Temperature Dependence of Pair Correlations in Nuclei in the Iron-Region

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Abstract

We use the shell model Monte Carlo approach to study thermal properties and pair correlations in $^{54,56,58}\text{Fe}$ and in $^{56}\text{Cr}$. The calculations are performed with the modified Kuo-Brown interaction in the complete $1p0f$ model space. We find generally that the proton-proton and neutron-neutron $J = 0$ pairing correlations, which dominate the ground state properties of even-even nuclei, vanish at temperatures around 1 MeV. This pairing phase transition is accompanied by a rapid increase in the moment of inertia and a partial unquenching of the M1 strength. We find that the M1 strength totally unquenches at higher temperatures, related to the vanishing of isoscalar proton-neutron correlations, which persist to higher temperatures than the pairing between like nucleons. The Gamow-Teller strength is also correlated to the isoscalar proton-neutron pairing and hence also unquenches at a temperature larger than that of the pairing phase transition.

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I. MOTIVATION

It has long being recognized that pairing correlations play an essential role in low-energy nuclear physics. In fact, mean-field theories like Hartree-Fock+BCS (which adds pairing as an additional degree of freedom to the mean-field solution) or the more consistent Hartree-Fock-Bogoliubov theory have proven to be quite successful in the general description of ground states of even-even nuclei. Although in many cases pairing among like nucleons is sufficiently well approximated by Cooper pairs (in which a nucleon is coupled to its time-reversed partner) phenomenology indicates that d-wave pairs of like nucleons play an important role in deformed heavier nuclei, such as those of the rare-earth region. This observation prompted the development of the Interacting Boson Model, which is remarkably successful in describing low-lying nuclear spectra [2].

The properties of nuclei at finite temperature have attracted recent experimental [3] and theoretical [4–6] interest. Although it is obvious that the influence of pairing decreases with temperature and must vanish in the high-temperature limit, the mean-field description of nuclei at finite temperature is inadequate due to the neglect of important quantum and statistical fluctuations [4]. Recently developed shell model Monte Carlo (SMMC) methods [7] do not have this shortcoming and also allow the consideration of model spaces large enough to account for the relevant nucleon-nucleon correlations at low and moderate temperatures ($T \leq 1.4$ MeV [8]).

A first study considered the thermal properties of $^{54}$Fe within the SMMC approach [8]. An important result was that the like-pair correlations, described by the BCS-like proton and neutron monopole pairs, vanish in a small temperature interval around $T = 1$ MeV. This pairing phase transition is accompanied by a rather sharp rise of the moment of inertia and a partial unquenching of the $B(M1)$ strength. However, we also found that the total Gamow-Teller strength $B(GT_+)$ remains roughly constant through the phase transition and does not unquench. It was conjectured [8] that the isoscalar proton-neutron correlations, which are known to be the main source for the quenching of the $B(GT_+)$ strength [9,10], persist to higher temperatures than the like-pair correlations.

The purpose of this paper is to demonstrate the validity of that conjecture. To that end we define improved measures for the strength of the various pair correlations and study their temperature dependence, as well as their correlation with such nuclear observables as the moment of inertia, and the total $B(M1)$ and $B(GT_+)$ strengths. Detailed SMMC calculations are presented for the nuclei $^{54,56,58}$Fe and $^{56}$Cr.

Our paper is organized as follows. After a brief discussion of the SMMC method in Section 2, we introduce our definition of the pairing correlation strengths. In Section 3 we present the results of our study. We begin by discussing the temperature dependence of the moment of inertia, the $B(M1)$ and $B(GT_+)$ strengths, and the monopole pairing fields for all four nuclei, demonstrating that the results found in Ref. [8] appear to be a general feature of even-even nuclei with $A \approx 56$. In Section 3.B we study the temperature dependence of the various pair correlations in the four nuclei, paying particular attention to the phase transition related to the breaking of monopole pairs as found in [8] and the presence of proton-neutron correlations at higher temperatures. Finally we relate in Section 3.C the calculated temperature dependences of the moment of inertia and the $B(M1)$ and $B(GT_+)$ strengths to the temperature dependences of selected pairing correlations.
II. THEORETICAL BACKGROUND

We exploit recently developed Monte Carlo techniques [7,11] to calculate the thermal properties of $^{54,56,58}$Fe and $^{56}$Cr in a complete $0\hbar\omega$ model space with a realistic interaction. The methods we use describe the nucleus by a canonical ensemble at temperature $T = \beta^{-1}$ and employ a Hubbard-Stratonovich linearization of the imaginary-time many-body propagator, $e^{-\beta H}$, to express observables as path integrals of one-body propagators in fluctuating auxiliary fields [7,12]. 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. To circumvent the notorious “sign problem” encountered in the Monte Carlo shell model calculations with realistic interactions [12], we adopted the procedure suggested in Ref. [8] which is based on an extrapolation from a family of Hamiltonians that is free of the sign problem to the physical Hamiltonian.

Our calculations include the complete set of $1_p^{3/2}, 1_p^{1/2}, 0_f^{7/2}, 5/2$ states interacting through the realistic Kuo-Brown Hamiltonian [13] as modified in [14]. Some $5 \times 10^9$ configurations of the valence neutrons and protons moving in these 20 orbitals are involved in the canonical ensemble. As in Ref. [8], the results presented below have been obtained in MC shell model studies with a time step of $\Delta\beta = 1/32$ MeV$^{-1}$ using about 5000 independent Monte Carlo samples at six values of the coupling constant $g$ spaced between $-1$ and 0 and the value $\chi = 4$ in the decomposition of the Hamiltonian. A linear extrapolation to the physical case ($g = 1$) has been adopted for the observables discussed below.

The results presented in this paper correspond to various nuclear observables at selected temperatures: the total $B(M1)$ and Gamow-Teller strengths and the moment of inertia $I$, given by $I = 3\langle J^2 \rangle / T$. The total $B(M1)$ strength is defined as $B(M1) = \langle \vec{\mu}^2 \rangle$, where the magnetic moment $\vec{\mu}$ is given by $\vec{\mu} = \sum_j N \{ g_l \vec{l} + g_s \vec{s} \}$, $\mu_N$ is the nuclear magneton and $g_l, g_s$ are the free gyromagnetic ratios for angular momentum and spin, respectively ($g_l = 1, g_s = 5.586$ for protons and $g_l = 0, g_s = -3.826$ for neutrons). The total Gamow-Teller strength is given by $B(GT^+_\pi) = \langle (\vec{\sigma}_\pi^+)^2 \rangle$. We also explore the isovector monopole pairing, as described in Section 3.A.

The main focus of this paper is on pairing correlations and their relation to nuclear observables. In our complete $0\hbar\omega fp$-shell model space, a pair of protons or neutrons with angular momentum quantum numbers $(JM)$ is generated by ($a = \pi$ for protons and $a = \nu$ for neutrons)

$$A^\dagger_{JM}(j_a, j_b) = \frac{1}{\sqrt{1 + \delta_{j_a,j_b}}} \left[ a^\dagger_{j_a} a^\dagger_{j_b} \right]_{(JM)}$$

where $\pi^\dagger_j$ ($\nu^\dagger_j$) creates a proton (neutron) in an orbital with total spin $j$. Proton-neutron pairs can have either isospin $T = 1$ or $T = 0$. The respective definitions for the pair operators are

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

for the isovector proton-neutron pairs and
\[ A_{JM}^\dagger(j_a,j_b) = \frac{1}{2\sqrt{1 + \delta_{ja,jb}}} \left[ \nu_{ja}^\dagger \pi_{jb}^\dagger - \pi_{ja}^\dagger \nu_{jb}^\dagger \right]_{JM} \]  

(3)

for the isoscalar pair.

A general description of a pair, \( \Delta_{JM}^\dagger \), is then given by a superposition of the pair operators:

\[ \Delta_{JM}^\dagger = \sum_{j_a \geq j_b} \beta_{JM}(j_a,j_b) A_{JM}^\dagger(j_a,j_b). \]  

(4)

In mean-field theories like Hartree-Fock+BCS or HFB, the weights \( \beta \) can be related to the two-body potential matrix elements by the variational minimization of the free energy in the mean-field model space. However, such a relation is not to our disposal in the complete shell model and thus the weights are apriori undetermined. To overcome this arbitrariness of the definition (4) we will define the pairing strength as follows. With (1-3) we build a generalized pair matrix

\[ M_{\alpha\alpha'}^J = \sum_M \langle A_{JM}^\dagger(j_a,j_b) A_{JM}(j_c,j_d) \rangle \]  

(5)

which corresponds to the calculation of the canonical ensemble average of two-body operators like \( \pi_1^\dagger \pi_2^\dagger \pi_3 \pi_4 \). The index \( \alpha \) distinguishes the various possible \((j_a,j_b)\) combinations (with \( j_a \geq j_b \)). For example, the square matrix \( M \) has dimension \( N_J = 4 \) for \( J = 0 \), \( N_J = 7 \) for \( J = 1 \), \( N_J = 8 \) for \( J = 2,3 \). In the second step, the matrix \( M^J \) is diagonalized \((\beta = 1, ..., N_J)\), labelling the eigenvectors and eigenvalues in decreasing order

\[ M_J^\chi_\beta = \lambda_\beta^J \chi_\beta. \]  

(6)

The presence of a pair condensate in a correlated ground state will be signaled by the largest eigenvalue for a given \( J \), \( \lambda_1^J \), being much greater than any of the others.

To discuss the temperature dependence of pairing correlations it is convenient to introduce an overall measure for the pairing strength. We define the pairing strength for pairs with spin \( J \) as the sum of the eigenvalues of the matrix \( M^J \),

\[ P^J = \sum_\beta \lambda_\beta^J = \sum_\alpha M_{\alpha\alpha}^J. \]  

(7)

We note that for a model space spanned by a single \( j \)-shell one finds a simple sum rule for proton and neutron pairs

\[ \sum_J P^J = \frac{1}{2} N_v(N_v - 1), \]  

(8)

where \( N_v \) is the number of valence protons or neutrons in the shell. This sum rule holds approximately at low temperatures to the protons of the nuclei studied in this paper, as the valence protons then occupy mainly the \( f_{7/2} \) orbital. The sum rule is not valid at higher temperatures as the valence particles are then spread out over several orbitals.

With our definition (7) the pairing strength is non-negative and indeed positive at the mean-field level. As we will focus on the pairing correlations beyond the mean field in this
paper, we also calculated the mean-field pairing strength, $P_{mf}^J$ by the same procedure as outlined above, however, replacing the expectation values of the two-body matrix elements in the definition of the generalized pair matrix $M^J$ by

$$\langle a_1^+ a_2^+ a_3 a_4 \rangle \rightarrow n_1 n_2 (\delta_{13} \delta_{24} - \delta_{23} \delta_{14}) \quad (9)$$

where $n_k = \langle a_k^+ a_k \rangle$ is the occupation number of the orbital $k$.

We then finally define the pairing correlation in the nucleus as the pairing strength beyond the mean field,

$$P_{corr}^J = P^J - P_{mf}^J. \quad (10)$$

### III. RESULTS

#### A. Signals for the phase transition

Ref. [8] reported on SMMC calculations of the thermal properties of $^{54}$Fe within the complete pf-shell. One quantity studied was the thermal response of BCS-like monopole-pair correlations among protons and neutrons, defined as ($a = \pi, \nu$ for protons and neutrons, respectively)

$$\Delta_{BCS}^\dagger = \sum_{m>0} a_m^+ a_{-m}^+. \quad (11)$$

It was observed that these BCS-like pairs break at temperatures near 1 MeV. Of the observables studied in Ref. [8] three exhibit a particularly interesting behavior with increasing temperature near the phase transition: a) the moment of inertia $I$ rises sharply; b) the M1 strength $B(M1)$ shows a sharp rise, but unquenches only partially; and c) the Gamow-Teller strength $B(GT_\pi)$ remains roughly constant and strongly quenched.

We will now show that the breaking of BCS-like pairs at temperatures near 1 MeV and the related behavior of the three observables (moment of inertia and M1 and Gamow-Teller strengths) is not a particular result for $^{54}$Fe, but is a more general feature of even-even nuclei in the $A=56$ mass region. To this end, we present the results of SMMC calculations for $^{56}$Cr and $^{54,56,58}$Fe at selected temperatures. Fig. 1 shows the temperature dependence of $I$, $B(M1)$ and $B(GT_\pi)$ for all four nuclei. Additionally, the expectation values for BCS-like pairing fields, $\langle \Delta_{BCS}^\dagger \Delta_{BCS} \rangle$, for both protons and neutrons are plotted as functions of temperature. It is obvious from Fig. 1 that the like-pair correlations disappear at around 1 MeV for all four nuclei. This phase transition is accompanied by the same behavior of $I$, $B(M1)$ and $B(GT_\pi)$ as discussed in Ref. [8] and summarized in points a)-c) above. We note that Ref. [8] employed a different residual interaction (the Brown-Richter interaction [15]) than used here; the temperature dependence of the quantities shown in Fig. 1 are apparently largely independent of the interaction.

While Ref. [8] presented results only up to $T = 2$ MeV, we have continued the calculations in this paper to higher temperatures. Although the quantitative results are expected to be affected by our finite model space at temperatures larger than about 1.4 MeV [8], the qualitative features of the observables are likely still meaningful. The moment of inertia
shows a $T^{-1}$-decrease with temperature at $T > 2$ MeV, as is expected from the definition $I = 3\langle J^2 \rangle / T$; our finite model space requires $\langle J^2 \rangle$ to approach a constant in the high-temperature limit. The $B(M1)$ strength unquenches in two steps. Following its partial unquenching at the pairing phase transition, it remains roughly constant up to $T = 2.6$ MeV, where it finally starts to fully unquench. Although not shown in Fig. 1, we have checked that in the high-temperature limit the $B(M1)$ strengths approach the appropriate values. Being roughly constant at lower temperatures, $B(GT_+)$ unquenches at $T > 2.6$ MeV. We observe that this happens simultaneously with the second step of the unquenching of $B(M1)$ and, as we will see below, the two phenomena have a common origin. Again we have checked that $B(GT_+)$ approaches the appropriate values in the high-temperature limit.

B. Pair correlations

We have studied the pair correlations in the four nuclei for the various isovector and isoscalar pairs up to $J = 4$. Detailed calculations have been performed for selected temperatures between $T = 0.5$ MeV and 8 MeV. As has been shown in Refs. [2,3], the SMMC studies at $T = 0.5$ MeV approximate the ground state properties for even-even nuclei well. We have checked that in the high-temperature limit, which in our calculations corresponds to $T = 1/(\Delta \beta) = 32$ MeV, the pairing correlations approach the appropriate mean-field values.

Although it is the pairing correlation $P^{J}_{\text{cor}}$ (i.e., pairing strength relative to the mean-field) that matters for the behavior of the physical observables, we will at first discuss some features of the pair matrix $M$ and its spectrum. In Fig. 2 we show the pair matrix eigenvalues $\lambda^J_{\alpha}$ for the three isovector $J = 0^+$ and the isoscalar $1^+$ pairing channels as calculated for the iron isotopes $^{54-58}$Fe. We compare the SMMC results with those derived on the mean-field level, as discussed in section 2. Additionally, Fig. 2 shows the diagonal matrix elements of the pair matrix $M_{\alpha,\alpha}$, where we use the notation $\alpha = 1, \ldots, 4$ for $J = 0^+$ pairs in the $f_{7/2}$, $p_{3/2}$, $f_{5/2}$ and $p_{1/2}$ orbitals. For the isoscalar pairs only the three largest diagonal matrix elements of $M$ are shown corresponding to pairs in $(f_{7/2})^2$ ($\alpha = 1$), $(p_{3/2})^2$ ($\alpha = 2$) and $(f_{7/2}f_{5/2})$ ($\alpha = 3$) proton-neutron configurations. As expected, the protons occupy mainly $f_{7/2}$ orbitals in these nuclei. Correspondingly, the $\langle A^\dagger A \rangle$ expectation value, $M_{11}$, is large for this orbital; the other diagonal elements of $M$ are small. For neutrons, the pair matrix is also largest for the $f_{7/2}$ orbital. The excess neutrons in $^{56,58}$Fe occupy the $p_{3/2}$ orbital, signalled by a strong increase of the corresponding pair matrix element $M_{22}$ in comparison to its value for $^{54}$Fe. Upon closer inspection we find that the proton pair matrix elements are not constant within the isotope chain. This behavior is mainly caused by the isoscalar proton-neutron pairing. The dominating role is played by the isoscalar $1^+$ channel, which couples protons and neutrons in the same orbitals and in spin-orbit partners. We thus find for $^{54,56}$Fe that the proton pair matrix in the $f_{5/2}$ orbital, $M_{33}$, is larger than in the $p_{3/2}$ orbital, although the latter is favored in energy. For $^{58}$Fe, this ordering is inverted, caused by the increasing number of neutrons in the $p_{3/2}$ orbital which in turn also increase the proton pairing in this orbital.

After diagonalization the proton pairing strength is essentially found in one large eigenvalue. Furthermore we observe that this eigenvalue is significantly larger than the largest eigenvalue on the mean-field level supporting the existence of a proton pair condensate in
the ground state of these nuclei. For the neutrons the situation is somewhat different. For $^{54}$Fe, little additional coherence is found beyond the mean-field value, reflecting the closed-subshell neutron structure of this nucleus. For the two other isotopes, the neutron pairing exhibits two large eigenvalues. Although the larger one exceeds the mean-field value and signals noticeable additional coherence across the subshells, the existence of a second coherent eigenvalue shows the limits of the BCS-like pairing picture.

In Fig. 3 we compare the SMMC pairing strengths $P_J$ (Eq. (7)) for the $^{54}$Fe ground state (calculated at $T = 0.5$ MeV) with the mean-field values. Although the largest values for $P_J$ are found for pairs with larger $J$-values (e.g. $J = 2$ and 4 for isovector pairs), these values simply reflect the larger combinatorial possibilities to make these $J$-pairs in our model space, as the mean-field values are close to the SMMC values, i.e. there are no true correlations. Fig. 3 also exhibits the expected odd-even staggering: in the isovector pairing channels, pairs with even $J$ are more likely than those with odd $J$, while it is vice versa for isoscalar pairs. It is also obvious from Fig. 3 that the most significant physical difference between the SMMC and mean-field pairing occurs in the isovector $J = 0$ proton-proton and neutron-neutron channels. Here, the SMMC calculations exhibit a significant excess of pairing correlations over the mean field, reflecting the well known coherence in the ground states of even-even nuclei. As the nucleus $^{54}$Fe is semimagic for neutrons, the excess is larger for protons than for neutrons. Due to the sum rule (8), which is approximately fulfilled for the $^{54}$Fe ground state, the excess of $J = 0$ pairs is counterbalanced by correlation deficiencies in the other isovector pairs.

In the following we will discuss the physically important pairing correlation as defined in Eq. (10). Fig. 4 shows the temperature dependence of the pair correlations for selected pairs, which, as we will see in the next subsection, play an important role in understanding the thermal behavior of the moment of inertia and the total $M1$ and Gamow-Teller strengths.

The most interesting behavior is found in the $J = 0$ proton and neutron pairs. As mentioned above, the large excess of this pairing at low temperatures reflects the ground state coherence of even-even nuclei. With increasing temperature, this excess diminishes, vanishing at around $T = 1.2$ MeV. This behavior is in agreement with the pairing phase transition deduced in Ref. and above from the temperature dependence of the BCS-like monopole pairs. We observe further from Fig. 4 that the temperature dependence of the $J = 0$ proton-pair correlations is remarkably independent of the nucleus, while the neutron pair correlations show interesting differences. First, the correlation excess is smaller in the semimagic nucleus $^{54}$Fe than in the others. Among the iron isotopes, the neutron $J = 0$ correlations vanish at higher temperatures with increasing neutron number. More quantitatively, we have fitted the correlation excess to a Fermi function,

$$P^J_{\text{corr}}(T) = P_0 \left[ 1 + \exp \left( \frac{(T - T_0)}{\Delta T} \right) \right]^{-1}. \quad (12)$$

We then find (in MeV) $T_0 = 0.82 \pm 0.13, \Delta T = 0.13 \pm 0.07$ for $^{54}$Fe, $T_0 = 0.96 \pm 0.03, \Delta T = 0.11 \pm 0.02$ for $^{56}$Fe, and $T_0 = 1.07 \pm 0.04, \Delta T = 0.18 \pm 0.04$ for $^{58}$Fe, while the fit for $^{56}$Cr is very similar to that for $^{58}$Fe, $T_0 = 1.06 \pm 0.04, \Delta T = 0.14 \pm 0.03$. Similar fits to the $J = 0$ proton pairing excess results in $T_0 \approx 0.9 \pm 0.04, \Delta T = 0.12 \pm 0.03$ for all nuclei. The vanishing of the $J = 0$ proton and neutron pair correlations is accompanied by a significant increase in the correlations of the other pairs.
The isovector $J = 0$ proton-neutron correlations are positive at all temperatures for all four nuclei, with a slight excess at low temperatures that increases by about a factor 3 after the $J = 0$ proton and neutron pairs have vanished. The correlation peak is reached at higher temperatures with increasing neutron number (about 1.3 MeV for $^{54}$Fe, 1.6 MeV in $^{58}$Fe), while the peak height decreases with neutron excess.

The isoscalar proton-neutron $J = 1$ pairs show an interesting temperature dependence. At low temperatures, when the nucleus is still dominated by the $J = 0$ proton and neutron pairs, the isoscalar proton-neutron correlations show a noticeable excess. But more interestingly, they are roughly constant and do not directly reflect the vanishing of the $J = 0$ proton and neutron pairs. However, at $T > 1$ MeV, when the proton and neutron-pairs are broken, the isoscalar $J = 1$ pair correlations significantly increase and have their maximum at around 2 MeV, with peak values of about twice the correlation excess in the ground state. A similar (but milder) increase is observed in the other isoscalar correlations. In contrast to the isovector $J = 0$ proton-neutron pairs, the correlation peaks are reached at lower temperatures with increasing neutron excess. We also observe that these correlations die out rather slowly with temperature.

In summary, our SMMC calculations of nuclei around $A = 56$ support the following temperature hierarchy of pairing correlations. In the ground state and at low temperatures, $J = 0$ proton and neutron pair correlations dominate. When these vanish at temperatures around 1 MeV, proton-neutron correlations become more important, with the isovector proton-neutron correlations, in our model space, vanishing at temperatures around 2 MeV. At high temperatures, isoscalar proton-neutron correlations dominate.

C. Pairing correlations and observables

In this subsection we will discuss the relationship between pairing correlations and the temperature response of the $M1$, and Gamow-Teller strengths, as well as of the moment of inertia. As in our definition of pairing, we will focus on the behavior of these observables beyond the mean-field values. In terms of the neutron and proton occupation numbers $n_n$ and $n_p$, respectively, the mean-field values for these observables are given by

$$\langle I \rangle_{mf} = \frac{3}{T} \sum_i \langle i | J^2 | i \rangle \left[ n_p(i) \bar{n}_p(i) + n_n(i) \bar{n}_n(i) \right]$$

$$B(M1)_{mf} = \sum_{i,j} \left[ |\langle i | \vec{\mu} (p) | j \rangle|^2 n_p(j) \bar{n}_p(i) + |\langle i | \vec{\mu} (n) | j \rangle|^2 n_n(j) \bar{n}_n(i) \right]$$

$$B(GT_+)_{mf} = \sum_{i,j} |\langle i | \vec{\sigma} \tau_+ | j \rangle|^2 n_p(j) \bar{n}_n(i)$$

where the blocking factors are

$$\bar{n}_p(i) = 1 - \frac{n_p(i)}{2j_i + 1};$$

8
\[ n_n(i) = 1 - \frac{n_n(i)}{2j_i + 1}; \]  

(17)

and \( \tilde{\mu}(p) \) and \( \tilde{\mu}(n) \) are the proton and neutron magnetic moments.

The SMMC results for all three observables are significantly smaller than the mean-field values. To quantify this suppression, we introduce quenching strengths

\[
\langle I \rangle_{\text{quench}} = \langle I \rangle_{\text{mf}} - \langle I \rangle; \tag{18}
\]

\[
B(M1)_{\text{quench}} = B(M1)_{\text{mf}} - B(M1); \tag{19}
\]

\[
B(GT_+)_{\text{quench}} = B(GT_+)_{\text{mf}} - B(GT_+). \tag{20}
\]

We expect the quenching strength of the observables to be larger when the relevant pairing correlations are. Fig. 5 shows the temperature dependence of the quenching strengths for the three observables and relates it to selected pairing correlations, where the latter are given in arbitrary units. The following observations are evident and apply to all four nuclei:

The quenching of the moment of inertia shows a sharp drop at around \( T = 1 \) MeV and then slowly diminishes; the SMMC and mean-field values are identical for \( T > 2 \) MeV. The drop at \( T \approx 1 \) MeV clearly signals a relation to the pairing phase transition observed in the \( J = 0 \) proton and neutron correlations (see Fig. 4). From the definition \( I \sim \langle J^2 \rangle = \langle (J_n + J_p)^2 \rangle \), where \( J_p, J_n \) are the proton and neutron angular momenta, respectively, we expect that the moment of inertia is sensitive to the proton, neutron and proton-neutron correlations. This expectation is confirmed in Fig. 5, which shows that the temperature dependence of the quenching is nearly identical to the sum of the isovector \( J = 0 \) pair correlations. The steep drop at \( T \approx 1 \) MeV is thus due to the \( J = 0 \) proton and neutron pair correlations. We note that the moment of inertia unquenches more slowly with temperature than the proton and neutron \( J = 0 \) pairs. This difference is due to the isovector \( J = 0 \) proton-neutron correlations.

The quenching of the M1 strength decreases significantly near \( T = 1 \) MeV. Following a minimum at \( T \approx 1.3 \) MeV, the quenching increases again and then, after a maximum near \( 2 \) MeV, decreases slowly. While the drop at \( T = 1 \) MeV again signals an association with the \( J = 0 \) proton and neutron pairing phase transition, the maximum at \( 2 \) MeV as well as the slow dying out clearly resembles the temperature dependence of the isoscalar \( J = 1 \) proton-neutron correlations. These two correlations reflect the two components in the M1 strength. The orbital part is sensitive to the \( J = 0 \) proton pairing correlations (the gyromagnetic moment \( g_l \) is zero for neutrons), while the quenching of the spin component is dominated by isoscalar proton-neutron correlations \[9,10\]. This conjecture is in fact nicely confirmed, as for all four nuclei the temperature dependence of the quenching of the M1 strength is well described by that of the sum of the \( J = 0 \) proton and isoscalar \( J = 1 \) proton-neutron correlations.

Our calculation reveals a close (linear) relation between the orbital part of the M1 strength and the moment of inertia at low temperatures, where both quantities are dominated by isovector \( J = 0 \) pairing correlations. Such a linear relation is experimentally known for heavier nuclei and is supported by QRPA calculations \[17–19\].

The quenching of the \( B(GT_+) \) strength is roughly constant at low temperatures (\( T < 1 \) MeV). It then increases slightly, before it slowly dies out following a maximum at \( T \approx 2.5 \) MeV. Fig. 5 shows that the temperature dependence of the Gamow-Teller strength is driven
by the isoscalar proton-neutron correlations, as the rough constancy at low temperatures, the maximum at around $T = 2.5$ MeV and the slow decrease of the correlations towards higher temperatures of the $B(GT_+)$ quenching qualitatively mimics the temperature dependence of the isoscalar $J = 1$ proton-neutron correlations. With increasing neutron excess the maximum in the $B(GT_+)$ quenching at $T \approx 2.5$ MeV is weakened, in qualitative agreement with the $J = 1$ proton-neutron correlations.

IV. SUMMARY

In a previous SMMC study of the nucleus $^{54}$Fe, a sharp rise in the moment of inertia and the M1 strength at a temperature $T \approx 1$ MeV were related to the vanishing of the BCS-like proton and neutron Cooper pairs. In this paper we have investigated in more details this phase transition and its connection to the temperature dependence of the moment of inertia and of the M1 and Gamow-Teller strength. To do so we have performed SMMC calculations for the iron isotopes $^{54,56,58}$Fe and $^{56}$Cr within the complete pf-shell using the KB3 interaction. To study the pairing correlations within the shell model, we have defined a generalized pair matrix for isovector and isoscalar pairs for a given angular momentum and have proposed the sum of the eigenvalues of this matrix (trace) as a measure of the pairing strength. Using the same formalism, but replacing the two-body pair operators in the generalized pair matrix by occupation numbers we have derived the mean-field pairing strength. The physically relevant pair correlations are then defined as the difference of the SMMC and mean-field pairing strengths.

A detailed investigation of the correlations in the various pairing channels gives the following qualitative picture.

At low temperatures the SMMC calculations show a strong excess of $J = 0$ proton and neutron pairs over the mean-field values. This excess drops sharply at around $T = 1$ MeV for all four nuclei studied here, confirming the pairing phase transition conjectured in Ref. $^{[8]}$. After the vanishing of the dominating $J = 0$ pairs, proton-neutron correlations show an excess over the mean-field values. We find that isoscalar proton-neutron correlations persist to higher temperatures than the isovector correlations and, within our model space, vanish slowly at temperatures larger than 3 MeV. We observe some evidence that the pairing correlations depend on the neutron excess of the nucleus. This nuclear isospin-dependence warrants more detailed explorations.

The temperature hierarchy of the pairing correlations and the $J = 0$ proton and neutron pairing phase transition manifests itself in the temperature dependence of the three observables we studied in detail. The moment of inertia of the nucleus correlates with the sum of the isovector $J = 0$ pair correlations. In particular, we find that the pairing phase transition is connected with a sharp rise of the moment of inertia. Due to its orbital and spin components, the M1 strength unquenches generally in two steps: the orbital part unquenches at the $J = 0$ proton and neutron pairing phase transition, while the spin part slowly unquenches at higher temperatures, in concert with the decrease of the isoscalar proton-neutron correlations. The temperature dependence of the Gamow-Teller quenching $B(GT_+)$ is well approximated by that of the isoscalar $J = 1$ proton-neutron pairs.

Although the present calculations have been performed in model spaces larger than any imagined tractable until only recently, the quantitative results suffer from finite model space
limitations at temperatures greater about 1.5 MeV. Although we believe that the qualitative results presented in this paper will persist in calculations performed in even larger model spaces, such work is certainly warranted for a quantitatively reliable description of the unquenching of the isoscalar correlations at high temperatures. Such calculations are feasible within the SMMC approach and, as a next step, we are planning studies in the complete \((pf+sdg)\) shells.

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REFERENCES

[1] P. Ring and P. Schuck, *The Nuclear Many-Body Problem*, (Springer, Heidelberg, 1980)
[2] A. Arima and F. Iachello, *The Interacting Boson Model*, (Cambridge Monographs on Mathematical Physics, Cambridge, England, 1987)
[3] E. Suraud, Ch. Gregoire, and B. Tamin, Prog. Nucl. Part. Phys. 23 (1989) 357; K. Snover, Ann. Rev. Nucl. Part. Sci. 36 (1986) 545.
[4] Y. Alhassid, in *New Trends in Nuclear Collective Dynamics*, edited by Y. Abe et al. (Springer Verlag, New York, 1991) p. 41–91;
[5] J. L. Egido and P. Ring, J. Phys. G 19 (1993) 1; J. L. Egido and P. Ring, Nucl. Phys. A388 (1982) 19;
[6] A. Goodman, Nucl. Phys. A352 (1981) 30; A. K. Ignatiuk et al., Nucl. Phys. 346 (1980) 191.
[7] G. H. Lang, C. W. Johnson, S. E. Koonin, and W. E. Ormand, Phys. Rev. C 48 (1993) 1518.
[8] D. J. Dean, P. B. Radha, K. Langanke, Y. Alhassid, and S. E. Koonin, Phys. Rev. Lett. 74 (1995) 2909.
[9] J. Engel, P. Vogel and M. R. Zirnbauer, Phys. Rev. C37 (1988) 1328.
[10] D. J. Dean, P. B. Radha, K. Langanke, Y. Alhassid, S. E. Koonin, and W. E. Ormand, Phys. Rev. Lett. 72 (1994) 4066.
[11] C. W. Johnson, S. E. Koonin, G. H. Lang and W. E. Ormand, Phys. Rev. Lett. 69 (1992) 3157.
[12] Y. Alhassid, D. J. Dean, S. E. Koonin, G. Lang, and W. E. Ormand, Phys. Rev. Lett. 72 (1994) 613.
[13] T. T. S. Kuo and G. E. Brown, Nucl. Phys. A114 (1968) 241.
[14] A. Poves and A. P. Zuker, Phys. Rep. 70 (1981) 235.
[15] W. A. Richter, M. G. Vandermerwe, R. E. Julies, and B. A. Brown, Nucl. Phys. A523 (1991) 325.
[16] K. Langanke, D. J. Dean, P. B. Radha, Y. Alhassid, and S. E. Koonin, Phys. Rev. C52 (1995) 718.
[17] W. Ziegler, C. Rangacharyulu, A. Richter and C. Spieler, Phys. Rev. Lett. 65 (1990) 2515.
[18] K. Heyde and C. De Coster, Phys. Rev. C44 (1991) R2262.
[19] N. Lo Iudice and A. Richter, Phys. Lett. B304 (1993) 193.
FIGURES

FIG. 1. Temperature dependence of the moment of inertia (left top), the $B(M1)$ strength (left bottom), the $B(GT_+)$ strength (right top), and the expectation values of the BCS proton and neutron pairing strength (right bottom). SMMC results are shown for $^{54}$Fe (part a), $^{56}$Fe (part b), $^{58}$Fe (part c), and $^{56}$Cr (part d).

FIG. 2. Diagonal elements (upper) and eigenvalues (middle) of the pair matrix $M$ in the three isovector $J = 0^+$ and the isoscalar $J = 1^+$ channels, as calculated for $^{54,56,58}$Fe at $T = 0.5$ MeV. Eigenvalues of the pair matrix on the mean-field level (see text) are shown in the lowest panels.

FIG. 3. Comparison of the SMMC ($P_J^J$) and mean-field ($P_{mfJ}^J$) pairing strengths in the $^{54}$Fe ground state for selected pairing channels.

FIG. 4. Temperature dependence of the pair correlations $P_{corr}^J$ as defined in Eq. (10) for selected pairing channels.

FIG. 5. Comparison of the temperature dependence of the quenching of the physical observables (see Eqs. (18-20)) with related pairing correlations for $^{54,56}$Fe (part a) and $^{58}$Fe, $^{56}$Cr (part b). Upper: moment of inertia and the sum of the isovector $J = 0$ pairing correlations, Middle: the M1 strength and the sum (solid line) of $J = 0$ proton (dashed) and isoscalar $J = 1$ proton-neutron (dotted) correlations; Lower: the $B(GT_+)$ strength and the isoscalar $J = 1$ proton-neutron correlations. The pairing correlations have been scaled arbitrarily.
$^{56}\text{Fe}$

- $I (\hbar^2/\text{MeV})$
- $B(\text{GT}_{+})$
- $\langle \Delta^+ \Delta \rangle$

- Protons
- Neutrons
Protons

T=0, pn

T=1, pn

Neutrons
