prediction is based only on a few Skyrme interactions, which implies that the pairing re-entrance is very sensitive to the size of the s.p. energy gap above the last occupied state.

Conflict of Interest

The authors have no conflict of interest.

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