The (theoretical) properties of very hot compound nuclei

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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

\[ D = \frac{1}{Z_0} \exp \left( -\sum_i \alpha_i a_i^\dagger a_i \right) \]

with \( Z_0 \) the grand canonical partition function, to define the thermodynamical potential

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

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 \( \mu_n \) and \( \mu_p \) 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.

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
\[
\Omega = T \sum_i \ln(1 - n_i)
\]
\[
\rightarrow T \sum_{i \in b} \ln(1 - n_i) + \frac{T}{\pi} \int_0^\infty \ln(1 - n(E)) \frac{d\delta}{dE} dE + 2R \frac{T}{\pi} \int_0^\infty \ln(1 - n(E)) \frac{dk}{dE} dE
\]
Continuum states II

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

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

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

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

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 $\rho_{NG}$;
- another corresponding to the gas, with nucleon density $\rho_G$.

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

$$\Delta \Omega (T, \mu, \rho_{NG} - \rho_G) = \Omega (T, \mu, \rho_{NG}, V_N) - \Omega (T, \mu, \rho_G, V_N)$$

$$+ \frac{1}{2} \int \left[ \rho_{NG,p}(\vec{r}) - \rho_{G,p}(\vec{r}) \right] \frac{e^2}{|\vec{r} - \vec{r}'|} \left[ \rho_{NG,p}(\vec{r}') - \rho_{G,p}(\vec{r}') \right] d^3 r d^3 r' + E_{CX}$$

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 $\rho_{NG} - \rho_G$.

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

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

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

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.
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 \( T=1.5 \text{ MeV} \).
Shell effects

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

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

where \( T_{\text{max}} = 6 \text{ MeV} \) and \( T_{\text{min}} \) 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 ≤ Z ≤ 82 and 12 ≤ A ≤ 250
- temperatures in the range 2 MeV ≤ T ≤ 6 MeV.
Liquid-drop model fit to the energy II

The parametrization:

\[ E = c_1 A + c_2 A^{2/3} + c_4 A d^2 + c_5 A^{1/3} + c_6 \frac{Z(Z-1)}{A^{1/3}} + (c_7 A + c_8 A^{2/3} + c_9 A d^2) T^2 \]

where

\[ d = \frac{1}{(1 + c_3 A^{-1/3})} \frac{N-Z}{A} \]

<table>
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<th>( c_1 )</th>
<th>( c_2 )</th>
<th>( c_3 )</th>
<th>( c_4 )</th>
<th>( c_5 )</th>
<th>( c_6 )</th>
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<td>0.0625</td>
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- 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

\[ E_{\text{sym}} \approx A d^2 \left( 30 - 0.1 T^2 \right) \text{ MeV} \]

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

\[ E_{\text{sym}} \approx E_{\text{sym},0} - c_m \bar{L} T^2 / 2 \]

where

\[ \bar{L} = 3 \rho_0 \frac{d E_{\text{sym}}}{d \rho} \bigg|_{\rho_0} \]
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

\[ \hbar / \tau_{eq} = \Gamma_{eq} \approx 20 \text{ MeV} \]


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.

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

\[ \Gamma_W = \frac{g \mu}{\pi^2 \hbar^2} \int e \sigma_{inv}(e) \frac{\rho_f(\varepsilon_0 - Q - e, 0)}{\rho_{cn}(\varepsilon_0, 0)} \, de \]
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

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

- Study fluctuations – in radius and deformation, at least

- Clusters – detailed balance?

\[ \omega_{fr}(\varepsilon_0) = \prod_{l=1}^{k} \frac{1}{N_l!} \left( \frac{V}{(2\pi \hbar)^3} \right)^{n-1} \int \prod_{j=1}^{n} d^3 p_j \delta \left( \sum_{j=1}^{n} \vec{p}_j \right) \]

\[ \times \int \prod_{j=1}^{n} \left( \omega_{b,j}(\varepsilon_j) d\varepsilon_j \right) \delta \left( \varepsilon_0 - B_0 - E_{c0} - \sum_{j=1}^{n} \left( \frac{p_j^2}{2m_j} + \varepsilon_j - B_j - E_{cj} \right) \right) \]