Thermal Properties of ^{54}Fe

D. J. Dean,[1] S. E. Koonin,[1] K. Langanke,[1] P. B. Radha,[1] and Y. Alhassid[2]
[1] *W. K. Kellogg Radiation Laboratory, California Institute of Technology, 106-38, Pasadena, California 91125*
[2] *Center for Theoretical Physics, Sloane Physics Laboratory Yale University, New Haven, Connecticut 06511*
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We study the thermal properties of ^{54}Fe with the Brown-Richter interaction in the complete $1p0f$ model space. Monte Carlo calculations show a peak in the heat capacity and rapid increases in both the moment of inertia and $M1$ strength near a temperature of 1.1 MeV that are associated with the vanishing of proton-proton and neutron-neutron monopole pair correlations; neutron-proton correlations persist to higher temperatures. Our results are consistent with a Fermi gas level density whose backshift vanishes with increasing temperature.

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The nuclear level density increases rapidly at excitation energies above several MeV, and it becomes difficult to resolve or calculate individual states. In this regime, it is more appropriate to employ a statistical description where observables are averaged over the many levels at a given energy. The concept of an equilibrated compound nucleus is among the most fundamental of nuclear reaction theories [1], and plays a central role in our understanding of processes induced by probes ranging from photons to heavy ions.

While the proper description of a compound nucleus is in terms of a microcanonical (fixed-energy) ensemble, it is often more convenient to consider a canonical ensemble whose temperature is chosen to reproduce the average excitation energy. In the past decade, there has been renewed experimental [2] and theoretical [3] effort to explore the properties of heavy nuclei at finite temperature and high spin. The properties of hot nuclei are also important in various astrophysical scenarios, particularly in the late stage of a supernova collapse and explosion [4].

Most theoretical approaches to hot nuclei devolve to a mean-field description based on an average configuration [5]. The realization that thermal and quantal fluctuations about the average can be important has prompted more sophisticated approximations [6], although even these have clear limitations. In principle, the nuclear shell model (which provides a complete spectrum and wave functions) offers a fully microscopic approach to the problem. However, conventional finite-temperature shell model calculations within a complete major shell are limited to light nuclei (^{20}Ne and ^{24}Mg) in the *sd* shell [7].

In this Letter, we exploit recently developed Monte Carlo techniques to calculate the thermal properties of ^{54}Fe 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 [8]. 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 nucleus we have chosen for this initial study (^{54}Fe) is among the most abundant in the presupernova core of a massive star, so that its thermal properties are of considerable astrophysical import. Further, the ground states of nuclei in the mid-pf-shell are dominated by nucleon-nucleon correlations (e.g., pairing) whose evolution with increasing temperature is of particular interest.

To circumvent the "sign problem" encountered in the Monte Carlo shell model calculations with realistic interactions, Alhassid *et al.* [9] suggested an extrapolation procedure from a family of Hamiltonians that are free of the sign problem to the physical Hamiltonian. One defines a set of Hamiltonians $H_g = H_G + gH_B$ such that $H_{g=1} = H$ is the physical Hamiltonian and $H_{G,B}$ are the "good" and "bad" parts of the Hamiltonian, respectively. For $g \leq 0$, H_g is free of the sign problem and calculated observables are extrapolated to $g = 1$. For ground state properties, this procedure was validated by comparison to direct diagonalization results in the *sd* and lower *pf* shells. However, it is impractical at intermediate temperatures due to the overly strong pairing interaction in H_g for $g < 0$, which suppresses the population of excited states. This problem can be corrected by scaling H_G as $[1 - (1 - g)/\chi]H_G$, together with a g-dependent compression of the single-particle spectrum; the value of χ is chosen to make the g extrapolation as smooth as possible. Note that, as before, the original Hamiltonian is recovered for $g = 1$.

Our calculations include the complete set of $1p_{3/2,1/2}0f_{7/2,5/2}$ states interacting through the realistic Brown-Richter Hamiltonian [10]. Some 5×10^9 configurations of the 8 valence neutrons and 6 valence protons moving in these 20 orbitals are involved in the canonical ensemble. The results presented below have been obtained in Monte Carlo shell model studies with a time step of $\Delta\beta = 1/32$ MeV $^{-1}$ using 5000–9000 independent Monte Carlo samples at seven values

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of the coupling constant g spaced between -1 and 0 and the value $\chi = 4$. A linear extrapolation to the physical case ($g = 1$) is justified by the quality of fit for most of the observables discussed below, although the quadrupole moments warranted a quadratic extrapolation. We have tested our procedure for the fp-shell nucleus ^{44}Ti against a calculation performed with the direct diagonalization code CRUNCHER [11] and were able to reproduce the excitation energy as a function of temperature for the temperature interval relevant for this Letter [12]. However, we note that an exact reproduction of the CRUNCHER energies is obtained only after a $\Delta\beta \rightarrow 0$ extrapolation, which lowers the absolute energies slightly compared to the calculation with the finite value $\Delta\beta = 1/32$ MeV $^{-1}$. For ^{54}Fe we have checked at several temperatures that our qualitative results are not changed by the $\Delta\beta$ extrapolation. We have also checked that using $\chi = 3$ in the g extrapolation does not change our results.

The calculated temperature dependence of various observables is shown in Fig. 1. In accord with general thermodynamic principles, the internal energy U steadily increases with increasing temperature [13]. It shows an inflection point around $T \approx 1.1$ MeV, leading to a peak in the heat capacity, $C \equiv dU/dT$, whose physical origin we will discuss below. The decrease in C for $T \gtrsim 1.4$ MeV is due to our finite model space (the Schottky effect [14]); we estimate that limitation of the model space to only the pf shell renders our calculations of ^{54}Fe quantitatively unreliable for temperatures above this value (internal energies $U \gtrsim 15$ MeV). The same behavior is apparent in the level density parameter, $a \equiv C/2T$. The empirical value for a is $A/8$ MeV $= 6.8$ MeV^{-1} which is in good agreement with our results for $T \approx 1.1-1.5$ MeV.

We also show in Fig. 1 the expectation values of the squares of the $J = 0$ proton-proton and neutron-neutron pairing fields, $\langle \Delta^\dagger \Delta \rangle$. Although the pair wave function we have used (the BCS form, in which all time-reversed pairs have equal amplitudes) is not necessarily optimal, these observables are a rough measure of the number of $J = 0$ pairs in the nucleus. At low temperatures, the pairing fields are significantly larger than those calculated for a noninteracting Fermi gas, indicating a strong coherence in the ground state. With increasing temperature, the pairing fields decrease; both approach the Fermi gas values for $T \approx 1.5$ MeV and follow it closely for even higher temperatures. Associated with the breaking of pairs is a dramatic increase in the moment of inertia I for $T = 1.0-1.5$ MeV; this is analogous to the rapid increase in magnetic susceptibility in a superconductor. At temperatures above 1.5 MeV, I is in agreement with the rigid rotor value, $10.7\hbar^2$/MeV; at even higher temperatures it decreases linearly due to our finite model space.

In Fig. 2, we show various static observables. The $M1$ strength unquenches rapidly with heating near the transition temperature. However, for $T = 1.3-2$ MeV $B(M1)$ remains significantly lower than the single-particle estimate ($41\mu_N^2$), suggesting a persistent quenching at temperatures above the like-nucleon depairing. This finding is supported by the near constancy of the Gamow-Teller β^+ strength, $B(\mathrm{GT}_+)$, for temperatures up to 2 MeV. As the results of Ref. [15] demonstrate that neutron-proton correlations are responsible for much of the GT quenching in iron nuclei at zero temperature, we interpret the present results as evidence that isovector proton-neutron

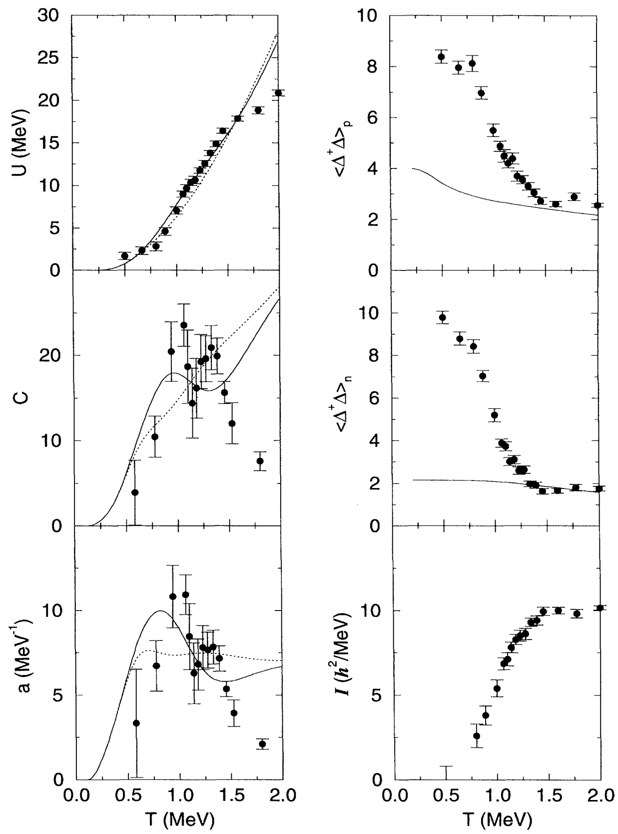

FIG. 1. Temperature dependence of various observables in ^{54}Fe. Monte Carlo points with statistical errors are shown at each temperature T. In the left-hand column, the internal energy U is calculated as $\langle H \rangle - E_0$, where H is the many-body Hamiltonian and E_0 the ground state energy. The heat capacity C is calculated by a finite-difference approximation to dU/dT, after $U(T)$ has been subjected to a three-point smoothing, and the level density parameter is $a \equiv C/2T$. The dashed and solid curves in these panels correspond to the constant- and temperature-dependent-backshift Fermi gas models, as described in the text. To eliminate the systematic error associated with the determination of E_0, we have chosen this parameter so that the Monte Carlo and Fermi gas results for U are equal at $T = 0.66$ MeV. In the right-hand column, we show the expectation values of the squares of the proton and neutron pairing fields, where $\Delta_p^+ = \sum p_{jm}^\dagger p_{j\bar{m}}^\dagger$ (and similarly for neutrons) and the sum is over all orbitals with $m > 0$. For comparison, the pairing fields calculated in an uncorrelated Fermi gas are shown by the solid curve. The moment of inertia is obtained from the expectation values of the square of the total angular momentum by $I = \beta\langle J^2 \rangle/3$.

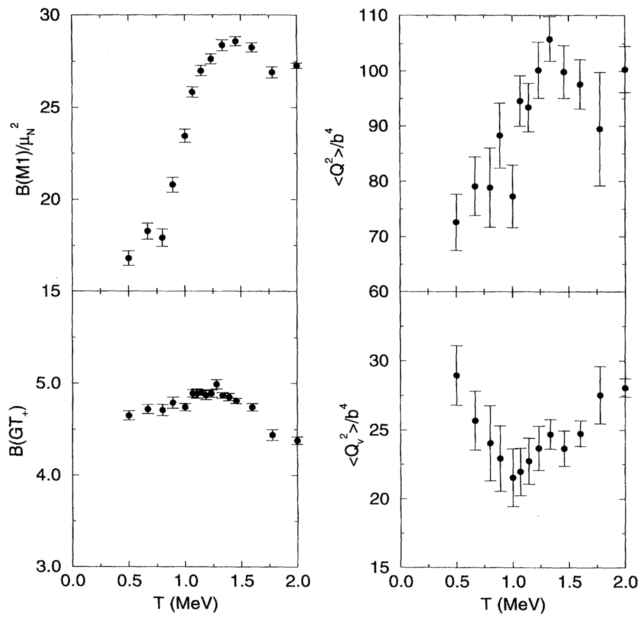

FIG. 2. The upper left panel shows the total magnetic dipole strength $B(M1)$ in units of nuclear magnetons; it is calculated using free-nucleon g factors. The lower left panel shows the GT β_+ strength. The low-temperature value of 4.7 ± 0.2 is somewhat larger than the 4.3 ± 0.2 given in Refs. [9,15], since the latter calculations were done with $\Delta\beta = 1/16\ \mathrm{MeV}^{-1}$. Calculations at $\Delta\beta = 1/64\ \mathrm{MeV}^{-1}$ indicate that the present low-temperature value is converged. The upper and lower right panels show the isoscalar ($Q = Q_p + Q_n$) and isovector ($Q_v = Q_p - Q_n$) quadrupole strengths, where the quadrupole operators are r^2Y_2 and results are given in terms of the oscillator length, $b = 1.96$ fm.

correlations persist to higher temperatures. We have verified that, in our restricted model space, both the GT$_+$ and $M1$ strengths unquench at temperatures above 2 MeV and that, in the high-temperature limit, they both approach the appropriate Fermi gas values of $10.8\mu_N^2$ and $41\mu_N^2$, respectively. We note that it is often assumed in astrophysical calculations that the GT strength is independent of temperature [4]; our calculations demonstrate that this is true for the relevant temperature regime ($T < 2$ MeV). We also note that a detailed examination of the occupation numbers of the various orbitals show no unusual variation as the pairing vanishes.

The isoscalar mass quadupole moment $\langle Q^2\rangle$ increases at temperatures near the phase transition (Fig. 2, upper right), while the isovector moment, $\langle Q_v^2\rangle$, decreases as the nucleus is heated, showing a minimum near $T = 1.1$ MeV (Fig. 2, lower right). The behaviors of $\langle Q^2\rangle$ and $\langle Q_v^2\rangle$ imply that $\langle Q_p \cdot Q_n\rangle = (\langle Q^2\rangle - \langle Q_v^2\rangle)/4$ increases near the phase transition ($Q_{p,n}$ are the proton and neutron quadrupole moments). Noting the relation between $\langle Q_p \cdot Q_n\rangle$ and the orbital part of the $M1$ strength [16], we interpret the partial unquenching of the $B(M1)$ near $T = 1.1$ MeV as related to the orbital part, while the spin part, dominated by the same operator as the GT strength, remains significantly quenched to higher temperatures.

We have compared our results for U with two simple models. As in Ref. [17], we define the partition function of the nucleus as

$$Z = \sum_i (2J_i + 1)e^{-\beta E_i} + \int_{E_0}^{\infty} \rho(E)e^{-\beta E}\,dE\,, \qquad (1)$$

where the sum runs over the experimentally known nuclear levels and the continuum state density $\rho(E)$ has been approximated by the backshifted Fermi gas model [18], where the backshift P accounts for the energy to break a pair; we adopted a level density parameter $a = 7.2\ \mathrm{MeV}^{-1}$ and chose $E_0 = 4$ MeV to smoothly match the two terms in Eq. (1). The first model had the conventional T-independent backshift $P_0 = 1.45$ MeV [18], while the second model simulated the vanishing of the pairing by a temperature-dependent P,

$$P(T) = P_0\left(1 + \exp\left\{\frac{T - T_0}{\alpha}\right\}\right)^{-1}. \qquad (2)$$

Our choice of the parameters $T_0 = 1.05$ MeV, $\alpha = 0.25$ MeV was motivated from the two upper right panels in Fig. 1. As seen from the solid curves in the left panels of Fig. 1, the $P(T)$ model exhibits clear maxima in both the heat capacity and the level density parameter related to the pairing phase transition. Whether the maxima observed in the Monte Carlo results are related to the pairing phase transition, as identified from other observables discussed above, will have to await calculations in larger model spaces. The dashed curves in these panels indicate that the assumption of a constant level density parameter is not quite appropriate at temperatures below the phase transition.

In conclusion, we have demonstrated that shell model Monte Carlo methods are well suited to studying the finite-temperature properties of nuclei using realistic effective two-body interactions. Our calculations of ^{54}Fe in the complete pf shell show clear signatures of a pairing phase transformation at a temperature of 1.1 MeV, but persistent quenching of the Gamow-Teller β^+ strength at higher temperatures. Results at temperatures above 1.5 MeV will become reliable only when two or more major shells are included in the calculations, an elaboration that is computationally quite feasible. The extension of these calculations to other interactions, heavier nuclei, and other observables should allow a more thorough understanding of nuclear properties at high excitation energies than is now possible by other methods.

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