Nuclear shell effects at high temperatures

N. J. Davidson and H. G. Miller
Department of Physics, University of Pretoria, Pretoria 0002, Republic of South Africa
(Received 8 April 1993)

In discussing the disappearance of nuclear shell effects at high temperatures, it is important to distinguish between the "smearing out" of the single-particle spectrum with increasing temperature and the vanishing of shell related structures in many-body quantities such as the excitation energy per nucleon. We propose a semiempirical method to obtain an upper bound on the temperature required to smooth the single-particle spectrum, and point out that shell effects in many-body parameters may persist above this temperature. We find that the temperature required to smear out the single-particle spectrum is approximately 1 MeV for heavy nuclei ($A \gtrsim 150$) and about 3–4 MeV for light nuclei ($A \lesssim 50$), in reasonable agreement with the estimate of $41/\pi A^{1/3}$ obtained from calculations with harmonic oscillator potentials. These temperatures correspond to many-body excitation energies of approximately 20 and 60 MeV, respectively.

PACS number(s): 21.10.Ma, 21.10.Dr

One of the interesting questions of nuclei at finite temperatures relates to the well-known phenomenon of shell structure. As the temperature (or the excitation energy) of the nucleus increases, it is believed that the visible effects of this structure will decrease, and finally disappear. However, it is important to distinguish between two cases, namely the disappearance of shell effects in a single nucleus, which we shall refer to as local shell effects, and the vanishing of effects across the entire periodic table (global effects). The purpose of the present paper is first to point out how the vanishing of local shell effects can be examined in a semiempirical manner, and second to highlight the problems associated with trying to quantify the disappearance of global effects.

The vanishing of local effects can be interpreted as the process by which the many-body spectrum of a particular nucleus becomes compatible with that generated by a single-particle spectrum which does not display shell structure. In the extreme example of an independent particle model, one might expect these shell effects to vanish when the temperature becomes comparable with the average shell spacing in the single-particle spectrum, since from this point on it is possible to (relatively) easily excite across the shell gaps.

To examine this more closely, a description of the many-body level density of nuclei is required. The low-energy portion of nuclear spectra are characterised by the presence of collective states (either rotational or vibrational) which are rather broadly spaced in energy. It is possible to obtain a reasonable fit to the many-body level density $\rho_{A,Z}(E)$ of most such spectra by the use of function of the form [1]

$$\rho_{A,Z}(E) = \frac{\sqrt{2\pi}\sigma}{\tau} \exp{(E - E_0)/\tau}, \tag{1}$$

where σ is the spin-dependence parameter and τ and E_0 are parameters to be fitted. At higher excitation energies, $\rho_{A,Z}(E)$ can be satisfactorily fitted by the usual first-order approximation for the many-body level density of a back-shifted Fermi gas:

$$\rho_{A,Z}(E) = \frac{\sqrt{\pi}}{12} \frac{\exp 2\sqrt{a_{A,Z}U}}{a_{A,Z}^{1/4} U^{5/4}}. \tag{2}$$

Here the level density parameter $a_{A,Z} = (\pi^2/6)g(\epsilon_F)$ with $g(\epsilon_F)$ the single-particle density of states at the Fermi surface and $U = E - P(N) - P(Z)$, where $P(N)$ and $P(Z)$ are the pairing corrections for neutron number N and proton number Z, respectively [1]. The Fermi gas model reflects the single-particle nature of nuclear excitation spectra at high energies, and does not include collective effects. In addition, the single-particle spectrum $g(\epsilon)$ is smooth, and therefore does not contain any shell structure.

It is this latter property of the Fermi gas which suggests a possible way to determine, in a semiempirical manner, an upper limit for the point at which local shell effects are "washed out". The excitation energy for the nucleus is calculated as a function of temperature and compared with the excitation energy of a pure Fermi gas spectrum with the same level density parameter as the nucleus in question. At some temperature, T_s, the two functions will coalesce due to the dominance of the single-particle levels in the nuclear spectrum at high energies. Thus, for temperatures above T_s, neither collective nor shell effects will be observed, and T_s may be considered as an upper bound for the vanishing of shell effects in the particular nucleus under investigation. The question is, of course, how to obtain a realistic estimate of the many-body excitation energy of a nucleus in a semiempirical manner; this will be discussed below.

The vanishing of local shell effects, however, does not imply the disappearance of global effects. The level density parameter $a_{A,Z}$, obtained from fits to low and medium energy neutron resonance data, shows distinct shell effects, with marked decreases near shell closures [1,2]. These effects can clearly be seen in the excitation energy per nucleon, which, for a Fermi gas at temperatures low compared to the Fermi energy, is given to good approximation by

$$\frac{E_{\rm ex}}{A} = \frac{a_{A,Z}}{A} T^2 \equiv \frac{T^2}{K_{A,Z}}. \tag{3}$$

In Fig. 1, we show E_{ex}/A as a function of A at a temperature of 3 MeV, which should be above the temperature required to remove local shell effects. The global shell effects are clearly visible, and are the result of the shell structure in $K_{A,Z}$.

So far in our discussions $a_{A,Z}$ has been assumed to be independent of the excitation energy. For a suitable energy dependence, $a_{A,Z}(E)$ might of course merge to a universal value independent of A, with the concomitant disappearance of shell effects in E_{ex}/A. The question is whether there is any indication that such a parameterization is justified.

Present experimental data covers three mass regions, namely $A \approx 40$ [3], $A \approx 120$ [4,5] and $A \approx 160$ [6–8]. The results obtained indicate that for the lowest mass region, $a_{A,Z}$ remains fairly constant at $\approx A/8$ for excitation energies up to 2 MeV per nucleon, whereas for $A \approx 120$, $a_{A,Z}$ changes from $\approx A/8$ to $\approx A/11$ and for $A \approx 160$, from $\approx A/8$ to $\approx A/13$ (the latter being very close to the ideal Fermi gas value) over the same range of excitation energies. This change is related to the temperature dependence of the effective mass m^* of the nucleons, as $a_{A,Z} \sim m^*/m$. However, m^* is not trivial to calculate. Calculations in the surface coupling model, in which the Hartree-Fock states are coupled to the collective random-phase approximation (RPA) modes has produced reasonable agreement with the experimental data for heavy nuclei [9], although similar calculations with realistic potentials for light systems [10] predict a decrease in $a_{A,Z}$ not seen in experimental data. On the other hand, a simple realistic model [11] has produced reasonable agreement with the experimental data for all three mass regions, although $a_{A,Z}$ still shows a decreasing tendency for small A. However, a general parameterization of $K_{A,Z}(E)$ is not easy to extract from any of these calculations, although the results of [11] suggest that $K_{A,Z}$ does not converge to a universal value with increasing E_{ex}. It therefore seems probable that shell effects in E_{ex}/A will remain visible right up to fragmentation, although the lack of a reliable parameterization of $K_{A,Z}(E)$ makes it impossible to make a firm statement on this.

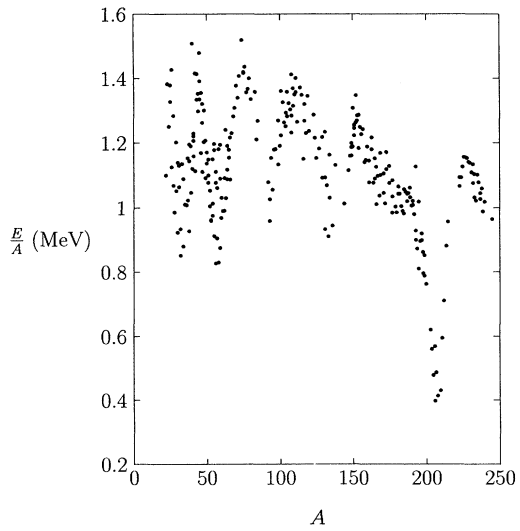

FIG. 1. The excitation energy of nuclei as a function of A for a temperature of 3 MeV. The global shell effects are clearly visible.

We return now to the question of shell effects in a particular nucleus. As we mentioned above, it is possible to obtain an estimate of the temperature at which such shell effects disappear from the form of the excitation energy of the nucleus. One way to do this is to calculate E_{ex} in the canonical ensemble using the experimental level data when available, supplemented by a continuum spectrum to account for the unmeasured, high-energy states. This approach has been used in the past to investigate low-temperature phase transitions in light nuclei [12], as well as to extend the semiempirical mass formula to finite temperatures [13]. The excitation energy is obtained in the canonical ensemble from

$$E_{ex} = -\frac{\partial \ln \mathsf{Z}}{\partial \beta} \tag{4}$$

where Z is the partition function given by

$$\mathsf{Z} = \sum_i g_i \exp(-\beta E_i) + \int_{E_n}^{E_{max}} dE \rho_{A,Z}(E) \exp(-\beta E) \tag{5}$$

with g_i the spin degeneracy and E_i the energy of the ith discrete state. The lower limit of the integral, E_n is taken to be 80% of the highest discrete energy, and the upper limit $E_{max} \sim 2$–3 GeV. The level density $\rho_{A,Z}(E)$ is either (1) or (2) depending on the energy. In many nuclei, there are insufficient data available to make the inclusion of the discrete states worthwhile. In these cases, the discrete states can be neglected altogether and the lower limit of the integral shifted to zero.

In our calculations, we have used the parameters of [1] for the nuclear many-body level densities. In particular, due to the lack of a general parameterization of $K_{A,Z}$, we have made no attempt to include an energy dependence in this quantity. However, since the temperatures of interest in our calculations are less than 2 MeV in the heavy nuclei and below about 4 MeV in the light nuclei, the neglect of this energy dependence should not be too serious.

To determine the temperature at which the excitation energy becomes compatible with that of a Fermi gas, we compare the excitation energy calculated from (4) with that obtained from a pure Fermi gas expression, and determine the temperature at which the relative difference between the two is less than 0.1%. This temperature is then an upper bound on the temperature at which shell effects vanish.

The choice of 0.1% for the convergence factor corresponds to differences of a few tens of keV between the energies of (4) and the Fermi gas. This is a few percent of the second-order contribution to the shell correction, which is estimated to be of the order of 1 MeV [14]. Decreasing the convergence factor to 0.01% results increases the tempertures at which the shell effects vanish by about

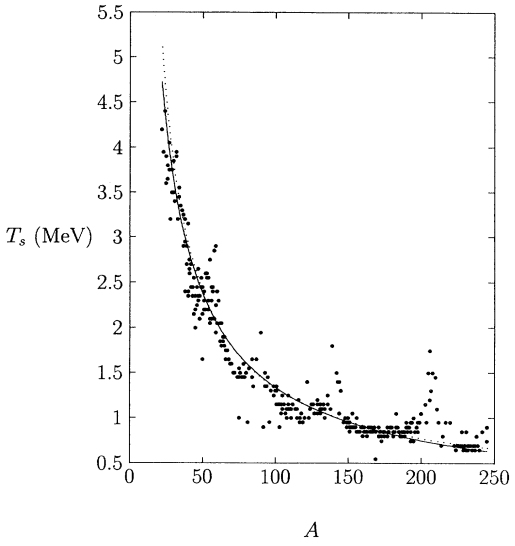

FIG. 2. The maximum temperature for local shell effects to be present, T_s, as a function of A. The solid line corresponds to $62A^{-5/6}$ and the dotted line to $[8/A\,(8+1400/A)]^{1/2}$.

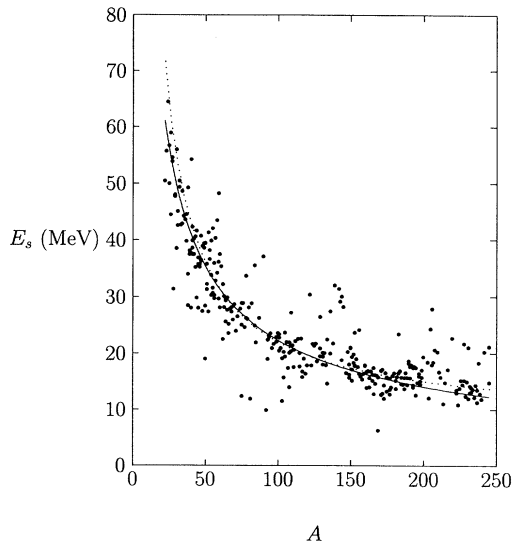

FIG. 3. The excitation energy E_s corresponding to T_s as a function of A. The solid line corresponds to $480A^{-2/3}$ and the dotted line to $(8+1400/A)$.

10–15%.

The temperatures resulting from these calculations are shown in Fig. 2, and the corresponding many-body excitation energies in Fig. 3. The major point of interest is the variation in T_s with A, where the effects of shell closures can clearly be seen. This emphasizes the distinction we drew earlier between local and global shell effects. The excitation energies E_s, although not constant for all A, nevertheless do not display as much structure at shell closures as the temperatures.

Quantitatively, the calculations indicate that local shell effects in heavy nuclei ($A \gtrsim 150$) have certainly vanished for temperatures in the order of 1 MeV, corresponding to excitation energies of 15–20 MeV. For lighter nuclei ($A \lesssim 50$), on the other hand, the temperatures required to wash out local shell effects are of the order of 2–4 MeV, or $E_x \sim 30$–60 MeV.

The temperatures which we obtain for the vanishing of the local shell effects are of the same order as the estimate of $41/\pi A^{1/3}$ obtained from calculations of the shell correction energy with a harmonic oscillator single-particle potential [15,16], although the values for large A differ by as much as a factor of two. This discrepancy can be understood in terms of the schematic nature of the harmonic oscillator model, which cannot be expected to reproduce the shell structure of real nuclei exactly.

There are definite systematics present in our results. In Fig. 3 we show two curves which fit the general trend in E_s well, namely $E_s = 480A^{-2/3}$ and $E_s = 8 + 1400A^{-1}$. These curves are not least squares fits, but are shown to guide the eye. The source of the systematics is the A dependence of the shifted (i.e., with pairing corrections subtracted) matching energy U_x between the low- and high-energy densities of states (1) and (2), which can be quite well described by an A^{-1} behavior [1]. As might be expected, this boundary between the regions of validity of the two expressions is reflected in E_s. Corresponding fits for the temperatures T_s can be found using the fits for E_s and (3) with $a_{A,Z} = A/8$.

The calculations described above allow for the extraction of information about shell effects at nonzero temperatures in a semiempirical manner. Although there are several approximations in the calculations, most notably the neglect of the energy dependence of the level density parameter, the temperatures of interest are low enough for these approximations to be valid. The results indicate that even though local shell effects in the single-particle spectrum are smeared out at temperatures of a few MeV, global shell effects remain visible in many-body quantities to considerably higher temperatures, and may survive right up to fragmentation.

The financial support of the Foundation for Research Development is gratefully acknowledged.

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