Pairing correlations in $N \sim Z$ pf-shell nuclei

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Abstract

We perform Shell Model Monte Carlo calculations to study pair correlations in the ground states of $N = Z$ nuclei with masses $A = 48 - 60$. We find that $T = 1, J^\pi = 0^+$ proton-neutron correlations play an important, and even dominant role, in the ground states of odd-odd $N = Z$ nuclei, in agreement with experiment. By studying pairing in the ground states of $^{52-58}$Fe, we observe that the isovector proton-neutron correlations decrease rapidly with increasing neutron excess. In contrast, both the proton, and trivially the neutron correlations increase as neutrons are added.

We also study the thermal properties and the temperature dependence of pair correlations for $^{50}$Mn and $^{52}$Fe as exemplars of odd-odd and even-even $N = Z$ nuclei. While for $^{52}$Fe results are similar to those obtained for other even-even nuclei in this mass range, the properties of $^{50}$Mn at low temperatures are strongly influenced by isovector neutron-proton pairing. In coexistence with these isovector pair correlations, our calculations also indicate an excess of isoscalar proton-neutron pairing over the mean-field values. The isovector neutron-proton correlations rapidly decrease with temperatures and vanish for temperatures above $T = 700$ keV, while the isovector correlations among like nucleons persist to higher temperatures. Related to the quenching of the isovector proton-neutron correlations, the average isospin decreases from 1, appropriate for the ground state, to 0 as the temperature increases.
I. INTRODUCTION

Proton-rich radioactive ion-beam facilities offer the novel possibility of exploring the structure of nearly self-conjugate ($N \sim Z$) nuclei in the medium mass range $Z \lesssim 50$. Special interest will be devoted to understanding the proton-neutron ($p_n$) interaction, which has long been recognized to play a particularly important role in $N = Z$ nuclei. The $p_n$ correlations can either correspond to isovector ($T = 1$) or isoscalar ($T = 0$) pairs. Like proton-proton (pp) and neutron-neutron (nn) pairing, isovector $p_n$ correlations in light to medium mass nuclei are assumed to involve a proton-neutron pair in time-reversed spatial orbitals, while the isoscalar correlations involve mainly pairing between identical orbitals and spin-orbit partners $^1$.

The importance of $p_n$ correlations in self-conjugate odd-odd nuclei is evident from the ground state spins and isospins. In the $sd$-shell, odd-odd $N = Z$ nuclei (with the exception of $^{34}$Cl) have ground states with isospin $T = 0$ and angular momenta $J > 0$, pointing to the importance of isoscalar $p_n$ pairing between identical orbitals. In contrast, self-conjugate $N = Z$ nuclei in the medium mass range ($A > 40$) have ground states with $T = 1$ and $J^{\pi} = 0^+$ (the only known exception is $^{58}$Co) indicating the dominance of isovector $p_n$ pairing.

Additional confirmation of the importance of $T = 1$ $p_n$-pairing in medium-mass odd-odd $N = Z$ nuclei is an experiment that identified the $T = 0$ and $T = 1$ bands in $^{74}$Rb $^2$. An isospin $T = 1$, arising from isovector $p_n$ correlations, has been assigned to the ground state rotational band in this nucleus. At higher rotational frequency, or equivalently higher excitation energy, a $T = 0$ rotational band becomes energetically favored.

The competition of isovector and isoscalar $p_n$ pairing has been extensively studied for $sd$-shell nuclei $^3$ and for nuclei at the beginning of the $pf$-shell $^4$ using the Hartree-Fock-Bogoliubov (HFB) formalism. A major result $^4$ is that $T = 0$ $p_n$ correlations dominate $T = 1$ correlations in the $N = Z$ nuclei studied; $T = 1$ $p_n$ pairing was never found to be important. As mentioned above, this is surprising since the $T = 1$ ground state isospin of most odd-odd $N = Z$ nuclei with $A \geq 40$ clearly points to the importance of $T = 1$ $p_n$ pairing in these nuclei. It has been pointed out recently that HFB calculations for intermediate mass nuclei can exhibit nearly degenerate minima that may or may not involve important $T = 1$ $p_n$ correlations $^3$. However, these studies assume that the $T = 1$ $p_n$ pairing strength is larger than the nn and pp pairing strengths.

Although HFB calculations have already pioneered the study of pairing in $N = Z$ nuclei, the method of choice to study pair correlations is the interacting shell model. Within the $sd$ shell $^3$ and at the beginning of the $pf$-shell $^4,5$ the interacting shell model has proven to give an excellent description of all nuclei, including the correct reproduction of the spin-isospin assignments of self-conjugate $N = Z$ nuclei. However, the conventional shell model using diagonalization techniques is currently restricted to nuclei with masses $A \leq 48$ due to computational limitations. These limitations are overcome by the recently developed Shell Model Monte Carlo (SMMC) approach $^6,7$. Using this novel method, it has been demonstrated $^8$ that complete $pf$ shell calculations using the modified Kuo-Brown interaction well reproduce the ground state properties of even-even and $N = Z$ nuclei with $A \leq 60$; for heavier nuclei an extension of the model space to include the $g_{9/2}$ orbitals is necessary. Additionally the SMMC approach naturally allows the study of
thermal properties. First studies have been performed for several even-even nuclei in the astrophysically interesting mass range $A = 54 - 60$ [12,13].

In this paper we extend SMMC studies to detailed calculations of the $N = Z$ nuclei with $A = 50 - 60$. The studies consider all configurations within the complete $pf$-shell model space. Special attention is paid to isovector and isoscalar pairing correlations in the ground states. To elucidate the experimentally observed competition between $T = 1$ and $T = 0$ correlations as a function of excitation energy, we have also performed SMMC studies of the thermal properties of an even-even and an odd-odd $N = Z$ nucleus ($^{52}$Fe and $^{50}$Mn, respectively). In particular, we discuss the differences in the thermal behavior of the pair correlations, and other selected observables, in these nuclei.

II. MODEL

The SMMC approach was developed in Refs. [9,10], where the reader can find a detailed description of the ideas underlying the method, its formulation, and numerical realization. As the present calculations follow the formalism developed and published previously, a very brief description of the SMMC approach suffices here. A comprehensive review of the SMMC method and its applications can be found in Ref. [14].

The SMMC method describes the nucleus by a canonical ensemble at temperature $T = \beta^{-1}$ and employs a Hubbard-Stratonovich linearization [15] of the imaginary-time many-body propagator, $e^{-\beta H}$, to express observables as path integrals of one-body propagators in fluctuating auxiliary fields [9,10]. Since Monte Carlo techniques avoid an explicit enumeration of the many-body states, they can be used in model spaces far larger than those accessible to conventional methods. The Monte Carlo results are in principle exact and are in practice subject only to controllable sampling and discretization errors. The notorious “sign problem” encountered in the Monte Carlo shell model calculations with realistic interactions [16] can be circumvented by a procedure suggested in Ref. [12], which is based on an extrapolation from a family of Hamiltonians that is free of the sign problem to the physical Hamiltonian. The numerical details of our calculation parallel those of Refs. [11,12].

As we will show below, isovector pair correlations depend strongly on the neutron excess in $N \sim Z$ nuclei, so that a proper particle number projection is indispensable for a meaningful study of these correlations. We stress that this important requirement is fulfilled by the present SMMC approach, which uses a canonical expectation value for all observables at a given temperature; i.e., the proper proton and neutron numbers of the nuclei are guaranteed by an appropriate number projection [10,14].

The main focus of this paper is on pairing correlations in the three isovector $J^\pi = 0^+$ channels and the isoscalar proton-neutron correlations in the $J^\pi = 1^+$ channel. In complete $0\hbar\omega$ shell model calculations, the definition of the pairing strength is somewhat arbitrary. In this paper, we follow Ref. [13] in our description of pairing correlation and define a pair of protons or neutrons with angular momentum quantum numbers $(JM)$ by ($c = \pi$ for protons and $c = \nu$ for neutrons)

$$A^\dagger_{JM}(j_a, j_b) = \frac{1}{\sqrt{1 + \delta_{j_aj_b}}} [c_{j_a}^\dagger c_{j_b}^\dagger]_{(JM)},$$  

(1)
where $\pi^+_j (\nu^+_j)$ creates a proton (neutron) in an orbital with total spin $j$. The isovector (plus sign) and isoscalar (minus sign) proton-neutron pair operators are given by

$$A^+_{JM}(j_a, j_b) = \frac{1}{\sqrt{2(1 + \delta_{j_a j_b})}} \left[ \nu^+_j \pi^+_j \pm \pi^+_j \nu^+_j \right]_{JM}.$$  

With these definitions, we build up a pair matrix

$$M_{\alpha\alpha'} = \sum_M \langle A^+_{JM}(j_a, j_b) A_{JM}(j_c, j_d) \rangle,$$

which corresponds to the calculation of the canonical ensemble average of two-body operators like $\pi^+_1 \pi^+_3 \pi^+_4$. The index $\alpha$ distinguishes the various possible $(j_a, j_b)$ combinations (with $j_a \geq j_b$). The square matrix $M$ for the $pf$ shell has dimension $N_J = 4$ for $J = 0$ and $N_J = 7$ for $J = 1$. In Ref. [13] the sum of the eigenvalues of the matrix $M^J$ (its trace) has been introduced as a convenient overall measure for the strength of pairs with spin $J$:

$$P^J = \sum_\beta \lambda^J_\beta = \sum_\alpha M^J_{\alpha\alpha},$$

where the $\lambda^J_\beta$ are eigenvalues of the matrix $M$.

An alternative often used to measure the overall pair correlations in nuclear wave functions, is in terms of the BCS pair operator

$$\Delta^+_{JM} = \sum_\alpha A^+_{JM}(\alpha).$$

The quantity $\sum_M \langle \Delta^+_{JM} \Delta_{JM} \rangle$ is then a measure of the number of nucleon pairs with spin $J$. We note that, for the results discussed in this paper, the BCS-like definition for the overall pairing strength yields the same qualitative results for the pairing content as the definition (4). Some SMMC results for BCS pairing in nuclei in the mass range $A = 48 - 60$ are published in Refs. [11,13,14,17].

With our definition (4) the pairing strength is non-negative, and indeed positive, at the mean-field level. The mean-field pairing strength, $P^J_{mf}$, can be defined as in (3,4), but replacing the expectation values of the two-body matrix elements in the definition of $M^J$ by

$$\langle c^+_1 c^+_2 c^+_3 c_4 \rangle \rightarrow n_1 n_2 (\delta_{15} \delta_{24} - \delta_{15} \delta_{24}) ,$$

where $n_k = \langle c^+_k c_k \rangle$ is the occupation number of the orbital $k$. This mean-field value provides a baseline against which true pair correlations can be judged.

**III. RESULTS**

Our SMMC studies for self-conjugate nuclei with $A = 48 - 60$ have been performed using the modified Kuo-Brown KB3 residual interaction [18]. Some results of these studies for observables like ground state energies and total Gamow-Teller, $B(M1)$, and $B(E2)$ strengths have already been presented in Ref. [11]. As for other $pf$-shell nuclei, the SMMC results for the self-conjugate nuclei are generally in very good agreement with data.
As is customary in shell model studies, the Coulomb interaction has been neglected, which we believe is a justified approximation in this mass range. Thus, our shell model Hamiltonian is isospin-invariant and, as a consequence, there are symmetries in the pairing strengths of the three isovector \( J^\pi = 0^+ \) channels. For even-even \( N = Z \) nuclei, \( P^{J=0} \) is identical for pp, pn and nn pairing. In odd-odd self-conjugate nuclei (with ground state isospin \( T = 1 \)), the equality of the pp and nn channels remains, but the pn part of the isovector multiplet \( P^{J=0} \) can differ from the other two components (\( P^{J=0}_{pp} = P^{J=0}_{nn} \neq P^{J=0}_{pn} \)). At the mean-field level, the three components of the isovector pairing multiplet are identical for both odd-odd and even-even \( N = Z \) nuclei.

A. Pairing in the ground states of self-conjugate pf-shell nuclei

Our SMMC calculations for the even-even nuclei have been performed at finite temperatures \( T = 0.5 \) MeV, which has been found sufficient in previous studies to guarantee cooling into the ground state. The odd-odd nuclei were studied at \( T = 0.4 \) MeV. Since the latter have experimentally a low-lying excited state with an excitation energy of about 0.2 MeV, our “ground state” calculations for these nuclei corresponds to a mixture of the ground and first excited states.

As expected, we calculate vanishing isospin and angular momentum expectation values (\( \langle T^2 \rangle \) and \( \langle J^2 \rangle \), respectively) for the ground states of the even-even nuclei. For the odd-odd nuclei our calculations yield isospin expectation values \( \langle T^2 \rangle = 2.2 \pm 0.3 \) for \( ^{50}\text{Mn} \), and \( 1.8 \pm 0.2 \) for \( ^{54}\text{Cu} \), in good agreement with experiment, as both \( ^{50}\text{Mn} \) and \( ^{54}\text{Co} \) have a \( T = 1 \) ground state, so that \( T(T+1) = 2 \). For \( ^{58}\text{Cu} \) we find \( \langle T^2 \rangle = 1.4 \pm 0.2 \), while the experimental level spectrum has a \( T = 0 \) \( 1^+ \) ground state and a \( T = 1 \) \( 0^+ \) first excited state at \( E_x = 0.2 \) MeV. The error bars in our calculations for the angular momentum expectation values (\( \langle J^2 \rangle = -1.4 \pm 4.5 \) for \( ^{50}\text{Mn} \), \( -7.0 \pm 7.5 \) for \( ^{54}\text{Co} \) and \( 3.0 \pm 4.0 \) for \( ^{58}\text{Cu} \)) prohibit meaningful comparison with experiment. We note that the SMMC also reproduces the \( T = 1 \) isospin of the \( ^{62}\text{Ga} \) and \( ^{74}\text{Rb} \) ground states (using the \( p, f_{5/2}, g_{9/2} \) model space [20]). Detailed calculations of the pairing in these two nuclei will be presented in [20].

We have calculated the isovector and isoscalar pairing strengths in the ground states of the self-conjugate nuclei with \( A = 48 - 60 \) using the definition (4). The results are presented in Fig. 1, where they are also compared to the mean-field values derived using Eq. (6). Discussing the isovector \( J = 0 \) pairing channels first, Fig. 1 shows an excess of pairing correlations over the mean-field values. For the even-even nuclei, this excess represents the well-known pairing coherence in the ground state. In addition, Fig. 1 exhibits a remarkable staggering in the \( J = 0 \) pp and nn pairing channels (\( P^{J=0}_{pp} = P^{J=0}_{nn} \)) and in the pn pairing channel (\( P^{J=0}_{pn} \)) when comparing neighboring even-even and odd-odd self-conjugate nuclei. In the latter, the isovector pn pairing clearly dominates the pp and nn pairing and is always significantly larger than in the neighboring even-even \( N = Z \) nuclei. In contrast, the like-nucleon pairing is noticeably reduced in the odd-odd nuclei relative to the values in the neighboring even-even nuclei.

The odd-even staggering is not visible in the total \( J = 0 \) pairing strength,

\[
P^{J=0}_{tot} = P^{J=0}_{pp} + P^{J=0}_{nn} + P^{J=0}_{pn},
\]
as can be seen in Fig. 1. Although the excess of $P_{J=0}^{I}$ over the mean-field value is significant, it is about equal for the “open shell” nuclei $^{48}\text{Cr}$, $^{50}\text{Mn}$, $^{52}\text{Fe}$ and $^{60}\text{Zn}$. Towards the $N = 28$ shell closure the excess decreases and becomes a minimum for the double-magic nucleus $^{56}\text{Ni}$. In fact, the excess of $P_{J=0}^{I}$ over the mean-field value is only $0.42 \pm 0.1$ in $^{56}\text{Ni}$ (or about 13% of $P_{J=0}^{I}$), while it is $2.1 \pm 0.1$ in $^{48}\text{Cr}$ (or about 35%). We thus conclude that the change in the total pairing strength in the $N = Z$ nuclei is governed by shell effects, but that there is a significant redistribution of strength between the like- and unlike-pairs in going from even-even to odd-odd nuclei, with pn pairing favored in the latter.

Our calculations indicate that the $J = 1$ pn channel is the most important isoscalar pairing channel in the ground states. As is shown in Fig. 1, there is a modest excess of $J = 1$ isoscalar pn pairing over the mean-field values in all nuclei studied. The calculations indicate a slight even-odd staggering in the pairing excess, with the excess being larger in the even-even nuclei. Apparently the strong isovector pn pairing decreases not only the isovector pairing between like nucleons, but also the isoscalar pn pairing. As in the isovector channels, the excess of isoscalar pairing is strongly decreased close to the $N = 28$ shell closure, where the nuclei become spherical. It is well-known that isoscalar $J = 1$ pn pairing is important in deformed nuclei like $^{48}\text{Cr}$. We note that within the uncertainties of the calculation, our studies do not show any pairing excess above the mean-field values in the $J = 3$, 5, and 7 isoscalar channels.

It is interesting to compare the present SMMC results for the isovector pairing strength with those of a simple seniority-like model with an isospin-invariant pairing Hamiltonian [17]. One finds that the magnitude of the isovector pairing correlations is smaller in the SMMC studies than in the simple pairing model, as in the realistic shell model these correlations compete with other nucleonic correlations (e.g. the isoscalar pairing, which had not been considered in Ref. [17]). However, it is remarkable that the simple pairing model reproduces the odd-even staggering seen in the SMMC studies.

Using the HFB approach, Wolter et al. have studied pairing in $^{48}\text{Cr}$, restricting themselves to considering isovector and isoscalar pairing separately [4]. These authors find the isoscalar pairing mode to be considerably stronger than the isovector [4]. This finding is not supported by our SMMC calculation; it might be caused by the fact that the HFB solutions had not been projected on the appropriate ground state angular momentum. In fact, the HFB solutions have $\langle J^2 \rangle \gg 0$, making the presence of aligned pairs necessary. The SMMC calculations, which have $\langle J^2 \rangle \approx 0$, do not show the importance of aligned pairing in the $^{48}\text{Cr}$ ground state.

To investigate how the various pairing strengths change if the proton-neutron symmetry of the $N = Z$ nuclei is broken by adding additional neutrons, we have performed a series of SMMC studies for the iron isotopes $^{52-58}\text{Fe}$; the results are shown in Fig. 2. The striking result is that the excess of isovector pn pairing over the mean-field values is decreased drastically upon adding neutrons and has practically vanished in $^{56,58}\text{Fe}$. In contrast the excess in both $J = 0$ pp and nn pairing is increased by moving away from charge symmetry. At the mean-field level pp pairing is virtually unchanged through an isotope chain, while adding neutrons increases the nn pairing. The excess in total pairing strength $P_{tot}^{I=0}$ within the isotope chain increases only slightly as neutrons are added. Fig. 2 also shows that the excess of $P_{pn}^{I=1}$ pairing decreases with neutron excess. However, this decline is less
dramatic than for $P_{pn}^{J=0}$ and it appears that in nuclei with neutron excess, isoscalar ($J = 1$) pn correlations are more important than isovector. This finding is in agreement with the observation that isoscalar pn pairing is mainly responsible for the quenching of the Gamow-Teller strength \cite{19}, as those SMMC investigations have been performed for nuclei with $N > Z$.

Note that $^{54}$Fe is exceptional as it is magic in the neutron number ($N = 28$). As a consequence, the excess of nn pairing, and also of isovector and isoscalar pn pairing, is low compared to the other isotopes.

Our SMMC results for pairing correlations as function of neutron excess thus yield the following simple picture. Adding neutron pairs apparently increases the collectivity of the neutron condensate so that there are fewer neutrons available to pair with protons. As a result, protons pair more often with other protons, in this way increasing the proton collectivity, although the total number of protons, of course, remains unchanged.

Based on the results of their simple pairing model, the authors of Ref. \cite{17} come to the same conclusions. In fact, the SMMC results for the changes of isovector pairing within an isotope chain again agree well with the simple pairing model. However, the ground state in the latter is nearly a product of pp and nn condensates (in the limit of large neutron excess), while protons and neutrons in the realistic SMMC calculations still couple via isoscalar (mainly $J = 1$) correlations.

\section*{B. Thermal properties of $^{50}$Mn and $^{52}$Fe}

To study the thermal properties of odd-odd and even-even $N = Z$ nuclei we have performed SMMC studies of $^{50}$Mn and $^{52}$Fe at selected temperatures $T \leq 2$ MeV; the results are presented in Figs. 3 and 4. As we will show in the following, the thermal properties of the two nuclei are dominated by the three isovector $J = 0$ and the isoscalar $J = 1$ proton-neutron correlations; differences between the two nuclei can be traced to differences in the thermal behavior of these correlations.

We note again that the three isovector $J = 0$ pairing correlations are identical in even-even $N = Z$ nuclei. As discussed above, these correlations show a strong coherence and dominate the ground state properties of $^{52}$Fe. The temperature dependence of the $J = 0$ pp correlations in $^{52}$Fe is very similar to those of the other even-even iron isotopes $^{54-58}$Fe, which have been discussed in Refs. \cite{12,13}. As in the other iron isotopes, the SMMC calculations predict a phase transition in a rather narrow temperature interval around $T = 1$ MeV, where the $J = 0$ pairs break. Due to $N = Z$ symmetry, this phase transition also occurs in the $J = 0$ pn channel. This behavior is different from the iron isotopes with neutron excess. There the pn $J = 0$ correlations have only a small excess at low temperatures, where $J = 0$ pairing among like nucleons dominates, and this excess actually increases slightly when the like-pairs break \cite{13}. We also observe that the excess in the isoscalar $J = 1$ pn correlations is about constant at temperatures below 2 MeV. Thus, these correlations persist to higher temperatures than the isovector $J = 0$ pairing, as has already been pointed out in Ref. \cite{13}.

The pairing phase transition is accompanied by a rapid increase in the moment of inertia, $I = \langle J^2 \rangle / (3T) \cite{13}$, and a partial unquenching (orbital part) of the total M1 strength. The total Gamow-Teller strength also unquenches partially at the phase transition, related
to the fact that the vanishing of the $J = 0$ pn correlations reduces the quenching for Gamow-Teller transitions between identical orbitals (mainly the $f_{7/2}$ proton to $f_{7/2}$ neutron transitions). The residual quenching of the Gamow-Teller strength at temperatures above the phase transition (the single particle value is 13.1 calculated from the various ground state occupation numbers) is caused by the isoscalar pn correlations, which persist to higher temperatures (see Fig. 3). We note that the temperature evolution of the Gamow-Teller transition is different in $^{52}$Fe than in the iron isotopes with neutron excess $^{12,13}$. In the latter, $J = 0$ pn correlations do not show any significant excess over the mean-field values, and in particular, do not exhibit the phase transition as in $^{52}$Fe. As a consequence, the Gamow-Teller strength in nuclei with neutron excess is roughly constant across the pairing phase transition, without any noticeable unquenching.

As required by general thermodynamic principles, the internal energy increases monotonically with temperature. The heat capacity $C(T) = dE/dT$ is usually associated with a level density parameter $a$ by $C(T) = 2a(T)T$. As is typical for even-even nuclei $^{12}$ $a(T)$ increases from $a = 0$ at $T = 0$ to a roughly constant value at temperatures above the phase transition. We find $a(T) \approx 5.3 \pm 1.2$ MeV$^{-1}$ at $T \geq 1$ MeV, in agreement with the empirical value of 6.5 MeV$^{-1}$ $^{21}$. At higher temperatures, $a(T)$ must decrease due to the finite model space of our calculation. The present temperature grid is not fine enough to determine whether $a(T)$ exhibits a maximum related to the phase transition, as suggested in $^{12}$.

As expected for an even-even nucleus, $\langle T^2 \rangle$ is zero at low temperatures and then slowly increases with temperature as higher isospin configurations are mixed in.

The thermal properties of $^{50}$Mn (Fig. 4) show some distinct differences from $^{52}$Fe, which we believe are typical for odd-odd $N = Z$ nuclei in this mass range. As already stressed in the last section, $J = 0$ pn correlations dominate the ground state properties. With increasing temperature these correlations decrease rapidly and steadily and have already dropped to the mean-field value at $T = 0.8$ MeV. (The fact that the correlations actually become slightly negative is unphysical and due to uncertainties in the extrapolation required to avoid the sign problem $^{14}$.) We have verified the qualitative results of our calculation for an isospin invariant pairing+quadrupole Hamiltonian which does not exhibit the sign problem $^{22}$. The $J = 0$ pp (and the identical nn) correlations show the same phase transition near $T = 1$ MeV, as in $^{52}$Fe and the other even-even nuclei $^{12,13}$. In contrast however, the excess of the $J = 0$ correlations between like nucleons in $^{50}$Mn is noticeably smaller at low temperatures. As in $^{52}$Fe, the moment of inertia of $^{50}$Mn increases drastically when the $J = 0$ pairs break.

We observe that the isoscalar $J = 1$ pairing in $^{50}$Mn is rather similar to that in $^{52}$Fe. In particular the excess of these correlations is roughly constant in the temperature range where the isovector $J = 0$ correlations vanish and persists to higher temperatures than the excess in the isovector correlations.

Related to the rapid decrease of isovector pn pairing with temperature, the isospin expectation value drops from $\langle T^2 \rangle = 2$ at $T \leq 0.5$ MeV to $\langle T^2 \rangle \approx 0.2 \pm 0.2$ at $T = 1.0$ MeV; the unpaired proton and neutron apparently recouple from an isovector $J = 0$ coupling to an isoscalar $J = 1$ coupling. At temperatures above $T = 1$ MeV (i.e., above the phase transition for like-nucleon pairs), the temperature dependences of the isospin expectation values in $^{50}$Mn and $^{52}$Fe are similar.

The temperature dependence of the energy $E = \langle H \rangle$ in $^{50}$Mn is significantly different
than that in the even-even nuclei. As can be seen in Fig. 4, $E$ increases approximately linearly with temperature, corresponding to a constant heat capacity $C(T) \approx 5.4 \pm 1 \text{ MeV}^{-1}$; the level density parameter decreases like $a(T) \sim T^{-1}$ in the temperature interval between 0.4 MeV and 1.5 MeV. We note that the same linear increase of the energy with temperature is observed in SMMC studies of odd-odd $N = Z$ nuclei performed with a pairing+quadrupole hamiltonian [22] and thus appears to be generic for self-conjugate odd-odd $N = Z$ nuclei.

From the discussion above, we conclude that the main effect of heating the nuclei $^{50}\text{Mn}$ and $^{52}\text{Fe}$ to temperatures around 1.5 MeV is to release the pairing energy stored in the isovector $J = 0$ correlations. From Fig. 1 (i.e., $P_{\text{tot}}^J$) we expect that this pairing energy is about the same for both nuclei. This is in fact confirmed by our calculation: Using a linear extrapolation to zero temperature, we find an internal excitation energy of about 8.6 MeV at $T = 1.6$ MeV in $^{50}\text{Mn}$, which agrees nicely with the value for $^{52}\text{Fe}$, if we approximate $E(T = 0) = E(T = 0.5 \text{ MeV})$. The apparent difference between the two nuclei is that, with increasing temperature, a strong pairing gap in the three isovector $J = 0$ channels has to be overcome in $^{52}\text{Fe}$, while no such strong gap in the dominant isovector $pn$ channel appears to exist in the odd-odd $N = Z$ nucleus $^{50}\text{Mn}$.

Associated with the decrease of the isovector $pn$ correlations, the Gamow-Teller strength in $^{50}\text{Mn}$ unquenches with heating to $T = 1 \text{ MeV}$. This is noticeably different than in even-even nuclei, where the Gamow-Teller strength is roughly constant at temperatures below the pairing phase transition. We stress that the $B(GT)$ strength, however, remains noticeably quenched even above $T = 1 \text{ MeV}$ due to the persistence of the isoscalar $pn$ correlations; the mean-field value for the Gamow-Teller strength increase only slightly from 11.1 at $T = 0.4 \text{ MeV}$ to 11.6 at $T = 2 \text{ MeV}$.

The $B(M1)$ strength in $^{50}\text{Mn}$ decreases when the isovector $pn$ correlations vanish. It unquenches at $T \geq 0.8 \text{ MeV}$, related to the breaking of the pp and nn pairs, as shown in [13]. As in even-even nuclei, the $B(M1)$ strength in $^{50}\text{Mn}$ remains quenched even for $T \approx 2 \text{ MeV}$ (the mean-field value is 33.6 $\mu_\text{N}^2$ at $T = 2 \text{ MeV}$) due to the persisting isoscalar $pn$ pairing.

IV. CONCLUSION

We have studied pairing correlations in self-conjugate nuclei in the middle of the $pf$ shell; our calculations are the first to take all relevant two-nucleon correlations into account. Our study is based on SMMC calculations of these nuclei within the complete $pf$ shell employing the realistic Kuo-Brown interaction KB3. Several results of our investigation are noteworthy.

The isovector $J = 0$ pairing correlations show a significant staggering between odd-odd and even-even $N = Z$ nuclei. While the three isovector channels have identical strengths in even-even $N = Z$ nuclei, the total isovector pairing strength is strongly redistributed in odd-odd self-conjugate nuclei, with a strong enhancement of the proton-neutron correlations. This redistribution manifests itself in a significantly different temperature dependence of observables like the $GT$ and $B(M1)$ strengths and the internal energy.

The importance of isovector proton-neutron correlations decrease drastically if neutrons are added. These additional neutrons increase the coherence among the neutron condensate, thus making less neutrons available for isovector proton-neutron correlations. At the
same time, the correlations among protons also increase if neutrons are added. Our calculations indicate that in nuclei with large neutron excess, isoscalar ($J = 1$) proton-neutron correlations dominate over isovector proton-neutron pairing.

We have studied the temperature dependence of the pairing correlations and of selected observables for $^{50}$Mn and $^{52}$Fe. While the even-even $N = Z$ nucleus $^{52}$Fe shows the same qualitative trends as other even-even nuclei in this mass region (including a pairing phase transition at temperatures near $T = 1$ MeV), the results for the odd-odd nucleus $^{50}$Mn differ in some interesting aspects. While the proton-proton and neutron-neutron correlations (although much weaker than in even-even nuclei) show a phase transition near $T = 1$ MeV, the dominant $J = 0$ proton-neutron correlations decrease steadily with increasing temperature. As a consequence the internal energy increases linearly with temperature, indicating that there is no pairing gap in the $J = 0$ proton-neutron channel to be overcome.

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FIGURES

FIG. 1. Pairing correlations $P^J$ in the ground state of the $N = Z$ nuclei with masses $A = 48 - 60$. The full circles show the SMMC results, while the open circles are the mean-field values. $P_{\text{tot}}^{J=0}$ gives the sum of the three isovector pair correlations in the $J = 0$ channel. Note that $P_{pp}^{J=0} = P_{nn}^{J=0}$ for $N = Z$ nuclei.

FIG. 2. Pairing correlations $P^J$ in the ground states of the even iron isotopes $^{52-58}\text{Fe}$. The full circles show the SMMC results, while the open circles are the mean-field values. $P_{\text{tot}}^{J=0}$ gives the sum of the three isovector pair correlations in the $J = 0$ channel.

FIG. 3. Thermal properties of $^{52}\text{Fe}$. The SMMC results are shown with error bars, while the lines indicate the mean-field values for the respective pair correlations.

FIG. 4. Thermal properties of $^{50}\text{Mn}$. The SMMC results are shown with error bars, while the lines indicate the mean-field values for the respective pair correlations.
