Thermal Response of Light Nuclei with a Realistic Effective Hamiltonian

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A realistic microscopic effective Hamiltonian (H_{eff}) is employed with the spherical finite-temperature Hartree-Fock approximation to evaluate the thermodynamic properties of ^{16}O and ^{40}Ca. We scale H_{eff} to accommodate the A-dependent effects. We then adjust the Hamiltonian slightly to reproduce appropriate ground-state properties in the Hartree-Fock approximation. We find the thermal response of these nuclei to be substantially greater than that obtained with zero-range phenomenological forces.

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A realistic, microscopically derived, nuclear equation of state for finite nuclei would be of great utility for interpreting current experiments in heavy-ion scattering and high-energy particle-nucleus collisions. A necessary and major step towards obtaining this equation of state involves solving for the thermal properties of nuclei without external constraints. A theoretical framework to explore the thermal properties of finite nuclei in the mean-field approximation has been introduced by Bloch and di Dominicis.[1] This framework and extensions to include the effects of superconductivity[2] have been applied to nuclei with phenomenological Hamiltonians.[3] We present results for two representative nuclei, ^{16}O and ^{40}Ca, in the finite-temperature Hartree-Fock approximation (FTHF) employing realistic effective Hamiltonians.

Given an effective Hamiltonian H_{eff} for a chosen model space, we minimize the free energy

$$F = \langle H_{\text{eff}} \rangle - TS, \tag{1}$$

assuming a mean-field approximation at fixed temperature T, and obtain the FTHF equations.[1,3] The fully self-consistent solutions of these equations provide the thermal properties of nuclei as a function of temperature.

The basic FTHF ingredients are defined as in the $T=0$ case but with a one-body operator

$$\rho = \textstyle\sum_\nu f_\nu |\nu\rangle\langle\nu|, \tag{2}$$

where $|\nu\rangle$ is an eigenstate of the Hartree-Fock Hamiltonian, corresponding to a single-particle (s.p.) energy e_ν, and f_ν is its occupation probability. For fermion systems,

$$f_\nu = \{1+\exp[(e_j-\mu)/T]\}^{-1}. \tag{3}$$

In this convention, temperature is given in energy units. The entropy is given by

$$S = -k \textstyle\sum_\nu [f_\nu \ln(f_\nu) + (1-f_\nu)\ln(1-f_\nu)].$$

The neutron and proton chemical potentials are determined separately in each iteration by requiring that the sums of neutron and proton occupation probabilities equal the desired numbers. The implementation of this constraint distinguishes FTHF treatment of finite systems from conventional applications to infinite systems. The equilibrium solution of the above equations at each T provides the entropy, excitation energy, free energy, neutron and proton chemical potentials, s.p. energies, occupation probabilities, and radial density distributions. In order to evaluate further features of the nuclear equation of state we must introduce constraints in the variational method but this is deferred to a later effort.

In principle, H_{eff} is also T dependent[4] but we have ignored this complication in our initial applications. Our approach is based on the philosophy that we will first develop the H_{eff} that would be appropriate to the full diagonalization of the no-core many-nucleon problem in the chosen finite model space. We have previously applied moment methods[5] to obtain spectral properties from these same effective no-core Hamiltonians. In brief, we write H_{eff} as

$$H_{\text{eff}} = T_{\text{rel}} + V_{\text{eff}} + V_c, \tag{4}$$

where T_{rel} is the relative kinetic energy operator between pairs of nucleons, V_C is the Coulomb interaction between protons, and V_{eff} is the sum of the Brueckner G matrix and the lowest-order folded diagram (second order in G) acting between pairs of nucleons in the model space.[5] The underlying nucleon-nucleon interaction is the Reid soft-core potential.[6] For evaluating matrix elements of H_{eff} we choose the harmonic-oscillator basis with $\hbar\omega = 14$ MeV and we select a sequence of model spaces abbreviated as the 2-space (0s, 0p, and 1s-0d shells), the 3-space (0s, 0p, 1s-0d, and 1p-0f shells), the 4-space (0s, 0p, 1s-0d, 1p-0f, and 2s-

1d-0g shells), and the 5-space (all shells through the 2p-1f-0h shell). This sequence of model spaces permits us to estimate convergence properties of physical quantities evaluated for many-nucleon systems.

In a recent application[7] of these same Hamiltonians we have introduced scaling rules that account for the major role of changing the harmonic-oscillator constant for the basis space in order to accommodate a change in nucleon number. With these scaling procedures we need only calculate $H_{\rm eff}$ for one representative value of the oscillator constant. Briefly, we showed that matrix elements of $T_{\rm rel}$ and $V_{\rm C}$ were exactly proportional to $\hbar\omega$ and $(\hbar\omega)^{1/2}$, respectively, while the matrix elements of phenomenological effective interactions were approximately proportional to $\hbar\omega$. It is then a simple matter to apply this same Hamiltonian to both ^{16}O and ^{40}Ca as we have done for these initial applications.

At $T=0$ we expect our results to be similar to those of the Brueckner-Hartree-Fock (BHF) approximation. Small differences may be ascribed to different choices for the Pauli operator and s.p. spectra in the two-particle propagators of the G matrix. Therefore, we expected and found the standard deficiencies in the $T=0$ ground-state solution for ^{16}O and ^{40}Ca in the spherical Hartree-Fock (SHF) approximation. Our philosophy is to adjust the $H_{\rm eff}$ in order to achieve agreement with measured ground-state properties in the SHF approximation before proceeding with the FTHF calculations. To do this we simply introduce overall factors λ_1 and λ_2 for the kinetic-energy and effective-interaction terms, respectively, in Eq. (5). We then adjust λ_1, λ_2, and $\hbar\omega$ simultaneously to achieve the correct rms radius and binding energy for a given nucleus within SHF for a fixed model space. The best-fit values are found to vary smoothly with increasing model-space size and increasing number of nucleons. For example, in the 5-space results for ^{16}O we obtian parameter values of 0.98, 1.30, and 9.71 MeV for λ_1, λ_2, and $\hbar\omega$, respectively. For ^{40}Ca ^{40}Ca in the 5-space the results are 0.98, 1.28, and 7.97 MeV.

We display in Fig. 1 the excitation energy of ^{16}O vs T for the 3-, 4-, and 5-spaces. The simplicity of this sequence of curves provides support for the sensibility of the entire procedure we have adopted. That is, the evaluation of a model-space-dependent realistic effective Hamiltonian, its phenomenological adjustment in the SHF approximation, and the solution of the self-consistent FTHF equations produce a sequence of excitation energy curves which agree to successively higher temperatures as the model-space sizes increase. Thus for low enough T even a small model space will provide useful results. We conclude that the 3-space results should be useful for $T \leqslant 4.5$ MeV, 4-space results for $T \leqslant 5.75$ MeV, and 5-space results for $T \leqslant 7$ MeV on the basis of the systematics shown in Fig. 1 and on a number of other systematic features in our results which we do not display here. From these results for ^{16}O and similar results for ^{40}Ca we can now extract with some confidence the parabolic dependence of excitation energy on T. We find a convenient parametrization $E^*(T)=0$ for $T \leqslant T_0$ and $E^*(T)=\sigma(T-T_0)^2$ for $T > T_0$. Then, with $T_0 = 1$ MeV we obtain $\sigma=0.185A$ for ^{16}O and $\sigma=0.104A$ for ^{40}Ca, where A represents the appropriate nucleon number. These results for ^{40}Ca follow the $\sigma \simeq 0.1A$ results obtained by Sauer, Chandra, and Mosel[3] with use of phenomenological Hamiltonians. However, our ^{16}O results display enhanced thermal sensitivity due to the larger surface-to-volume ratio.

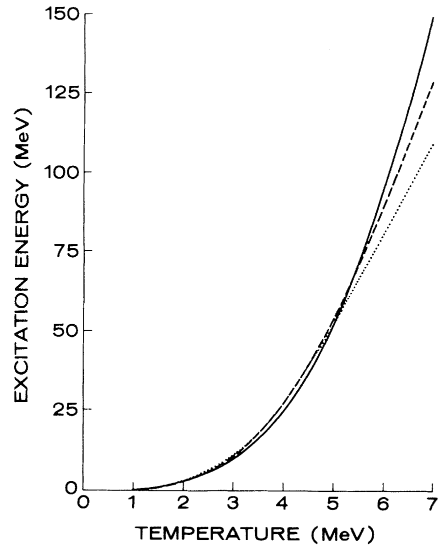

FIG. 1. Excitation energy E^* as a function of nuclear temperature T for ^{16}O for different sizes of the model space. The dotted line indicates the 3-space results while the dashed and solid lines show the 4- and 5-space (lowest six oscillator shells) results, respectively.

We display the FTHF results for the rms radii of ^{16}O and ^{40}Ca as a function of temperature in Fig. 2. These results and those of Fig. 3 are obtained in the 5-space. For low temperatures, $T \leqslant 2$ MeV in ^{16}O and $T \leqslant 1$ MeV in ^{40}Ca, the radius exhibits almost no thermal response because of the shell-closure effects. Then with increasing T, both nuclei undergo a radial expansion proportional to T^2. The behavior

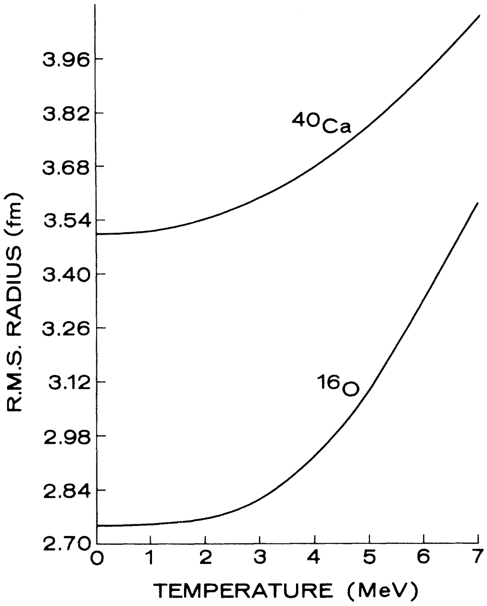

FIG. 2. Root-mean-square radii as a function of temperature T for ^{16}O and ^{40}Ca.

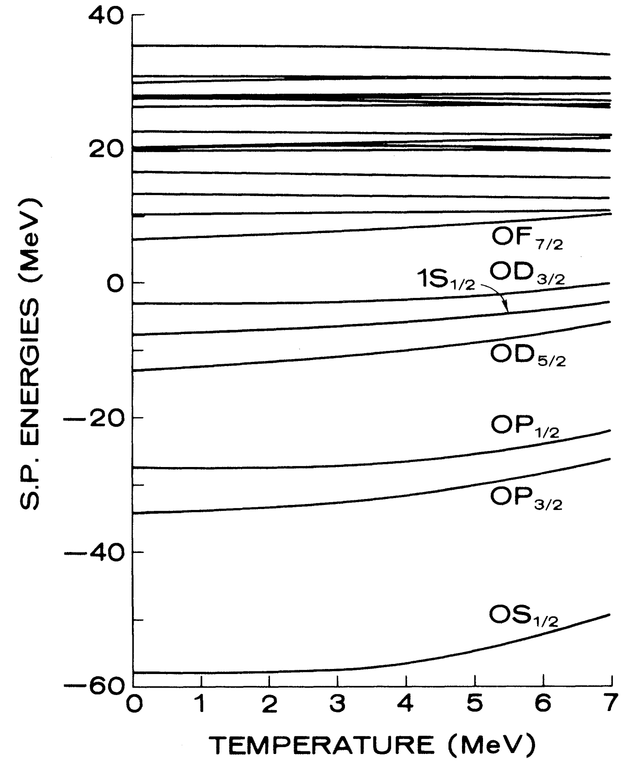

FIG. 3. Single-particle neutron states as a function of nuclear temperature T for ^{40}Ca in the 5-space. The unlabeled levels are approximately consistent with the expected shell-model ordering at $T=0$ MeV.

of the rms radii with T can be parametrized by $r(T)=r_0(1+bT^2)$, and we find that $r_0=2.74$ fm and $b=5.6\times10^{-3}$ MeV^{-2} for ^{16}O and $r_0=3.50$ fm and $b=3.3\times10^{-3}$ MeV^{-2} for ^{40}Ca. The thermal response is far more substantial than the results obtained with the zero-range phenomenological effective Hamiltonians.[3] These earlier results obtained essentially no change in the rms radii for $T\leqslant 5$ MeV while our results yield a 14% increase and an 8% increase in the ^{16}O and ^{40}Ca radii, respectively, at $T=5$ MeV.

In Fig. 3 we present the neutron s.p. energies for ^{40}Ca as a function of T. At $T=0$ we obtain self-consistent s.p. energies which are in the order expected from a phenomenological shell model and the results are reminiscent of the earlier BHF s.p. energies.[8] Recall that the effective Hamiltonian has no one-body component so that the appearance of a sensible single-particle spectrum at $T=0$ provides further justification for this approach to obtain thermal properties. Note especially that with increasing T the spin-orbit splitting decreases fast enough to actually preserve the shell gaps to higher temperatures than might have otherwise been expected. Here also we find more substantial changes with T than reported for phenomenological Hamiltonians.[3]

We conclude that our approach to evaluating the thermal properties of nuclei satisfies smoothness criteria as a function of model-space size and leads to predictions of thermal properties for finite nuclei which differ substantially from results based on phenomenological Hamiltonians. The realistic microscopic effective Hamiltonians in the mean-field approach yield predictions for substantially greater thermal response of light nuclei.

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