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Caloric curve for finite nuclei in Thomas-Fermi theory

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In a finite temperature Thomas-Fermi theory with realistic nuclear interactions, we construct caloric curves for finite nuclei enclosed in a sphere of about 4 to 8 times the normal nuclear volume. The specific heat capacity C_v shows a peaked structure that is possibly indicative of a liquid-gas phase transition in finite nuclear systems. [S0556-2813(97)50704-7]

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The equation of state (EOS) of nuclear matter with realistic effective interactions shows a typical Van der Waals type behavior and a critical temperature of $\approx 15-20$ MeV [1-3]. Supported by the experimental observation of a power law behavior in the mass or charge distribution in proton [4,5] and heavy ion induced reactions [6,7], the idea of liquid-gas phase transition in nuclear matter or finite nuclear systems [2,8-10] has gotten considerable interest in the literature. Theoretical speculations and possible experimental indications of a limiting temperature [11-15] in finite nuclei at \approx 5–7 MeV, above which the nucleus becomes unstable and breaks up into many fragments, also calls for a possible connection between the limiting temperature and the phase transition. Phase transitions are normally signaled by peaks in the specific heat at constant volume, C_v as temperature increases. Fragmentation calculations in the microcanonical algorithm of Gross [16] and in the Copenhagen canonical description [17,18] show such peaks. Recent calculations by Das Gupta et al. [19] in the lattice gas model for fragmentation also show such a structure. Renewed interest in this subject was further fueled by the recent experimental observation [20] in the caloric curve of a near constancy of temperature in the excitation energy range of $\approx 4-10$ MeV/ nucleon in Au + Au collisions. This prompted us to find out whether the trends in the caloric curve as seen in the experiment or in fragmentation calculations are reproduced in a finite temperature Thomas-Fermi (TF) theory. To our knowledge this is the first calculation of its kind with a realistic effective interaction. In the context of an exactly solvable Fermion model, Rossignoli *et al.* [21] have earlier calculated the specific heat of a finite nucleus in the grand canonical mean field theory with Lipkin's model Hamiltonian, but found no structure in it as a function of temperature. The structure appeared in the canonical calculation, with inclusion of correlations.

In our refined Thomas-Fermi (TF) model, the interaction density is calculated with a Seyler-Blanchard type [22] momentum and density dependent finite range two-body effective interaction [13]. The interaction is given by

$$v_{\text{eff}}(r,p,\rho) = C_{l,u}[v_1(r,p) + v_2(r,\rho)], \qquad (1)$$
$$v_1 = -(1 - p^2/b^2)f(\mathbf{r_1},\mathbf{r_2}),$$
$$v_2 = d^2[\rho_1(r_1) + \rho_2(r_2)]^n f(\mathbf{r_1},\mathbf{r_2}), \qquad (2)$$

with

$$f(\mathbf{r}_1,\mathbf{r}_2) = \frac{e^{-|\mathbf{r}_1 - \mathbf{r}_2|/a}}{|\mathbf{r}_1 - \mathbf{r}_2|/a}.$$
(3)

Here *a* is the spatial range and *b* the strength of repulsion in the momentum dependence of the interaction, $r = |\mathbf{r}_1 - \mathbf{r}_2|$ and $p = |\mathbf{p}_1 - \mathbf{p}_2|$ are the relative distance and relative momenta of the two interacting nucleons. The subscripts *l* and *u* in the strength *C* refer to like pair (*n*-*n* or *p*-*p*) or unlike pair (*n*-*p*) interaction, respectively, *d* and *n* are measures of the strength of the density dependence of the interaction, and ρ_1 and ρ_2 are the densities at the sites of the two nucleons.

The potential parameters are determined for a fixed value of n from a fit of the well-established bulk nuclear properties and the value of n is determined [13] from a fit of the giant monopole resonance energies over a broad mass spectrum.

The Coulomb interaction energy density is given by the sum of the direct and exchange terms. They are given by

$$\varepsilon_D(r) = e^2 \pi \rho_p(r) \int dr' r'^2 \rho_p(r') g(r,r'), \qquad (4)$$

and

$$\varepsilon_{\rm ex}(r) = -\frac{3e^2}{4\pi} (3\pi^2)^{1/3} \rho_p^{4/3}(r).$$
 (5)

Here $\rho_p(r)$ is the proton density and

$$g(r,r') = \frac{(r+r') - |r-r'|}{rr'}.$$
 (6)

With the potential chosen, the total energy density at a temperature T is then written as

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FIG. 1. The proton density profile for the system ¹⁵⁰Sm calculated at four temperatures in the volume $V=8.0V_0$. The dashed, dotted, dash-dot, and full lines correspond to temperatures T=5,9,9.5, and 10 MeV, respectively.

$$\varepsilon(r) = \sum_{\tau} \rho_{\tau}(r) \{ T J_{3/2}[\eta_{\tau}(r)] / J_{1/2}[\eta_{\tau}(r)] \\ \times [(1 - m_{\tau}^{*}(r)V_{\tau}^{1}(r)] + \frac{1}{2}V_{\tau}^{0}(r) \}.$$
(7)

Here τ refers to neutron or proton, the J's are the usual Fermi integrals, V_{τ}^0 is the single particle potential (for protons, it includes the Coulomb term), V_{τ}^1 is the potential term that comes with momentum dependence and is associated with the effective mass m_{τ}^* . The fugacity $\eta_{\tau}(r)$ is defined as

$$\eta_{\tau}(r) = [\mu_{\tau} - V_{\tau}^{0}(r) - V_{\tau}^{2}(r)]/T, \qquad (8)$$

where μ_{τ} is the chemical potential and V_{τ}^2 is the rearrangement potential that appears for a density-dependent interaction. The total energy per particle at any temperature is then given by

$$E(T) = \int \varepsilon(r) \, \mathrm{d}^3 r / A. \tag{9}$$

Once the interaction energy density is known, the nuclear density can be obtained self-consistently and other observables of physical interest calculated. For details on the finite temperature TF theory, we refer to Ref. [13].

Since the continuum states of a nucleus at nonzero temperature are occupied with a finite probability given by a Fermi factor [23], the particle density does not vanish at large distances. The observables then depend on the size of the box in which the calculations are performed. Guided by the practice that many calculations for heavy ion collisions are done by imposing that thermalization occurs in a freezeout volume, we fix a volume and find out the excitation energy as a function of temperature which allows for the determination of the specific heat at constant volume.

We choose two systems, namely ¹⁵⁰Sm and ⁸⁵Kr. In the context of very heavy ion collisions at intermediate or higher energies, this mass range is of experimental interest. The calculations have been done for two confinement volumes, one at $V=4.0V_0$ and the other at $V=8.0V_0$, where V_0 is the normal volume of the nucleus at zero temperature. The cal-



FIG. 2. The proton density profile for the system ¹⁵⁰Sm calculated at temperature T = 10 MeV in two different volumes. The full and dashed lines correspond to calculations at $V = 4.0V_0$ and $V = 8.0V_0$, respectively.

culations at zero temperature are independent of the volumes taken; at low temperature of $\approx 1-2$ MeV, the observables are nearly independent of the volume. As the temperature increases, the central density is depleted. In Fig. 1, the proton densities for ¹⁵⁰Sm calculated in the volume $V = 8.0V_0$ are displayed for four temperatures, T=5 MeV (dashed curve), T=9 MeV (dotted curve), T=9.5 MeV (dash-dotted curve), and T = 10 MeV (full curve). At T = 5 MeV, the central density is depleted by $\approx 4\%$ compared to zero temperature density, but has a long thin tail spread to the boundary. The behaviors at T=9 and 9.5 MeV are qualitatively the same, but with further depletion in the central density and a thicker tail. Beyond T=9.5 MeV, the change in the density starts being abrupt and the whole system looks like a uniform distribution of matter inside the volume. This is shown by a representative density distribution at T = 10 MeV. The slight bump seen in the outer edge of the density is due to the Coulomb force. In Fig. 2, the proton density at T = 10 MeV for the system at $V = 8.0V_0$ (dashed curve) is compared with that calculated at $V=4.0V_0$ (full curve). The density calculated in smaller volume still shows a structure and the central density is depleted by only about 20% even at this high temperature.

The excitation energy per particle E^* is defined as $E^* = E(T) - E(T=0)$. In Fig. 3, we display the caloric curve for the system ¹⁵⁰Sm. The upper dashed curve corresponds to $V=4.0V_0$, while the lower full curve corresponds to $V=8.0V_0$. At lower density, the excitation energy rises faster. For both volumes, initially the temperature rises faster with excitation energy, then its rise is slower. For the lower density, a kink is observed in the caloric curve at $T\approx 10$ MeV, after which the excitation energy rises almost linearly with temperature. For the higher density, the kink is much smaller and appears at a somewhat higher temperature. In Fig. 4, the corresponding specific heats C_v defined as

$$C_n = (\mathrm{d}E^*/\mathrm{d}T)_n \tag{10}$$

are displayed. Since we use units of MeV for both energy and temperature, the calculated C_v is dimensionless. For



FIG. 3. The temperature plotted as a function of excitation energy per particle (caloric curve) for the system ¹⁵⁰Sm. The dashed curve corresponds to calculations with volume $V=4.0V_0$, while the full curve corresponds to $V=8.0V_0$.

both volumes, the specific heat shows a peak, the peak being much sharper for the case of a larger volume. For the smaller volume, the peak is at $T \approx 10.5$ MeV, while for the large volume the peak is shifted down by ≈ 1 MeV. We believe that the kink in the caloric curve or the peak in the specific heat are related to a phase transition in finite nuclei. From our calculations, we find that this transition temperature is weakly dependent on the confinement volume beyond $V=8V_0$, e.g., for V as high as $20V_0$, the transition temperature is shifted down further by only ≈ 1 MeV. The classical value of $C_v = 3/2$ is reached at $T \approx 11$ MeV for the case with $V=8.0V_0$ while for the smaller volume, it is reached at $T \approx 13$ MeV. This is expected as the interaction becomes weaker either with increased volume or with increased temperature.

In Fig. 5, the caloric curve for the lower mass system ⁸⁵Kr is shown. The trends are nearly the same as in Fig. 3. Figure 6 displays the specific heat for this system. In the calculation with $V=4V_0$, a broad bump in the specific heat



FIG. 5. Same as Fig. 3 for the system ⁸⁵Kr.

at $T \approx 11$ MeV is seen. In calculations with expanded volume $(8V_0)$, the system shows a sharp peak at $T \approx 10.5$ MeV. This peak is, however, not as sharp as the one for the heavier system. In calculations on limiting temperature in the model of liquid-gas phase equilibrium, the influence of Coulomb forces has often been emphasized [3,24] in the instability of the system. For example, for infinite nuclear matter, with isospin asymmetry equal to that for ¹⁵⁰Sm, we find that the critical temperature is ≈ 13 MeV with the present interaction. However, the limiting temperature for the aforesaid nucleus comes down to as low as ≈ 5 MeV in the refined TF calculation [13] which is basically due to Coulomb interaction. In the present calculation, we see a relatively small effect of the Coulomb forces on the transition temperature. With the Coulomb force switched off, the transition temperature is shifted up by ≈ 1 MeV for both the confinement volumes $4V_0$ and $8V_0$ and the matter density becomes more uniform. This is true for both the systems we have studied.

To summarize, we have calculated the caloric curve and the specific heat for two systems in a self-consistent Thomas-Fermi theory at two volumes, namely at 4 and 8 times the normal nuclear volume. The specific heat C_v shows a peaked structure possibly signaling a liquid-gas phase transition at a temperature of ≈ 10 MeV which is lower than the calculated critical temperature for infinite nuclear matter, but larger



FIG. 4. The specific heat per particle plotted as a function of temperature for the system ¹⁵⁰Sm. The dashed curve corresponds to calculations with volume $V=4.0V_0$, while the full curve corresponds to $V=8.0V_0$.



FIG. 6. Same as Fig. 4 for the system ⁸⁵Kr.

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compared to the calculated limiting temperature for finite real nuclei [13]. In simplistic model calculations [21], it has been shown that the inclusion of correlations brings in features reminiscent of a phase transition in a system when no phase transition is evident in the usual mean field calculation; it would therefore be interesting to see whether fluctuations with two-body correlations bring down the phase transition temperature obtained in our TF calculation. The authors acknowledge fruitful discussions with Dr. E. Ramakrishnan. One of the authors (J.N.D.) gratefully acknowledges the hospitality of the Cyclotron Institute, Texas A&M University where this work was completed. This work is supported by the U.S. Department of Energy under Grant No. DE-FE05-86ER40256, by the Natural Sciences and Engineering Research Council of Canada and by the U.S. National Science Foundation under Grant No. PHY-9413872.

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