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Gross features of finite nuclei at finite temperatures

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Abstract. A simple expression is obtained for the low-temperature behaviour of the energy and entropy of finite nuclei for $20 \leq A \leq 250$. The dependence on A of these quantities is for the most part due to the presence of the asymmetry energy.

In nuclei the nuclear force between the nucleons is short ranged which leads to saturation of the binding energy, $E(A, Z)$, per nucleon. Empirically, it is known that for the stable isotopes

$$\frac{E(A, Z)}{A} \approx \alpha, \qquad (1)$$

where $\alpha \approx 8\,\text{MeV}$ and $A \geq 20$. This fundamental gross property of nuclei is well accounted for by the semi-empirical mass formula [1–3] which provides a simple parametrization of the binding energy per nucleon for all known nuclei. Qualitatively, it is also consistent with the simple Fermi gas model prediction [4,5]

$$\frac{\mathcal{E}(A)}{A} = \frac{3}{5}\epsilon_f, \qquad (2)$$

where $\mathcal{E}$ is the ground-state energy and ϵ_f is the Fermi energy which is constant as long as the particle density remains constant. It is interesting to note that at low temperatures ($T < T_f$) the excitation energy in the Fermi gas model is given by [4,6]

$$\frac{\mathcal{E}(A, T)}{A} = \frac{3}{5}\epsilon_f + \frac{\pi^2}{4}\frac{T^2}{\epsilon_f}, \qquad \text{or} \qquad (3)$$

$$= a + bT^2, \qquad (4)$$

where a and b are constant again as long as the particle density remains constant. Although the Fermi gas model may be an oversimplified model which ignores the existence of low-lying collective states, nonetheless it underscores the relevance of independent particle (or quasiparticle) methods in nuclear-structure physics. Modifications to the Fermi gas model expressions for the nuclear

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level density such as the back-shifted Bethe formula give good fits to the experimental data [7–9] with only a few parameters which have to be adjusted for each nuclei and are in good agreement with recent shell model Monte Carlo calculations [10].

Mean-field methods have been used throughout the periodic table, both at zero temperature and at finite but low temperatures, and typically yield a T^2 behaviour of the energy density. A similar temperature behaviour in Sm isotopes has also been observed in the Thomas-Fermi approximation in the relativistic non-linear Walecka model [11]. Recently, correlations have also been included [12] which bring added structure not seen in mean-field calculations [13]. Furthermore, experimentally extracted level densities in rare-earth nuclei [14] used in the calculation of the caloric curve show evidence of weak collective pairing vibrations as well as smooth underlying T^2 behaviour. This suggests that perhaps at low but finite temperatures a simple scaling relation might also exist for the excitation energy, $\mathcal{E}(A, T)$, of finite nuclei. Such relationships are of great interest for simulating nuclear reactions under extreme conditions [15].

Clearly some care must be exercised as most nuclei as well as nuclear matter at finite temperatures display two phases which are dominated by different degrees of freedom. At low temperatures collective degrees of freedom are important while at higher temperatures independent particle degrees of freedom dominate [13,16–18]. In Fermi gas models the low-temperature collective degrees of freedom are completely ignored even if interactions are included [19,20]. On the other hand, the empirically based finite-temperature extension of the semi-empirical mass formula [17] most certainly includes both phases. Although as we shall show both approaches yield at higher temperatures roughly the same temperature dependence for finite nuclei, not surprisingly, differences occur in coefficients of the volume and surface contributions. As has been pointed out, however, the extended Fermi gas model

results are extremely dependent on some of the parameters in the model and the parametrization of the surface energy [19]. At higher temperatures one would expect the surface energy to decrease not increase and eventually to vanish at the critical temperature at which the liquid-to-gas phase transition takes place. However, a reasonable fit to the empirical nuclear level density parameter is still possible which probably accounts for the aforementioned agreement.

Extended Thomas-Fermi model calculations at low temperatures in Pb [21] which ignore the contributions from both pairing and the continuum agree well with Hartree-Fock calculations and also yield a T^2 behaviour for the excitation energy. The level density parameter obtained at higher temperatures, however, agrees with the simple Fermi gas model prediction.

In order to test the validity of eq. (4) in the case where both the continuun as well as collective states are taken into account we have made use of a finite-temperature extension of the semi-empirical mass formula [17]. The following form for the temperature-dependent binding energy [3,22] has been assumed

$$E(A,Z,T) = \overbrace{\alpha(T)A}^{1} + \overbrace{\beta(T)A^{\frac{2}{3}}}^{2}$$
$$+ \overbrace{\left(\gamma(T) - \frac{\eta(T)}{A^{\frac{1}{3}}}\right)\left(\frac{4t_\zeta^2 + 4|t_\zeta|}{A}\right)}^{3}$$
$$+ \underbrace{\kappa(T)\frac{Z^2}{A^{\frac{1}{3}}}\left(1 - \frac{0.7636}{Z^{\frac{2}{3}}} - \frac{2.29\,\kappa^2(T)}{(0.8076)^2 A^{\frac{2}{3}}}\right)}_{4}$$
$$+ \underbrace{\delta(T)f(A,Z)A^{-\frac{3}{4}}}_{5}, \tag{5}$$

where $A = N + Z$, $t_\zeta = \frac{1}{2}(Z - N)$ and $f(A,Z) = (-1, 0, +1)$ for (even-even, even-odd, odd-odd) nuclei. Here 1 is the volume energy, 2 is the surface energy, 3 is the asymmetry energy, 4 is the Coulomb energy and 5 is the pairing energy contribution to the temperature-dependent binding energy. Note that no symmetry skin effects have been included in the surface energy [23]. In this parametrization the temperature dependence of the contributions to the Coulomb energy term which arise from exchange and surface effects [3,24] was ignored. Also, no attempt has been made to include shell effects in the finite-temperature expression.

The excitation energy per particle is given by

$$\frac{\mathcal{E}(A,Z,T)}{A} = \frac{E(A,Z,0) - E(A,Z,T)}{A}. \tag{6}$$

At $T = 0$ the coefficients are given by [3] $\alpha(0) = -16.11$ MeV, $\beta(0) = 20.21\,\text{MeV}$, $\gamma(0) = 20.65\,\text{MeV}$, $\eta(0) = 48.00\,\text{MeV}$, and $\kappa(0) = 0.8076\,\text{MeV}$ obtained from a fit to the experimental nuclear ground-state energies of 488 odd mass nuclei. The $T = 0$ coefficient for the pairing term is taken as $\delta(0) = 33.0\,\text{MeV}$ [22].
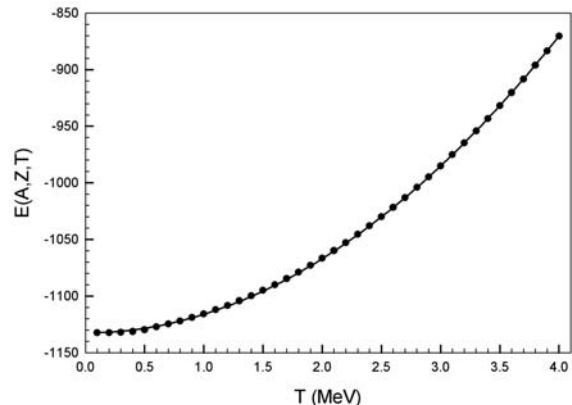

Fig. 1. Quadratic fit of the calculated binding energy of Xe ($A = 130$) using eq. (5). The fit to the Xe data is representative of the fits obtained for other nuclei.

To obtain the temperature dependence of the coefficients, the available experimental information about the excited states of nuclei throughout the periodic table was used to determine the partition function, $\mathcal{Z}(A,Z,T)$, of each nucleus in the canonical ensemble. The coefficients in the mass formula have been determined by a least-squares fit of (6) to the ensemble average of the excitation energy

$$\mathcal{E}(A,Z,T) = -\frac{\partial}{\partial\beta}\ln\mathcal{Z}(A,Z,T) \tag{7}$$

determined from a total of 313 nuclei in the mass region $22 \leq A \leq 250$ for temperatures $T \leq 4\,\text{MeV}$. The details of the determination of $\mathcal{Z}(A,Z,T)$ and the temperature dependence of the six coefficients are given in ref. [17]. This finite-temperature parametrization has been used to identify the pairing phase transition in symmetric nuclear matter [18]. The same techniques have also been successfully employed to identify the remnants of the pairing phase transition in finite nuclei [16].

The excitation energy, $\mathcal{E}(A,Z,T)$, has been calculated for a number of stable isotopes in the mass region $20 \leq A \leq 250$ using the temperature-dependent coefficients determined in ref. [17]. For each stable isotope, the constant b in eq. (4) was determined from a quadratic fit of $\mathcal{E}(A,Z,T)$ versus T. These fits were in general excellent, as shown in fig. 1 with only occasional small deviations from the quadratic fit occurring at low temperature. This is not surprising given that the continuum contributions are given by Fermi gas expressions. However, this alone in no way guarantees any simple dependence of b on A. Note also that no attempt has been made in the fits to take into account the presence of low-temperature collective to non-collective phase transitions [13,16]. Essentially, the fits reflect the temperature dependence in the excitation energy above the aforementioned phase transition. The coefficient b was then plotted as a function of A, as shown in fig. 2. As can be seen in figs. 2 and 3 there is a relatively simple dependence of b on A. In order to determine the effect on b of the different terms in the temperature-dependent binding energy (5), various combinations of the five terms were plotted against T, then quadratically fitted to obtain
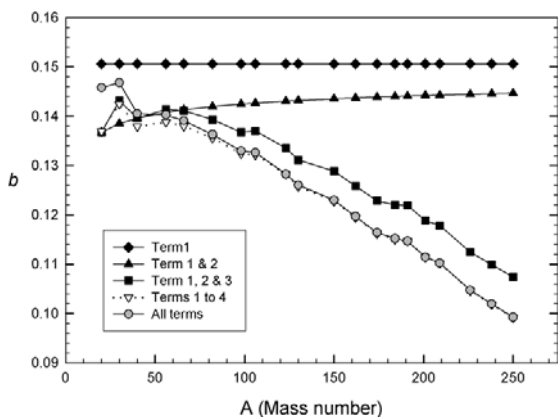
Fig. 2. The resultant b from various combinations of terms in eq. (5) has been plotted against A, thereby illustrating the linearity of all five cases.

Fig. 3. Plot of the linear fit of the b resulting from eq. (5), and eq. (5) without term 3.

b for each A and finally these points were linearly fitted, as shown in figs. 2 and 3. Although only 20 stable nuclei were used these were chosen at random to cover the range from $A = 20$ to $A = 250$. In fig. 3 the equations for the fits are $b = -2.032 \times 10^{-4}A + 0.152$ with a root mean square (RMS) deviation of 0.99 when all terms of eq. (5) are used and $b = -1.617 \times 10^{-5}A + 0.140$ with an RMS deviation of 0.72 if term 3 of eq. (5) is excluded. This latter value is in agreement with the results obtained from an earlier extended Fermi gas model calculation [19]. The gradient is small in both cases but especially small when term 3 is excluded, with b gradually varying from 0.141 to 0.137 for nuclei larger than $A = 40$. Surface effects become significant in nuclei smaller than $A = 40$ and the pairing effects are most likely overestimated. This most probably accounts for the deviation of the corresponding points from the fit in fig. 3 and subsequently prompted the exclusion of these points from the linear fit. These results demonstrate that the asymmetry term (*i.e.* term 3) is largely responsible for the A-dependence of b.

Furthermore in the canonical ensemble the specific heat is given by

$$C = \frac{\partial \mathcal{E}}{\partial T} \tag{8}$$

$$= T \frac{\partial S}{\partial T}. \tag{9}$$

At low T up to an A-dependent additive constant the entropy, S, for finite nuclei in the mass range $20 \leq A \leq 250$ is therefore given simply by

$$\frac{S}{A} = 2bT \tag{10}$$

with $b = -2.032 \times 10^{-4}A + 0.152$. This is to be compared with the value $b \approx \frac{1}{11}$, obtained in a two-fluid Thomas Fermi calculation at finite temperature using a Skyrme interaction [25]. Again the discrepancy is probably due to the neglect of pairing correlations.

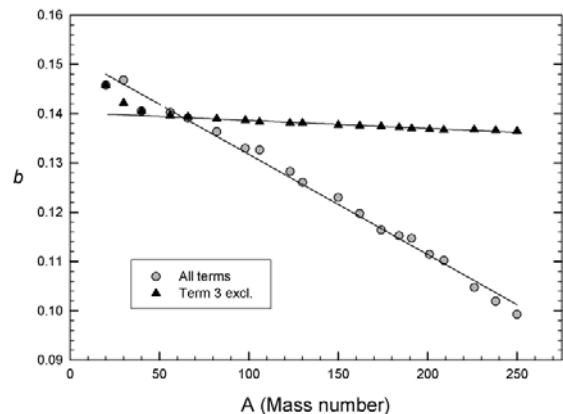It is interesting to note that the simple Fermi gas model does not take properly into account that the nucleus is composed of protons and neutrons and that therefore the effects of the Coulomb force must be considered. Were only the nuclear force present one might expect b to be independent of A. The presence of the Coulomb force gives rise to the asymmetry term which at $T = 0$ leads to a displacement of the island of stability away from nuclei with $N = Z$ and at finite temperature is largely responsible for an A-dependence in b.

Recently, it has been noted that there is a similarity in the binding energy E of polymers containing A monomers and nuclei containing A nucleons [26]. In both cases E/A is linear and in the case of polymers, where only the Coulomb force is present and the asymmetry term does not exist, the linearity is almost exact when compared with large-scale microscopic DFT-based calculations. In spite of the fact that the interactions are very different in both cases, nearest-neighbour interactions dominate in both cases. It would be of great interest to know how the excitation energy behaves at higher temperatures (where the electronic degrees of freedom are important) in polymers. Such finite-temperature calculations as a function of A are extremely computationally expensive to perform in polymers. If indeed these similarities are relevant, the present calculations suggest that in polymers a simple scaling in the excitation energy might take place.

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