Shape of ^{24}Mg at zero and finite temperature

B. J. Cole,* R. M. Quick, and H. G. Miller
Department of Physics, University of Pretoria, Pretoria 0002, South Africa
(Received 27 February 1989)

Hartree-Fock-Rothaan calculations with realistic effective interactions in the *sd* shell consistently yield an ellipsoidal ground-state deformation for ^{24}Mg. The predictions of the present mean-field calculations are supported by experiment and exact shell-model calculations. For a deformed ground state with ellipsoidal symmetry two shape transformations are observed in the finite-temperature Hartree-Fock approximation as the temperature is increased, firstly from ellipsoidal to axially symmetric and finally to a spherical shape.

The long-standing controversy concerning the shape of ^{24}Mg has been revived in two recent publications,[1,2] with some calculations now indicating an axially-symmetric ground state whilst others suggest a triaxial shape. We have carried out a series of calculations for ^{24}Mg with both the shell-model and Hartree-Fock techniques, using realistic effective interactions in the *sd*-shell-model space, which enable us to clarify the situation. In addition, our recent work[3] on the finite-temperature properties of nuclei allows us to extend this discussion to the changes in shape which ^{24}Mg experiences when the temperature is increased, i.e., to the phase transitions which the nucleus undergoes.

Bonche *et al.*[1] imply that mean-field calculations with more realistic Skyrme interactions will yield an axially-symmetric deformation for the ground-state band of ^{24}Mg, rather than the triaxiality produced by simple density-dependent interactions.[4,5] Previous no-core realistic effective interactions defined in large model spaces[6] also appeared to yield a ground-state band in ^{24}Mg which has a prolate deformation.[7] In contrast, the use of effective interactions defined in the *sd* shell, whether phenomenological[8] or more realistic,[9] consistently, as we will demonstrate, lead to predictions that the ground-state band has ellipsoidal symmetry. These smaller model-space calculations have the advantage that their results can be compared directly with exact shell-model calculations with the same interaction in the same space; as shown below, the nonaxial nature of the ground-state band seems to be supported by such calculations as well as by experiment. In the case where the ground-state band possesses ellipsoidal symmetry, ^{24}Mg undergoes two shape transformations as the temperature is increased,[3] firstly from ellipsoidal to axially symmetric and finally to a spherical shape; this second transformation may be indicative of the liquid-to-gas phase transition which appears if the effects of the continuum are considered.[10,11]

The shape of ^{24}Mg is apparently quite sensitive both to the choice of effective interaction and also to the details of the computational technique used. Bonche *et al.*[1] solved the self-consistent cranked Hartree-Fock plus BCS equations using several parametrizations of the Skyrme interaction. Using the Skyrme III interaction, which incorporates a spin-orbit coupling term, they found that the ground-state deformation was predicted to be prolate; this contrasted with their earlier calculations which omitted the spin-orbit force and which produced a triaxial shape.[5] Other interactions which they tried also lead to a prolate deformation. The fact that strong spin-orbit coupling tends to oppose deviations from axial symmetry is not unexpected.[12] A prolate ground-state deformation was also obtained in very large model space no-core Hartree-Fock-Rothaan calculations.[7] These calculations used a realistic effective interaction obtained from the two-particle $\mathcal{G}$ matrix with folded-diagram corrections;[6] matrix elements were scaled to $A=24$ and minor adjustments were applied to predict more accurately the correct ground-state binding energy and rms radius. However, we recently repeated these calculations with a more extensive search for further Hartree-Fock (HF) solutions and discovered an ellipsoidal ground-state solution which lies 3 MeV below the previously found solution of lowest energy.

Hartree-Fock-Rothaan calculations using the simple Rosenfeld interaction in a model space (the *sd* shell) had in any case previously indicated that the lowest-energy solution for ^{24}Mg possesses ellipsoidal symmetry;[13,14] the first axially-symmetric solution lies about 3 MeV higher in energy. In this work we have carried out a series of similar calculations employing the more realistic *sd*-shell effective interaction of Vary and Yang.[9] This interaction includes additional third-order corrections to the $\mathcal{G}$ matrix to provide a more complete accounting of core-polarization effects,[15] and is used in conjunction with the following single-particle energies:

$$\epsilon(d_{5/2})=-5.00 \text{ MeV} ,$$

$$\epsilon(d_{3/2})=0.08 \text{ MeV} ,$$

$$\epsilon(s_{1/2})=-4.13 \text{ MeV} .$$

As already indicated, the solution of lowest energy found in Hartree-Fock-Rothaan calculations using this interaction has ellipsoidal symmetry; the first axially-symmetric solution lies about 2 MeV higher.

In order to establish the reliability of this interaction we also calculated the spectrum of the lowest even $J^+, T=0$ states with a shell-model diagonalization in the full *sd*-shell model space; the results are displayed in Fig. 1 together with the experimental spectrum.[16,2] Although the agreement with data is not comparable to that found for this nucleus with fitted interactions (see, for example, Refs. 17, 18, and 2), it is nonetheless surprising, with an rms deviation of approximately 0.8 MeV for excitation energies up to about 10 MeV, giving confidence in the ability of this interaction to describe adequately ^{24}Mg at low excitation energies. The calculated quadrupole moment of the first 2^+ state, $Q=-0.19\ e$ b with an effective charge of 0.5e, is also in reasonable agreement with the measured value, $Q=-0.25\ e$ b.[16]

There are also indications in the experimental data that an axially-asymmetric solution is not unreasonable. The low-lying states are usually assigned to either the ground-state $K=0$ band or a $K=2$ band based on the 2^+ state at 4.24 MeV; in the shell-model calculations reported here this 2^+ state is lowered to 3.23 MeV. The Hartree-Fock calculations must in some way incorporate effects from both these bands which necessarily have different intrinsic structures; mixing of two such bands leads naturally to a solution of undefined K, i.e., to a solution with nonaxial symmetry. Further evidence of nonaxial symmetry is provided by the macroscopic-microscopic calculations of Sheline *et al.*;[2] the potential energy surfaces computed with the extended Nilsson-Strutinsky formalism clearly indicate that the various members of the ground-state band are in fact triaxial. In addition, as pointed out by Sheline *et al.*, the unexpectedly large γ-decay rates which have been measured for some interband transitions can be easily explained if the ground-state band itself is not pure $K=0$.

The thermal response of ^{24}Mg has been studied both in finite-temperature Hartree-Fock calculations (FTHF) and in the exact canonical ensemble;[3] these calculations extend the previously discussed HF-Rothaan and shell-model calculations to finite temperatures. The FTHF results for the ensemble average of the energy are presented in Fig. 2, which displays the behavior of the three lowest HF solutions as the temperature is increased. The symmetry of each solution can be determined by studying the coefficients of its wave function expanded in a spherical basis. This reveals, for example, that the lowest-lying solution changes from ellipsoidal shape to prolate at $T \simeq 1.9$ MeV and from prolate to spherical at about 3 MeV; in fact all solutions merge finally into a single spherical solution in a global shape transition at $T \simeq 3$ MeV. For comparison, the canonical ensemble average of the energy

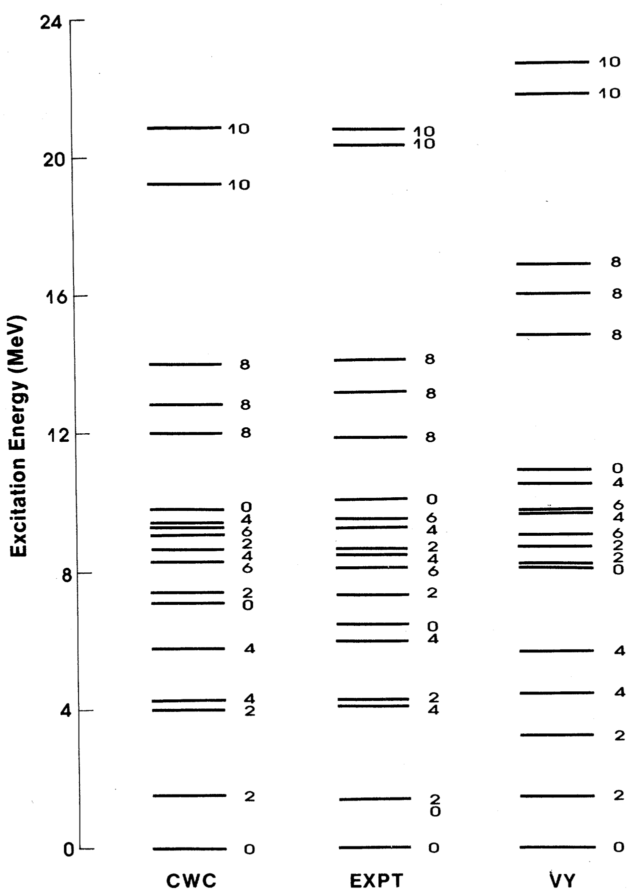

FIG. 1. Shell-model spectra of ^{24}Mg calculated with the Chung-Wildenthal plus Coulomb (CWC) interaction (Ref. 18) and the Vary-Yang (VY) interaction (this work). The experimental spectrum (EXPT) includes all states of even J, $T=0$ below 9.0 MeV and selected states above 9.0 MeV (Ref. 16).

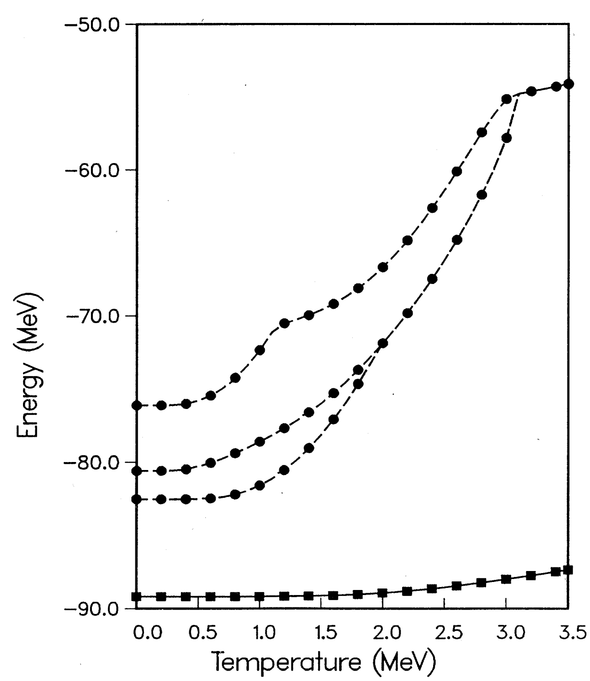

FIG. 2. The ensemble average of the energy as a function of temperature in the exact canonical ensemble (■) and the FTHF approximation (●). At $T=0$ the solutions of the FTHF equations with increasing energy have ellipsoidal, axial and ellipsoidal symmetry, respectively.

$$\langle E \rangle = \sum_{\nu} (2J+1) E_\nu \exp(-E_\nu/T) / \sum_{\nu} (2J+1)\exp(-E_\nu/T)$$

is also given. The sums in this equation run over the low-lying $J^+ =$even, $T=0$ states predicted in the shell-model calculations. The temperature dependence of the canonical ensemble results is quite different from that obtained in the FTHF approximation. Nonetheless, if the specific heat, $C = \partial\langle E \rangle / \partial T$, is computed, a broad peak is seen at $T=2.5$ MeV, signaling a change in the predicted spectrum from essentially rotational to basically harmonic;[3] this peak therefore corresponds to the global shape transition seen in the FTHF approximation.

Two of us (B.J.C. and H.G.M.) acknowledge the support of the Foundation for Research Development, Pretoria and, in addition, B.J.C. acknowledges the hospitality and financial support of the University of Pretoria.

*On leave from Department of Physics, University of the Witwatersrand, Johannesburg, South Africa.

[1] P. Bonche, H. Flocard, and P. H. Heenen, Nucl. Phys. **A467**, 115 (1987).
[2] R. K. Sheline, I. Ragnarsson, S. Aberg, and A. Watt, J. Phys. **14**, 1201 (1988).
[3] H. G. Miller, R. M. Quick, and B. J. Cole, Phys. Rev. C **39**, 1599 (1989).
[4] P. Bonche, S. Koonin, and J. W. Negele, Phys. Rev. C **13**, 1226 (1976).
[5] H. Flocard, P. H. Heenen, S. J. Krieger, and M. S. Weiss, Prog. Theor. Phys. **72**, 1000 (1984).
[6] G. Bozzolo and J. P. Vary, Phys. Rev. C **31**, 1909 (1985).
[7] H. G. Miller, R. M. Quick, G. Bozzolo, and J. P. Vary, Phys. Lett. **168B**, 13 (1986).
[8] L. Rosenfeld, *Nuclear Forces* (North-Holland, Amsterdam, 1958), p. 233.
[9] J. P. Vary and S. N. Yang, Phys. Rev. C **15**, 1545 (1977).
[10] H. G. Miller, B. J. Cole, and R. M. Quick (unpublished).
[11] B. J. Cole, H. G. Miller, and R. M. Quick (unpublished).
[12] A. Bohr and B. R. Mottelson, *Nuclear Structure* (Benjamin, New York, 1975), Vol. 2.
[13] J. Bar-Touv and I. Kelson, Phys. Rev. **138**, B1035 (1965).
[14] G. Ripka, *Advances in Nuclear Structure,* edited by M. Baranger and E. Vogt (Plenum, New York, 1958), Vol. 1, p. 183.
[15] M. S. Sandel, R. J. McCarthy, B. R. Barrett, and J. P. Vary, Phys. Rev. C **17**, 777 (1978).
[16] P. M. Endt and C. Van der Leun, Nucl. Phys. **A310**, 1 (1978).
[17] B. J. Cole, A. Watt, and R. R. Whitehead, J. Phys. A **7**, 1374 (1974).
[18] D. Kelvin, A. Watt, and R. R. Whitehead, J. Phys. G **3**, 1539 (1977).