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Nuclear shape transitions at finite temperature

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Changes in shape in ^{24}Mg are studied at $T \neq 0$ both in finite-temperature mean-field calculations and in the exact canonical ensemble. With increasing temperature the canonical ensemble average of the rotational energy spectrum tends toward a more equispaced harmonic spectrum. This deformed to spherical transition gives rise to a peak in the specific heat which is also seen in finite-temperature Hartree-Fock approximation albeit at a slightly higher temperature. The canonical ensemble average of the quadrupole moment does not, however, appear to vanish at the critical temperature as is the case in the finite-temperature Hartree-Fock approximation.

INTRODUCTION

At zero temperature deformed nuclei exhibit a rotational spectrum. This can be approximated microscopically in a mean-field treatment most simply by a cranking calculation for each angular momentum of the band. A simple constraint of the form $\langle \hat{j}_x \rangle = \sqrt{J(J+1)}$ is generally sufficient to ensure that the cranked energy-level spacings provide a reasonable first-order approximation to the exact energy-level spacings. At nonzero temperatures an interesting situation develops. As the system heats up it tends to become less deformed on the average, and in unconstrained mean-field calculations at a certain critical temperature undergoes a deformed to spherical phase transition.[1-6] Clearly this cannot happen in a cranked mean-field calculation as the equation of constraint must be satisfied for each angular momentum. Instead as the critical temperature is approached it becomes impossible to find solutions of the cranked mean-field equations. This behavior has been demonstrated previously in Hartree-Fock calculations in which a constraint on the total angular momentum has been used.[7]

In the present work we have investigated the thermal response of a rotational band in ^{24}Mg in both the cranked finite-temperature Hartree-Fock approximation and in the exact canonical ensemble. In both cases we are interested in examining the phase structure of the rotational band as a function of temperature. Recently it has been pointed out[8] that in the canonical ensemble the specific heat

$$C_N = \frac{\partial}{\partial T}\langle E \rangle \tag{1a}$$

$$= \beta^2(\langle E^2 \rangle - \langle E \rangle^2) \tag{1b}$$

must exhibit a peaked structure at low temperature for systems with a rotational spectrum. Here

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

$$\langle E^2 \rangle = \sum_{J,\nu(J)} (2J+1) E^2_{J,\nu(J)} e^{-\beta E_{J,\nu(J)}} / Z(\beta) , \tag{3}$$

$$Z(\beta) = \sum_{J,\nu(J)} (2J+1) e^{-\beta E_{J,\nu(J)}} . \tag{4}$$

$\beta = 1/T$; $\nu(J)$ labels the states in each irreducible representation with angular momentum J, and the subscript N on C indicates that the specific heat is evaluated in the canonical ensemble with the number of particles N in the system fixed. In the present work we see evidence of this peak in the specific heat at $T \simeq 0.5$ MeV but it is obscured by a larger peak at $T \simeq 2.6$ MeV. We note also that with increasing temperature the exact canonical ensemble average of the rotational energy spectrum tends towards a more equispaced harmonic spectrum associated with a spherical nucleus which suggests that the larger peak at $T \simeq 2.6$ MeV is associated with a deformed to spherical phase transition. In the uncranked finite-temperature Hartree-Fock (FTHF) calculations in deformed systems a similar peaked structure is observed and has been interpreted as the onset of a phase transition.[6,13] Furthermore, the ensemble average of the quadrupole moment goes to zero at roughly the same critical temperature.[5] In the present work this vanishing of the quadrupole moment at the critical temperature is not seen in the exact canonical ensemble results. As has been noted previously in model calculations[6] work we find that the critical temperature of the deformed to spherical phase transition is predicted to lie higher in temperature in the FTHF approximation than in the canonical ensemble calculations.

The same peaked structure occurs in the specific heat calculated in both the canonical ensemble and the uncranked FTHF approximation as well as for each angular momentum of the rotational band in both the canonical ensemble and the cranked finite-temperature Hartree-Fock (CFTHF) approximation. Unfortunately, before the critical temperature is reached it is no longer possible to find solutions of the CFTHF equations for $J \neq 0$; however, the onset of the phase transition appears to be reasonably well predicted.

NUMERICAL RESULTS

In order to perform the exact diagonalization, in the present work we consider ^{24}Mg as an inert ^{16}O core plus eight valence particles in the 2s-1d shell. The total number of states with even spin and isospin $I=0$ is 4082. Clearly the number of states in the system is not large, but recent model studies of quantum spin chains have demonstrated that quantum systems with few degrees of freedom display quantum-statistical behavior. Numerical studies of such systems[9] have shown that they could be adequately described by the canonical ensemble in spite of the fact that only 2^7 states were present and the density of states was too irregular to be described by a Boltzmann distribution. Furthermore, in finite-temperature mean-field calculations at low temperature,[5] only the valence particles are thermally excited and it seems reasonable, therefore, to neglect the thermal excitation of the core.

In the CFTHF calculations the thermodynamic potential

$$\Omega=\langle H\rangle_T-TS-\mu N \tag{5}$$

is minimized with respect to the Hartree-Fock (HF) orbitals and the single-particle thermal occupation probabilities f_ν, subjected to the constraints

$$\sum f_\nu=N \tag{6}$$

and

$$\langle\hat{j}_x\rangle_T=\sqrt{J(J+1)}\ . \tag{7}$$

Here $\langle\ \rangle_T$ denotes the ensemble average at temperature T, the chemical potential is given by μ, the number of particles by N, and the entropy by S, where

$$S=-\sum[f_\nu\ln f_\nu+(1-f_\nu)\ln(1-f_\nu)]\ . \tag{8}$$

In the 2s-1d shell we used an effective Hamiltonian with the Vary-Yang interaction,[10] including additional third-order corrections to the G matrix to provide a more complete accounting of the core-polarization effects[11] and the following single-particle energies:

$$\epsilon_{d_{5/2}}=-5.00\text{ MeV}\ ,$$

$$\epsilon_{d_{3/2}}=0.08\text{ MeV}\ ,$$

$$\epsilon_{s_{1/2}}=-4.13\text{ MeV}\ .$$

Only the thermal response of the states of total isospin $I=0$ were considered in the present calculations in ^{24}Mg. Relaxing this constraint is not expected to be overly important since the $I\neq 0$ spectrum lies significantly higher in energy.

The exact diagonalization of the effective Hamiltonian was performed by means of the Lanczos algorithm.[12] Because of the presence of the Boltzmann factor, the lowest-lying eigenstates are most heavily weighted in the exact canonical ensemble calculations. Previous calculations[13] have demonstrated that using roughly 10% or less of the eigenspectrum produced results at low temperatures which are indistinguishable from those obtained with the compete eigenspectrum. In the present work we have used only those eigenstates which lie in the first 10–15 MeV of excitation energy for each angular momentum.

DISCUSSION OF RESULTS

The numerical results for the ensemble average of the energy are given in Fig. 1. In the FTHF approximation the ensemble average of the energy rises more steeply as a function of energy than in the full canonical ensemble and is shifted up in energy. A similar behavior was noted in previous uncranked calculations in ^{20}Ne.[13] The simple smearing out of the occupation of the single-particle orbitals does not appear to approximate very well the temperature dependence of the results obtained in the exact canonical ensemble. Furthermore, in the FTHF approximation more structure is seen than in the canonical results. At $T\simeq 3.1$ MeV the abrupt change in slope is usually interpreted as the signal of a deformed to spherical phase transition. This agrees reasonably well with a critical temperature of about 2.8 MeV obtained previously in a realistic no-core calculation in ^{24}Mg.[5] The change of slope at $T\simeq 1.7$ MeV signals a change in the system from a triaxial to an axially symmetric shape.[14]

The numerical results for the ensemble average of the energy of the $J=0$, 2, 4, 6, and 8 states as a function of

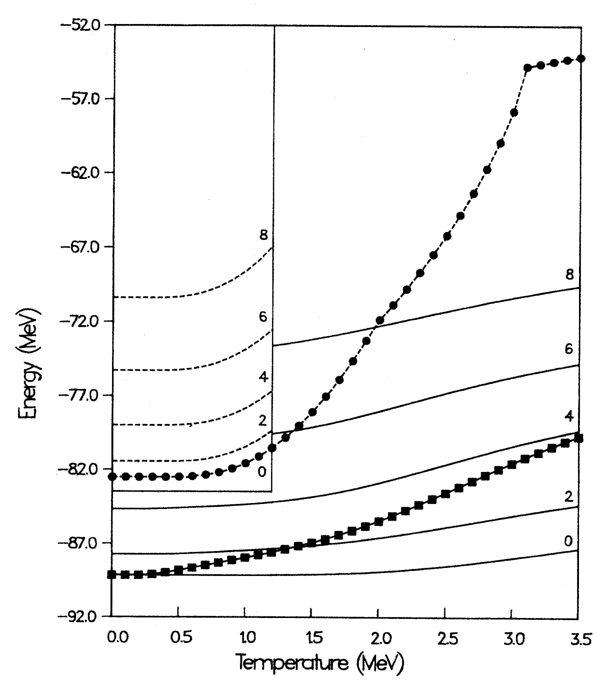

FIG. 1. The ensemble average of the energy as a function of temperature in the exact canonical ensemble (■) and the FTHF approximation (●). For the angular momenta $J=0$, 2, 4, 6, and 8 the ensemble average of the energy in the canonical ensemble and the CFTHF approximation (inset) are indicted by solid and dashed lines, respectively. The $J=0$ solution of the CFTHF equations corresponds to the FTHF solution.

temperature are also given in Fig. 1 for the exact canonical ensemble and for the CFTHF approximation. The canonical ensemble average of the energy has been calculated using Eq. (2) by summing over $\nu(J)$ only for each value of J individually. Note that the $J=0$ solution of the CFTHF equations is the same as that obtained in the FTHF approximation since the cranking term in this case is identically equal to zero. For $T \geq 1.2$ MeV we were unable to find solutions of the FTCHF equations for $J \neq 0$. This is most likely due to the fact that with increasing temperature the system on the average becomes more spherical and it becomes increasingly more difficult to fulfill the equation of constraint. Aside from an overall shift in energy the FTCHF results rise more steeply with increasing temperature than those obtained in canonical ensemble.

The temperature dependence of the moment of inertia has been determined (see Fig. 2) by fitting the energy spectrum in the canonical ensemble and the CFTHF approximation at each temperature to that of a rotor. In both cases the moment of inertia decreases as a function of temperature. For $T < 1.2$ MeV the errors in the fits in the CFTHF approximation are negligibly small and not significantly larger in the canonical ensemble which confirms that the ensemble average of the spectrum remains rotational in nature. The ensemble average of the energy spectrum obtained in the canonical ensemble has also been fitted to an equispaced harmonic spectrum in which the level spacing has been adjusted at each temperature to give the best fit (see Fig. 2). At lower temperatures the errors in this fit are rather large but they decrease with increasing T and become less than those obtained for the fit to the energy spectrum of a rotor for $T > 2.4$ MeV. This strongly suggests that a deformed to spherical phase transition has taken place at a critical temperature of $T_c \simeq 2.6$ MeV.

In order to try to further verify that a phase transition has indeed occurred we have calculated the specific heat as a function of temperature (see Figs. 3 and 4). The specific heat has also been calculated in the FTHF approximation (see Fig. 3). In this case we have used the definition

$$C = \frac{\partial \langle \hat{H} \rangle_T}{\partial T} \tag{9}$$

and not that given in Eq. (1b). The two definitions are inequivalent for finite-temperature mean-field calculations,[15] and the definition given above is believed to be more accurate.[16] The derivative has been determined by fitting a smooth curve to the values of $\langle \hat{H} \rangle_T$ and differentiating. In the FTHF approximation two prominent peaks are seen in the specific heat at the same temperatures at which the changes in slope is observed in the ensemble average of the energy (see Fig. 1). The peaks in the specific heat at $T \simeq 1.7$ and 3.1 MeV correspond to an average change in shape of the system from ellipsoidal to axially symmetric and from axially symmetric to spheri-

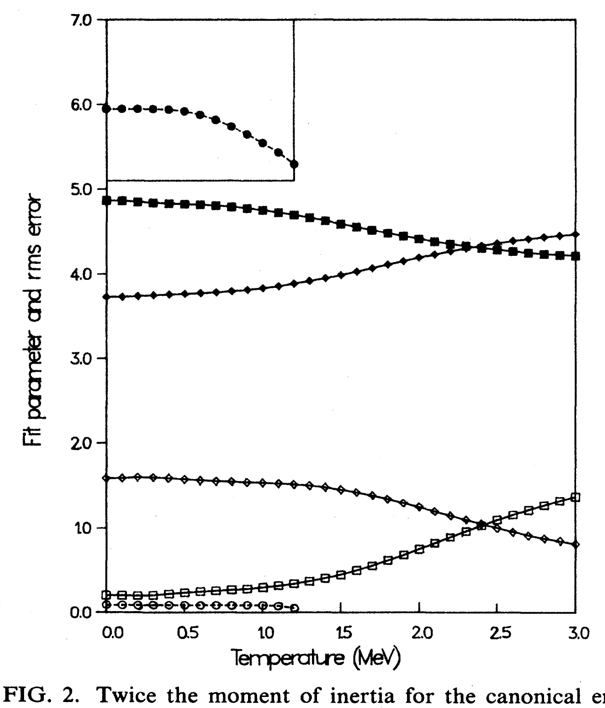

FIG. 2. Twice the moment of inertia for the canonical ensemble (■) and the CFTHF solutions (●) together with the respective rms errors in the fit to a rotational spectrum (□) and (○) (×10) as a function of temperature. Also shown is the energy spacing (♦) for the best fit to a harmonic spectrum and the rms error in this fit (◇).

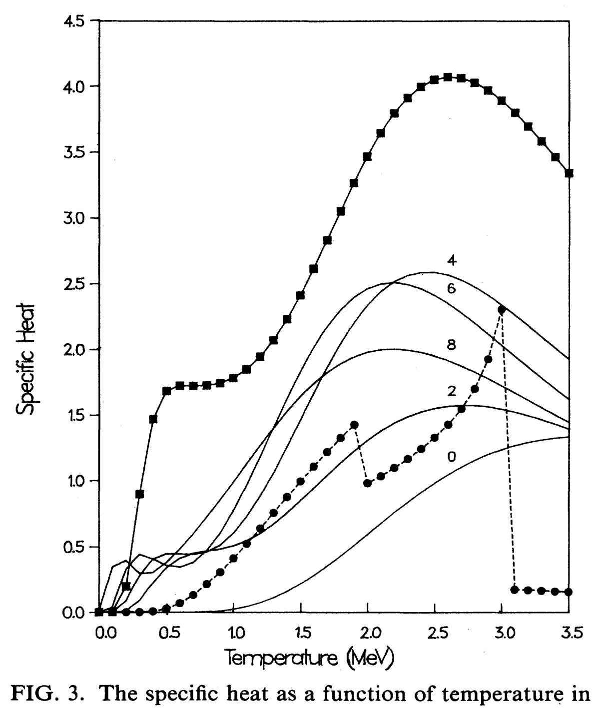

FIG. 3. The specific heat as a function of temperature in the canonical ensemble (■) and in the FTHF approximation (●). One should note that the values for the FTHF approximation have been divided by a factor of 10 in order to display them on the same plot. For the angular momenta $J=0$, 2, 4, 6, and 8 the specific heat calculated in the canonical ensemble is also given by the appropriately labeled solid lines.

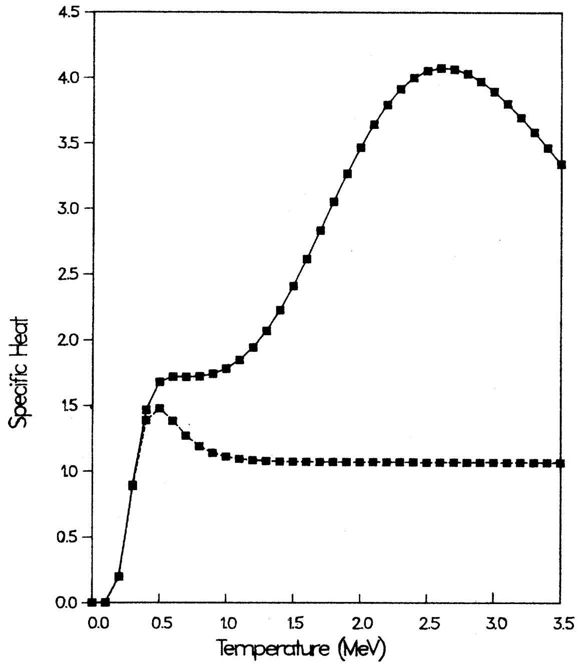

FIG. 4. The specific heat as a function of temperature calculated in the full canonical ensemble (solid curve) and for the eigenstates in the ground-state rotational band only (dashed curve).

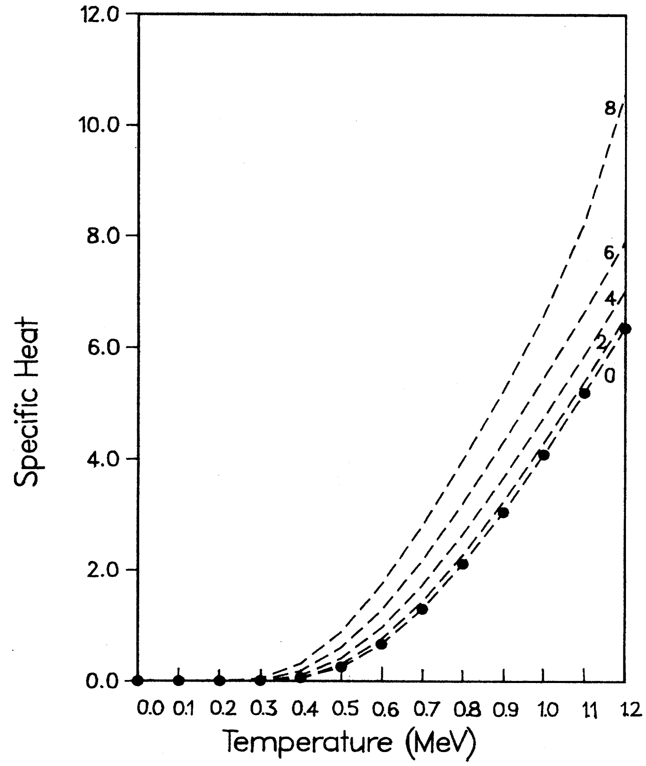

FIG. 5. The specific heat as a function of temperature in the CFTHF approximation for the angular momenta $J=0$, 2, 4, 6, and 8. Again the $J=0$ results are identical to the FTHF results (●).

cally symmetric, respectively.

In the canonical ensemble average one can also see a peak in the specific heat at $T \simeq 2.6$ MeV corresponding to the observed change in the energy spectrum discussed previously and lending further support to our conjecture that a deformed to spherical phase transition has indeed taken place. There is also a shoulder at $T \simeq 0.5$ MeV which, in spite of the slight loss of numerical accuracy in the calculation at low temperature, is probably due to the presence of the ground-state rotational band. In Fig. 4 we compare the full canonical ensemble calculation of the specific heat with that calculated using only the eigenstates in the ground-state rotational band. The specific heat in the latter case exhibits a small peak at $T \simeq 0.5$ MeV and appears to go asymptotically with increasing temperature to roughly unity as expected.[8] In the full canonical ensemble results this asymptotic behavior is obscured by the presence of the larger peak. The specific heat for each angular momentum J in the canonical ensemble has been calculated using the expression

$$C_J = \frac{\langle \hat{H}^2 \rangle_{T,J} - \langle \hat{H} \rangle_{T,J}^2}{T^2} . \qquad (10)$$

The same structure (see Fig. 3) seen in the complete canonical ensemble calculations are observed in the specific heat calculated for each individual angular momentum. The specific heat has also been calculated for the different angular momenta in the FTCHF approximation (see Fig. 5). In this case we have used the definition

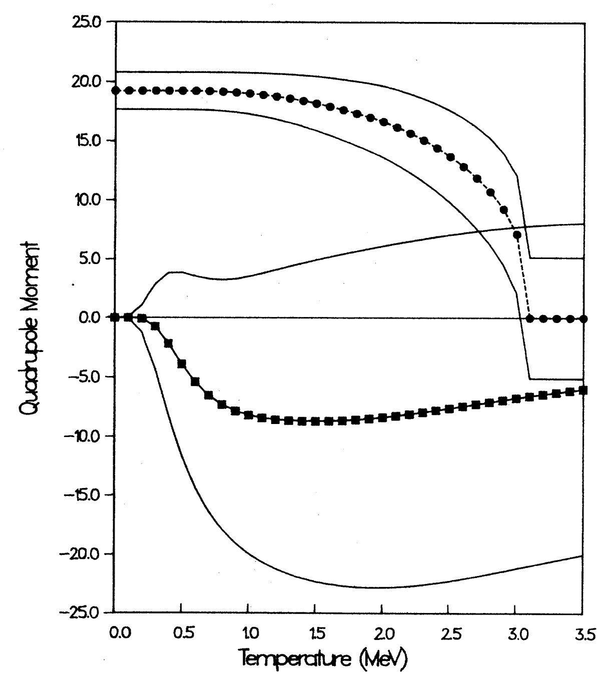

FIG. 6. The ensemble average of the quadrupole moment in the FTHF approximation (●) and in the canonical ensemble (■). The fluctuations in both calculations are indicated by the adjacent solid curves.

$$C_J = \frac{\partial \langle \hat{H} \rangle_{T,J}}{\partial T} . \tag{11}$$

The derivative has been determined by fitting a smooth curve to the values of $\langle \hat{H} \rangle_{T,J}$ and differentiating it for each value of the angular momentum. For all angular momenta the specific heat increases rapidly with increasing temperature. Unfortunately we were only able to find solutions for $T \leq 1.2$ MeV. Hence we are only able to see the onset of the deformed to spherical phase transition without being able to ascertain the critical temperature at which it occurs.

Lastly we have calculated the ensemble average of the quadrupole moment and its fluctuations in the canonical ensemble and in the FTHF approximation (see Fig. 6). At $T \simeq 0$ the canonical ensemble average of the quadrupole moment is zero because the spin of the groundstate in ^{24}Mg is zero. With increasing temperature it becomes negative and never vanishes. It is most unlikely that the canonical ensemble average of the quadrupole moment vanishes at higher temperatures since with increasing temperature the states of higher angular momenta become more important and their quadrupole moments are predominantly negative. Furthermore, the fluctuations are extremely large and clearly no indication of the deformed to spherical transition occurs. On the other hand, in the FTHF approximation the ensemble average of the quadrupole moment, which has opposite sign, vanishes at $T \simeq 3.1$ MeV. At this temperature as discussed above the FTHF solution becomes spherically symmetric.

In conclusion we feel that there is ample evidence in support of the existence of a deformed to spherical phase transition in ^{24}Mg at $T \simeq 2.6$ MeV. At this temperature the peak in the specific heat in the canonical ensemble has been shown to arise from a change in the ensemble average of the energy spectrum from rotational to harmonic. Somewhat surprisingly this change in the nature of the energy spectrum is not reflected in the ensemble average of the quadrupole moment which neither vanishes nor becomes significantly smaller in the canonical ensemble. The critical temperature of the phase transition is predicted to lie slightly higher in the FTHF approximation. Again the presence of a phase transition is signaled unambiquously by the presence of peaks in the specific heat calculated in this case as the numerical derivative of the ensemble average of the energy as well as the vanishing of the ensemble average of the quadrupole moment.

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[1]M. Brack and Ph. Quentin Phys. Scr. A **10**, 163 (1974); Phys. Lett. **52B**, 159 (1974).
[2]S. Levit and Y. Alhasid, Nucl. Phys. **A413**, 439 (1984).
[3]H. G. Miller and J. P. Vary, Phys. Lett. **150B**, 11 (1985).
[4]U. Mosel, P. G. Zint, and K. H. Passler, Nucl. Phys. **A236**, 252 (1974).
[5]H. G. Miller, R. M. Quick, G. Bozzolo, and J. P. Vary, Phys. Lett. B **168**, 13 (1986).
[6]E. D. Davis and H. G. Miller, Phys. Lett. B **196**, 277 (1987).
[7]R. M. Quick and H. G. Miller, Phys. Rev. C **34**, 1458 (1986).
[8]R. K. Bhaduri and W. van Dijk, Nucl. Phys. **A485**, 1 (1988).
[9]R. V. Jenson and R. Shankar, Phys. Rev. Lett. **54**, 1879 (1985).
[10]J. P. Vary and S. N. Yang, Phys. Rev. C **15**, 1545 (1977).
[11]M. S. Sandel, R. J. McCarthy, B. R. Barrett, and J. P. Vary, Phys. Rev. C **17**, 777 (1978).
[12]R. R. Whitehead, A. Watt, B. J. Cole, and I. Morrison, Adv. Nucl. Phys. **9**, 123 (1977).
[13]R. M. Quick, H. G. Miller, and B. J. Cole (unpublished).
[14]B. J. Cole, R. M. Quick, and H. G. Miller (unpublished).
[15]R. Rossignoli, A. Plastino, and J. P. Vary, Phys. Rev. **C37**, 314 (1988).
[16]R. M. Quick and H. G. Miller (unpublished).