Proton-neutron pairing energies in $N = Z$ nuclei at finite temperature

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Thermal behavior of isoscalar ($\tau=0$) and isovector ($\tau=1$) proton-neutron (pn) pairing energies at finite temperature are investigated by the shell model calculations. These pn pairing energies can be estimated by double differences of "thermal" energies which are extended from the double differences of binding energies as the indicators of pn pairing energies at zero temperature. We found that the delicate balance between isoscalar and isovector pn pairing energies at zero temperature disappears at finite temperature. When temperature rises, while the isovector pn pairing energy decreases, the isoscalar pn pairing energy rather increases. We discuss also the symmetry energy at finite temperature.

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The proton-neutron (pn) pairing energies have become one of hot topics in the study of the nuclear structure for proton-rich nuclei. In particular, interests are increasing in studying isovector ($\tau=1$) and isoscalar ($\tau=0$) pn pairing energies in medium mass $N = Z$ nuclei produced at the radioactive nuclear beam facilities. The study of pn pairing energies is also important in the astrophysical context. These nuclei lie along the explosive rp-process nucleosynthesis path and the nuclear properties such as masses, halflives, and isomers have a strong influence on modeling the rp-process and identifying possible nucleosynthesis sites. Odd-odd $N = Z$ nuclei are an ideal experimental laboratory for the study of pn pairing energies. It is well known that the lowest $\tau = 0$ and $\tau = 1$ states compete for the ground state changing the sign of the energy difference $E_{\tau=1} - E_{\tau=0}$ in odd-odd $N = Z$ nuclei, while all even-even $N = Z$ nuclei have the $\tau = 0$ ground states. Several authors [1, 2, 3, 4, 5, 6, 7] already pointed out that this degeneracy in odd-odd $N = Z$ nuclei reflects the delicate balance between the symmetry energy and the like-nucleon neutron-neutron (nn) (or proton-proton (pp)) pairing energy. On the other hand, it has recently been shown that this degeneracy is attributed to competition between the isoscalar and isovector pairing energies [9, 10, 25].

It has been recently reported [11, 12] that the canonical heat capacities extracted from observed level densities in ^{162}Dy, ^{166}Er and ^{172}Yb display the S shape with a peak around $T \approx 0.5$ MeV, which is interpreted as the breaking of like-nucleon $J = 0$ pairs because the BCS critical temperature corresponds to $T_c \approx 0.57\Delta_n(T = 0) \approx 0.5$ MeV, where the like-nucleon pairing gap $\Delta_n(T = 0)$ is calculated at zero temperature by the BCS theory. Thus it seems that the S shape is a signature of pairing transition at the critical temperature. For the finite Fermi system like a nucleus, however, since the nuclear radius is much smaller than the coherence length of the Cooper pair, statistical fluctuations beyond the mean field in the BCS theory become large. The fluctuations smooth out the sharp phase transition, and then the like-nucleon pairing gap Δ_n does not quickly become zero at the BCS

critical temperature but decreases with increasing temperature. There are many approaches to treat the fluctuations beyond the mean field. The shell model calculation can take into account the large fluctuations beyond the mean field. Recently the shell model Monte Carlo (SMMC) calculation [13, 14] using the $fp + g_{9/2}$ shell has been performed in the even- and odd-mass Fe isotopes.

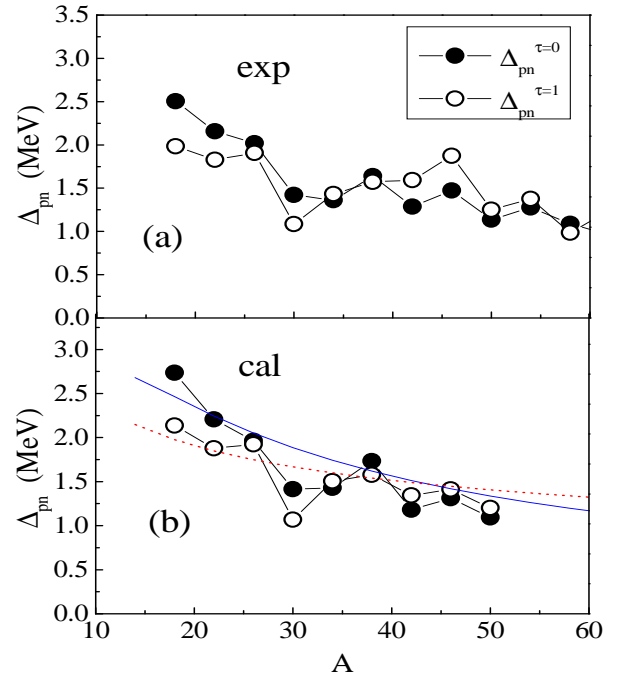We recently proposed [15] "thermal" odd-even mass

FIG. 1: $\tau = 0$ and $\tau = 1$ pn pairing gaps estimated from double differences of binding energies for odd-odd $N = Z$ nuclei: (a) experimental ones; (b) those of shell model calculations. The solid and dotted curves show $122.25(1 - 1.67A^{-1/3})/A$ and $5.18A^{-1/3}$, respectively.

difference to estimate the like-nucleon pairing energy at finite temperature, and showed in the spherical shell model calculations that the drastic suppression of like-nucleon pairing energy due to finite temperature brings about the S shape in the heat capacity arround the temperature $T_c \approx 0.57\Delta_n(T=0)$ MeV. In this rapid communication, we study the pn pairing energies at finite temperature in odd-odd $N=Z$ nuclei. Does pairing transition due to the breaking of pn pairs take place when temperature increasing? It is now interesting to investigate thermal behavior of the pn pairing energies in $N=Z$ nuclei.

We start from the double difference of binding energies [16, 17, 18] defined as

$$\Delta_{pn}^{\tau}(Z,N) = \frac{1}{2}[B(Z,N)^{\tau} - B(Z,N-1)$$
$$-B(Z-1,N) + B(Z-1,N-1)], \qquad (1)$$

where $B(Z,N)$ is the binding energy. The indicator $\Delta_{pn}^{\tau=1}$ gives the $\tau=1$ pn pairing gap in $N=Z$ nuclei. The $\Delta_{pn}^{\tau=0}$ can be regarded as the $\tau=0$ pn pairing gap as well. Figure 1 (a) shows the $\tau=0$ and $\tau=1$ pn pairing gaps estimated from the double differences of experimental binding energies (1) in odd-odd $N=Z$ nuclei with $A=18-58$. The $\tau=0$ pn energy is somewhat larger than the $\tau=1$ pn energy in the sd shell nuclei and *vice versa* in the pf shell nuclei. Over a wide range of odd-odd $N=Z$ nuclei, however, basically Fig. 1 shows almost the same magnitude of the $\tau=0$ and $\tau=1$ pn pairing gaps. We carried out shell model calculations using isospin-invariant interactions such as the unified sd (USD) interaction [19] for odd-odd $N=Z$ nuclei in sd shell and the GPFX1 interaction [20] for ^{42}Sc, ^{46}V, and ^{50}Mn in fp shell. On the mean-field level the ratio between the strengths of pp-, nn-, and pn-pair fields is given by the orientation of the pair field. The relative strengths of three types of pair fields becomes only definite when isospin symmetry is restored. Note that the shell model calculations with isospin invariance show $\Delta_{pp}^{\tau=1} = \Delta_{nn}^{\tau=1} = \Delta_{pn}^{\tau=1}$ in odd-odd $N=Z$ nuclei.

In Fig. 1(b), we can see that the shell model results reproduce well the experimental pn pairing gaps, and describe the characteristic behavior in Fig. 1(a). The pn pairing gaps are closely realted to the energy difference $B(Z,N)^{\tau=1} - B(Z,N)^{\tau=0}$ between the lowest $\tau=0$ and $\tau=1$ states in odd-odd $N=Z$ nuclei, because the energy difference satisfies the following identity [9],

$$B(Z,N)^{\tau=1} - B(Z,N)^{\tau=0} = 2(\Delta_{pn}^{\tau=0} - \Delta_{pn}^{\tau=1}). \quad (2)$$

Odd-odd $N=Z$ nuclei with $A < 40$ have the ground states with $\tau=0, J>0$ except for ^{34}Cl, while the ground states of odd-odd $N=Z$ nuclei with $40<A<74$ are $\tau=1$ and $J=0$ except for ^{58}Cu. Several authors [1, 2, 3, 5, 6, 7] discussed that this degeneracy is attributed to the delicate balance between the symmetry energy $a(A)\tau(\tau+1)/A$ and pairing gap Δ and that the energy difference $\delta B = B(Z,N)^{\tau=1} - B(Z,N)^{\tau=0}$ is ex-

pressed as $\delta B = 2(a(A)/A - \Delta)$. However, if we employ the symmetry energy coefficient $a(A) = 134.4(1 - 1.52A^{-1/3})$ and pairing gap $\Delta = 5.18A^{-1/3}$ of Duflo and Zuker mass formula [21], the energy difference δB becomes larger than the experimental value. As suggested in our previous paper, the isoscalar pairing gap $\Delta_{pn}^{\tau=0}$ is approximately written as $122.25(1 - 1.67A^{-1/3})/A$ and the isovector one $\Delta_{pn}^{\tau=1}$ is equal to the like-nucleon nn pairing gap $\Delta_n \approx 5.18A^{-1/3}$. These two curves are shown in Fig. 1(b) for comparison. Since $\delta B = 2(\Delta_{pn}^{\tau=1} - \Delta_{pn}^{\tau=0})$, the degeneracy between the lowest $\tau=0$ and $\tau=1$ states in odd-odd $N=Z$ nuclei comes from the delicate balance between the isoscalar and isovector pn pairing energies.

Let us next describe the pn pairing gaps at finite temperature. We introduce the canonical partition function defined by

$$Z(T) = \text{Tr}(e^{-H/T}) = \sum_{i=0}^{\infty} e^{-E_i/T}, \qquad (3)$$

where E_i is the energy of the ith eigenstate with degeneracies based on symmetries for the Hamiltonian H of a system. All the eigenvalues E_i are obtained by solving the eigenvalue equations $H\Psi_i = E_i\Psi_i$. Then, the partition function in the canonical ensemble is calculated from Eq. (3), and any thermodynamical quantities $O(T)$ can be evaluated from

$$O(T) = \langle O \rangle = \text{Tr}(Oe^{-H/T})/Z(T), \qquad (4)$$

where $\langle O \rangle$ stands for the average value of operator O over the range of eigenstates. For instance, the thermal energy is expressed as

$$E(Z,N,T) = \langle H \rangle = \sum_{i=0}^{\infty} E_i e^{-E_i/T}/Z(T). \qquad (5)$$

The heat capacity is then given by

$$C(Z,N,T) = \frac{\partial E(Z,N,T)}{\partial T}. \qquad (6)$$

We now introduce the following double difference of "thermal" enegies $E(Z,N,T)$ analogous to Eq. (1) as an indicator of pn pairing energies,

$$\Delta_{pn}^{\tau}(Z,N,T) = \frac{1}{2}[E(Z,N,T)^{\tau} - E(Z,N-1,T)$$
$$-E(Z-1,N,T) + E(Z-1,N-1,T)]. \quad (7)$$

The double differences of binding energies at zero temperature in Eq. (1) are known theoretically and experimentally as important quantities in evaluation of the pn pairing energies in a nucleus [16, 17, 18]. The double differences of thermal energies in Eq. (7) are also indicators of the pn pairing energies and can be regarded as the pn pairing gaps at finite temperature.

Let us evaluate the double difference of thermal energies (7) for $N=Z$ sd shell nuclei. We make numerical

calculations by way of two steps. First, we carry out the exact shell model calculations in the sd shell using the USD interaction [19], and calculate the correlated thermal energy $E_{v,tr}$ from Eq. (5). Secondly, we extend the model space to a larger one ($sd + fp + s_{1/2}d_{5/2}$) in order to display the double difference of thermal energies in a broader range of temperature using an independent-particle approximation [14]. The single-particle energies of the extended space are obtained by diagonalizing the Woods-Saxon potential with the spin-orbit interaction, where the harmonic-oscillator (H.O.) eigenfunctions are used. The Woods-Saxon parameters are chosen so as to reproduce the single-particle energies estimated from ^{17}O, because it is necessary to reasonably extrapolate the single-particle energies of the sd shell to those of the larger space. In this way, we combine the correlated thermal energy $E_{v,tr}$ in the truncated space with the thermal energy E_{sp} calculated using the independent-particle approximation in the larger space. The thermal energy which takes account of the interaction effects in the sd shell is estimated as follows [14]:

$$E = E_{v,tr} + E_{sp} - E_{sp,tr}, \qquad (8)$$

where $E_{sp,tr}$ is the thermal energy of the sd shell within the independent-particle approximation. We now obtain the double difference of thermal energies Δ_{pn}^{τ} by substituting E of Eq. (8) for $E(Z, N, T)$ in Eq. (7).

Figure 2 shows the calculated thermal pn pairing gaps for odd-odd $N = Z$ nuclei, ^{22}Na, ^{26}Al, ^{30}P, and ^{34}Cl at temperature $T = 2.0$ MeV. The $\tau = 1$ and $\tau = 0$ pn pairing gaps are largely separated at $T = 2.0$ MeV. Comparing Fig. 2 with Fig. 1(b), we notice that the $\tau = 1$ pn pairing gap decreases but the $\tau = 0$ pn pairing gap keeps the magnitude from zero temperature to high temperature.

Figure 3 shows the variation of the thermal pn pairing gaps depending on temperature T for ^{22}Na, ^{26}Al, ^{30}P, and ^{34}Cl. In all graphs, we can see increase of the $\tau = 0$ pn pairing gap and decrease of the $\tau = 1$ pn pairing gap. As mentioned above, at zero temperature the $\tau = 0$ and $\tau = 1$ pn pairing gaps are almost the same, and the lowest $\tau = 0$ and $\tau = 1$ states are degenerate. As increasing temperature, the $\tau = 1$ pn pairing gap decreases and $\tau = 0$ one rather increases. Thus, we know that the $\tau = 0$ pairing energy becomes dominant at high temperature.

It would be valuable to discuss the symmetry energy $\sim 4a_{\text{sym}}(T)\tau(\tau+1)/A$ at finite temperature because it is closely related to the $\tau = 0$ pairing energy. In our previous paper [18], we suggested that the dominant part of the symmetry energy comes from the $\tau = 0$ pairing energy part in the shell-model interaction energy. For the application of the symmetry energy in core-collapse supernova simulations, Donati et $al.$ [23] pointed out a possibility that the symmetry energy coefficient a_{sym} at the finite temperature has been estimated to be somewhat larger than that of stable nuclei at zero temperature. The increase ($\sim 3\%$) of the symmetry energy between $T = 0.0$ and $T = 1.0$ MeV after implementing the correction in the SMMC calculations is smaller than that
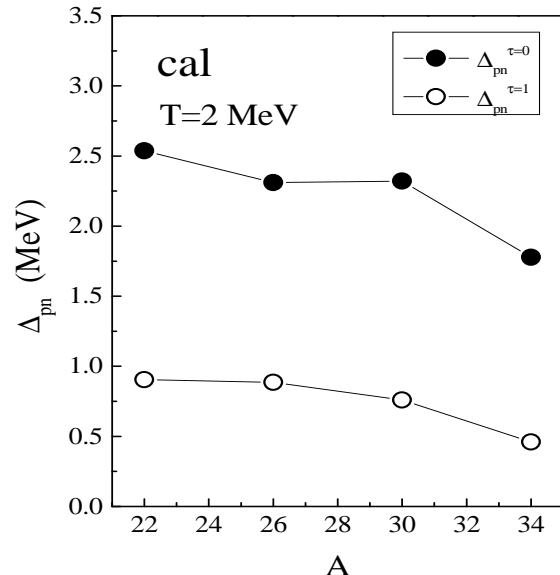

FIG. 2: Calculated thermal pn pairing gaps for odd-odd $N = Z$ nuclei at temperature $T = 2.0$ MeV. The solid circles denote the $\tau = 0$ pn pairing gap, and the open circles the $\tau = 1$ pn pairing gap.

($\sim 8\%$) of the quasiparticle random phase approximation (QRPA) with temperature [24]. We now calculate the temperature dependence of the symmetry energy using the shell model calculations. We estimate the symmetry energy coefficient from the thermal energy $E(Z, N, T)^{\tau}$ with isospin τ and temperature T obtained in the shell model calculations as follows:

$$a_{\text{sym}}(T) = \frac{E(Z, N, T)^{\tau} - E(Z, N, T)^{\tau'}}{\tau(\tau+1) - \tau'(\tau'+1)}A, \qquad (9)$$

where τ and τ' are different isospins for isobaric nuclei with same mass number A. At zero temperature, the calculated symmetry energy coefficient $a_{\text{sym}}(T = 0) \sim 16$ MeV for $A=24$ is in good agreement with the value determined from experimental masses and with the empirical value of Duflo and Zuker mass formula.

Figure 4 shows the symmetry energy coefficient a_{sym} as a function of the temperature for even-even $N \approx Z$ nuclei with mass number $A = 20$, 24, and 28, where several isobaric pairs of $N \approx Z$ nuclei such as (^{20}Ne,^{20}O), (^{24}Mg,^{24}Ne), and (^{28}Si,^{28}Mg) are chosen. This figure shows that the symmetry energy coefficients increase with increasing temperature in these three cases. Moreover, we can see that the symmetry energy coefficient depends on the mass A which is empirically fitted by adding the surface contribution with the $A^{-1/3}$ dependence at zero temperature. This mass dependence ap-

change of the symmetry energy coefficient $\delta a_{\mathrm{sym}}(T)$ does not change by this replacement.

In conclusion, we investigated the $\tau=0$ and $\tau=1$ pn pairing energies at finite temperature using the shell
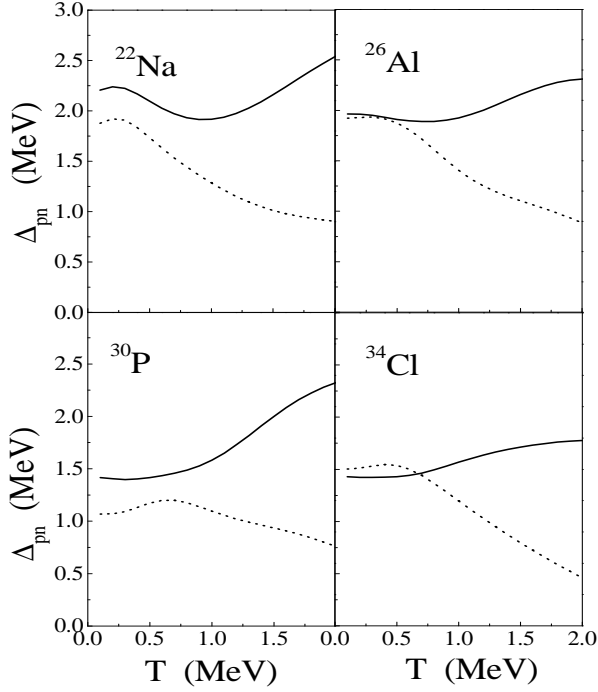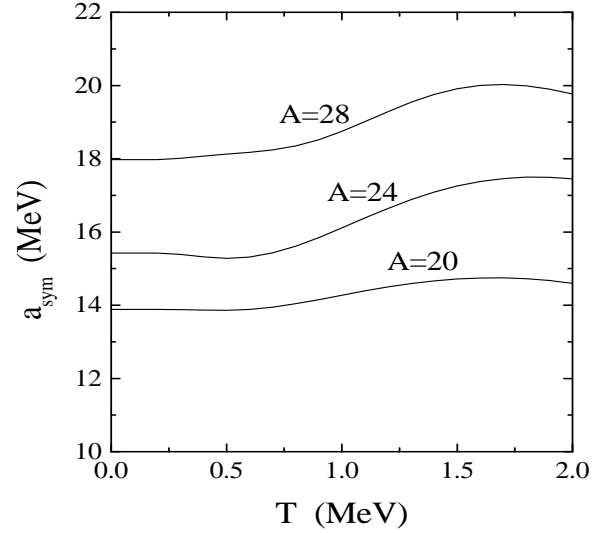

FIG. 3: Calculated thermal pn pairing gaps for odd-odd $N = Z$ nuclei as a function of temperature. The solid line denotes the $\tau=0$ pn pairing gap, and the dotted line the $\tau=1$ pn pairing gap.

pears in the $\tau = 0$ pn pairing gap estimated from the double difference of binding energies, in Fig. 1(b). Figure 4 also suggests that the mass dependence changes as temperature increases. To see the temperature dependence of the symmetry energy coefficient, we define the relative change of the symmetry energy coefficient with respect to temperature as

$$\delta a_{\mathrm{sym}}(T) \;=\; \frac{a_{\mathrm{sym}}(T) - a_{\mathrm{sym}}(T=0)}{a_{\mathrm{sym}}(T=0)}. \qquad (10)$$

Averaging the $\delta a_{\mathrm{sym}}(T)$ at $T = 1.0$ MeV over various pairs of nuclei, we obtain an increase $\sim 4\%$. This is in agreement with the SMMC result $\sim 3\%$ obtained after implementing the correction. We used here the form of symmetry energy $\tau(\tau + 1)$, which is motivated by the charge independence of the nuclear force. But as a phenomenological parametrization the isospin dependence $\tau(\tau + \alpha)$ with $\alpha \neq 1$ is also possible, where the linear term in τ is so-called Wigner term. Recently, empirical fitting to the Wigner term gave $\alpha = 1.25$ in the vicinity of the $N = Z$ line [2, 25]. However, the symmetry energy coefficient is affected little by replacing $\tau(\tau + 1)$ with $\tau(\tau + 1.25)$. Moreover, by definition the relative

FIG. 4: Symmetry energy coefficient a_{sym} as a function of temperature for $N \approx Z$ nuclei with mass number $A =$20, 24, and 28.

model calculations. The pn pairing gaps at finite temperature were estimated from the double differences of thermal energies defined by Eq. (7), which is analogous to the double differences of binding energies as indicators of the pn pairing energies at zero temperature. It was shown that as temperature increases the isoscalar pn pairing energy rather increases, while the isovector pn pairing energy decreases. Almost the same pn pairing gaps of stable $N = Z$ nuclei at zero temperature are separated with increasing temperature. We also studied the temperature dependence of the symmetry energy in $N \approx Z$ nuclei. The symmetry energy coefficients increase with increasing temperature. The increase of the calculated symmtery energy coefficient between $T = 0.0$ and $T = 1.0$ MeV is in good agreement with that of the SMMC calculations. We suggest that the pn pairing energies can be estimated using Eqs. (5) and (7) from the measured level densities of nuclei. We expect that the pn pairing energies play an important role in the astrophysics.

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