Effects of Finite Size on Thermodynamic Properties of Nuclei

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Introduction

An important ingredient of the theory of nuclear structure and nuclear reactions is the single-particle (SP) level density, $g(\varepsilon)$, associated with the nucleus mean field. This summer, I investigated the calculation of this quantity for various nuclei using the Thomas Fermi approximation and compared my results with the Fermi gas model. I also used the single particle level density to calculate thermodynamic properties of the nucleus, including entropy and excitation energy.

Quantum Mechanics

To find the wave function of a system, (such as the nucleus), you have to solve the many body Schrödinger equation

$$\hat{H}\psi_A = E\psi_A \;\rightarrow\; \psi\left(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_A\right),\; E$$

Nucleons in the nucleus can be described by the many body Hamiltonian:

$$H = \sum_{k=1}^{A} \frac{p_k^2}{2m_k} + \sum_{i<j} V\left(\vec{r}_i, \vec{r}_j\right).$$

$$\vec{p} \rightarrow -i\hbar\vec{\nabla} = \hat{p}$$

Mean Field Approximation

$$H = \sum \frac{p_i^2}{2m} + \sum_{i<j} V_{ij}$$

$$V(\vec{r}_i) \cong \sum_j V_{ij}$$

$$H \cong H_0 = \sum_i h_i \qquad h_i = \frac{p_i^2}{2m} + V(\vec{r}_i)$$

$$\hat{h}\phi_i = \varepsilon_i \phi_i \qquad \psi_A = \phi_1(\vec{r}_1)\,\phi_2(\vec{r}_2)\cdots\phi_A(\vec{r}_A)$$

Slater Determinant

The wave function for the whole nucleus will be a product of the wave functions for the individual nucleons. Due to the Pauli exclusion principle, we have:

$$\psi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_2(\vec{r}_1) & \cdots & \phi_A(\vec{r}_1) \\ \phi_1(\vec{r}_2) & \phi_2(\vec{r}_2) & \cdots & \phi_A(\vec{r}_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(\vec{r}_A) & \phi_2(\vec{r}_A) & \cdots & \phi_A(\vec{r}_A) \end{vmatrix}$$

Level Density

Let $N(E_x)$ be the number of excited states of the many body system up to E_x.

The level density of a system gives the number of states within an interval of energy.

$$\rho(E) = \frac{dN}{dE}$$

$$\hat{\rho}(E) = Tr\left[\delta\left(E - \hat{H}\right)\right]$$

$$\rho(E) = \sum_n \delta\left(E - E_n\right)$$

Nuclear Level Density

In the independent particle model the nuclear level density is given by

$$\rho(E_x) \cong \frac{1}{E_x}\exp\left[2\sqrt{aE_x}\right]$$

where E_x is the excitation energy an *a* is the so called level density parameter.

$$a = \tfrac{1}{6}\pi^2 g_s(\varepsilon_F).$$

$g_s(\varepsilon_F)$ is the value of the smoothed single particle level density at the Fermi energy, ε_F.

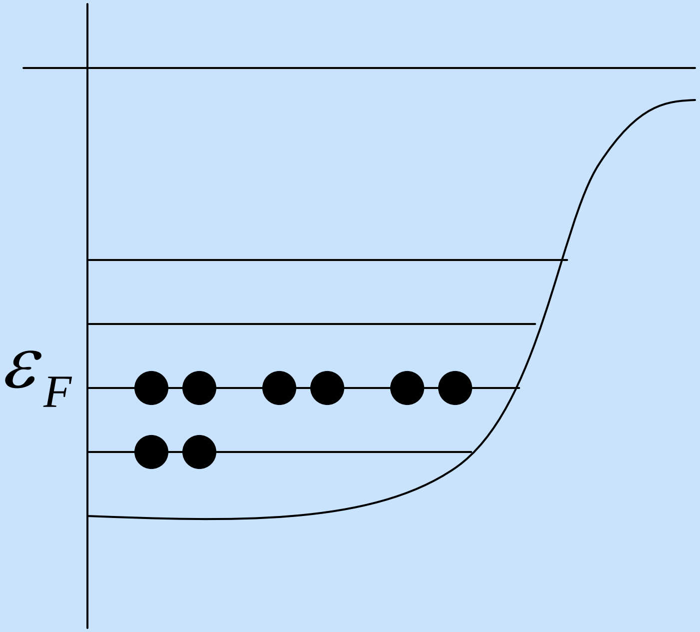
Single Particle Level Density

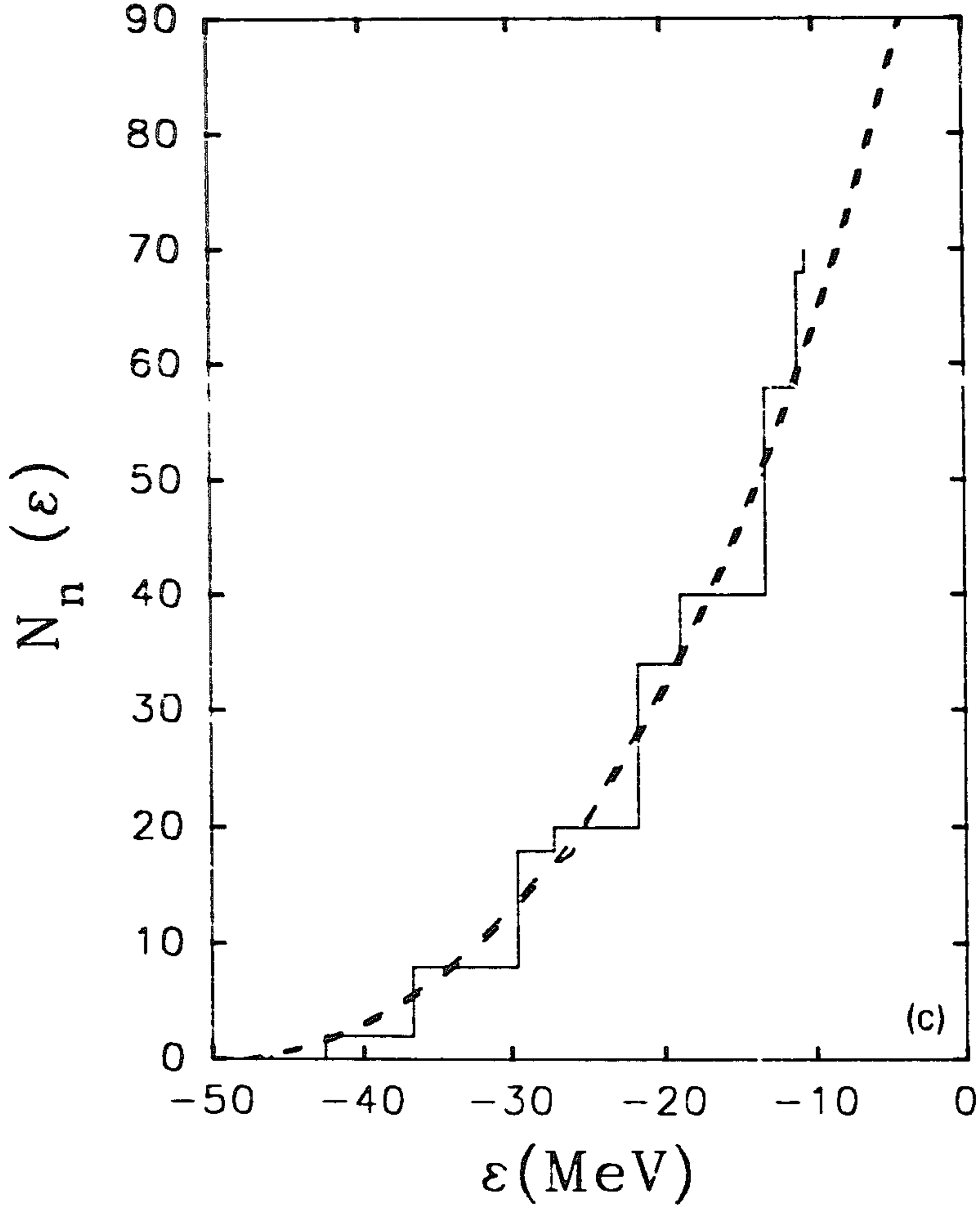
The single particle level density is calculated using the energies from the single particle states.

$$\hat{h}\phi_i = \varepsilon_i \phi_i$$

$$g(\varepsilon) = \sum \delta(\varepsilon - \varepsilon_i)$$

$$N(\varepsilon) = \int^{\varepsilon} g(\varepsilon)\, d\varepsilon$$





90
80
70
60
50
40
30
20
10
0
−50
−40
−30
−20
−10
0
N n (ε)
ε(MeV)
(c)

Thomas-Fermi Approximation

In a semi-classical calculation of g(ε), we have the Thomas-Fermi Approximation

$$g(\varepsilon) = \frac{1}{(2\pi\hbar)^3} \int d\vec{r}\, d\vec{p}\; \delta\left[\varepsilon - \left(\frac{p^2}{2m} + V(r)\right)\right],$$

Integrating over p, we have

$$g_{TF}(\varepsilon) = \frac{1}{\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int d^3\vec{r}\,(\varepsilon - V)^{1/2}\,\Theta(\varepsilon - V).$$

Fermi Gas Model

The Thomas-Fermi approximation, evaluated with a square well potential of depth V_0, gives the Fermi Gas model result for the level density

$$g_f = \frac{1}{2\pi^2}\Omega\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon - V_0}$$

For finite V, we must subtract the contribution of the free gas states above ε=0

$$g_f = \frac{1}{2\pi^2}\Omega\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} \qquad \varepsilon > 0$$

Thermodynamic Properties

Using the single-particle level density, we can calculate various thermodynamic properties of the system within the IPM.

$$S(T) = -\int g(\varepsilon)[f \ln f + (1-f)\ln(1-f)]d\varepsilon$$

$$E(T) = \int \varepsilon g(\varepsilon) f(\varepsilon, \mu, T)\, d\varepsilon$$

$$A = \int g(\varepsilon) f(\varepsilon, \mu, T)\, d\varepsilon .$$

$$f\left(\varepsilon, \mu, T\right) = \frac{1}{1 + e^{\frac{\varepsilon - \mu}{T}}}$$

Zero Temperature Limit

In the zero temperature limit, the entropy is

$$S = 2aT \, ,$$

And the excitation energy is

$$E^* \equiv E(T) - E(0) = aT^2 \, ,$$

$$a = \tfrac{1}{6}\pi^2 g_s(\varepsilon_F).$$

Harmonic Oscillator Potential

The HO potential is of the form

$$V^{HO}(r) = \tfrac{1}{2} m\omega^2 r^2,$$

Using the Thomas-Fermi approximation, we obtain for the single-particle level density

$$g_{TF}^{HO}(\varepsilon) = \varepsilon^2 / (\hbar\omega)^3.$$

Trapezoid Potential

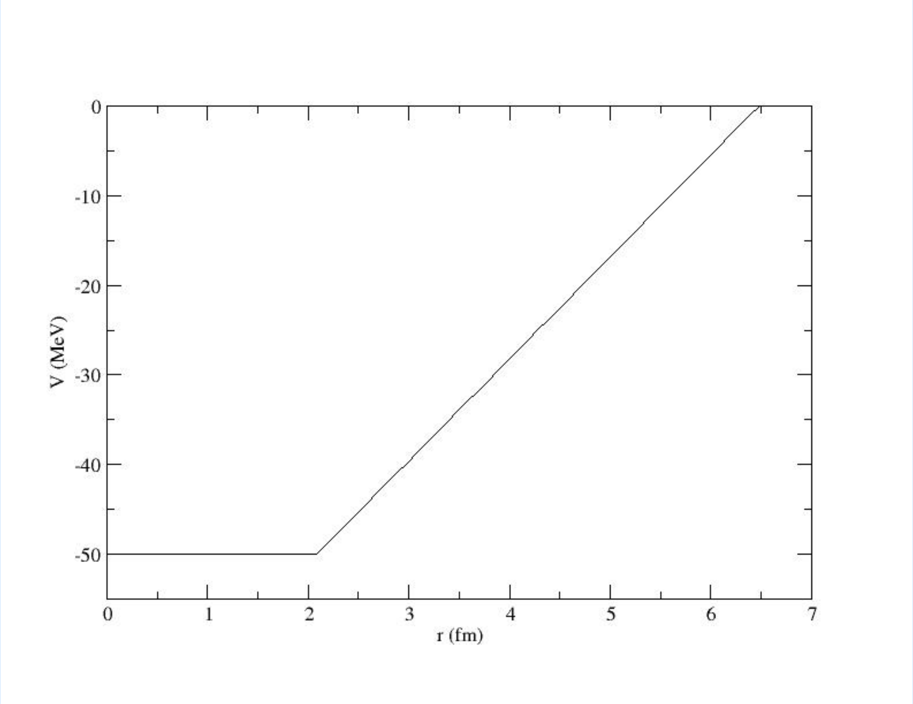
$$V^{TR}(r) = \begin{cases} V_0 & r < R - D \\ \frac{1}{2} V_0 [1 - (r - R)/D] & r > R - D \\ 0 & r > R + D \end{cases}$$

$$V_0 = -50 \text{ MeV}$$

$$D = 0.70\pi \text{ fm}$$

$$R = R_v / [1 + (D/R)^2]^{1/3}$$

$$R_v = 1.12 A^{1/3} + 0.80 \text{ fm}$$



Level Density in TR Potential

In the trapezoid potential, the single particle level density is

$$g_{TF}^{TR}(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{4\pi(R-D)^3}{3}\sqrt{\varepsilon - V_0}\left[1 + 2x + \tfrac{8}{5}x^2 + \tfrac{16}{35}x^3\right]$$

with

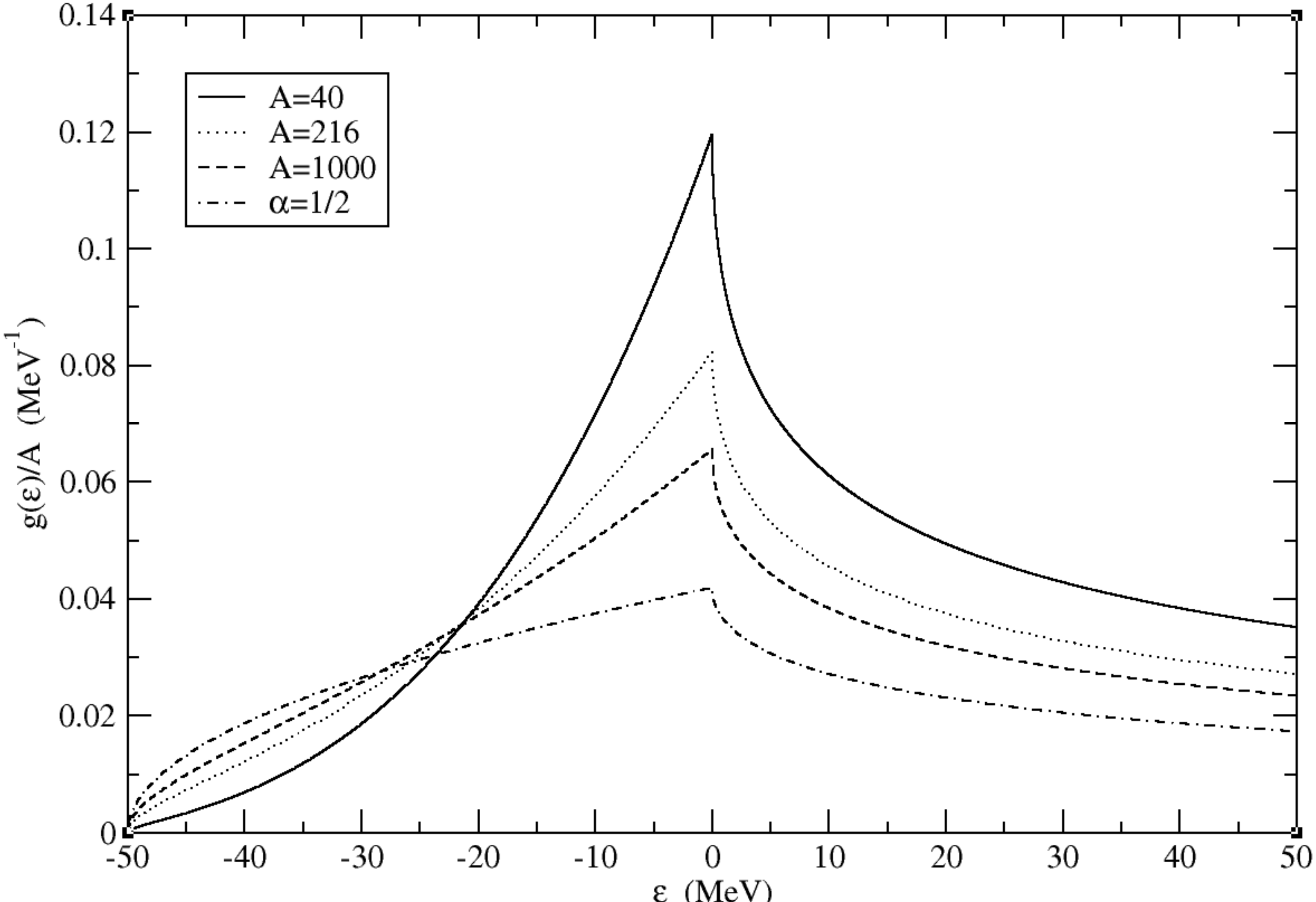
$$x = -\frac{2D(\varepsilon - V_0)}{(R-D)V_0}.$$

Subtracting the Free Gas States

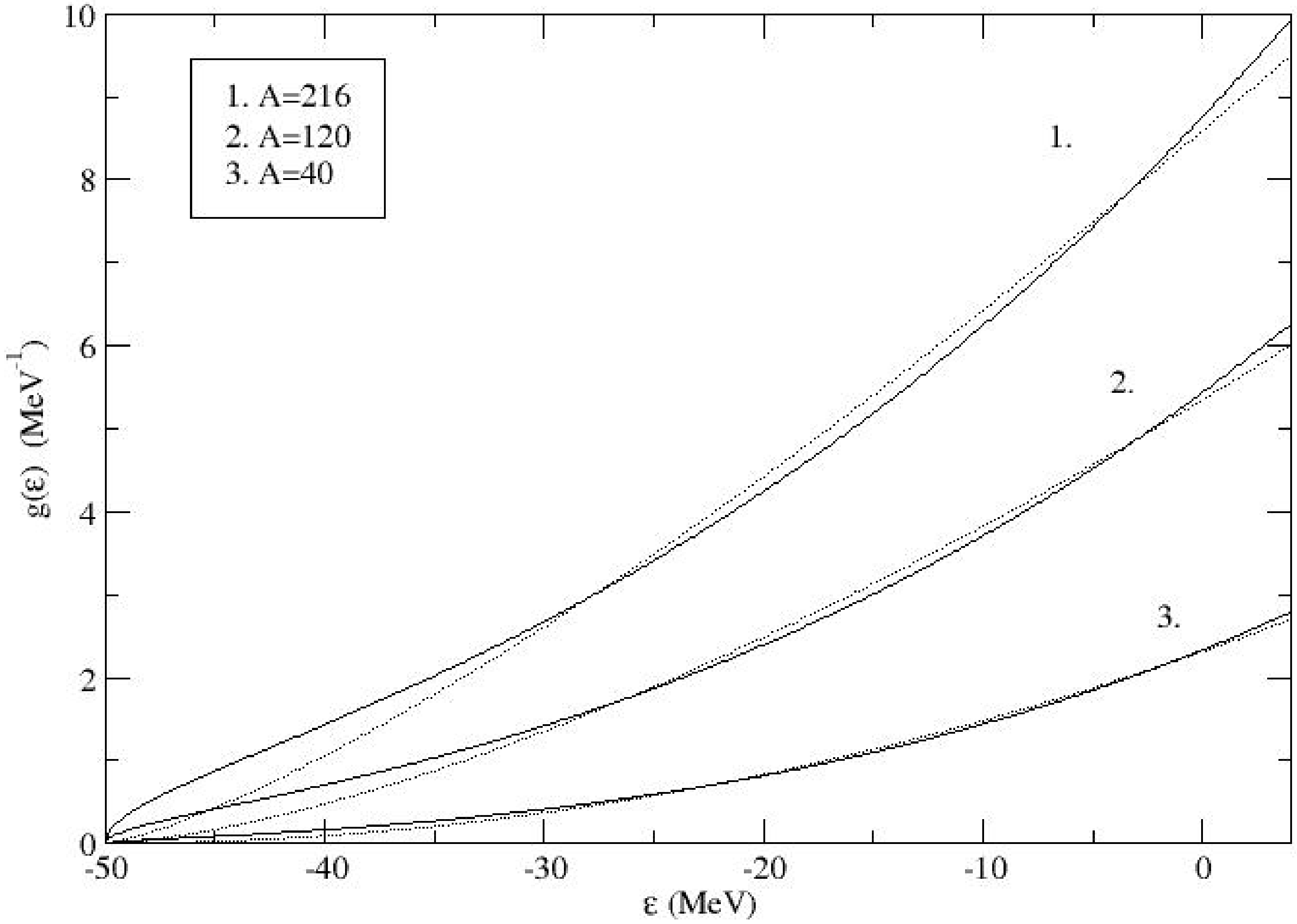
Since the SP potential is finite, the level density must be corrected above ε=0 by subtracting the contribution of the free gas states:

$$\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{4\pi\left(R-D\right)^3}{3}\sqrt{\varepsilon}\left[1+2u+\tfrac{8}{5}u^2+\tfrac{16}{35}u^3\right],$$

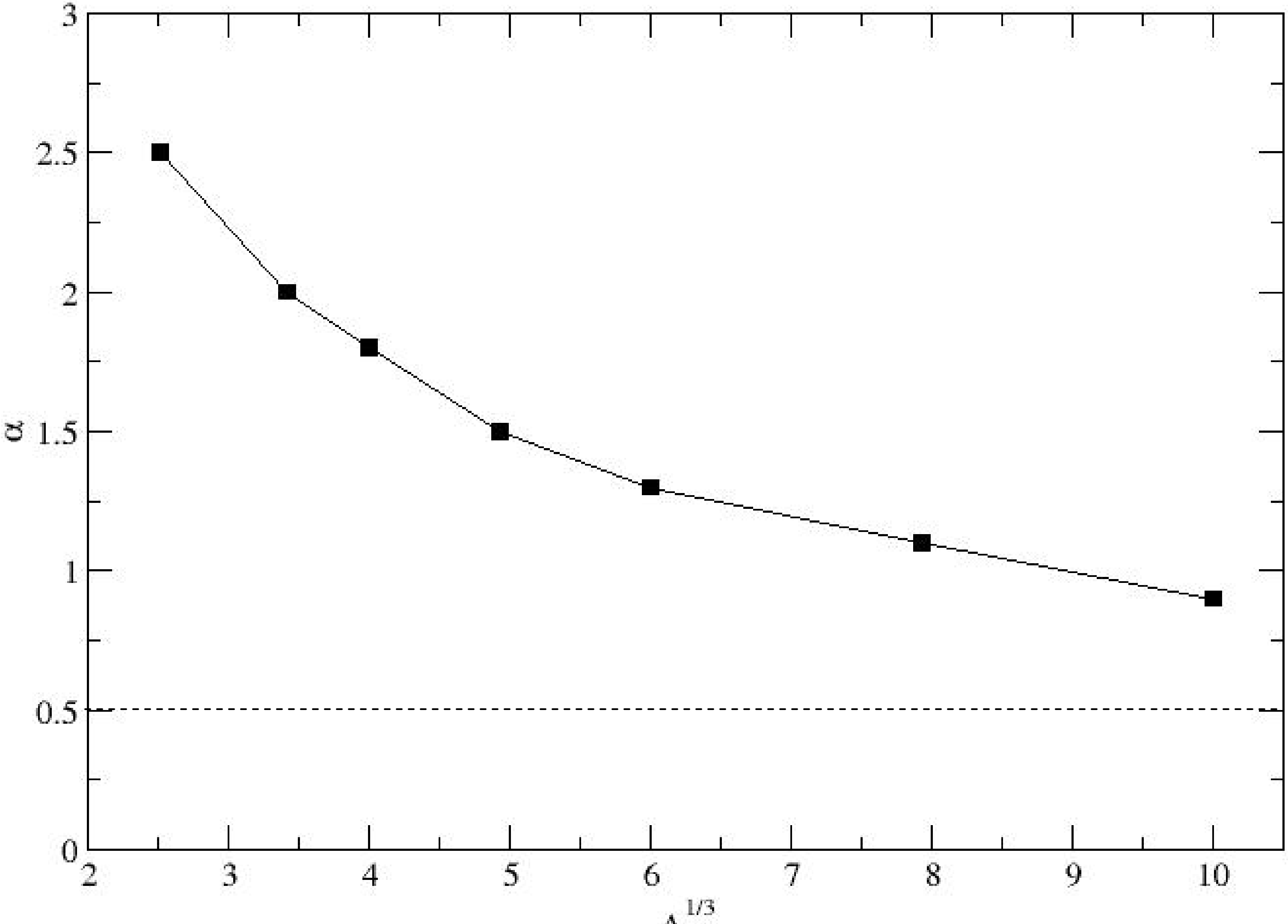
$$\text{with}\quad u=-\frac{2D\varepsilon}{(R+D)V_0},\quad \text{for } \varepsilon>0.$$



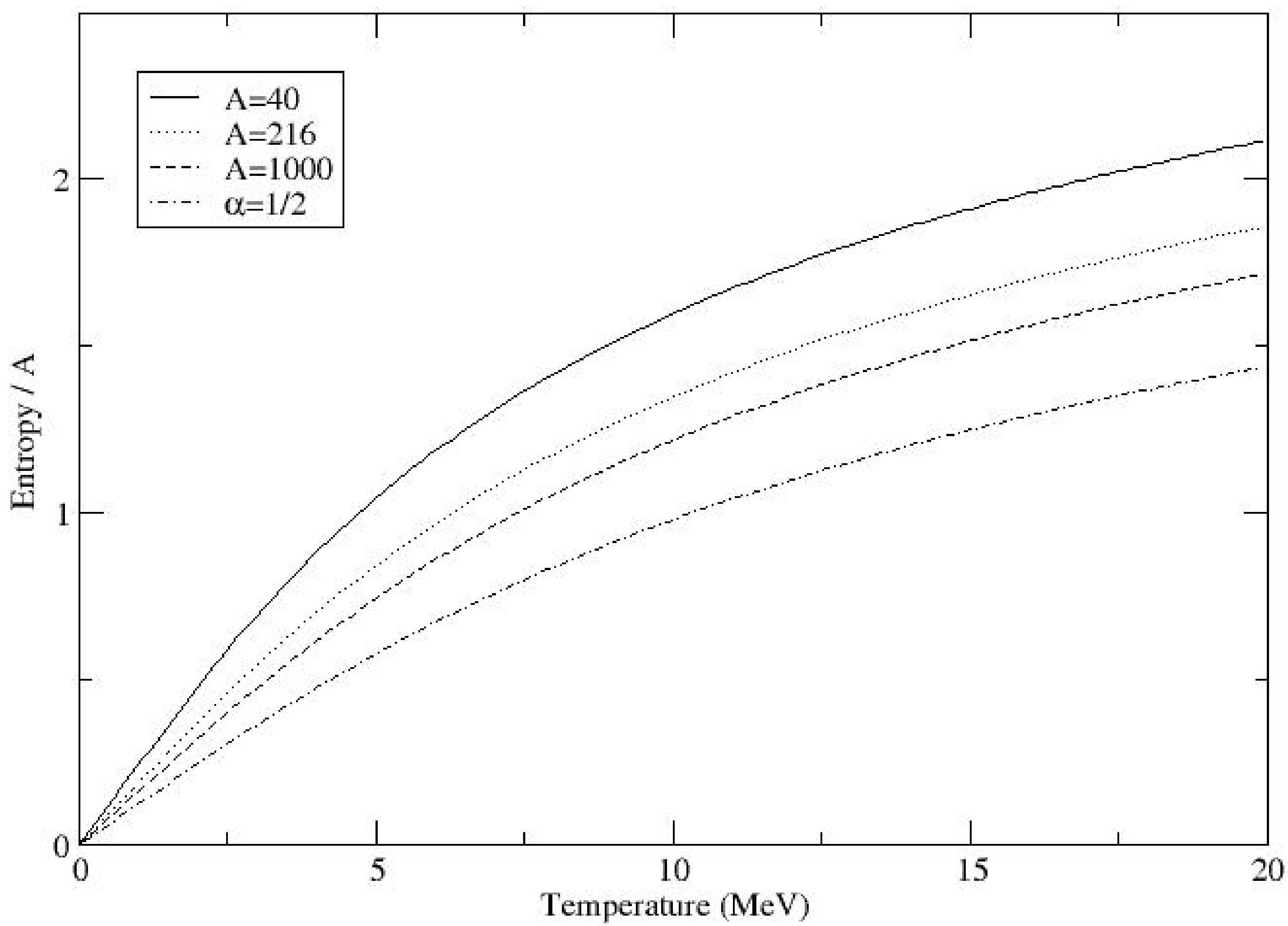
SP Level Density per Nucleon



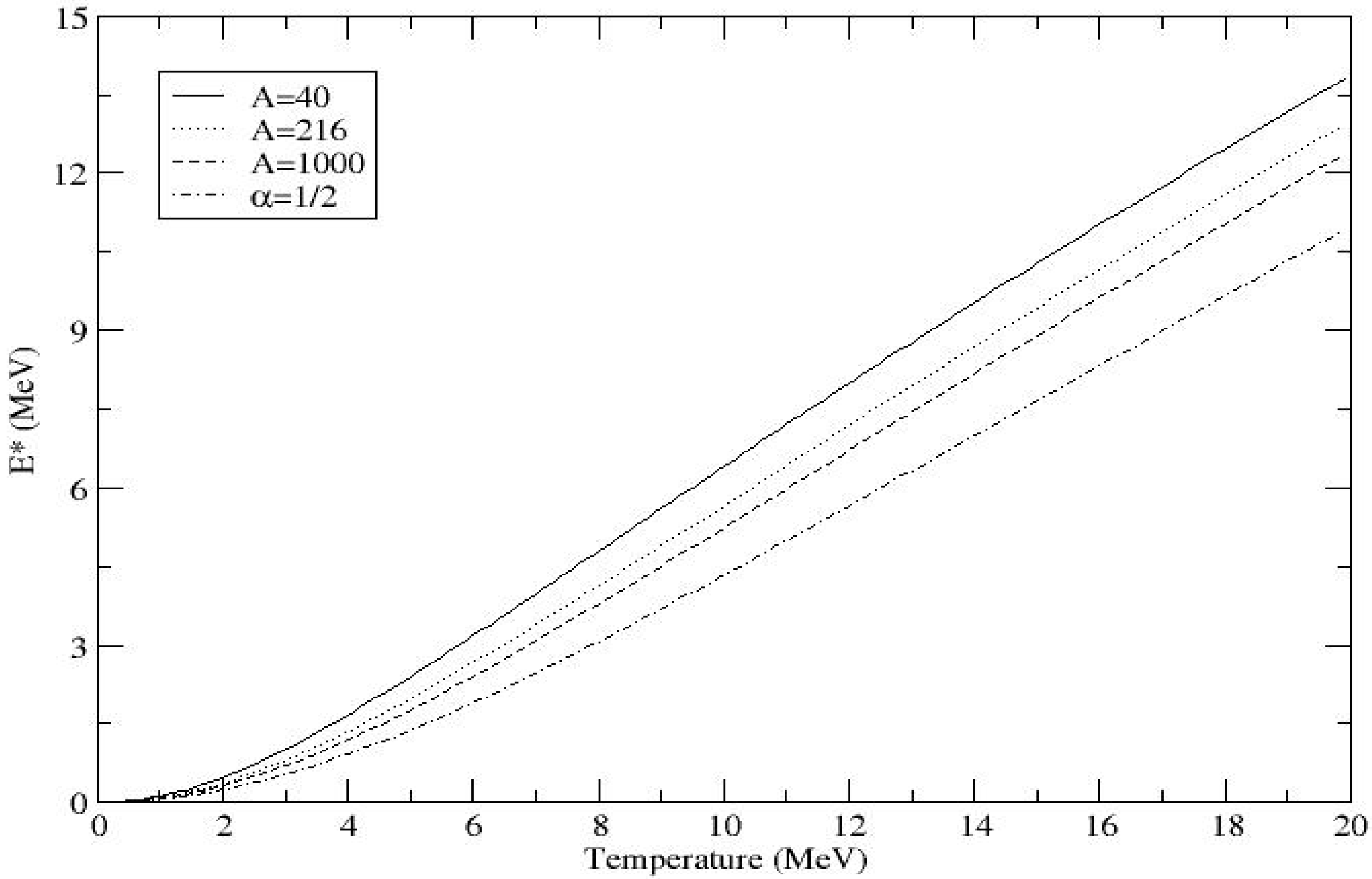
SP Level Densities in a Trapezoid potential fit to $g = C\varepsilon^{\alpha}$



α vs. $A^{1/3}$



Entropy per Nucleon



Excitation Energy per Nucleon

Conclusion

We have calculated the smooth single-particle level density, entropy and excitation energy for several nuclei, using a realistic potential well and properly accounting for the continuum. We demonstrated that the commonly adopted Fermi gas model, $g(\varepsilon) = C\sqrt{\varepsilon}$, is not appropriate for finite nuclei. The effect of finite size of the nucleus leads to an increase in the entropy and excitation energy by more than 50%.

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