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SHELL-MODEL MONTE CARLO STUDIES OF NUCLEI

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Shell Model Monte Carlo Studies of Nuclei

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Abstract

The pair content and structure of nuclei near $N = Z$ are described in the framework of shell-model Monte Carlo (SMMC) calculations. Results include the enhancement of J=0 T=1 proton-neutron pairing at N=Z nuclei, and the marked difference of thermal properties between even-even and odd-odd N=Z nuclei. Additionally I present a study of the rotational properties of the T=1 (ground state), and T=0 band mixing seen in ^{74}Rb.

I. INTRODUCTION AND FORMALISM

As new radioactive beam facilities become operational a wealth of information on nuclei near the N=Z line has emerged. These experimental facilities will continue to increase our understanding of the in medium isoscalar ($T = 0$) and isovector ($T = 1$) proton-neutron (*pn*) interaction. Several physical features in these nuclei are of interest. In their ground states, even-even nuclei are dominated by isovector pair correlations. In the absence of isospin-breaking forces like the Coulomb interaction, isospin symmetry enforces identical proton-proton (*pp*), neutron-neutron (*nn*), and *pn* correlations in self-conjugate nuclei. With increasing neutron (or proton) excess, the isovector *pn* correlations decrease sharply and the ground state of even-even nuclei near β-stability is dominated by isovector $J = 0$ pairing among like nucleons [1,2]. This is the reason why *pn* correlations are rather difficult to explore in stable medium-mass nuclei which have a moderate neutron excess.

On the other hand, *pn* pairing plays a particularly important role in odd-odd $N = Z$ nuclei. With the exception of ^{34}Cl, all $N = Z$ nuclei with $A \leq 40$ are dominated by isoscalar pairing involving pn pairs in identical orbitals, and so have ground states with $T=0$, $J>0$. However, the experimental ground state spins and isospins of virtually all odd-odd $N=Z$ nuclei with $A>40$ are $T=1$ and $J=0$ (the only known exception is ^{58}Cu), indicating the dominance of isovector pn pairing in these nuclei.

Further experimental information, including the identification of the spin, parity, and isospin of the ground and excited states of nuclei from ^{66}As through ^{98}In, will shed light on the isospin structure of pairing for $A>60$. At the present, ^{74}Rb is the only odd-odd $N=Z$ nucleus in that region that has been studied with any spectroscopic detail [3]. Interestingly, there is a change in the dominance between isovector and isoscalar pn pairing with rotational frequency. While the ground state band is identified as isovector (proposed to be the isobaric analogs of states in ^{74}Kr), $T=0$ states become energetically favored at about 1.0 MeV of excitation energy.

In this contribution, I will attempt to describe these interesting properties using the tools of shell-model Monte Carlo (SMMC) [4,5]. SMMC offers an alternative way to calculate nuclear structure properties, and is complementary to direct diagonalization. SMMC cannot find, nor is it designed to find, every energy eigenvalue of the Hamiltonian. It is designed to give thermal or ground-state expectation values for various one- and two-body operators. Indeed, for larger nuclei, SMMC may be the only way to obtain information on the thermal properties of the system from a shell-model perspective. We are interested in finding the partition function of the imaginary-time many-body propagator $U=\exp(-\beta\hat{H})$ where $\beta=1/T$ and T is the temperature of the system in MeV. We calculate expectation values of any observable $\hat{\Omega}$ with

$$\langle\hat{\Omega}\rangle=\frac{\mathrm{Tr}\hat{U}\hat{\Omega}}{\mathrm{Tr}\hat{U}} . \quad (1)$$

Since $\hat{H}$ contains many terms that do not commute, one must discretize $\beta=N_t\Delta\beta$. Finally, two-body terms in $\hat{H}$ are linearized through the Hubbard-Stratonovich transformation, which introduces auxiliary fields over which one must integrate to obtain physical answers. The method can be summarized as

$$Z = \mathrm{Tr}\hat{U} = \mathrm{Tr}\exp(-\beta\hat{H}) \to \mathrm{Tr}\left[\exp(-\Delta\beta\hat{H})\right]^{N_t}$$
$$\to \int \mathcal{D}[\sigma]G(\sigma)\mathrm{Tr}\prod_{n=1}^{N_t}\exp\left[\Delta\beta\hat{h}(\sigma_n)\right] , \qquad (2)$$

where σ_n are the auxiliary fields (there is one σ-field for each two-body matrix-element in $\hat{H}$ when the two-body terms are recast in quadratic form), $\mathcal{D}[\sigma]$ is the measure of the integrand, $G(\sigma)$ is a Gaussian in σ, and $\hat{h}$ is a one-body Hamiltonian. Thus, the shell-model problem has been transformed from the diagonalization of a large matrix to one of large dimensional quadrature. Dimensions of the integral can reach up to 10^5 for rare-earth systems, and it is thus natural to use Metropolis random walk methods to sample the space. Such integration can most efficiently be performed on massively parallel computers. Further details are discussed in [5].

Realistic interactions often have a Monte Carlo sign problem, that is they have complex actions. We have found that a certain class of Hamiltonians has good Monte Carlo sign properties, and one performs calculations with these Hamiltonians. Fortunately in nuclear physics good Hamiltonians, such as pairing plus quadrupole, are not too far removed from realistic Hamiltonians so that the extrapolation is a gentle function of the coupling constant, g [6].

The residual nuclear interaction builds up pairing correlations in a nucleus. Introducing nucleon creation operators $a^\dagger$, these correlations can be studied by defining pair creation operators

$$A^\dagger_{JM}(j_a, j_b) = \frac{1}{\sqrt{1+\delta_{ab}}}\left[a^\dagger_{j_a} \times a^\dagger_{j_b}\right]_{JM} \qquad (3)$$

for proton-proton or neutron-neutron pairs, and

$$A^\dagger_{JM}(j_a, j_b) = \frac{1}{\sqrt{2(1+\delta_{ab})}}\left\{\left[a^\dagger_{pj_a} \times a^\dagger_{nj_b}\right]_{JM} \pm \left[a^\dagger_{nj_a} \times a^\dagger_{pj_b}\right]_{JM}\right\} , \qquad (4)$$

for proton-neutron pairs where "$+(-)$" is for $T = 0(T = 1)$ pn-pairing. With these definitions, I construct a pair matrix

$$M^J_{\alpha\alpha'} = \sum_M \langle A^\dagger_{JM}(j_a, j_b)A_{JM}(j_c, j_d)\rangle , \qquad (5)$$

where $\alpha = \{j_a, j_b\}$ and $\alpha' = \{j_c, j_d\}$ and the expectation value is in the ground state or canonical ensemble at a prescribed temperature. The pairing strength for a given J is then given by

$$P(J) = \sum_{\alpha \geq \alpha'} M^J_{\alpha,\alpha'}. \tag{6}$$

With this definition (4) the pairing strength is non-negative, and indeed positive, at the mean-field level. The mean-field pairing strength, $P_{\rm MF}(J)$, 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

$$\langle a_1^\dagger a_2^\dagger a_3 a_4 \rangle \rightarrow n_1 n_2 \left(\delta_{13}\delta_{24} - \delta_{23}\delta_{14}\right), \tag{7}$$

where $n_k = \langle a_k^\dagger a_k \rangle$ is the occupation number of the orbital k. This mean-field value provides a baseline against which true pair correlations can be judged. Genuine pair correlations can then be defined as those in excess of the mean-field values

$$P_{\rm corr}(J) = P(J) - P_{\rm MF}(J)\ . \tag{8}$$

Note that this is a different definition of the correlations than that used in Ref. [2]; however, it leads to the same qualitative results.

In the following I will describe ground state pairing properties in nuclei in the mass $A = 40 - 80$ range. I will then present SMMC results of thermal pairing properties in ^{50}Mn and ^{52}Fe. and discuss rotational properties of ^{74}Rb. I will conclude with a future outlook for large calculations within the SMMC framework.

II. INTERACTIONS AND MODEL SPACES

SMMC calculations of pf shell nuclei were performed to study ground-state [7] and thermal [8,9] properties of nuclei using the Kuo-Brown [10] interaction modified in the monopole terms [11]. (The interaction has subsequently been dubbed KB3.) Excellent agreement between theory and experiment was observed, indicating the usefulness of this interaction for pf shell nuclei up to $A = 60$. The KB3 interaction also successfully reproduces many of the ground-state properties and spectra of nuclei in the lower pf shell [7,12]. As an example, Fig. 1 displays the SMMC calculations of the mass excesses in this model space, relative to the ^{40}Ca core (top panel), and the deviation between theory and experiment (bottom panel). Investigations of B(E2)'s, B(M1)'s, and Gamow-Teller operators were also carried out, and good agreement in comparison to experimental data has been demonstrated [5,7].

In order to investigate heavier systems, the $0g_{9/2}$ was included in the pf model space [10]. However, we found that the coupling between the $0f_{7/2}$ and $0g_{9/2}$ causes fairly significant center-of-mass contamination to the ground state, and we therefore close the $0f_{7/2}$. The model space is thus $0f_{5/2}1p0g_{9/2}$. This appears to be a good approximation in systems where both the neutrons and protons completely fill the $f_{7/2}$ level. The monopole terms of this new interaction were modified [13] to give a good description of the spectra of nuclei in the Ni isotopes. Since ^{56}Ni is the core of this model space, the single-particle energies were determined from the ^{57}Ni spectrum. Mass excesses (top panel) and differences between experiment and theory (bottom panel) are shown in Fig. 2 for this new interaction.

III. PAIR CORRELATIONS NEAR N=Z

It has long been anticipated that $J = 0^+$ proton-neutron correlations play an important role in the ground states of $N = Z$ nuclei. These correlations were explored with SMMC for $N = Z$ nuclei in the mass region $A = 48 - 58$ in the pf-shell, and $A = 64 - 74$ in the $0f_{5/2}1p0g_{9/2}$ space. As the even-even $N = Z$ nuclei have isospin $T = 0$, the expectation values of $A^\dagger A$ are identical in all three isovector 0^+ pairing channels. This symmetry does not hold for the odd-odd $N = Z$ nuclei in this mass region, which usually have $T = 1$ ground states, and $\langle \hat{A}^\dagger \hat{A} \rangle$ can be different for proton-neutron pairs than for like-nucleon pairs. (The expectation values for proton and neutron pairs are identical.)

We find the proton-neutron pairing strength significantly larger for odd-odd $N = Z$ nuclei than in even-even nuclei, while the 0^+ proton and neutron pairing shows the opposite behavior, in both cases leading to a noticeable odd-even staggering, as displayed in Fig. 3, for the pf shell. Due to the strong pairing of the $f_{7/2}$, all three isovector 0^+ channels of the pairing matrix essentially exhibit only one large eigenvalue which is used as a convenient measure of the pairing strength in Fig. 3. This staggering is caused by a constructive interference of the isotensor and isoscalar parts of $\hat{A}^\dagger \hat{A}$ in the odd-odd $N = Z$ nuclei, while they interfere destructively in the even-even nuclei. The isoscalar part is related to the pairing energy and is found to be about constant for the nuclei studied here.

Fig. 4 shows the correlated pairs for $N = Z$ nuclei in the $A = 64 - 74$ region of the $0f_{5/2}1p0g_{9/2}$ space. Note that ^{64}Ge exhibits little $J = 0$ pairing, indicating that the $p_{3/2}$ subshell is relatively closed for this system. The correlated pairs exhibit a strong $J = 0$, $T = 1$ like-particle staggering for the even-even and odd-odd $N = Z$ systems, while the number of correlated proton-neutron pairs is much larger than the like-particle pairing for the odd-odd systems. The correlated pairing behavior of $N = Z$, $N = Z + 2$, $N = Z + 4$ nuclei is shown in Fig. 4, where one clearly sees the decrease in T=1 proton-neutron pairing as one moves away from $N = Z$.

Another striking feature of proton-neutron pairing can be found through studying the thermal properties of these systems [5,8,9]. In the case of ^{52}Fe $J = 0$, proton-neutron and like-particle pairing decrease quickly to fermi-gas values at a temperature of approximately 1.1 MeV (corresponding to an excitation energy of approximately 4 MeV) (see Fig. 5). This decrease in pairing behaves like $P(T) = P_0 \left(1 + \exp\left\{\frac{T-T_0}{\alpha}\right\}\right)^{-1}$, where $T_0 \approx 1.1$ MeV, and $\alpha = 0.25$ MeV, and is the same for both like-particle and proton-neutron T=1 pairing. For the case of ^{50}Mn (shown in Fig. 6), the proton-neutron pairing decreases much more quickly, and is almost zero at approximately a temperature of 0.75 MeV, while the like-particle pairing remains until 1.1 MeV. One also sees a dramatic drop in the dependence of the isospin $< T^2 > [= T(T+1)]$ on temperature. Since ^{50}Mn has a $T = 1$ ground-state, $< T^2 >= 2$ at very low temperatures, but decreases towards zero as the system is heated, indicating a thermal mixture of T=1 and T=0 states.

As required by general thermodynamic principles, the internal energy increases steadily with temperature. The heat capacity $C(T) = dE/dT$ is usually associated with the level density parameter a by $C(T) = 2a(T)T$. As is typical for even-even nuclei [8] $a(T)$ 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} [14] for ^{52}Fe. 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 [8].

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. 6, E increases approximately linearly with temperature, corresponding to a constant heat capacity $C(T) \approx 5.4 \pm 1$ 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 [15] and thus appears to be generic for self-conjugate odd-odd $N = Z$ nuclei.

IV. PAIR CORRELATIONS IN ^{74}RB

The band mixing seen in ^{74}Rb can be measured within SMMC by adding a cranking term to the shell-model Hamiltonian [16]. Thus $H \leftarrow H + \omega J_z$. Note that since J_z is a time-odd operator, the sign problem is reintroduced, and good statistical sampling requires the cranking to be carried out only to finite ω. For the calculations shown in Fig. 7, the largest cranking frequency was $\omega = 0.4$. A signature of the band mixing is a change in the isospin $< T^2 >$ as a function of $< J_z >$, which is shown in the figure. We see that at about a spin of $J_z = 4\hbar$, $< T^2 >$ moves away from its initial value of 2. A mixing of $T = 0$ and $T = 1$ states forces the expectation value to decrease. Thus in a full shell-model calculation, we predict the onset of this mixing at approximately $J_z = 4\hbar$, consistent with the spectrum found in Ref. [3].

To understand the apparent crossing of the $T = 1$ and $T = 0$ bands, we have studied the various pair correlations as a function of rotational frequency. We find that the isovector $J = 0$ correlations and the aligned isoscalar $J = 9$ pn correlations are most important in this transition. These correlations are plotted in Fig. 7 as a function of $\langle J_z \rangle$, where we have defined pair correlations by Eq. (8). Strikingly the largest pair correlations are found in the isovector $J = 0$ and isoscalar $J = 9$ proton-neutron channels at low and high frequencies, respectively. Furthermore, the variation of isospin with increasing frequency reflects the relative strengths of these two pn correlations. Our calculation clearly confirms that proton-neutron correlations determine the behavior of the odd-odd $N = Z$ nucleus ^{74}Rb, as already supposed in [3].

With increasing frequency the isovector $J = 0$ pn correlations decrease rapidly to a constant at $\langle J_z \rangle \approx 3$. This behavior is accompanied by an increase of the pn correlations in the maximally aligned channel, $J = 9, T = 0$ which dominates ^{74}Rb at rotational frequencies where the $J = 0$ pn correlations become small. Furthermore, although $J = 8$, $T = 1$ pairs exist, they do not exhibit correlations beyond the mean field, as shown in Fig. 8.

Since $J = 9$ pn pairs can be formed only in the $g_{9/2}$ orbitals of our model space, the pairing results suggest increasing occupation of this orbital with increasing ω. To demonstrate this increase, Fig. 8 shows the $g_{9/2}$ proton occupation number (equal to the neutron occupation number) as a function of $\langle J_z \rangle$. While the ground state has roughly one proton in the $g_{9/2}$ orbital, this number increases by some 50% at the highest $\langle J_z \rangle$ values we study and tracks the $J = 0$ pn pairing correlations. It should be noted that although the increased $g_{9/2}$ occupation number increases the mean-field value of the pair correlations [see Eq. (8)], the $J = 9$ pn correlations as shown in Fig. 8, reflect genuine pairing beyond the mean field values.

V. CONCLUSIONS AND FUTURE PROSPECTS

In these Proceedings I have indicated some of the studies of pairing that are accessible using SMMC techniques. As the above results indicate, strong $J = 0$, $T = 1$ proton-neutron correlations exist for odd-odd $N = Z$ nuclei, and die off quickly as one adds neutrons. Thermal studies of $N = Z$ even-even and odd-odd systems indicate that proton-neutron isovector pairs break more readily with increasing temperature than do the like-particle pairs. Finally, an odd-odd $N = Z$ system such as ^{74}Rb should exhibit a $T = 1$ to $T = 0$ band mixing as one cranks the system. Both studies indicate that isoscalar pairing is more resistant to both thermal and rotational excitation of the nucleus.

In this procedings I have endeavored to demonstrate by concentrating on a particular problem, which demonstrates that with the SMMC approach a microscopic method is now at hand which allows detailed studies of many correlations in nuclei in the mass range $A = 60 - 100$. These nuclei will be the focus of future experimental interest at radioactive ion-beam facilities. Space does not permit me to discuss other exciting applications of SMMC to nuclear systems. I will simply list them here. We have made a detailed study of the ground state properties of pf-shell nuclei including the quenching of the Gamow-Teller strength [7]. We have calculated $\beta\beta$-decay matrix elements for ^{76}Ge [17]. We have studied the γ-softness of ^{124}Xe [18]. We have also begun programs in multi-major shell calculations, and in calculations for rare earth nuclei.

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FIGURES

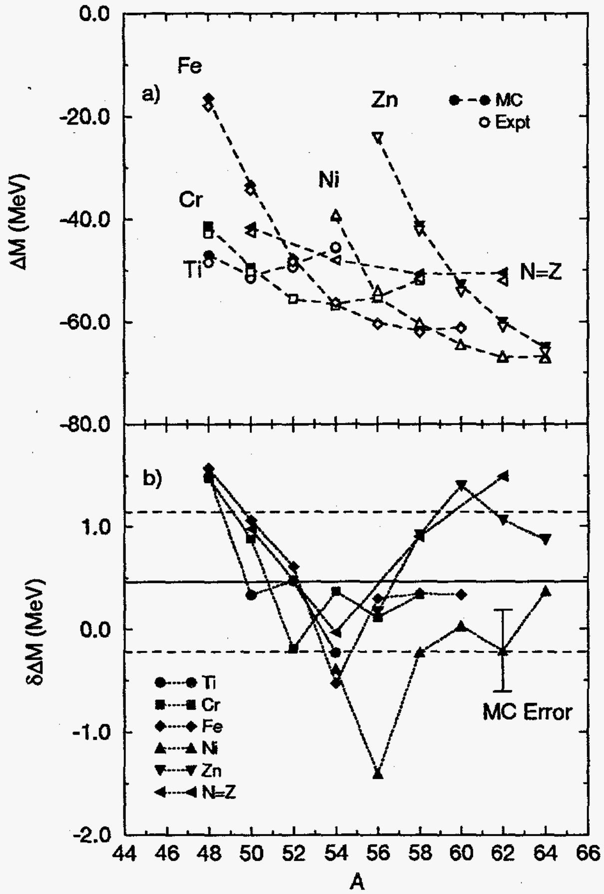

Fig 1. Upper panel (a): Comparison of the mass excesses ΔM as calculated within the SMMC approach with data. Lower panel (b): Discrepancy between the SMMC results for the mass excesses and the data, $\delta\Delta M$. The solid line shows the average discrepancy, 450 keV, while the dashed lines show the rms variation about this value (from [7]).

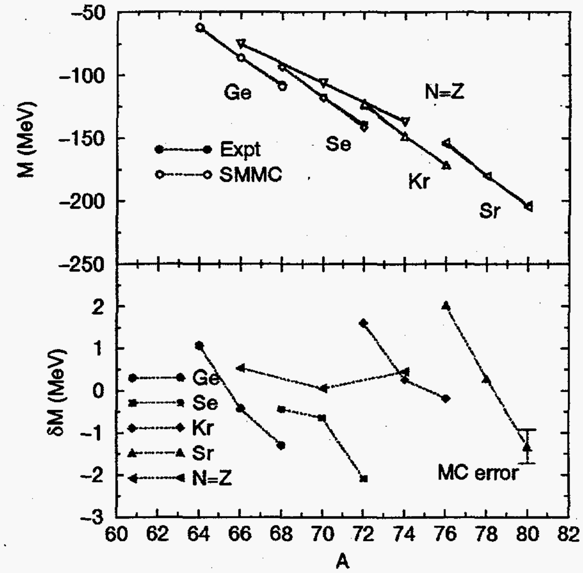

Fig 2. Calculated mass excesses are compared with experiment (top panel), and the difference between experiment and theory is shown (bottom panel).

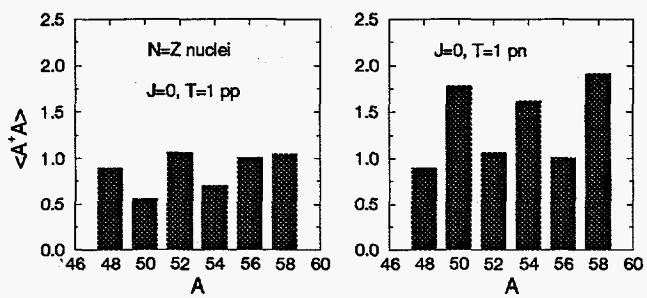

Fig 3. Largest eigenvalues for the $J = 0$, $T = 1$ proton-proton (left) and proton-neutron (right) pairing matrix as a function of mass number.

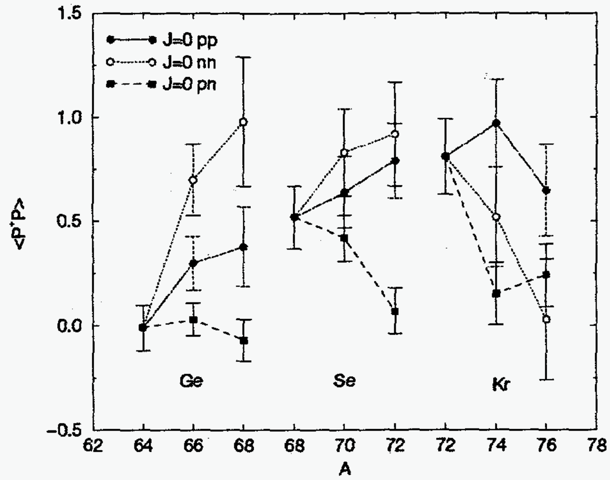

Fig 4. Correlated $J = 0$, $T = 1$ pairs in the proton-proton and proton-neutron channel for $N = Z$ nuclei in the $0f_{5/2}1p0g_{9/2}$ model space.

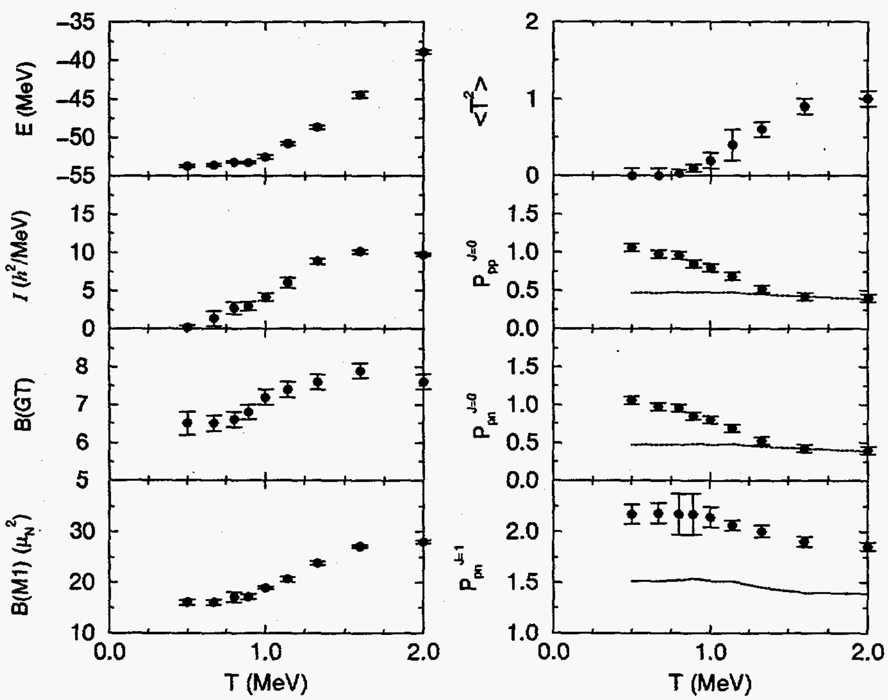

Fig. 5. Thermal properties of ^{52}Fe. The SMMC results are shown with error bars, while the lines indicate the mean-field values for the respective pair correlations.

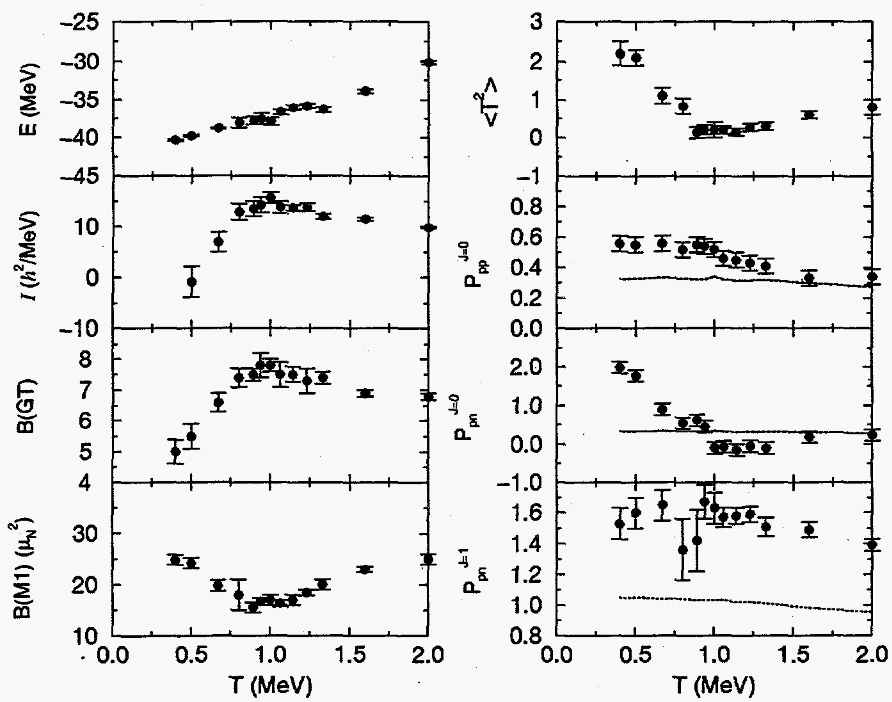

Fig. 6. Thermal properties of ^{50}Mn. The SMMC results are shown with error bars, while the lines indicate the mean-field values for the respective pair correlations.

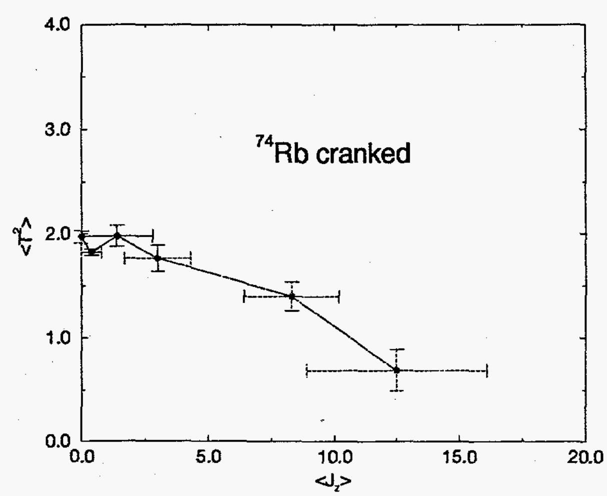

Fig 7. $< T^2 >$ as a function of J_z for ^{74}Rb.

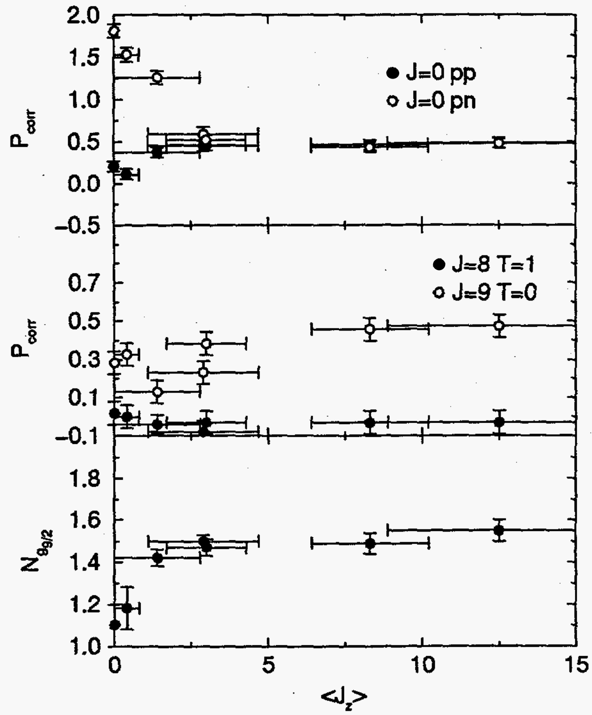

Fig 8. Selected pair correlations and the proton $g_{9/2}$ occupation number (bottom panel) as a function of $\langle J_z \rangle$. The top panel shows the isovector $J = 0$ *pp* and *pn* correlations, while the isoscalar $J = 9$ and isovector $J = 8$ *pn* correlations are shown in the middle panel.