

The (theoretical) properties of very hot compound nuclei

B.V. Carlson, F.T. Dalmolin, M. Dutra – ITA, Brazil

S. R. Souza – IF - UFRGS and IF - UFRJ, Brazil

R. Donangelo – IF - UFRJ, Brazil and IF – Universidad de la República, Uruguay

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Motivation

- One would expect nuclei to grow bigger as they become hotter. How much bigger?
- How does the change in size affect statistical properties? What is the relationship between excitation energy, entropy and temperature?
- What is the limiting excitation energy or temperature above which the nucleus does not exist?
- In short, what can we expect when a nucleus gets hotter and hotter?

Finite temperature formalism

In the Hartree-Fock approximation, one uses the single-particle density operator

$$D = \frac{1}{Z_0} \exp \left(- \sum_i \alpha_i a_i^\dagger a_i \right) \quad \text{with } Z_0 \text{ the grand canonical partition function,}$$

to define the thermodynamical potential

$$\Omega(D) = \text{Tr}[DH] - TS(D) - \mu_n N(D) - \mu_p Z(D)$$

where the entropy is given by

$$S = \text{Tr}[D \ln D]$$

and $N(D)$ and $Z(D)$ are the neutron and proton number operators and μ_n and μ_p the associated chemical potentials.

The Hartree-Fock equations are obtained by minimizing the thermodynamical potential with respect to the wavefunctions,

$$|i\rangle = a_i^\dagger |0\rangle$$

The single-particle occupations that result are

$$n_i = \text{Tr} \left[D a_i^\dagger a_i \right] = \frac{1}{1 + \exp[(e_i - \mu)/T]}$$

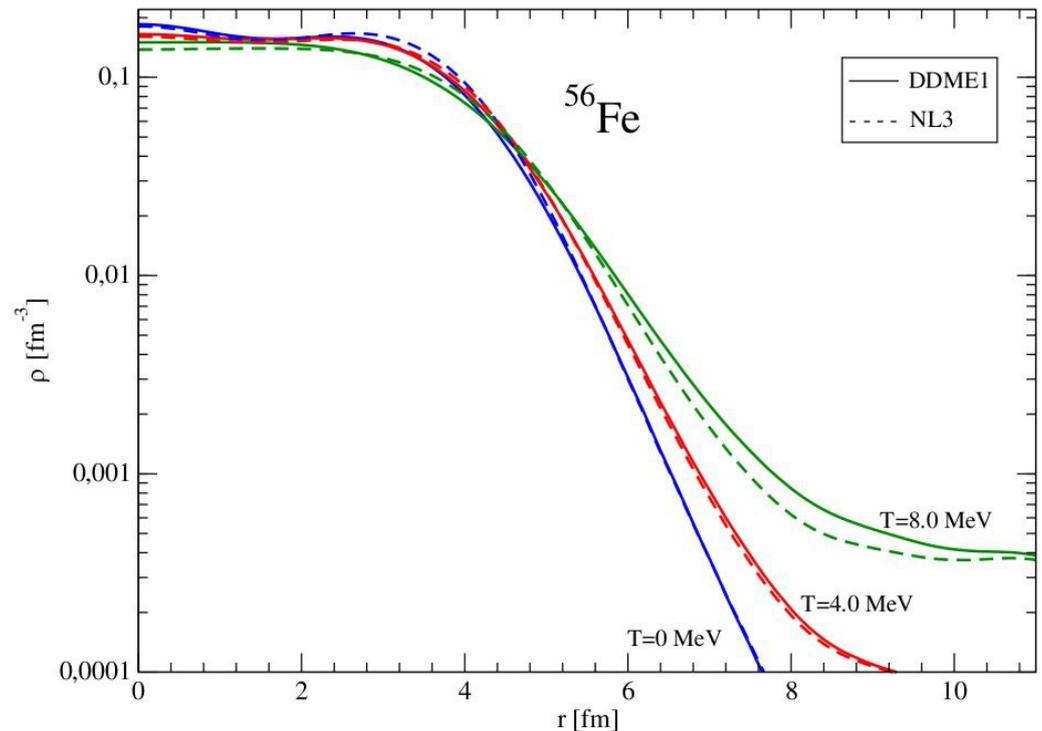
Bound states only

At low temperature, only bound single particle states have non-negligible occupations.
At higher temperatures, we can artificially restrict the occupations so that only bound single-particle states are occupied.

Two calculations:

- Hartree RMF;
- NL3 and DD-ME1 parameter sets;
- Harmonic oscillator basis;
- 30 major shells.

Anomalous behavior at 8 MeV, but
artificially restricted anyway.



NL3 – G.A. Lalazissis, J. König and P. Ring, Phys.Rev. C 55, 540 (1997).

DD-ME1 – T. Niksic, D. Vretenar, P. Finelli, and P. Ring, Phys. Rev. C 66, 024306 (2002).

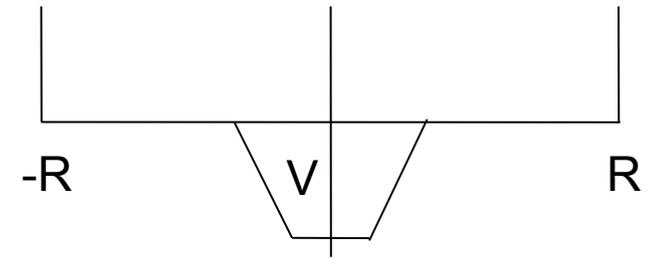
Continuum states

Consider scattering from a potential $V(x)$ in a 1-D box $[-R, R]$ with the condition that the wave function is zero on the edges of the box.

For a positive energy continuum state, this implies that

$$2kR + \delta(E) = n\pi$$

where $\delta(E)$ is the phase shift due to scattering from the potential.



The density of continuum single-particle states is

$$\rho(E) = \frac{dn}{dE} = \frac{2R}{\pi} \frac{dk}{dE} + \frac{1}{\pi} \frac{d\delta}{dE}$$

so that the thermodynamic potential can be written as the sum of three contributions

$$\begin{aligned} \Omega &= T \sum_i \ln(1 - n_i) \\ &\rightarrow T \sum_{i \in b} \ln(1 - n_i) + \frac{T}{\pi} \int_0^\infty \ln(1 - n(E)) \frac{d\delta}{dE} dE + 2R \frac{T}{\pi} \int_0^\infty \ln(1 - n(E)) \frac{dk}{dE} dE \end{aligned}$$

Continuum states II

The first term in the thermodynamical potential is the contribution of the bound states,

$$\Omega = T \sum_{i \in b} \ln(1 - n_i) + \frac{T}{\pi} \int_0^\infty \ln(1 - n(E)) \frac{d\delta}{dE} dE + 2R \frac{T}{\pi} \int_0^\infty \ln(1 - n(E)) \frac{dk}{dE} dE$$

The second term furnishes the contribution of resonances – the phase shift near a resonance can be written as

$$\delta(E) \approx \delta_0 + a \tan\left(\frac{\Gamma/2}{E_R - E}\right)$$

and its derivative as

$$\frac{d\delta}{dE} \approx \frac{\Gamma/2}{(E - E_R)^2 + \Gamma^2/4} \approx \pi \delta(E - E_R)$$

which contributes to the thermodynamic potential as

$$\Omega_R = T \ln(1 - n_R)$$

The last term - the continuum contribution – diverges and is the same when $V=0$.

We can extract the finite contribution due to the potential by taking the difference,

$$\Delta\Omega(T, \mu) = \Omega(T, \mu, V) - \Omega(T, \mu, V = 0)$$

Two solutions

In 3-D, including the Coulomb interaction, this is

$$\Delta\Omega(T, \mu) = \Omega(T, \mu, V + V_C) - \Omega(T, \mu, V = V_C)$$

For given values of the chemical potentials, the Hartree-Fock equations have two solutions:

- one corresponding to a nucleus + gas, with nucleon density ρ_{NG} ;
- another corresponding to the gas, with nucleon density ρ_G .

However, the solutions are unstable due to the Coulomb repulsion of the gas particles on themselves. To remedy this, only the Coulomb repulsion from the particles in the nucleus, $\rho_{NG} - \rho_G$, are included.

The thermodynamic potential is given by

$$\begin{aligned} \Delta\Omega(T, \mu, \rho_{NG} - \rho_G) = & \Omega(T, \mu, \rho_{NG}, V_N) - \Omega(T, \mu, \rho_G, V_N) \\ & + \frac{1}{2} \int [\rho_{NG,p}(\vec{r}) - \rho_{G,p}(\vec{r})] \frac{e^2}{|\vec{r} - \vec{r}'|} [\rho_{NG,p}(\vec{r}') - \rho_{G,p}(\vec{r}')] d^3r d^3r' + E_{CX} \end{aligned}$$

Nuclear densities

Two self-consistent calculations are performed
– for the nucleus + gas and the gas.

The chemical potentials are such that Z and A correspond to $\rho_{\text{NG}} = \rho_{\text{G}}$.

RMF calculations w/pairing

- Harmonic oscillator basis – 30 major shells;

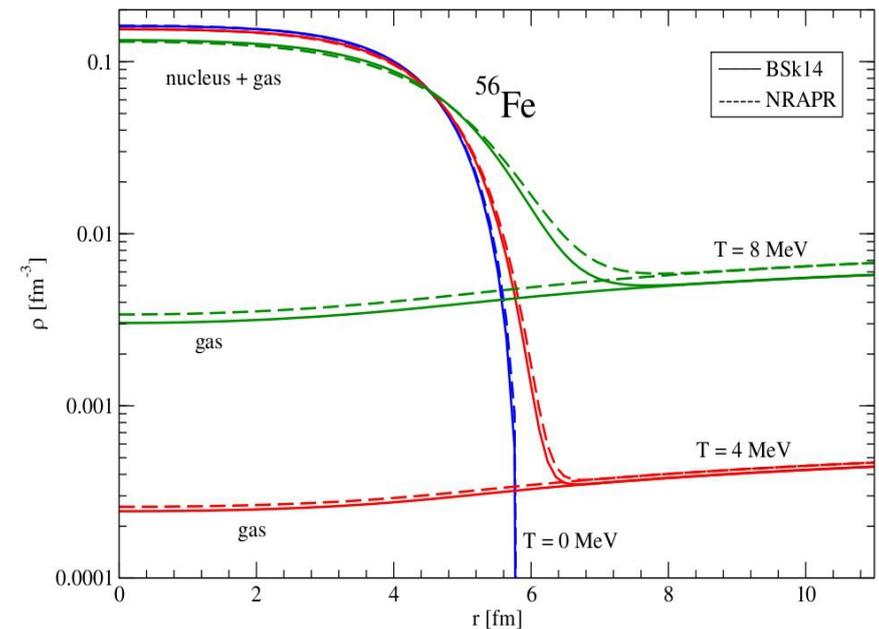
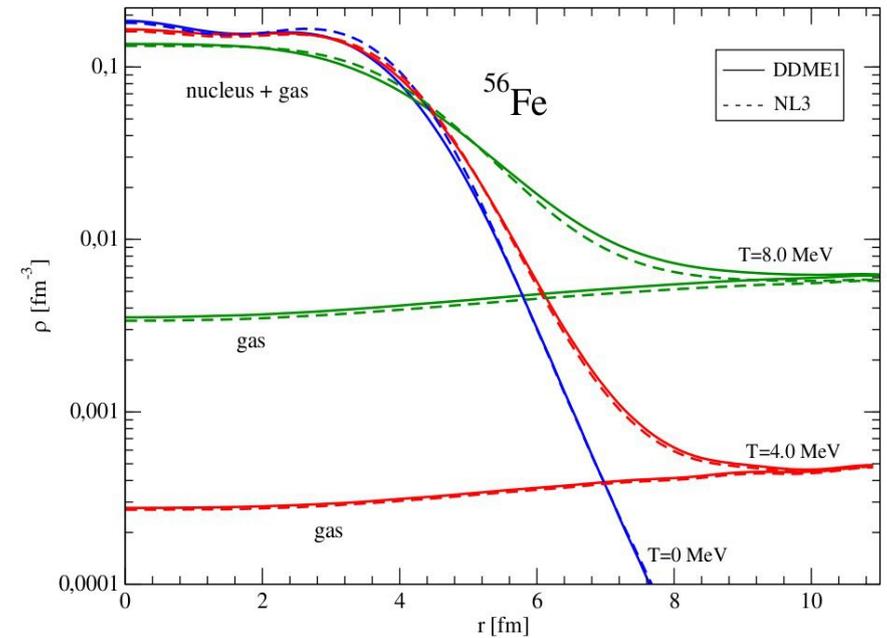
Skyrme Thomas-Fermi calculations

- Regular grid in a 1-D box;

- BSk14 and NPAPR parameter sets

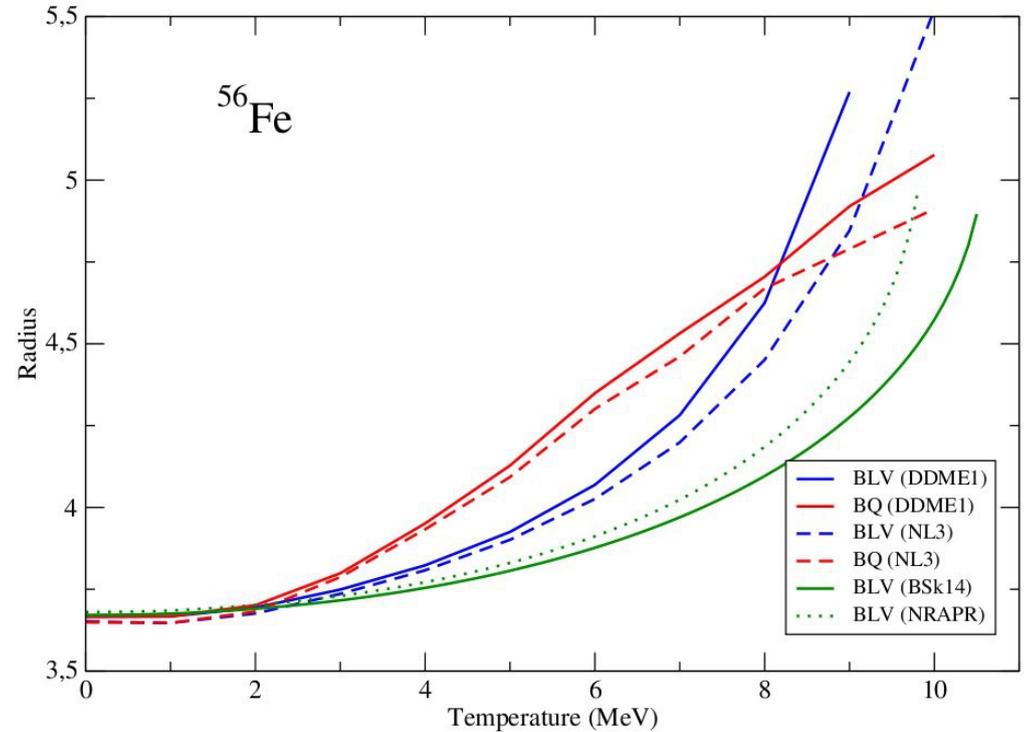
BSK14 - S. Goriely, M. Samyn, J. Pearson, Phys. Rev. C 75, 064312 (2007).

NPAPR - A. W. Steiner, M. Prakash, J. M. Lattimer, P. J. Ellis, Phys. Rep. 411, 325 (2005)



Rms radii

- Radii including only bound states increase fastest but saturate.
- Thomas-Fermi radii increase the slowest.
- The BLV radii diverge between 9 and 11 MeV, depending on the interaction.
- Without Coulomb, the BLV radii diverge at about 12 MeV.



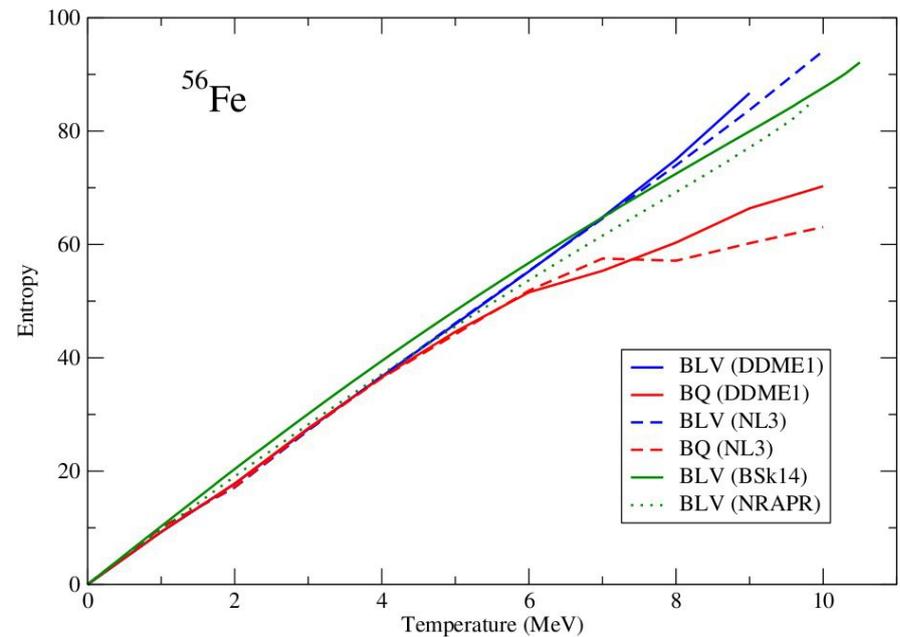
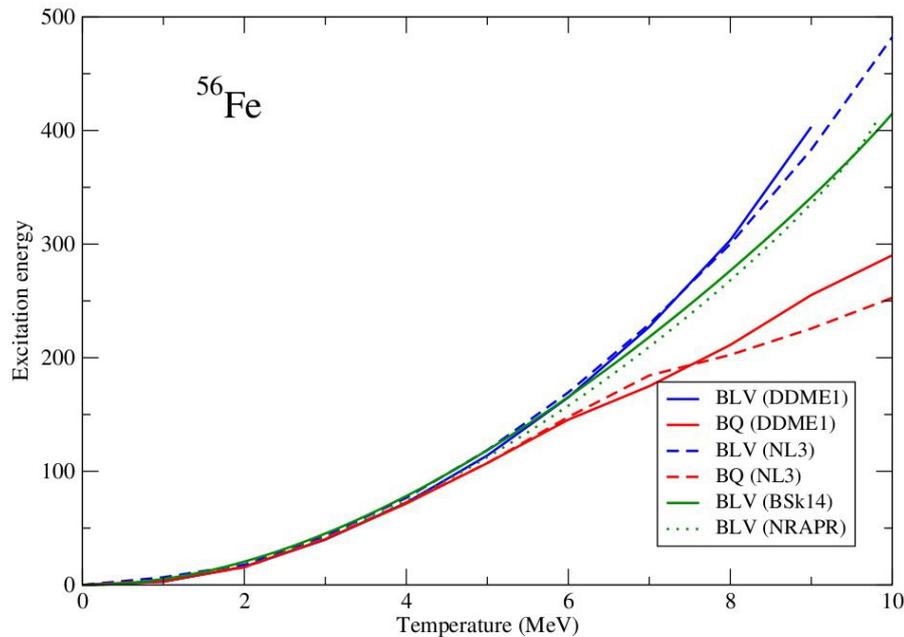
The BLV matter radii are well fit at $T < 6$ MeV by

$$\langle r_m^2 \rangle = r_{m0}^2 A^{2/3} (1 + c_m T^2)$$

with

$$r_{m0} = 0.95 \pm 0.05 \text{ fm} \quad c_m = 0.005 \pm 0.001 \text{ MeV}^{-2}$$

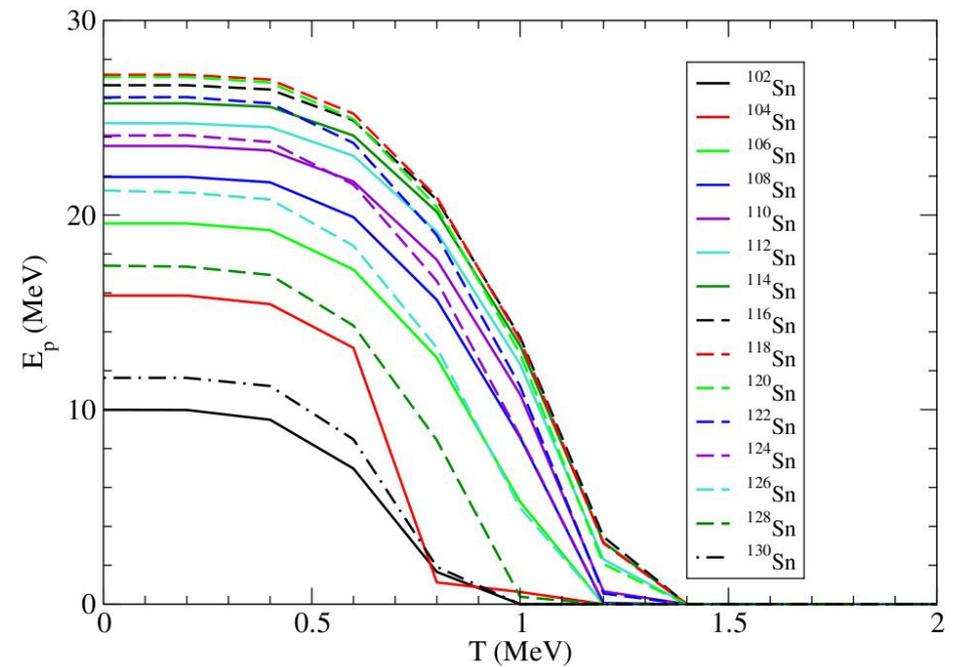
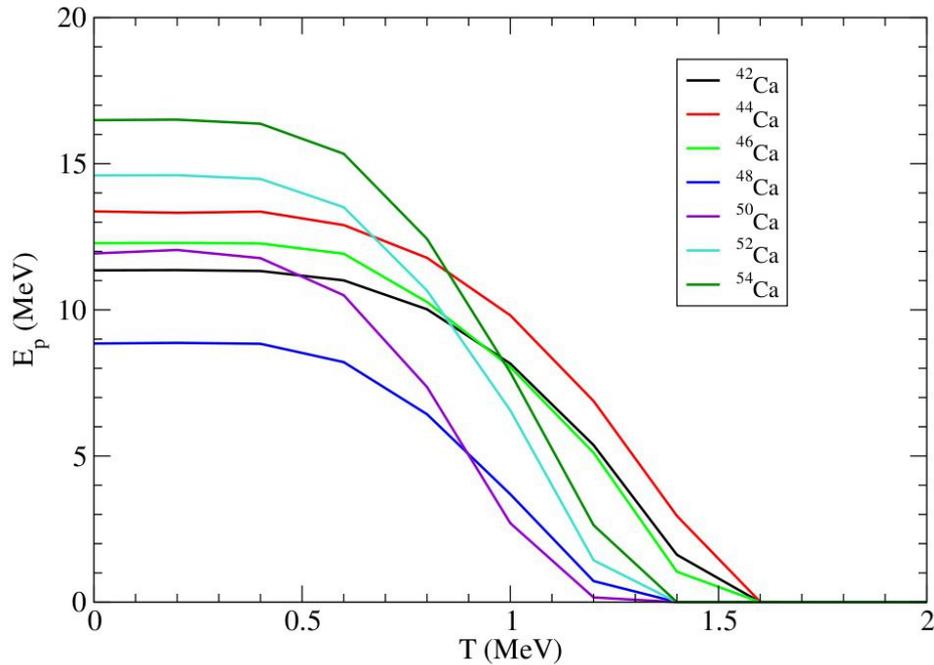
Excitation energy and entropy



On the scale shown here,

- the excitation energy appears to vary quadratically and the entropy linearly with the temperature, in all cases, up to about 5 MeV (Fermi gas behavior);
- above 5 MeV, the calculations including only bound states begin to show saturation effects;
- Pairing and shell effects enter at low temperatures.

Pairing



The RMF calculations were performed using an extended BCS approximation and a relativistic zero-range pairing interaction. (BVC and D. Hirata, Phys. Rev. C62 (2000) 054310.)

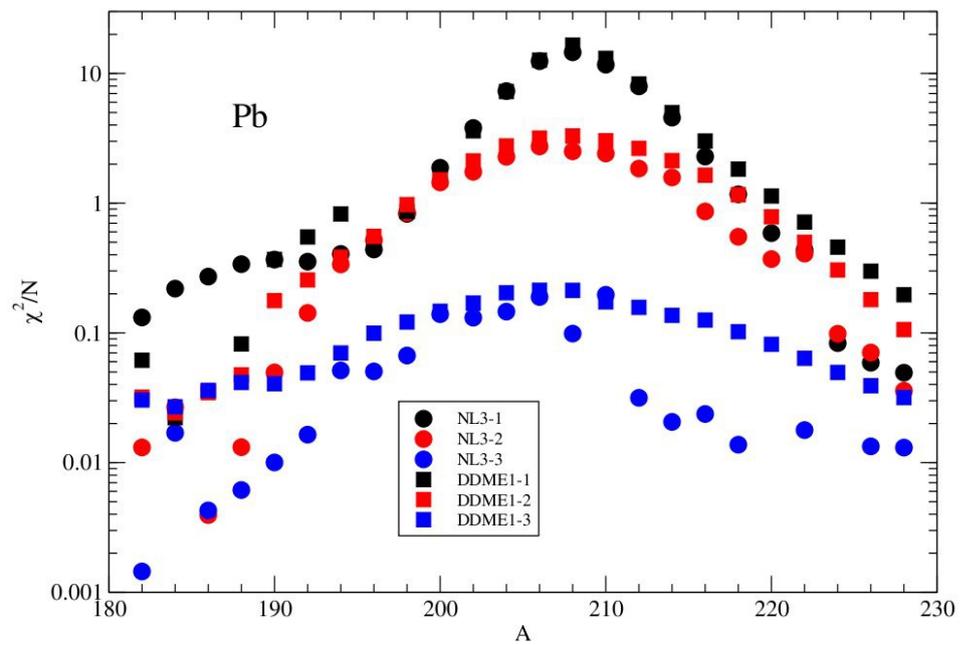
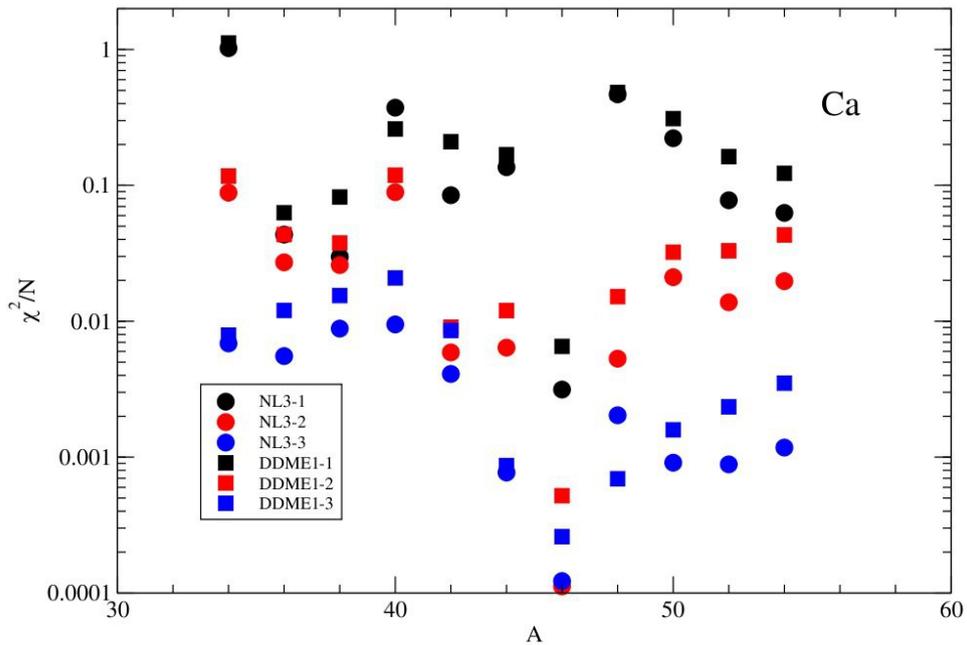
The pairing energy has the typical energy dependence and decreases to zero below $T=1.5$ MeV.

Shell effects

The RMF calculations also showed the effects of shell closures. To get an idea of their importance we looked at

$$\chi^2 = \sum_{T_{min}}^{T_{max}} \left(E_{RMF}(T) - E_0 - c_0 T^2 \right)^2$$

where $T_{max} = 6$ MeV and T_{min} was varied between 1 and 3 MeV.



Liquid-drop model fit to the energy

- Due to the effects of pairing and shell closures, ground state energies cannot be used as a reference for the functional dependence of the excitation energy at high energy.
- Both the constant and temperature dependent terms must be fit.
- We take

$$E = c_1A + c_2A^{2/3} + c_4Ad^2 + c_5A^{1/3} + c_6\frac{Z(Z-1)}{A^{1/3}} + (c_7A + c_8A^{2/3} + c_9Ad^2)T^2$$

where

$$d = \frac{1}{(1 + c_3A^{-1/3})} \frac{N - Z}{A}$$

Fits were performed using

- RMF and Skyrme T- F calculations
- 180 nuclei with $8 \leq Z \leq 82$ and $12 \leq A \leq 250$
- temperatures in the range $2 \text{ MeV} \leq T \leq 6 \text{ MeV}$.

Liquid-drop model fit to the energy II

The parametrization:

$$E = c_1A + c_2A^{2/3} + c_4Ad^2 + c_5A^{1/3} + c_6\frac{Z(Z-1)}{A^{1/3}} + (c_7A + c_8A^{2/3} + c_9Ad^2)T^2$$

where

$$d = \frac{1}{(1 + c_3A^{-1/3})} \frac{N - Z}{A}$$

Modelos	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	χ^2/N
BSk14	-14.71	11.73	0.655	27.29	6.94	0.664	0.064	0.077	-0.091	3.5
NRAPR	-14.35	9.98	0.718	28.24	9.17	0.649	0.057	0.087	-0.095	3.6
DD-ME1	-15.83	21.16	1.042	32.79	-7.79	0.675	0.062	0.093	-0.112	7.0
NL3	-15.27	17.68	1.145	32.47	-1.88	0.650	0.059	0.090	-0.085	6.6
G.S.	-15.8	18.3	0.0	23.7	0.0	0.714	0.0625	0.139	0.0	--

- Skyrme volume and surface terms are smaller than those in G.S. fit;
- Symmetry energy term c_4 is higher because of c_3 dependence not in G.S. Fit;
- Temperature-dependent volume and surface terms – c_7 and c_8 – smaller.

Symmetry energy

The symmetry energy is found to be

$$E_{sym} \approx Ad^2 \left(30 - 0.1T^2 \right) \text{ MeV}$$

It is about 10% below its ground state value at a temperature of 6 MeV.

Why does it decrease? The principal effect is the volume expansion.

With

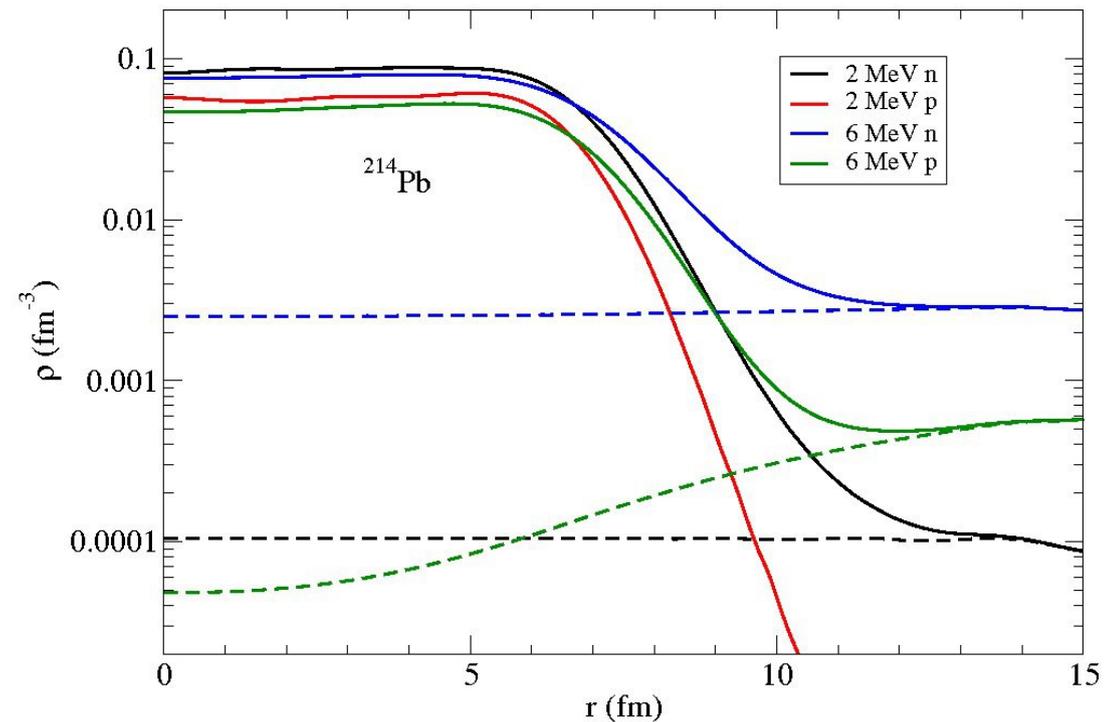
$$\langle r_m^2 \rangle = r_{m0}^2 A^{2/3} \left(1 + c_m T^2 \right)$$

we have

$$E_{sym} \approx E_{sym,0} - c_m \tilde{L} T^2 / 2$$

where

$$\tilde{L} = 3\rho_0 \left. \frac{dE_{sym}}{d\rho} \right|_{\rho_0}$$



Equilibrium

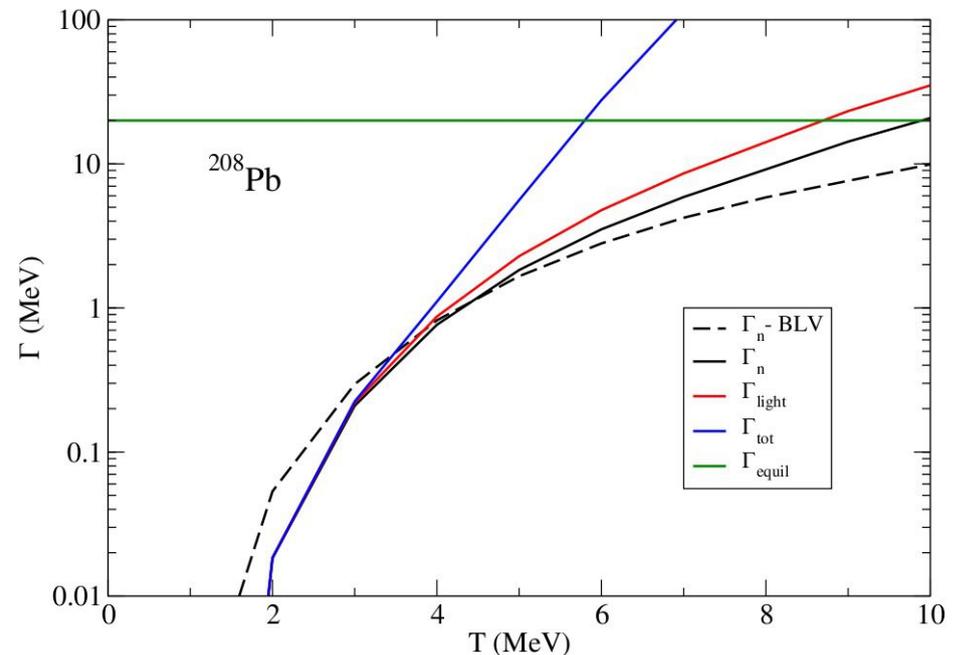
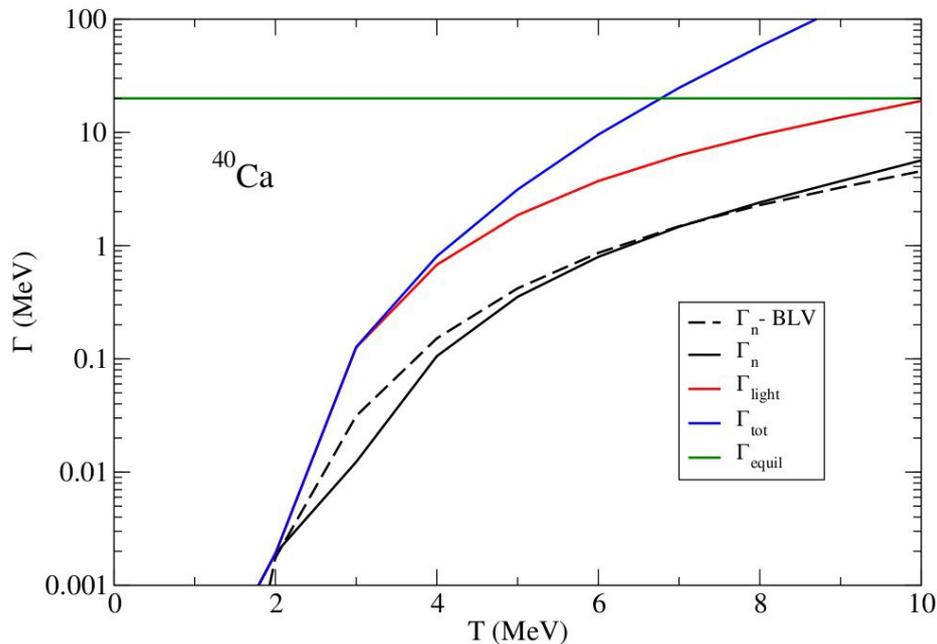
The compound nucleus is assumed to be in equilibrium. We estimate the local equilibration time in terms of the typical width of a shell-model state

$$\hbar/\tau_{eq} = \Gamma_{eq} \approx 20 \text{ MeV} \quad \text{N. Frazier, B.A. Brown, V. Zelevinsky, Phys. Rev. C54 (1996) 1665.}$$

The width of the BLV nucleus can be estimated in terms of the incident gas flux $n(e)$ as well as in terms of its Weisskopf decay width.

$$\Gamma_{BLV} \approx \hbar \langle \sigma v n \rangle = \frac{g\mu}{\pi^2 \hbar^2} \int e \sigma(e) n(e) de$$

$$\Gamma_W = \frac{g\mu}{\pi^2 \hbar^2} \int e \sigma_{inv}(e) \frac{\rho_f(\epsilon_0 - Q - e, 0)}{\rho_{cn}(\epsilon_0, 0)} de$$



Summary

- As expected, a nucleus expands as it is heated. The nuclear radius grows approximately quadratically with the temperature and is about 10% larger than the ground state radius at 6 MeV.
- The excitation energy also grows approximately quadratically with the temperature, except at temperatures below about 2 MeV, where pairing and shell effects are important.
- The symmetry energy is temperature dependent and decreases by about 10% from the ground state value at a temperature of 6 MeV.
- The calculations suggest that nuclei are unstable due to Coulomb repulsion at temperatures above about 8 MeV.
- Decay times suggest that an equilibrated hot nucleus cannot exist at temperatures of more than 5 or 6 MeV.

Things to do

- Improve the description of the geometry

$$\langle r^2 \rangle \rightarrow \frac{1}{1 + \exp[(r - R)/a]}$$

- Study fluctuations – in radius and deformation, at least
- Clusters – detailed balance?

$$\begin{aligned} \omega_{fn}(\varepsilon_0) &= \prod_{l=1}^k \frac{1}{N_l!} \left(\frac{V}{(2\pi\hbar)^3} \right)^{n-1} \int \prod_{j=1}^n d^3 p_j \delta \left(\sum_{j=1}^n \vec{p}_j \right) \\ &\times \int \prod_{j=1}^n (\omega_{bj}(\varepsilon_j) d\varepsilon_j) \delta \left(\varepsilon_0 - B_0 - E_{c0} - \sum_{j=1}^n \left(\frac{p_j^2}{2m_j} + \varepsilon_j - B_j - E_{cj} \right) \right) \end{aligned}$$