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Thermal quasiparticle correlations and continuum coupling in nuclei far from stability

Nguyen Dinh Dang[a] [b] and Akito Arima[c]

[a]RI-beam factory project office, RIKEN, 2-1 Hirosawa, Wako, 351-0198 Saitama, Japan

[b]Institute for Nuclear Science and Technique, VAEC, Hanoi, Vietnam

[c]House of Councilors, 2-1-1 Nagatacho, Chiyoda-ku, Tokyo 100-8962, Japan

The contributions of quasiparticle correlations and continuum coupling upon the superfluid properties of neutron-rich Ni isotopes are studied within the modified BCS approximation at finite temperature. The effect of quasiparticle correlations is included using a secondary Bogoliubov transformation explicitly involving the quasiparticle occupation numbers at temperature T. The effect of continuum coupling is taken into account via the finite widths of the single-particle resonant states. It is shown that the combination of these effects washes out the sharp superfluid-normal phase transition given by the standard finite-temperature BCS calculations. It is also found that the two-neutron separation energy for ^{84}Ni drops to zero at $T \simeq 0.8$ MeV.

1. INTRODUCTION

It is well known that there exists a sharp phase transition from the superfluid phase to the normal-fluid one in infinite Fermi systems at a critical temperature $T_c \approx 0.567\Delta(0)$, where $\Delta(0)$ is the pairing gap at zero temperature $T = 0$ [1]. In finite Fermi systems like nuclei, fluctuations due to the finiteness of the system become large. Several papers took into account thermal fluctuations in the pairing field [2–5]. Their results showed that, although the gap $\Delta(T)$ decreases with increasing temperature, it remains finite even at rather high temperature.

In nuclei close to the drip line, the Fermi level is close to the continuum threshold. With increasing T, the nucleons are easily promoted into the continuum part of the single-particle spectrum, mainly into the single-particle resonant states, which are trapped by the centrifugal and/or Coulomb barrier inside the nucleus. The resonant states have a continuous energy spreading (finite width) and, therefore, the Pauli blocking, responsible for the superfluidity suppression at $T \neq 0$, is less effective than for a spectrum formed only by bound states. As a result, the critical temperature T_c is reduced [6].

Recently, an improved treatment of ground-state correlations called the modified RPA (MRPA) has been proposed in Ref. [7], which employs the modified quasiparticles obtained by a secondary canonical transformation of usual quasiparticles explicitly involving the quasiparticle occupation numbers. This approach is applied in this work to study how the continuum coupling and the quasiparticle correlations at finite temperature simulta-

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neously affect the properties of the superfluid-normal phase transition in neutron-rich Ni isotopes.

2. FORMALISM

We consider a system of fermions described by the particle creation and destruction operators, $a^{\dagger}_{jm}$ and a_{jm}, in a spherical mean field, where the single-particle orbitals are labeled by the total angular-momentum quantum numbers j and m. The pairing correlations of the system is induced by an attractive two-body force with the pairing constant G. Using the canonical Bogoliubov transformation from the particle operators, $a^{\dagger}_{jm}$ and $a_{j\widetilde{m}} \equiv (-1)^{j-m}a_{j-m}$, to the quasiparticle ones, $\alpha^{\dagger}_{jm}$ and $\alpha_{j\widetilde{m}}$, the pairing Hamiltonian of this system is transformed into the quasiparticle representation, whose explicit form is given in [8,9]. On top of that, following Ref. [7], the quasiparticles are modified by the correlations in the quasiparticle ground state according to the following secondary canonical transformation between the quasiparticle operators $\alpha^{\dagger}_{jm}$, α_{jm}, and the modified ones $\bar{\alpha}^{\dagger}_{jm}$, $\bar{\alpha}_{jm}$:

$$\bar{\alpha}^{\dagger}_{jm} = \sqrt{1-n_j}\alpha^{\dagger}_{jm} + \sqrt{n_j}\alpha_{j\widetilde{m}} \ , \quad \bar{\alpha}_{j\widetilde{m}} = \sqrt{1-n_j}\alpha_{j\widetilde{m}} - \sqrt{n_j}\alpha^{\dagger}_{jm} \ , \tag{1}$$

where n_j are the quasiparticle occupation numbers of orbitals j in the correlated ground state $|\bar{0}\rangle$: $n_j = \langle\bar{0}|\alpha^{\dagger}_{jm}\alpha_{jm}|\bar{0}\rangle \neq 0$. Using Eq. (1), the transformation from the original particle operators to the modified quasiparticle operators $\bar{\alpha}^{\dagger}_{jm}$, $\bar{\alpha}_{jm}$ becomes

$$a^{\dagger}_{jm} = \bar{u}_j\bar{\alpha}^{\dagger}_{jm} + \bar{v}_j\bar{\alpha}_{j\widetilde{m}} \ , \quad a_{j\widetilde{m}} = \bar{u}_j\bar{\alpha}_{j\widetilde{m}} - \bar{v}_j\bar{\alpha}^{\dagger}_{jm} \ , \tag{2}$$

with the coefficients $\bar{u}_j$ and $\bar{v}_j$ related to the conventional Bogoliubov coefficients u_j and v_j as

$$\bar{u}_j = u_j\sqrt{1-n_j} + v_j\sqrt{n_j} \ , \quad \bar{v}_j = v_j\sqrt{1-n_j} - u_j\sqrt{n_j} \ . \tag{3}$$

We see that the transformation (2) has the same form as the usual Bogoliubov transformation, where the coefficients u_j and v_j are replaced with $\bar{u}_j$ and $\bar{v}_j$. Therefore, the pairing Hamiltonian expressed in terms or the modified quasiparticles operators $\bar{\alpha}^{\dagger}_{jm}$ and $\bar{\alpha}_{jm}$ has the same form as that of the usual quasiparticle Hamiltonian in [8,9] with (u,v) and $(\alpha^{\dagger},\alpha)$ replaced with $(\bar{u},\bar{v})$, and $(\bar{\alpha}^{\dagger},\bar{\alpha})$, respectively. Hence, the modified BCS (MBCS) equations, derived with respect to $|\bar{0}\rangle$, also has the same form as that of the standard BCS equation, namely

$$\bar{\Delta} = G\sum_j \Omega\bar{u}_j\bar{v}_j = G\sum_j \Omega_j[(1-2n_j)u_jv_j - \sqrt{n_j(1-n_j)}(u_j^2 - v_j^2)] \ , \tag{4}$$

$$N = 2\sum_j \Omega_j\bar{v}_j^2 = 2\sum_j \Omega_j[(1-2n_j)v_j^2 + n_j - 2\sqrt{n_j(1-n_j)}u_jv_j] \ , \tag{5}$$

using Eq. (3). The quasiparticle occupation number n_j can be determined from the backward amplitudes $Y_j^{(\nu)}$ of the renormalized RPA (RRPA) equation by solving it self-consistently with Eqs. (4) and (5) following the procedure discussed in [7,10]. At $T \neq$

0, the statistical approach is often used. Its major assumption is the replacement of the individual compound systems, each with a given intrinsic excitation energy and particle number, by the grand canonical ensemble of nuclei in thermal equilibrium. The nuclear temperature T and chemical potential λ determine the average excitation energy and average particle number of the system, respectively. The probability for a quantum system to have a given eigenenergy is determined by the density matrix $\mathcal{D}$ rather than by a pure wave function. Solving the MBCS and MRPA equations (obtained using a Hamiltonian with monopole pairing) for neutron-rich Ni isotopes at $T \neq 0$, we found that the quasiparticle occupation number n_j is very close to the one given by the Fermi-Dirac distribution of non-interacting Fermi gas

$$n_j(T) = Tr\{\alpha^{\dagger}_{jm}\alpha_{jm}\mathcal{D}\} = \frac{1}{e^{E_j/T}+1} , \quad (6)$$

where E_j is the quasiparticle energy. Therefore, we approximate $n_j = n_j(T)$ in all further numerical calculations. Within this approximation, the MBCS equations (4) and (5) become the finite-temperature MBCS (FT-MBCS) equations.

The extension of the conventional FT-BCS equations to include the contribution of the continuum single-particle states has been performed in Ref. [6]. Using the same prescription we can also include the effect of the continuum coupling into the FT-MBCS equations (4) and (5) with $n_j = n_j(T)$:

$$\bar{\Delta} = G\Big\{\sum_j \Omega_j[(1-2n_j)u_jv_j - \sqrt{n_j(1-n_j)}(u_j^2 - v_j^2)]$$

$$+\frac{1}{2}\int g(\epsilon)[(1-2n(\epsilon))u(\epsilon)v(\epsilon) - \sqrt{n(\epsilon)(1-n(\epsilon))}(u^2(\epsilon) - v^2(\epsilon))]d\epsilon\Big\} , \quad (7)$$

$$N = 2\sum_j \Omega_j[(1-2n_j)v_j^2 + n_j - 2\sqrt{n_j(1-n_j)}u_jv_j]$$

$$+\int g(\epsilon)\Big[(1-2n(\epsilon))v^2(\epsilon) + n(\epsilon) - 2\sqrt{n(\epsilon)(1-n(\epsilon))}u(\epsilon)v(\epsilon)\Big]d\epsilon , \quad (8)$$

where $n(\epsilon)$ is obtained from $n_j(T)$ replacing the discrete single-particle energy ϵ_j with the integration parameter ϵ. In the resonant-continuum BCS equations, the variation of the matrix elements of the interaction in the energy region of a resonance is in fact taken into account through the continuum level density $g(\epsilon)$. The continuum usually contributes through a few narrow and well separated resonant states [6]. Therefore one can replace in the equations above the continuum level density with [11]

$$g(\epsilon) = \frac{1}{\pi}\sum_j (2j+1)\frac{\frac{1}{2}\Gamma_j}{(\epsilon-\epsilon_j)^2 + (\frac{1}{2}\Gamma_j)^2} . \quad (9)$$

where ϵ_j and Γ_j are the energy and the width of the resonance state with angular momentum j, respectively. In the limit of zero widths, the RHS of Eq. (9) becomes a sum of δ-functions, recovering the level density of the bound spectrum.

3. NUMERICAL RESULTS

TABLE I. Neutron single-particle states used in calculations for $^{68-84}$Ni isotopes.

shell	state	ϵ_j (MeV)	$\Gamma_j/2$ (MeV)
	$1g_{7/2}$	4.229	0.171
50-82	$2f_{7/2}$	3.937	1.796
	$1h_{11/2}$	3.334	0.014
	$2d_{3/2}$	1.338	0.489
	$3s_{1/2}$	-0.284	
	$2d_{5/2}$	-0.80	
28-50	$1g_{9/2}$	-4.398	
	$1f_{5/2}$	-5.623	
	$2p_{1/2}$	-5.649	
	$2p_{3/2}$	-7.836	

The neutron single-particle states used in the present calculations are shown in Table I. They were calculated using a Woods-Saxon potential with the depth $V_0 = 40$ MeV, radius $R_0 = 1.27$ fm, and surface thickness $a = 0.67$ fm. For the spin-orbit interaction we use a Woods-Saxon potential with the same values for the radius R_0 and surface thickness a, but the depth is changed to the value $V_{so} = 21.43$ MeV. These parameters are chosen so that the obtained single-particle spectrum for ^{78}Ni is similar to that given by the Skyrme - HF calculations. The widths of these resonant states are shown in the fourth column of the Table I. Their effects on the pairing correlations, both in resonant-continuum BCS and MBCS equations, appear through the continuum level density. In order to see these effects we perform also a calculation in which the resonant states are treated as quasibound states, i.e., replacing in the BCS equations the continuum level density with the Dirac δ-function. These calculations will be quoted below as quasibound BCS and quasibound MBCS. The pairing matrix elements are considered equal with the constant $G = 0.214$ MeV in all the calculations. This value gives within the quasibound BCS a pairing gap of 1.3 MeV for ^{84}Ni at $T = 0$, as in Ref. [6].

The pairing gaps for some Ni isotopes are plotted in Fig. 1 as a function of temperature. As in [6], one notices a reduction of the gap due to the finite widths of the resonant states. This effect is enhanced in the vicinity of the drip line. Although T_c is significantly diminished due to the finite widths of the resonant states, the ratio $T_c/\Delta(0)$ remains close to 0.57 in both calculations. The situation changes when together with the continuum coupling we introduce the effect of the thermal quasiparticle correlations. As compared to the quasibound BCS, the quasibound-modified BCS predicts a slower decrease of pairing gap with increasing temperature. The sharp superfluid-normal phase transition occurs at a much higher temperature. However, as the thermal quasiparticle correlations decrease with increasing the particle number, the slopes of two curves are getting closer. Taking the widths of the resonant states into account, the MBCS predicts a slower decrease of the gap than that given by the quasibound MBCS as the temperature increases. This is due to the fact that, with increasing the temperature, the Pauli blocking becomes less effective due to the spreading of the resonant states. The gap obtained within the resonant-continuum MBCS remains finite as a long tail extended to $T > 2$ MeV. It is important to point out that, in contrast to the quasibound-MBCS calculations, the values of the gap obtained within the resonant-continuum MBCS never cross zero. In general, we found that by introducing the width of the resonances into the MBCS equations the sharp superfluid-normal phase transition is washed out for all the isotopes under consideration.

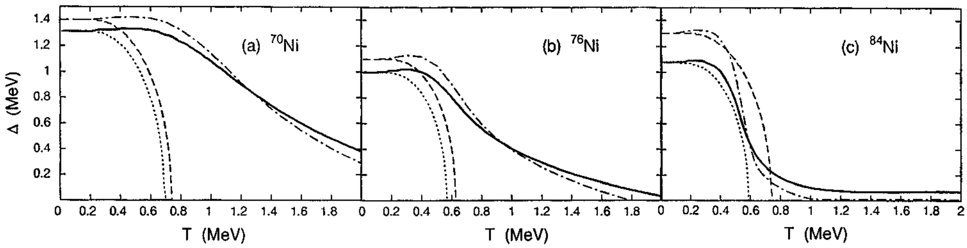

Figure 1. Pairing gaps for as a function of temperature. The dashed, dotted, dash-dotted, and solid lines represent the solutions of the quasibound BCS, resonant-continuum BCS, quasibound MBCS, and resonant-continuum MBCS, respectively.

A particular interest in the study of unstable nuclei is the identification of the location of the two-neutron drip line. One of the quantities that provide the relevant information of the two-neutron drip line is the two-neutron separation energy $S_{2n} = \mathcal{E}(N-2,Z) - \mathcal{E}(N,Z)$, where $\mathcal{E}$ is the total energy of the system. A nucleus with N neutrons is beyond the two-neutron drip line if S_{2n} becomes negative. Using this quantity, it has been found by the recent continuum HFB calculations in Ref. [12] that the heaviest bound Ni isotope is ^{86}Ni.

The two-neutron separation energies S_{2n} calculated within the BCS and MBCS approximations with continuum coupling via the widths of resonant states are plotted in Fig. 2 (a) and (b), respectively, against the mass number A for the Ni isotopes under consideration at several temperatures. It is seen that the decrease of S_{2n} with increasing A is smoother within the MBCS approximation than the BCS one, especially with increasing temperature. This is a direct consequence of the smooth temperature dependence of the pairing gap within the MBCS discussed previously. A particular interesting feature revealed by this figure is the reduction of two-neutron separation energy with increasing T within the MBCS approximation for the isotopes close to the drip line. Thus, the value of S_{2n} for ^{84}Ni drops from around 1 MeV at $T = 0.3$ MeV to almost zero at $T = 0.8 \sim 1$ MeV (See Fig. 2 (b)). This does not happen within the BCS approximation (See Fig. 2 (a)). This observation suggests that thermal quasiparticle correlations, which are taken into account within the MBCS approximation, may cause the two-neutron drip line to be reached at ^{84}Ni, i.e. at two mass units earlier, at $T = 0.8 \sim 1$ MeV.

In conclusion we have studied how the thermal quasiparticle fluctuations and the continuum coupling affect the pairing correlations in neutron-rich Ni isotopes. The results show that the combined effect of the thermal quasiparticle correlations and of continuum

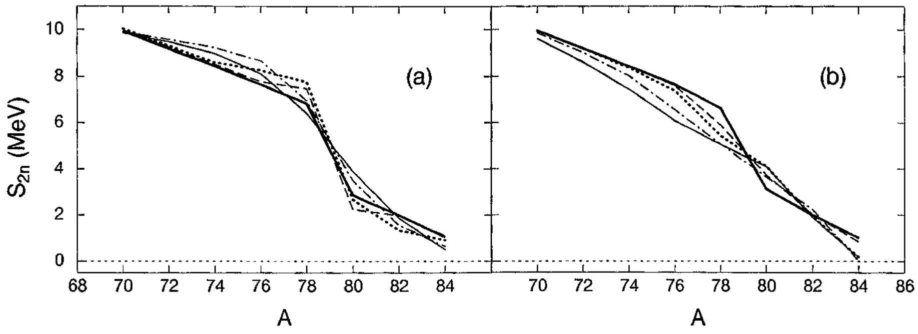

Figure 2. Two-neutron separation energies as a function of the mass number A for Ni isotopes at temperatures $T = 0.3$ (thick solid line), 0.5 (dashed line), 0.6 (dotted line), 0.8 (dash-dotted line), and 1 MeV (thin solid line). (The lines are drawn just to connect the points at given values of A in order to make the trend more visible). The results obtained within the resonant-continuum BCS and resonant-continuum MBCS are shown in (a) and (b), respectively.

coupling reduces the pairing gap in the low-temperature region and washes out the sharp superfluid-normal phase transition found in the standard FT-BCS and FT-HFB calculations, which neglect these effects. We also observed that the two-neutron separation energy obtained within the MBCS approximation for ^{84}Ni reaches zero at temperature around $T = 0.8 \sim 1$ MeV. This suggests that the thermal quasiparticle fluctuations may cause the drip line to be reached earlier in mass units compared to the zero temperature case.

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