Hartree-Fock Mass Formulas 
and the $\tau$-Process

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Relevance of Mass Formula to $\alpha$-Process

Masses as such not needed, but differential quantities are crucial:

$s_n$, neutron separation energy, determines position of $\alpha$-process path for given physical conditions (at least in canonical model).

$Q_{13}$, beta-decay energy, necessary for $\beta$-decay rates, which determine relative elemental abundances along $\alpha$-path.

NB Determination of $\beta$-decay rates requires also microscopic nuclear wave functions.
elucidating the r-process requires also a knowledge of fission barriers

any mass formula that minimizes
binding energy w.r.t. deformation
can be adapted to calculation of barriers.
Macroscopic - Microscopic

\[ [ \text{MM} ] \]

droplet

(refinement of
liquid-drop model)

shear effects

(Skrotinsky)

pairing effects

(BCS)

Shell Corrections

Suppose that droplet generates s.p.
field \( \hat{\mathcal{V}} \) (non-local and spin-dependent)

\[ (-\frac{\hbar^2}{2M} + \hat{\mathcal{V}}) \phi_i = \varepsilon_i \phi_i \]
Strutinsky Theorem

\[ E_{\text{tot}} = E_{\text{mac}} + \sum_i \epsilon_i - \sum_i \epsilon_i \]

\[ \sum_i \epsilon_i \] - smoothed sum of s.p. energies

Theorem gives a precise expression, but evaluation impossible for a DM starting point
- replaced by smoothing procedures
- plateau condition

Finte-Range Droplet Model (FROM)

Möller, Nix, Myers, and Swiateckz

A0040 T 59 195 (1995)

1654 masses fitted

\[ \sigma_{\text{rms}} = 0.669 \text{ MeV} \]
Excellent fit to data
- but how reliable are extrapolations?

1. No unambiguous choice of \( \tilde{U} \)
   - how to relate it to macro. term?

2. Scrutinizing smoothing procedures
   very ambiguous at n-deep line
   require a more fundamental approach,
   more closely related to basic
   nucleonic interactions
   i.e., more microscopic approach
   both sources of ambiguity avoided with
   Hartree-Fock - our approach
S. Cassedy, F. Tondeur, J.M. Pearson

ADNRT 34, 311 (2001)

Skyrme force - conventional 10 param.

\[ v_{ij} = t_0(1 + x_0 P_0) \delta(r_{ij}) + t_1(1 + x_1 P_0) \frac{1}{2\hbar^2} \left\{ p^2_{ij} \delta(r_{ij}) + h.c. \right\} \\
+ t_2(1 + x_2 P_0) \frac{1}{\hbar^2} p_{ij} \cdot \delta(r_{ij}) p_{ij} + \frac{1}{6} t_3(1 + x_3 P_0) \rho^3 \delta(r_{ij}) \\
+ \frac{i}{\hbar^2} W_0(\sigma_i + \sigma_j).p_{ij} \times \delta(r_{ij}) p_{ij} \]

Many Skyrme forces already on market S3, SHT*, S4P, Skym... but this is first time that essentially all mass data are fitted.
Pairing term

\[ \nu_{\text{pair}} = \sqrt{\frac{\lambda}{\pi g}} \delta(\pi \varepsilon_f) \]

treated in BCS approx.

Wigner term

\[ E_w = N_w \exp \left( -\lambda \frac{\ln(A-1)}{A} \right) \]

T = 0 pairing?

Combinations of Skyrme params. corresponding to \( M_s^* \) and \( M_v^* \) (isoscalar and isovector effective masses) constrained such that

\[ M_{s}^{*} = M_{v}^{*} \]

\[ \Rightarrow 15 \text{ degrees of freedom} \]
Fit to Audi-Wapstra (1998)

1768 nuclei with $Z, N \geq 8$

$\sigma_{\text{rms}} (1768) = 0.718 \text{ MeV}$

[ From $\sigma_{\text{rms}} (1768) = 0.678 \text{ MeV} $ ]

$\sigma(S_n) = 0.489 \text{ MeV}$

$\sigma(Q_2) = 0.614 \text{ MeV}$

Charge radii: 523 measured values

$\text{rms error} = 0.024 \text{ fm}$

Quadrupole deformation parameter $\beta_2$

274 measured values

$\text{rms error} = 0.100$

$(-0.5 \leq \beta \leq 0.5)$
HFB - 1
Well known problems with BCS at neutron drip line
Replace BCS by Bogoljubov
new mass formula


Same form of Skyrme + pairing forces
Same pairing cutoff (≈ 100 MeV)
With original force MSR1 (force HFBcs-3) quality of data fit deteriorates in HFB.

- new fit: force BSR1

\[ \sigma (1768) = 0.740 \text{ MeV} \]
\[ (0.718 \text{ MeV before}) \]

Extrapolation to neutron-deep line

\[ | M(\text{HFB-1}) - M(\text{HFBcs-3}) | < 2 \text{ MeV} \]

- usually much smaller.

Also shifts in \( S_n \) and \( Q_B \) very small e.g. shell gaps at magic neutron numbers.
This suggests that BCS might be sufficient — for masses

(radius of nucleii at neutron-drop
line are slightly smaller in
HFB — as expected.)
NEW DATA!

Sept. 2001

Preliminary version of new Audi-Wapstra compilation

382 new nuclei, \( N, Z \geq 8 \)

HFBCS-21 and HFB-1 both extrapolate badly to these new data—tendency to strongly overbind "exotic" nuclei.
Two sources of overbinding

1. Wigner term

\( A < 60 \), but this is where many of new data lie.

2. Cutoff of pairing spectrum

(with a 8-function pairing force, there will be a divergences if no cutoff)

See how HFB-I can be improved
Wigner Energy

originally had

\[ E_w = V_w \exp \left( -\lambda \frac{|N-21|}{A} \right) \]

now write

\[ E_w = V_w \exp \left\{ -\lambda \left( \frac{N-2}{A} \right)^2 \right\} \]

\[ + V'_w |N-2| \exp \left( -\frac{A}{A_b} \right)^2 \]

\[ SU(4) \text{ spin-isospin symmetry} \]

- confined to light nuclei;
  - best fit with \( A_b = 20 \)
Pairing Cutoff

$\epsilon_n = \hbar \omega = 41 A^{-1/3} \text{ MeV}$

**Alternative Scenario**

$\epsilon_n$ specified w.r.t. $\epsilon_F$

We optimized both models.
Latter scenario favoured

\[ E_{\Lambda} = E_{F} + 15 \text{ MeV} \]

Fit to 1995 data improves by 0.051 MeV

Extrapolation

Fit is 0.192 MeV

New data are far enough away from stability line to tell us something about cutoff

- cannot change this and maintain the fit by changing other parameters.
Errors of fits to the masses of the 1768 nuclei of the 1995 data compilation and of extrapolations to the 382 new nuclei of the 2001 data compilation. $\sigma$ denotes rms error, $\epsilon$ denotes mean error; all errors in MeV.

<table>
<thead>
<tr>
<th></th>
<th>1995 data (1768 nuclei)</th>
<th>new data (382 nuclei)</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>$\sigma$</td>
<td>$\epsilon$</td>
</tr>
<tr>
<td>FRDM</td>
<td>0.678</td>
<td>0.023</td>
</tr>
<tr>
<td>HFBCS-1</td>
<td>0.718</td>
<td>0.102</td>
</tr>
<tr>
<td>HFB-1</td>
<td>0.740</td>
<td>0.040</td>
</tr>
<tr>
<td>HFB-1'</td>
<td>0.651</td>
<td>-0.039</td>
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</table>
N.B.
We have adopted very simple parametrizations for pairing cutoffs. More elaborate parametrizations, e.g., different treatment of $n$ and $p$, may lead to better fits and may be required by future data.

A better microscopic understanding of pairing could provide a valuable guide.

But already we have established that cutoff energy does not have to be high — computer time!
So make a fit to complete new data set of 2135 nuclei with this new model, i.e. new Wigner term --- cutoff prescription

new mass formula

HFB-2

<table>
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<th>new data (382 nuclei)</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$\sigma$</td>
<td>$\epsilon$</td>
</tr>
<tr>
<td>FRDM</td>
<td>0.676</td>
<td>0.072</td>
</tr>
<tr>
<td>HFB-2</td>
<td>0.674</td>
<td>0.000</td>
</tr>
</tbody>
</table>

\[ \text{NB.} \]

From fitted to only 1654 masses (1993). So if refitted to new data it would almost certainly out-perform HFB-2.
Of particular interest to $r$-process magic neutron-shell gap

$$\Delta(N_0) = S_{2n}(N_0,2) - S_{2n}(N_0+2,2)$$

possibility of gap quenching as $n$-drip line is approached, i.e., as protons are removed for the given $N_0$
HFBCS-2 and HFB-2 quite similar
but HFB-2 follows distinct trend

⇒ Quenching depends on pairing cutoff

Treatment of pairing in FRDM
parametrization of pairing gap

\[ \Delta_{n\text{-pair}} \propto \frac{1}{N^{1/3}} \]

\[ \Delta_{p\text{-pair}} \propto \frac{1}{Z^{1/3}} \]
Symmetry Coefficient of INM

INM: Infinite nuclear matter

Weizsäcker mass formula

\[
\frac{E}{A} = a_0 + a_A A^{-1/3} + a_2 \frac{Z^2}{A^{2/3}} + a_{\text{sym}} \left( \frac{N-Z}{A} \right)^2
\]

All Skyrme-HF mass formulas lead to

\[
a_{\text{sym}} \approx 28 \text{ MeV}
\]

FROM \[\text{32 - 35 MeV}\]

Very important to have an independent determination of \( a_{\text{sym}} \)
if $\rho_{\text{sym}} > 2.9$ MeV, say, then bad news for Skyrme forces - would have to turn to finite-range forces -

much more complicated

Theory:

Calculation INM with Argonne 18 force

$\rho_{\text{sym}} = 28.7$ MeV

Zuo et al.

mass-independent measurement required for neutron-skin thickness

\[ \delta_n = R_m - R_p \]

measurement of \( R_m \) is difficult

old measurement of scattering of protons

208 Pb: \( \delta_n = 0.14 \pm 0.04 \) fm


\[ \Delta_{\text{sym}} = 29 \pm 2 \text{ MeV} \]

- hardly conclusive!

new experiment proposed:

parity-violating e-scattering
CONCLUSIONS

• Two mass formulas giving very similar global fits to the data can extrapolate quite differently to the highly neutron-rich region.

• “Ultimate” mass formula must be microscopic, but Skyrme-form force may not be the last word.

• Mass measurements have now reached the region of the nuclear chart where one can begin to distinguish between different cutoff prescriptions if δ-function pairing force is used.

• Treatment of pairing is crucial, but question of HFBCS vs. HFB is less important than prescription for cutoff.

• Need a better theory of pairing.

• Need more data, particularly data relevant to quenching

• Importance of symmetry coefficient.