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To cite this article: H Nam and D J Dean 2013 J. Phys.: Conf. Ser. 445 012029

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Re-entrance in nuclei: competitive phenomena

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Abstract. Using the shell-model Monte Carlo method, we investigate how temperature and rotation affect pairing properties for nuclei in the fp - gds region. The re-entrance of pairing correlations with temperature is predicted at high rotational frequencies. It manifests through an anomalous behavior of the specific heat and level density.

1. Introduction

Phase transitions, as seen in superconductivity, superfluidity or ferromagnetism, are the result of competition between the order interaction and thermal fluctuations. Ordered phases (less symmetric) usually reside at lower temperatures and transition to disordered phases (more symmetric) at higher temperatures due to thermal fluctuations. Re-entrance (or partial order) phenomena manifests itself in successive phase transitions as a function of temperature or other extensive quantity. For example, re-entrance was discovered experimentally for liquid crystals in 1975 [1], showing a higher symmetry nematic phase occurring at a lower temperature than the lower symmetry smectic phase. Interestingly, the discovery of this phenomena led to many technological applications in electronic displays. Other condensed matter systems that display re-entrant phenomena include ferromagnetic insulators [2] and orbital antiferromagnetism [3].

The properties of nuclei are governed by the nuclear interactions. The singlet-S and triplet-P channels in the nucleon-nucleon interaction generate global nuclear pairing properties. Indeed, a large even-even nucleus will exhibit specific pairing properties, such as a large pairing gap from the ground state to the first excited state [4]. The nuclear Hamiltonian also generates other phenomena such as intrinsic deformation, with an experimental signature of the energy of a band of states increasing like $E(J) \sim J(J+1)$ where J is the spin of the state. Pairing and deformation are competitive phenomena in nuclei. One can heat a nucleus thermally and induce a pairing transition. This transition occurs at around a temperature of T = 0.7 - 1.5 MeV where thermal fluctuations overcome the effects of pairing [5–8]. A clearly defined peak occurs in the specific heat at these temperatures. If the nucleus is well deformed, that peak structure can be smeared. Early work on thermally assisted pairing predicted by Kammuri in 1964 [9], describes a local increase of pairing correlations in a rotating nucleus with excitation energy. One can also enhance or suppress structures in a nucleus through cranking, which practically involves adding to the Hamiltonian a time-reversal breaking term ωJ_z , where ω is the cranking frequency, and J_z is the projection of spin along the axis of rotation. As the cranking frequency increases, pairing within the nucleus should decrease due to spin alignment [10].

The objective of this work is to present a short survey on our studies using the shell-model Monte Carlo method to examine how temperature and rotation affect pairing properties on the

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N = 40 systems, ⁶⁸Ni, ⁷⁰Zn, ⁷²Ge and ⁸⁰Zr, which exhibit distinct phase-transitional behavior [10, 11]. Interestingly, we have found one system, ⁷²Ge in which a re-entrant phenomena occurs where at high cranking frequency there is a small window in temperature where pairing actually increases at a critical temperature [10]. This leads to a specific heat that shows a sharp decrease with temperature. We also present early results on current work investigating the phase-transitional behavior of the odd-odd N = Z nuclei, ⁷⁰Br, ⁷⁴Rb and ⁷⁸Y.

2. The Shell-Model Monte Carlo Method

The shell-model Monte Carlo (SMMC) method [12] allows investigations of nuclei at finite temperatures with the relevant degrees of freedom included. This makes it possible to account for the thermal and quantal fluctuations which are important to describe phase transformations in finite-size systems. The SMMC approach describes nuclear observables at finite-temperature as thermal averages

$$\langle A \rangle = \frac{Tr_N(Ae^{-\beta H})}{Tr_N e^{-\beta H}} \tag{1}$$

where $\beta = 1/T$ is the inverse temperature, Tr_N is the many-body trace at fixed particle number N, and $-\beta H$ is the imaginary-time many-body propagator. For certain classes of residual nucleon-nucleon interactions [13], like the attractive pairing+quadrupole force employed in this work, the evaluation of observables is exact, subject only to statistical errors related to the Monte Carlo integration. As we are concerned here with a description of collective quadrupole and pairing correlations at relatively low energies, we have employed a pairing+quadrupole-quadrupole Hamiltonian

$$H = \sum_{jmt_z} \epsilon(j) a_{jmt_z}^{\dagger} a_{jmt_z} - \frac{G}{4} \sum_{\alpha, \alpha', t_z} P_{JT=01, t_z}^{\dagger}(\alpha) P_{JT=01, t_z}(\alpha') - \chi \sum_{\mu} (-1)^{\mu} Q_{2\mu} Q_{2-\mu}, \qquad (2)$$

where $Q_{2\mu}$ is the mass quadrupole moment operator given by

$$Q_{2\mu} = \frac{1}{\sqrt{5}} \sum_{ac} \langle j_a \| \frac{dV}{dr} Y_2 \| j_c \rangle [a_{j_a}^{\dagger} \times \tilde{a}_{j_c}]^{2\mu}$$
(3)

with projection μ , $a_{jmt_z}^{\dagger}(a_{jmt_z})$ creates (destroys) a nucleon of isospin t_z in the orbital jm, and $\tilde{a}_{jm} = (-1)^{j+m} \hat{a}_{j-m}$, and the seniority pairing operator P^{\dagger} is defined as

$$P_{JT=01,t_{z}}^{\dagger}(\alpha) = (-)^{l} [a_{\alpha,t_{z}}^{\dagger} \times a_{\alpha,t_{z}}^{\dagger}]^{JM=00,T=1}$$
(4)

with $\alpha = \{n, l, j\}.$

The details of our SMMC calculations follow those of Refs. [10, 11]. Namely, calculations were performed in the complete (0f1p - 0g1d2s) model space for protons and neutrons. The singleparticle (s.p.) energies have been determined from a Woods-Saxon potential parametrization of ⁵⁶Ni. Using the parameters G = 0.106 MeV and $\chi = 0.0104$ MeV⁻¹ fm², we reproduce the lowenergy spectrum of ⁶⁴Ni and ⁶⁴Ge. Nuclei are described by valence protons and neutrons outside the closed core of ⁴⁰Ca. In order to generate the angular momentum polarization, we consider the Routhian $\hat{H}^{\omega} = \hat{H} - \omega \hat{J}_z$, where the cranking frequency ω (in units of MeV) enters through the cranking term. Our SMMC calculations were performed on Jaguar, a Cray XT5 at Oak Ridge National Laboratory (ORNL) with 18,688 nodes containing dual hex-core AMD Opteron processors, totalling 224,256 cores. Simulations investigated cranking frequencies $\omega = 0.0$ to 0.5 MeV and the temperature parameter β was split into $N_{\beta}\Delta\beta$ slices with $\Delta\beta = 1/32$ MeV⁻¹. Each parameter set was run with up to 15 840 statistical samples, requiring a total of 190,080 cores for 4 hours for a full parameter study of a single nucleus.

International Symposium on Exotic Nuclear Structure From Nucleons	(ENSFN 2012)	IOP Publishing
Journal of Physics: Conference Series 445 (2013) 012029	doi:10.1088/1742-	-6596/445/1/012029

3. Nuclei in the *fp-gds* region

To understand the competition between nuclear pairing correlations as a function of the rotational frequency and temperature for nuclei, we first apply the SMMC method to look at known nuclei in the fp - gds region where sizable pairing correlations dominate in their ground state without the effects of rotation. Studying the temperature-induced interplay between deformation and pairing in four N = 40 isotones, ⁶⁸Ni, ⁷⁰Zn, ⁷²Ge, and ⁸⁰Zr shows that shape and pairing contribute to the specific heat of the nucleus [11]. Theoretical studies to identify phase transitions in nuclei have focused on the relationship between pairing correlations and an associated peak in the specific heat $C_v = dE/d(kT)$. To assess the magnitude of pairing correlations, it is convenient to employ the J = 0 pair operator

$$\Delta^{\dagger} = \sum_{jm>0} a^{\dagger}_{jm} a^{\dagger}_{j\bar{m}}, \tag{5}$$

where we sum over orbitals with m > 0 and the time-reversed creation operator is $a_{j\bar{m}}^{\dagger} = (-)^{j-m} a_{j-m}^{\dagger}$. The observable $\langle \Delta^{\dagger} \Delta \rangle$, referred to as the J = 0 pairing strength, measures the number of J = 0, T = 1 pairs in the correlated nuclear state.



Figure 1. (color online). Neutron and proton J = 0 pairing strength $\langle \Delta^{\dagger} \Delta \rangle$ as a function of temperature for the four N = 40 isotones. Shown are proton and neutron pairing content with (Q+P) and without (Q) the pairing term included. Taken from [11].



Figure 2. (color online). Specific heat calculated as a function of temperature for the four N = 40 isotones. The squares (dashed line) indicate calculations with only the $Q \cdot Q$ part of the interaction present, while the circles (solid line) show both $P^{\dagger}P$ and $Q \cdot Q$ terms included. Taken from [11].

Figure 1 shows the neutron and proton J = 0 pairing strength and Fig. 2 shows the corresponding specific heat calculations for the four N = 40 isotones. Only for the full interaction (Q + P) do peaks appear in the specific heat corresponding to the increase in pairing strength at low temperatures. In the case of ⁶⁸Ni, proton pairing correlations are very weak and the peak in the C_v is associated with the collapse of the neutron pairing with temperature. For ⁷⁰Zn, the two peaks in the specific heat can be associated separately with the proton pairing and neutron pairing transitions to normal phase, which occur at different rates with temperatures, resulting in a pronounced single peak in C_v . In the strongly deformed ⁸⁰Zn, there is an absence of a sharp maxima in C_v with a pairing strength equal for proton and neutron that is significantly reduced from the lighter N = 40 isotones.

3.1. Re-entrance in ^{72}Ge

In the absence of rotation, the SMMC calculations [11] gives clear evidence for the breaking of isovector pairs at temperatures around $kT_c \approx 0.6$ MeV in ⁷²Ge which is reflected by a noticeable peak in the specific heat C_v . To study the effects of rotation, we employ the cranking term from $\omega = 0.0$ to 0.5 MeV. In a model of non-interacting particles, the neutrons in ⁷²Ge would completely occupy the fp shell. However, correlations induced by the residual interaction make it energetically favorable to scatter neutrons across the N=40shell gap which is about 2.5 MeV. From Ref. [10], we see the effects of rotating the nucleus. Figure 3 shows single-neutron occupations in the wave function of ⁷²Ge as a function of rotational frequency at two temperatures: kT = 0.47 meV (slighly above g.s.) and 1.6 MeV (well above T_c). In the g.s. configuration, the total neutron occupation of the gds shell is about 3.5, with about 3 neutrons in the $g_{9/2}$ orbital. Upon rotating the nucleus, the s.p. cranking term $\omega \hat{j}_z$, representing the combined effect of the Coriolis and centrifugal force, generates angular momentum polarization by lifting the magnetic *m*-degeneracy of s.p. states.



Figure 3. (color online). Neutron occupations of the individual $f_{7/2}, f_{5/2}$, and $g_{9/2}$ s.p. orbits as a function of cranking frequency ω in the wave function of ⁷²Ge for temperatures (a) kT = 0.47 MeV and (b) kT = 1.6 MeV. The angular momentum alignment in the nucleus is generated by the gradual increase of occupations of positive-*m* orbits (solid lines) at the expense of negative-*m* states (dashed lines). The doubled magnetic quantum numbers, 2m, of individual orbits are marked. Taken from [10].

The highly symmetric pattern of s.p. occupations seen in Fig.3(a) is due to an interplay between the Coriolis force, which tries to align individual single-particle angular momenta along the axis of rotation, thus introducing spatial polarization of the system, and the symmetry-restoring pairing force. At low temperatures, the occupations of the various m substates of the $g_{9/2}$ and $f_{5/2}$ orbitals do not follow a simple thermal ordering. In fact, the occupations of the substates with largest m values are largest, as expected from energy considerations, but far from one (the extreme s.p. limit). On the other hand, the states with the lowest negative m values have very similar reduced (but nonzero) occupations, indicating that the residual population, although disfavored by the cranking term, allows the system to gain energy through pairing.

If the nucleus is heated above T_c , or if the rotation is rapid, pairing correlations are dramatically reduced, as seen in Fig. 4. The neutron pairing locally increases with temperature at low values of T and high rotational frequencies. This is a clear signal of thermally assisted pairing. One of the signatures of re-entrance of the partial order is the anomalous specific heat behavior seen

in Fig. 5. At $\omega = 0.5$ MeV, the specific heat exhibits a clear local dip associated with the pairing re-entrance. A pronounced low-temperature, high-frequency irregularity is also seen in the level density ρ , shown in the inset of Fig. 5.





Figure 4. (color online). Neutron and proton J = 0 pairing strength $\langle \Delta^{\dagger} \Delta \rangle$ as a function of temperature for ⁷²Ge at four values of ω (in MeV). At higher rotational frequencies, neutron pairing locally increases at low temperatures reaching a maximum (marked by arrows). Taken from [10].

Figure 5. (color online). Specific heat calculated in SMMC for ⁷²Ge as a function of temperature at $\omega = 0.2$ and 0.5 MeV. At $\omega = 0.5$ MeV, C_v shows a local dip at low temperatures; this is a signature of pairing reentrance. The inset shows the calculated level density. Taken from [10].

3.2. Odd-odd, N = Z nuclei

We extend our studies on the effects of rotation and temperature on pairing correlations by exploring medium mass (A > 40) odd-odd self-conjugate N = Z nuclei. The proton-neutron (pn) interaction has long been recognized to play an important role in N = Z nuclei. The pn correlations can either correspond to isovector (T = 1) or isoscalar (T = 0) pairs. The pnpairing correlations are particularly important in self-conjugate odd-odd nuclei, evident in the ground state spins and isospins. The experimental ground state spins and isospins of virtually all odd-odd N = Z nuclei with $A \leq 40$ (with the exception of ³⁴Cl) have ground states with T = 0, J > 0 and are dominated by isoscalar pairing involving pn pairs in identical orbitals. In contrasts, medium mass odd-odd N = Z nuclei have T = 1 and J = 0 ground state isospins and spins (with the exception of ⁵⁸Cu), indicating the dominance of isovector pn pairing. The competition between isovector and isoscalar pairing is highlighted in the odd-odd N = Z nuclei ⁷⁴Rb, where experimental results identified the T = 0 and T = 1 bands [14]. The ground state band is identified as isospin T = 1, arising from isovector pn correlations, with T = 0 states favored at higher rotational frequency, or equivalently higher excitation energy at about 1.0 MeV.

To study the effects of rotation and temperature on pn pairing correlations in odd-odd N = Z nuclei, we performed SMMC calculations of ⁷⁴Rb and two adjacent odd-odd selfconjugate nuclei ⁷⁰Br and ⁷⁸Y. ⁷⁸Y has a highly deformed J = 0, T = 1 ground state with considerable quenching of the pn pairing compared to ⁷⁴Rb [15] and ⁷⁰Br is predicted to have a J = 0, T = 1 ground state [16], which has not been verified experimentally. Figure 6 shows SMMC calculations for (a) the heat capacity, C_v , (b) the J = 0 pairing strength, $\langle \Delta^{\dagger} \Delta \rangle$, and (c) the squared isospin $\langle T^2 \rangle$ as a function of temperature at different cranking frequencies of $\omega = 0.0, 0.2$, and 0.5 MeV. Results show that all three nuclei exhibit similar isospin behavior. At low temperature and small frequencies T = 1, so that T(T + 1) = 2 and at high frequency, T = 0 and T(T + 1) = 1, shown in Fig.6(c).



Fig.6(b) shows contrasting behavior to that seen in 72 Ge, where a local increase in the pairing strength occurs at low frequency and low temperature rather than at high frequency. A clear indicator of a phase transition, such as the dip seen for 72 Ge, does not appear for these nuclei seen in Fig 6(a). The high frequency specific heat exhibits interesting behavior for 74 Rb and 78 Y, by crossing the low frequency specific heat and remaining unusually high. Understanding of these new behaviors requires additional study.

The J = 0 pairing strength seen in

4. Conclusions

In summary, using the SMMC tech-Figure 6. (a) Specific heat, (b) the J = 0 pairing nique we explored the interplay bestrength, $\langle \Delta^{\dagger} \Delta \rangle$, and (c) $\langle T^2 \rangle$ calculated in SMMC for tween temperature and rotation in odd-odd N = Z nuclei ⁷⁰Br, ⁷⁴Rb, and ⁷⁸Y as a function fp - qds nuclei and its effect on pairing resulting in phase transitions. Our calculations demonstrate

the presence of the partial order phenomenon associated with the reappearance of pairing at high rotational frequencies and intermediate temperatures for 72 Ge. Similar behavior is not currently seen for odd-odd N = Z nuclei, but requires further studies to adequately understand results.

Acknowledgments

Supported by the U.S. Department of Energy under Contract No. DE-AC05-000R22725 with UT-Battelle, LLC (Oak Ridge National Laboratory). Computational resources provided by the Oak Ridge Leadership Computing Facility.

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