Evidence for Phase Transitions in Finite Systems

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A canonical-ensemble calculation of the specific heat in ^{20}Ne using the eigenstates of a number of realistic interactions and the energies of the states obtained experimentally exhibits a prominent peak at $T \simeq 1.7$–2.5 MeV which is associated with the deformed-to-spherical phase transition seen in finite-temperature mean-field calculations. This phase transition arises from a change in the relevant degrees of freedom describing the system and will occur for any nucleus which has a low-lying collective spectrum. Including a continuum in addition to the discrete spectrum does not produce an additional peak in the specific heat at low temperatures.

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One of the interesting questions which arises in the finite-temperature description of nuclei is whether or not phase transitions really do occur. Finite-temperature mean-field calculations have addressed this question but have not been able to provide a definitive answer because of the large fluctuations inherent in such calculations. The vanishing of an order parameter such as the gap parameter in superconducting nuclei[1] or the quadrupole moment in deformed nuclei[2] has been offered as evidence of the existence of a phase transition in such systems. When the fluctuations, which are partly thermal and partly due to the nuclear-structure approximation, are calculated they are generally large enough to obscure the presence of such a phase transition.[3-5]

Perhaps a more meaningful quantity to study in this respect is the specific heat.[6] Model studies in an SU(2) $\times$SU(2) system show that, in the thermodynamic limit, this system exhibits a singularity in the specific heat characteristic of a true phase transition.[7,8] Furthermore, the remnant of this singularity remains in the form of a peak in finite systems of this type. The presence of this peak in the specific heat has been used to map out the phase structure in such a model.[9]

In deformed nuclear systems, however, it has recently been pointed out[10] that one must obtain in the canonical-ensemble calculation of the specific heat a peak which is due simply to the presence of the ground-state rotational band. Furthermore, if one includes only the states in the ground-state rotational band the asymptotic high-temperature behavior of the specific heat in the canonical ensemble yields, as it should from the law of Dulong and Petit,[11] correct information about the relevant degrees of freedom in the system. The peak, as we have shown in a canonical-ensemble calculation of the specific heat in ^{24}Mg,[5] occurs at a low temperature and is given solely by the contribution of the ground-state band to the specific heat. The high-temperature contribution of the ground-state rotational band is obscured by a much more prominent peak which we associate with a deformed-to-spherical phase transition. In this calculation of the specific heat in ^{24}Mg,[5] however, only the even-J, positive-parity, $I=0$ states were considered.

In this Letter we provide more convincing evidence that phase transitions do indeed take place in deformed systems and discuss in some detail their meaning. We have performed an exact diagonalization of ^{20}Ne in the *sd* shell for a number of realistic effective interactions[12-15] and have used the exact shell-model eigenstates as well as the energies of the states obtained experimentally to calculate the specific heat. In the canonical ensemble, the partition function is given by

$$Z(\beta)=\sum_{J,I,\nu(J,I)}(2I+1)(2J+1)e^{-\beta E_{J,I,\nu(J,I)}}, \tag{1}$$

where $\beta=1/T$ and $\nu(J,I)$ labels the states in each irreducible representation with angular momentum J and isospin I. Here only the ground state is populated at zero temperature and not the entire yrast band. The latter case is more appropriate for nuclei formed in heavy-ion collisions since the kinetic energy can be converted into collective energy before thermalization. The ensemble average of the energy is formally defined by $\langle E\rangle=-\partial(\ln Z)/\partial\beta$ and the specific heat is calculated as the square of the fluctuation in the energy multiplied by β^2; alternatively

$$C_N=\frac{\partial}{\partial T}\langle E\rangle, \tag{2}$$

where the subscript N indicates that the specific heat is evaluated in the canonical ensemble, with the number of particles N in the system fixed. Admittedly the number of states in these systems is not large, but recent model studies of quantum spin chains[16] have demonstrated that quantum systems with few degrees of freedom display quantum-statistical behavior and can be described adequately by the canonical ensemble in spite of the fact that only 2^7 states are present and the density of states is too irregular to be described by a Boltzmann distribution.

In Fig. 1 the low-lying part of the positive-parity eigenspectra for the various *sd*-shell effective interac-

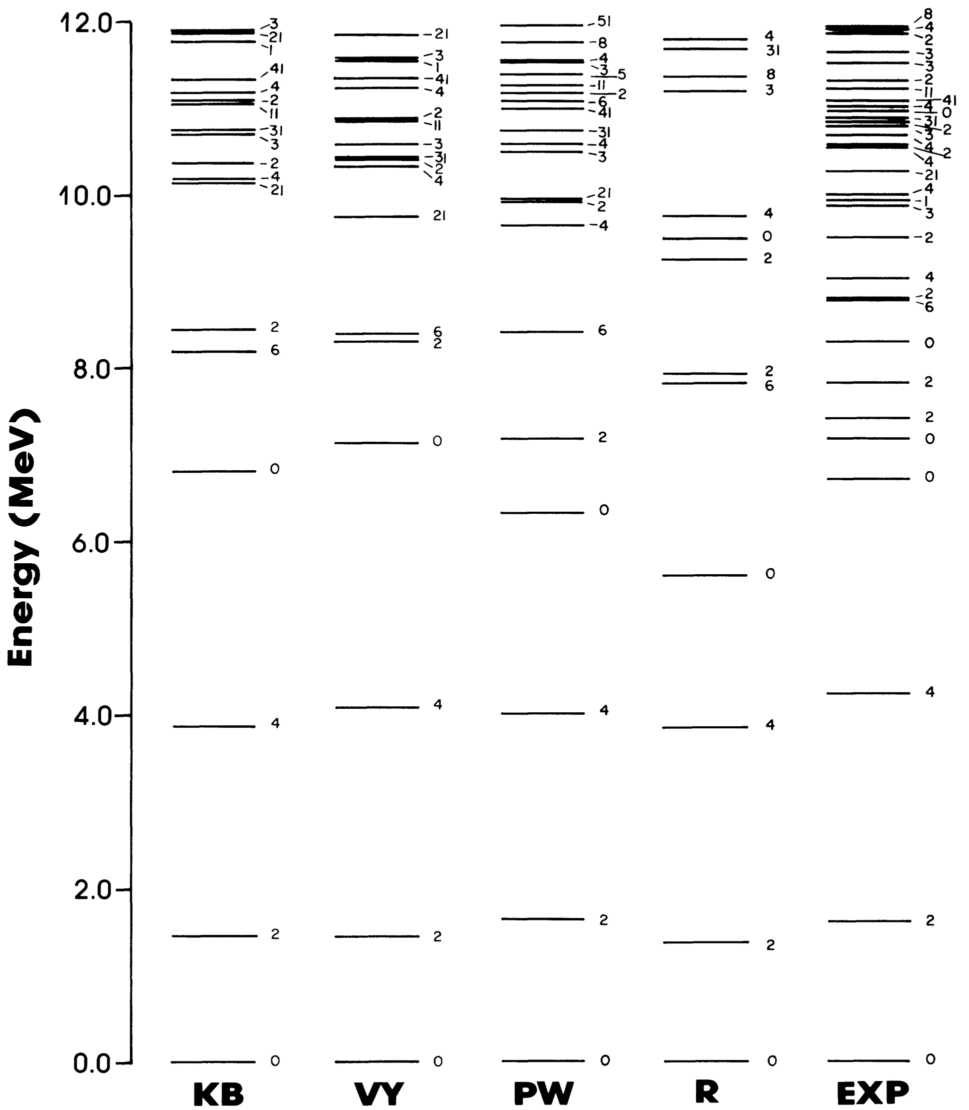

FIG. 1. Shell-model spectra for the positive-parity states in ^{20}Ne calculated with the Kuo-Brown (KB) interaction (Ref. 12), the Vary-Yang (VY) interaction (Ref. 14), the Preedom-Wildenthal (PW) interaction (Ref. 13), and the Rosenfeld (R) interaction (Ref. 15). The experimental spectrum (Ref. 17) (EXP) includes only the positive-parity states.

tions[12-15] are compared with the experimental spectrum. More energy levels occur in the experimental spectrum as no attempt has been made to isolate the states arising primarily from *sd*-shell configurations. All of the effective interactions appear to provide a reasonable description of the low-lying excitation spectrum.

The specific heats as a function of temperature calculated in the canonical ensemble from the eigenstates of the various effective interactions are given in Fig. 2. In all cases the specific heats calculated from the complete eigenspectra are almost identical and exhibit the same structure: a small peak at $T \simeq 0.5$ MeV and a much larger peak at $T \simeq 2.4$ MeV. The temperature at which the maximum of the larger peak occurs differs by less than a few hundred keV for the different effective interactions. In the finite-temperature Hartree-Fock (FTHF) approximation for the Vary-Yang (VY) interaction[14] a similar peak occurs in the specific heat at $T \simeq 2.1$ MeV, indicating quite dramatically that a deformed-to-spherical shape transition has taken place. The change of symmetry is evident in the expansion coefficients of the FTHF solutions.

If only the states in the ground-state rotational band are used in the calculation of the specific heat, this is sufficient to reproduce the smaller peak at the lower temperature and to yield roughly unity at higher temperatures. This behavior is identical for all of the effective interactions and is shown in Fig. 2 for the Preedom-

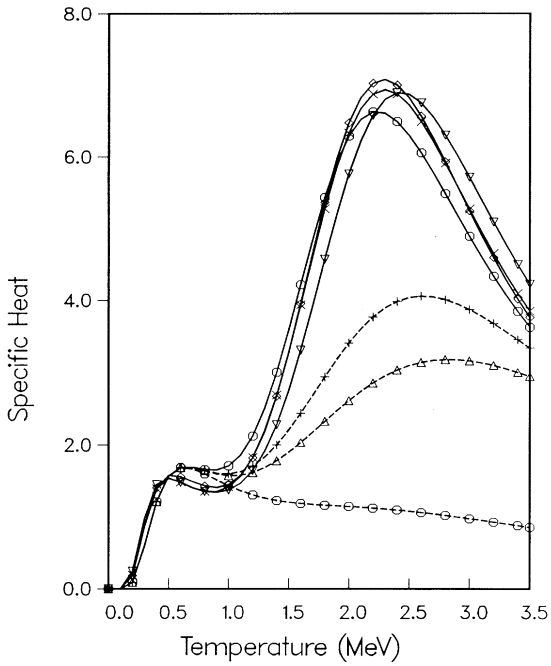

FIG. 2. The specific heat as a function of temperature in the canonical ensemble calculated, solid lines, from the complete eigenspectra of the KB (Ref. 12) (◇), VY (Ref. 14) (×), PW (Ref. 13) (○), and R (Ref. 15) (▽) interactions and, dashed lines, using the eigenstates of the PW (Ref. 13) interaction in the ground-state rotational band (○), and the following sets of eigenstates of J and I: even J, $I=0$ (△) and all J, $I=0$ (+).

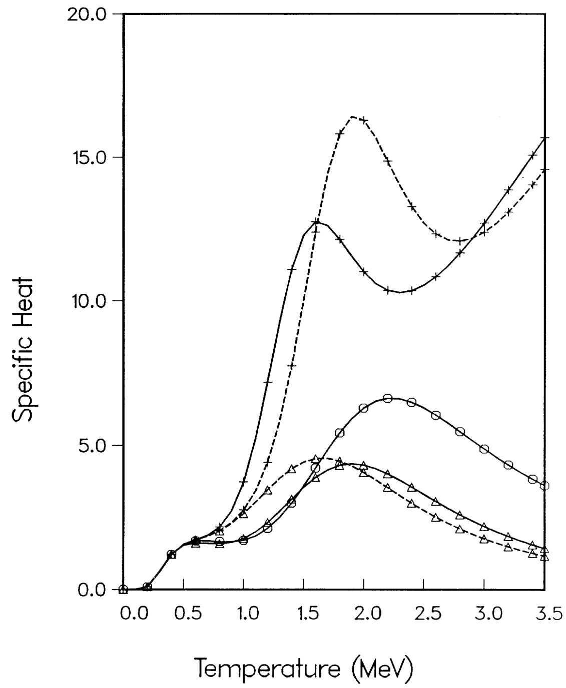

FIG. 3. The specific heat as a function of temperature calculated using the complete eigenspectrum of the PW interaction (solid line plus circles), and using all of the experimental energy levels (dashed line plus triangles) with excitation energy below 14.5 MeV (Ref. 17) and only those with positive parity (solid line plus triangles). The curves labeled with crosses include the effects of continua starting at 10 (solid curve) and 14.5 MeV (dashed curve), respectively.

Wildenthal (PW) interaction. The asymptotic behavior thus gives the correct value for the number of relevant degrees of freedom, namely two for a rotor—each degree of freedom contributes one-half in units of the Boltzmann constant to the asymptotic value of the specific heat. Note also that if only the states in the ground-state rotational band are used in the calculation of the specific heat, the larger peak at $T \simeq 2.4$ MeV is no longer present. As soon as the states with higher excitation energies are used in the calculation of the specific heat a prominent peak appears at $T \simeq 2.5$–3.0 MeV. Regardless of which subset of eigenstates of J and I are included in the ensemble the specific heat shows a large peak which obscures the high-temperature contribution from the states in the ground-state rotational band. Furthermore, as more states are included in the ensemble this peak becomes more pronounced. This behavior may be understood in the following manner: As the system is heated up a transition occurs in the states populated in the canonical ensemble from those associated with the purely collective ground-state rotational band to those of a more random nature. This peak in the specific heat arises from the change in the level density associated with the thermal excitation (see Fig. 1). It signals a change in the relevant degrees of freedom of the system and therefore may be regarded as indicative of a phase transition. This phase transition must occur in all deformed nuclei and is more evident when more states are included in the ensemble. In the FTHF approximation the transition manifests itself as a deformed-to-spherical shape transition, the spherical shape arising from averaging over random deformations which are the result of thermal excitations of different single-particle orbitals.

The specific heat has also been calculated using the experimental energy spectrum of ^{20}Ne[17] (see Fig. 3). The specific heat was computed using just the positive-parity states and using states of both parties to see the effect of the negative-parity states which are not included in the shell-model calculations. In both cases the specific-heat curves obtained resemble in shape those obtained using the shell-model eigenstates. The differences in the magnitudes of the peaks are probably due to the fact that at higher excitation energies the experimental level spectrum is denser than those obtained theoretically (see Fig. 1). For the positive-parity states the position of the maximum is in good agreement with the shell-model results; including the negative-parity states shift the position of the maximum to a slightly lower temperature.

In calculations with the experimental spectrum only those energy levels whose excitation energy is less than 14.5 MeV have been considered since above this energy the assignment of spins and parities of the various levels is less certain. To ensure that this truncation of the spectrum does not affect our conclusions we have added to the discrete spectrum two continua starting at 10 and 14.5 MeV, respectively. As shown in Fig. 3, the main effect of the continuum is to enhance the peak in the specific heat. We have employed for the density of states in the continuum a modification of the usual Fermi-gas-model prediction[18] with level-density parameter $e_0 = 8$ MeV. The qualitative results presented here should not be influenced by the detailed form of the density-of-states function.

In conclusion, we would like to point out that a phase transition of the type described here will occur for any nucleus which has a low-lying collective spectrum, regardless of the nature of the collectivity. Eventually, at some excitation energy, the energy-level spectrum will become denser and more random and a peak will occur in the specific heat which indicates that the relevant degrees of freedom in the system are no longer purely collective. Furthermore, we find it remarkable that no additional peak in the specific heat is produced by the inclusion of the continuum; there is no evidence in the specific heat of the particle-emission thresholds which exist below 18 MeV and which should mark the beginning of a liquid-to-gas phase transition.

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