Home Page

Title Page

Contents

Page 1 of 109

Go Back

Full Screen

Close

Quit

Nuclear Mass Models

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PLAN

1. Introduction
2. Weizsäcker semi-empirical mass formula, with ramifications
3. Nuclear many-body problem: the fundamentalist's approach
4. Hartree-Fock-Bogoliubov model
5. Macroscopic-microscopic mass models: the FRDM and FRLDM
6. Comparison of models
7. Conclusions

1. Introduction

- Interest in nuclear masses lies entirely in **binding energy**

$$B(N,Z) = \left\{ NM_n + ZM_p - M(N,Z) \right\} c^2$$

$< 1\%$ of total mass

– hence need for great precision

$$B = -E \quad ,$$

where

$$H\Psi = E\Psi \quad .$$

- "Mass defect" first noted by Aston (1920)

$$\text{H: } 1.008 \qquad\qquad {}^{4}\text{He: } 4.000$$

(at the time believed that $^{4}\text{He} = 4\text{H} + 2\text{e}$)

- Eddington (1920) made connection with $E = mc^2$ and at the same time saw that conversion of H to He could be source of stellar energy

– a long-standing puzzle solved.

- Eddington's comment marks birth of nuclear astrophysics;

link to nuclear masses established right at the outset.

N.B. ATOMIC masses

•Tabulated masses are for *neutral atoms* not *bare nuclei.*

e.g., Atomic Mass Evaluation (AME) of Audi *et al.* (2003)

$$M_{at}(N,Z) = M(N,Z) + Z\,m_e - B_{el}(Z)/c^2 \quad ,$$

where

$$B_{el}(Z) = 14.4381\,Z^{2.39} + 1.55468 \times 10^{-6}\,Z^{5.35}\ \mathrm{eV}$$

is binding energy of electrons in atom.

•Actually, it is *mass excess* $\Delta(N,Z)$ that is tabulated:

$$\Delta(N,Z) = \left\{ M_{at}(N,Z) - \frac{A}{12} M_{at}(6,6) \right\} c^2$$

(in keV)

What have we learned from mass measurements?

1. B/A roughly constant, around 8 MeV per nucleon.

   This, along with $R \propto A^{1/3}$, led to idea of saturation of nuclear forces, i.e., each nucleon interacts only with its nearest neighbors (aside from Coulomb force between protons).

   Nuclear matter. Liquid-drop model (charged).

2. Pairing.

   From systematics of even-A beta-decay chains.

3. Generalized shell model (including deformations).

   From two-neutron separation energies

$$S_{2n}(N, Z) = M_{at}(N-2, Z) - M_{at}(N, Z) + 2M_n \quad .$$

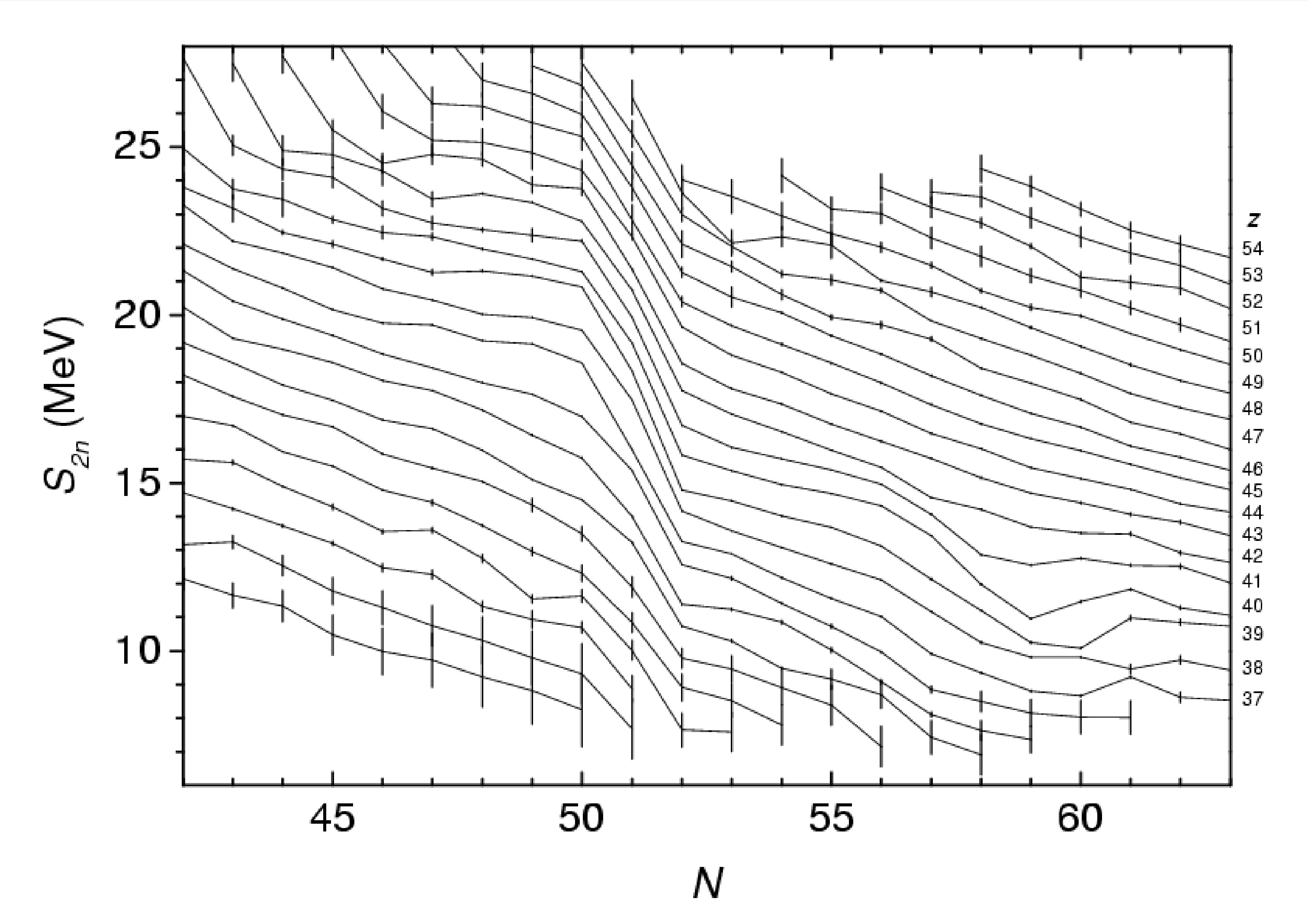


Fig. 1.1. Two-neutron separation energy S_{2n} of several elements in the range $Z \sim 30$-50, as a function of neutron number N.

Mass measurements made crucial contribution to our understanding of nuclear structure in the 1930's.

Diminishing contribution since 1948.

So why the current interest in mass measurements?

Astrophysics

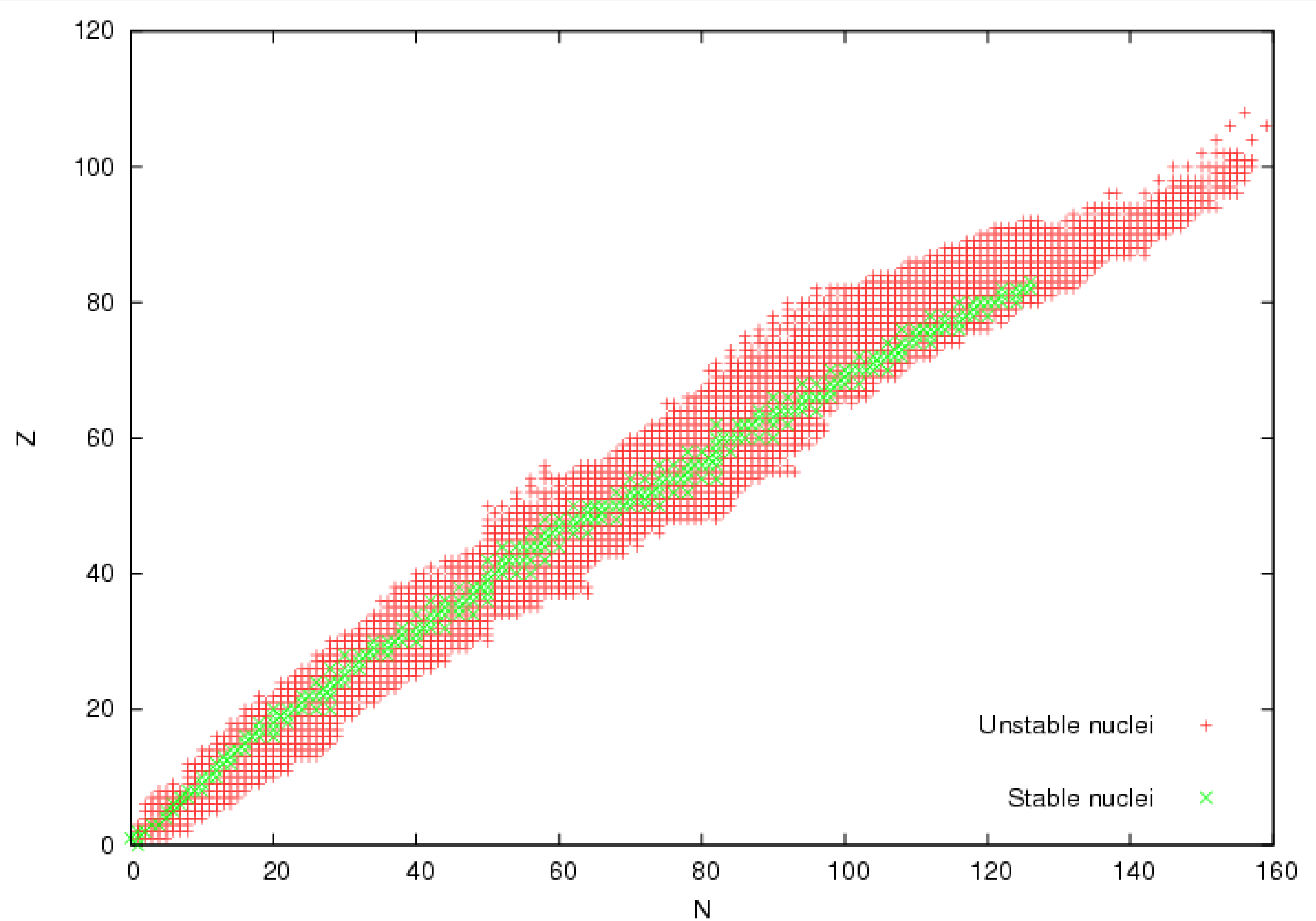


Fig. 1.2. Nuclei with measured masses according to 2003 AME. NOT shown: nuclei for which quoted mass is an estimate based on local systematics (indicated by # in table).

2221 measured nuclei in 2003 AME

1964 measured nuclei in 1995 AME

Any limit on nuclei that can exist and in principle have mass determined?

Increasing β^- instability as we add neutrons and move off to the right, because beta-decay energy Q_β increases,

$$Q_\beta = M_{at}(N, Z) - M_{at}(N-1, Z+1)$$

More seriously, neutron separation energy S_n decreases,

$$S_n = M_{at}(N-1, Z) - M_{at}(N, Z) + M_n$$

When $S_n = 0$ impossible to add any more neutrons.

Likewise increasing β^+ instability as we add protons and move off to the left of beta-stable nuclei. Also, decreasing proton separation energy S_p,

$$S_p = M_{at}(N, Z-1) - M_{at}(N, Z) + M_H$$

When $S_p = 0$ impossible to add any more protons.

Neutron drip line:

Z fixed, add neutrons, first nucleus with $S_n = 0$.

Proton drip line:

N fixed, add protons, first nucleus with $S_p = 0$

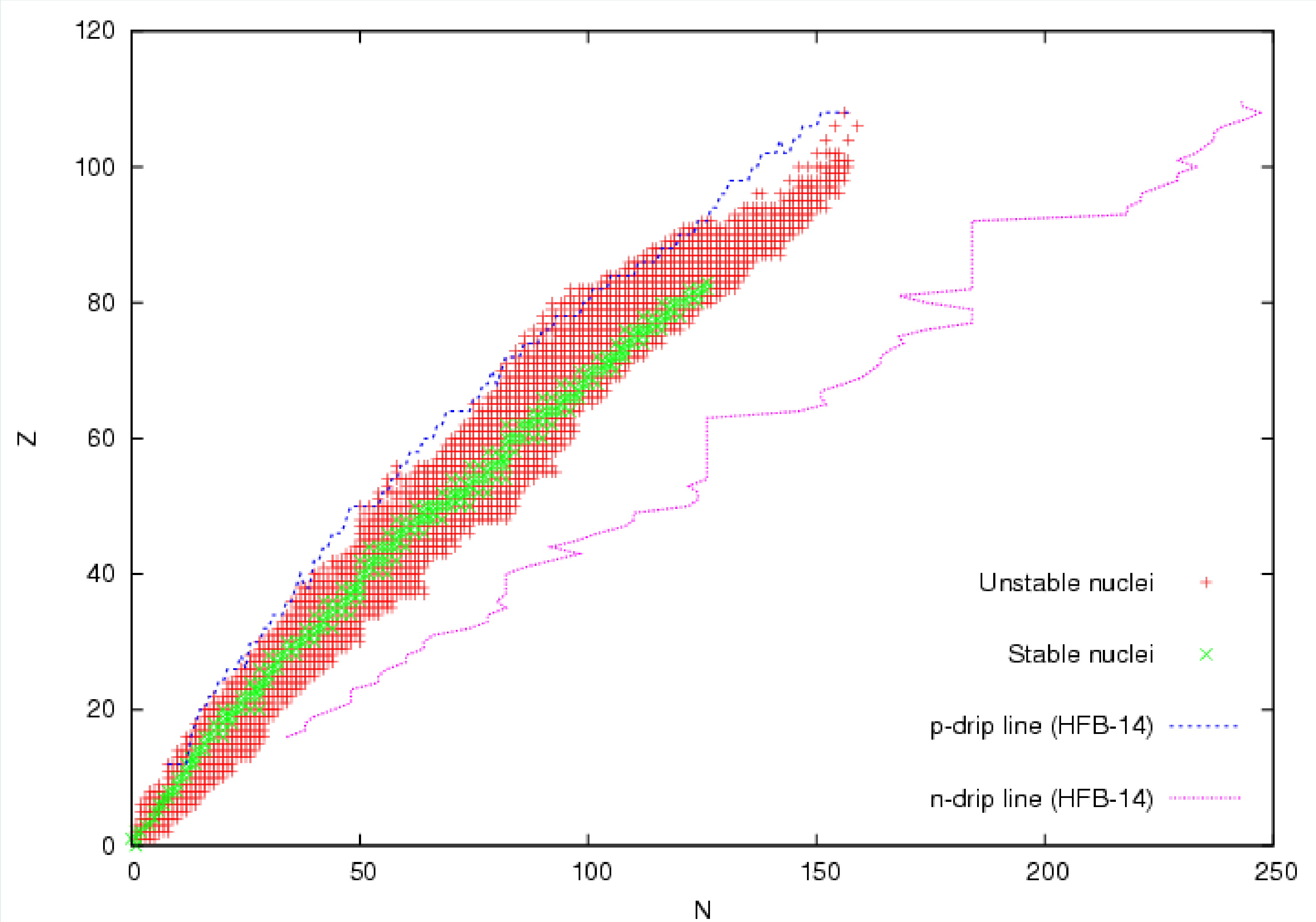


Fig. 1.3.

HFB-14 is the most recent Hartree-Fock Bogoliubov mass model of the Brussels-Montreal (B-M) group: Goriely *et al.* (2007).

Fig. 1.4.

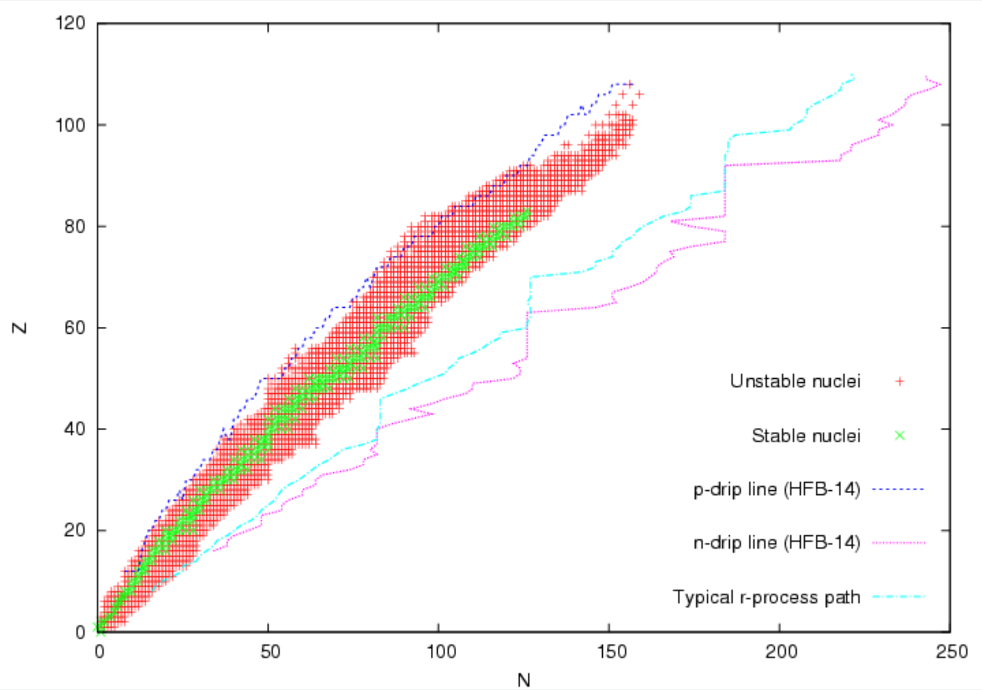
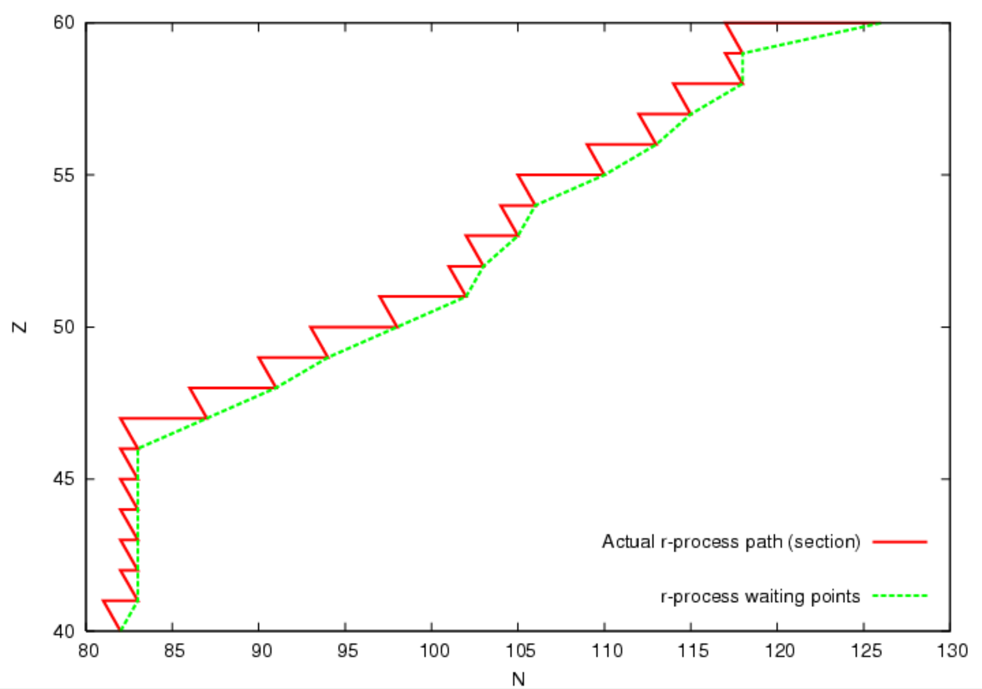

Z
N
Unstable nuclei
Stable nuclei
p-drip line (HFB-14)
n-drip line (HFB-14)
Typical r-process path
0
20
40
60
80
100
120
0
50
100
150
200
250

Fig. 1.5.


Z
N
Actual r-process path (section)
r-process waiting points
40
45
50
55
60
80
85
90
95
100
105
110
115
120
125
130

Mass dependence of r-process

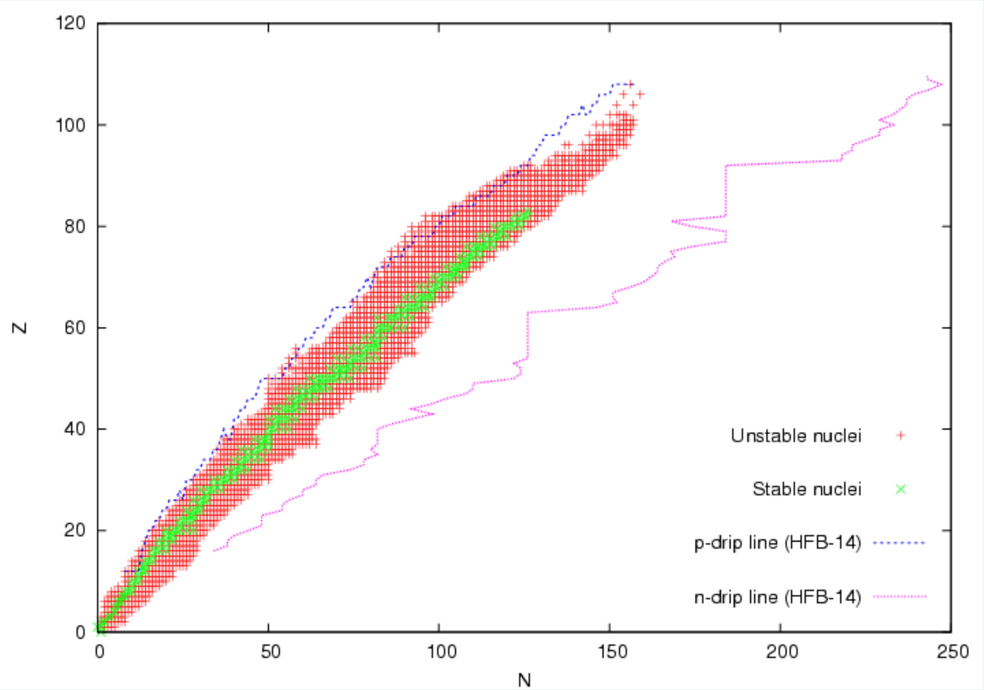
$$S_n = M_{at}(N-1, Z) - M_{at}(N, Z) + M_n$$

$$Q_\beta = M_{at}(N, Z) - M_{at}(N-1, Z+1)$$

only differential quantities

absolute masses not required

Fig. 1.3.


Unstable nuclei
Stable nuclei
p-drip line (HFB-14)
n-drip line (HFB-14)
Z
N
0
20
40
60
80
100
120
0
50
100
150
200
250

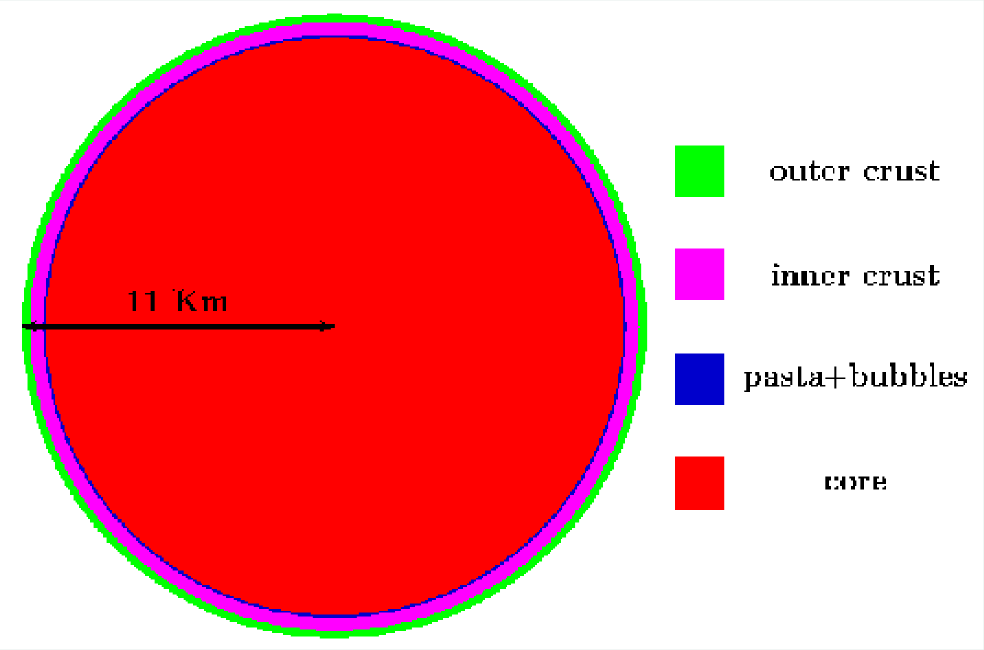

11 Km
outer crust
inner crust
pasta+bubbles
core

Fig. 1.6.

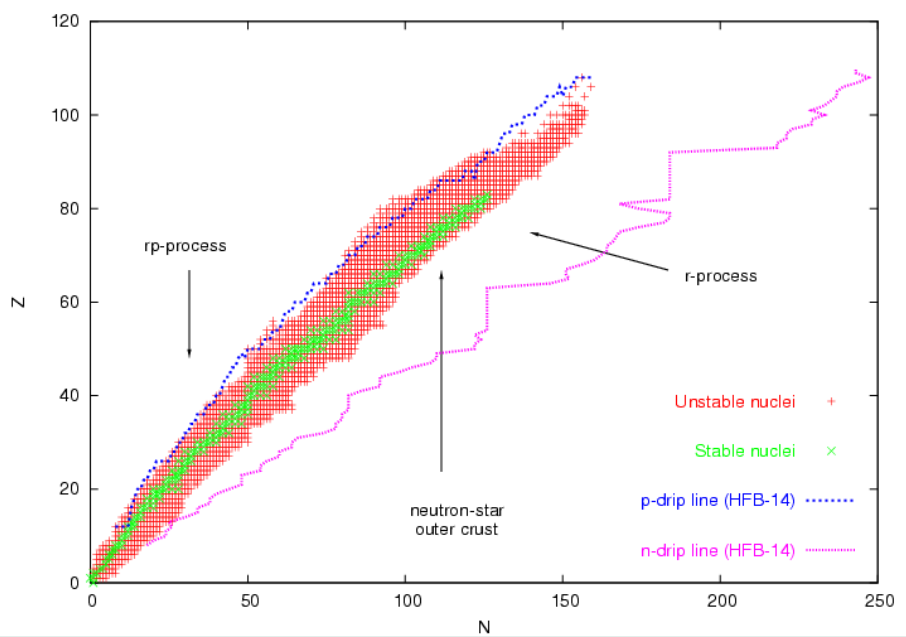
Outer crust. $\simeq$ 300 meters thick. $0 < \rho < 1.2 \times 10^{-3}\, \rho_0$
– n-rich nuclei (+ electrons); within neutron drip line.
Composition depends only on S_n and Q_β: **absolute masses again not required.**

Inner crust. $\simeq$ 500 meters thick. $1.2 \times 10^{-3}\, \rho_0 < \rho < 0.4\, \rho_0$
– nuclear clusters (+ electrons) floating in neutron vapour; beyond neutron drip line (**EOS sensitive to mass fit).**

Core. 10 km radius (roughly). ρ up to about $4\, \rho_0$
– homogeneous gas of n and p (+ electrons). About 97 % n at ρ around ρ_0; other particles (including possibly free quarks) towards center.

Electrical neutrality everywhere assured by electron gas: beta-equilibrated with nucleons.

Fig. 1.7.



Lack of data on n-rich side: serious problem for astrophysics.

Semi-empirical **global** mass models.
For reliable extrapolations into the unknown n-rich region underlying theory must be sound: not enough to have a good fit.

rp process. Very few holes in data on p-rich side; can rely on **local** models, of which best are those of AME (#), when available. Otherwise, Garvey-Kelson, etc.

I will talk only about semi-empirical global mass models.

Masses not the only nuclear quantity of astrophysical interest.

r-process, for example requires:

β-decay rates
Level densities
Fission barriers

Fission leads to high-A termination of r-process path (and subsequent recycling).

Fission also occurs during β-decay cascade back towards stability line.

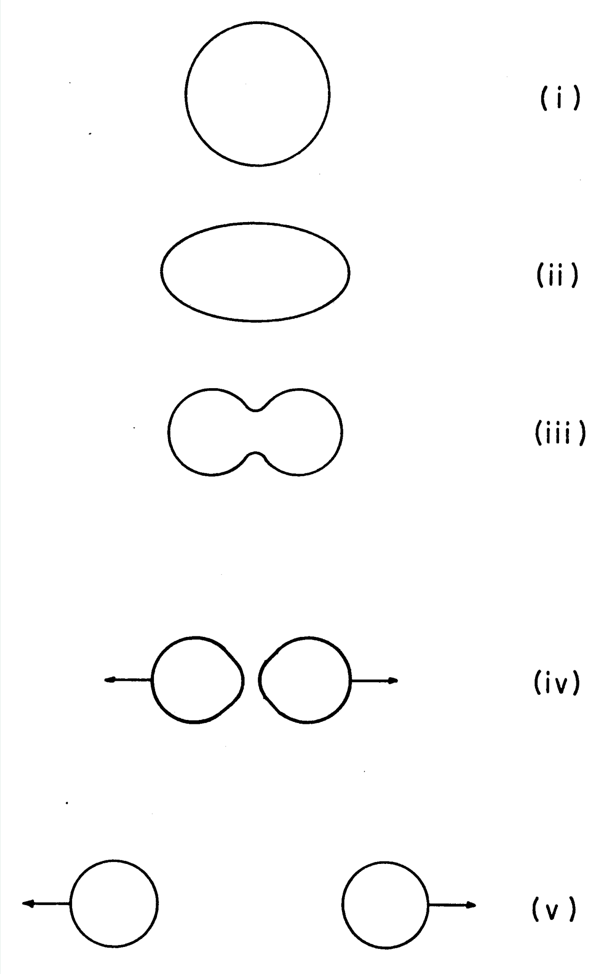


Fig. 1.8.

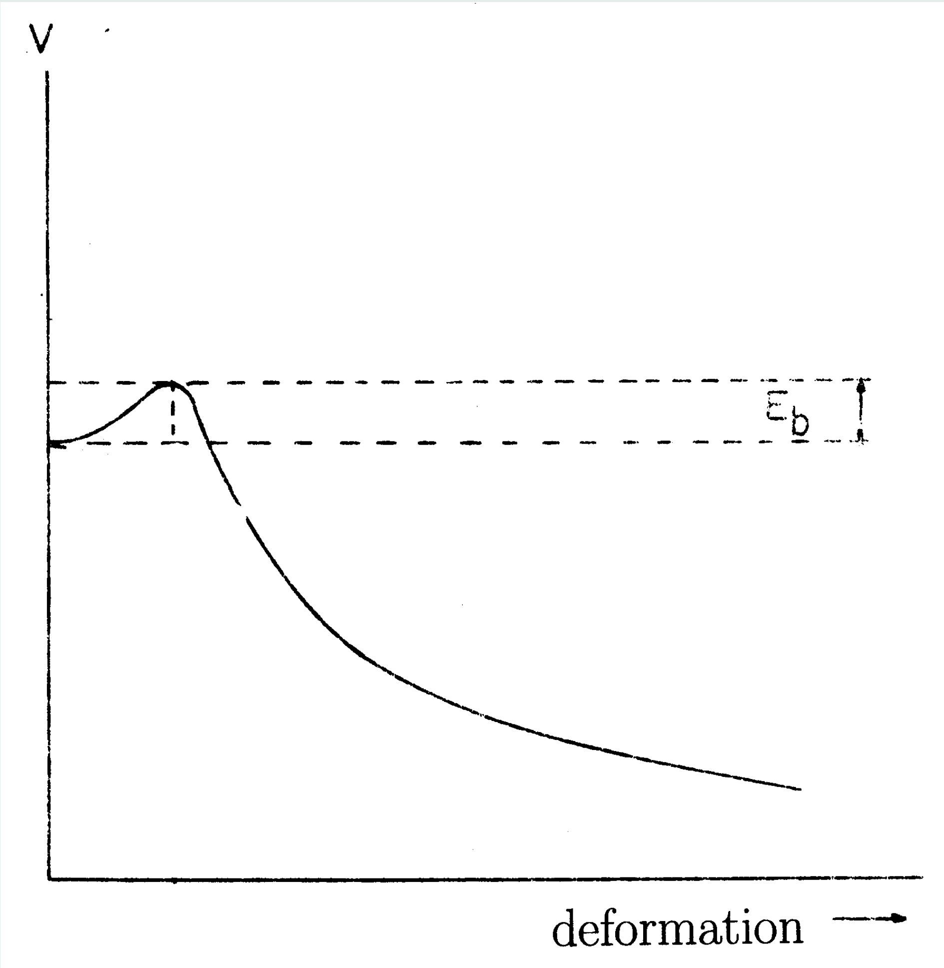


Fig. 1.9.

Any model of fission is automatically a mass model: energy calculated as function of deformation, so just look for minimum.

Converse is almost true: most mass models have been adapted, more or less successfully, to calculation of barriers.

Mass models relevant also for EOS of inner crust of neutron star (see Section 4)

Need a unified treatment: same model, with same parameters, for fission and masses – and for many other nuclear properties.

2. Semi-empirical mass formula

Weizsäcker(1935). Also Bethe and Bacher (1936).

$$E = a_{vol}A + a_{sf}A^{2/3} + \frac{3e^2}{5r_0}Z^2A^{-1/3} + \left(a_{sym}A + a_{ss}A^{2/3}\right)I^2 + \Delta_n + \Delta_p$$

$\Delta_{n,p} = \pm\delta$ as N, Z even or odd.

(rms charge radius given by $R_{ch} = r_0 A^{1/3}$)

$$I = \frac{N - Z}{A}$$

a_{ss} term is due to Myers and Swiatecki (1966).

Fit the six parameters to all 2149 measured masses for $N, Z \geq 8$ given in 2003 AME.

$$a_{vol} = \text{-}15.697550 \text{ MeV} \qquad a_{sf} = 17.662690 \text{ MeV}$$

$$a_{sym} = 26.308165 \text{ MeV} \qquad a_{ss} = \text{-}17.003132 \text{ MeV}$$

$$r_0 = 1.221897 \text{ fm} \qquad \delta = \text{-}1.250000 \text{ MeV}$$

$$e^2 = 1.43985 \text{ MeV.fm}$$

Mean deviations

$$\sigma = 2.75 \text{ MeV}, \qquad \bar{\epsilon} = 0.022 \text{ MeV}$$

$$\sigma(\delta\, \mathrm{E}/\mathrm{E}) = 0.4\%$$

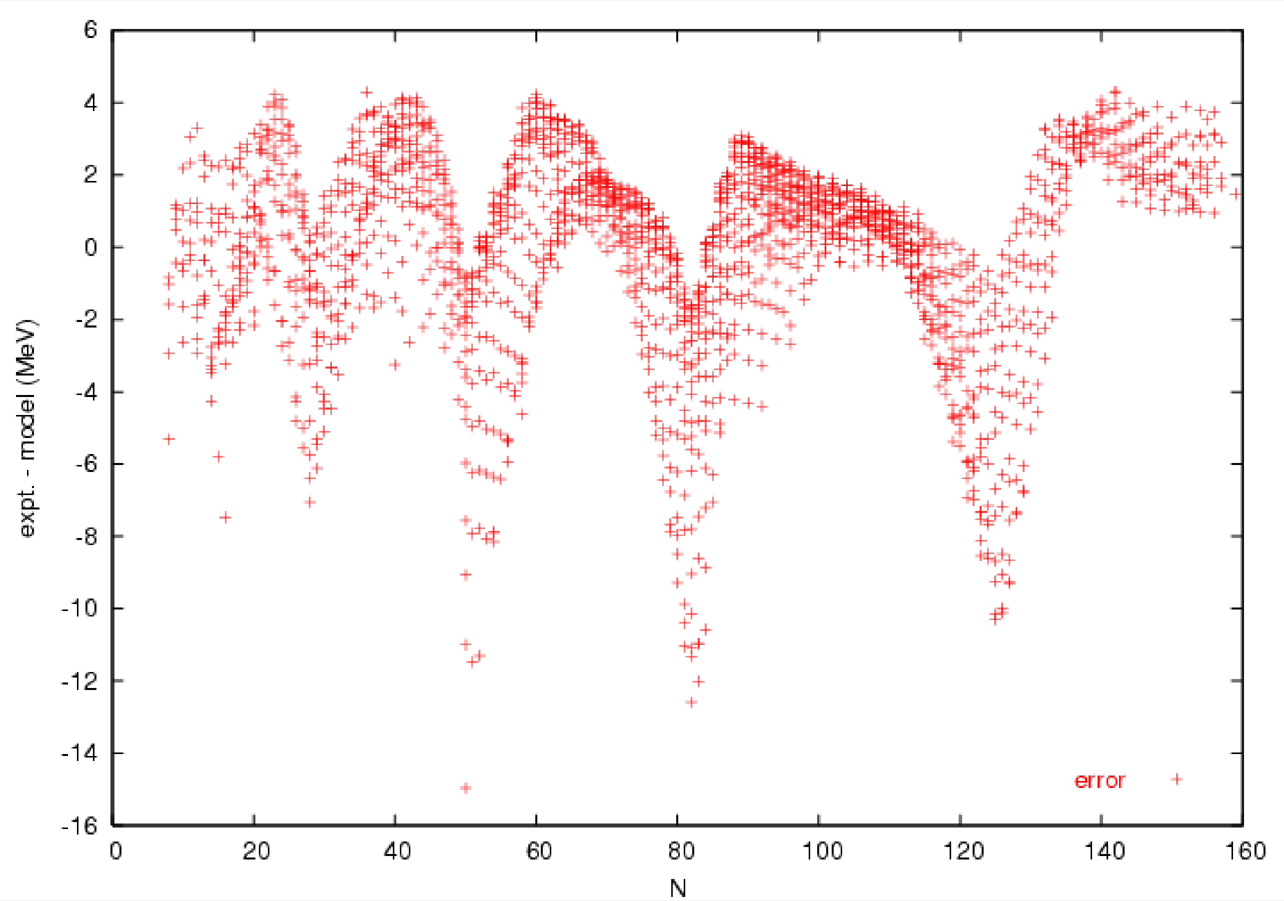


Fig. 2.1. Deviation of Weizsäcker formula from experiment.

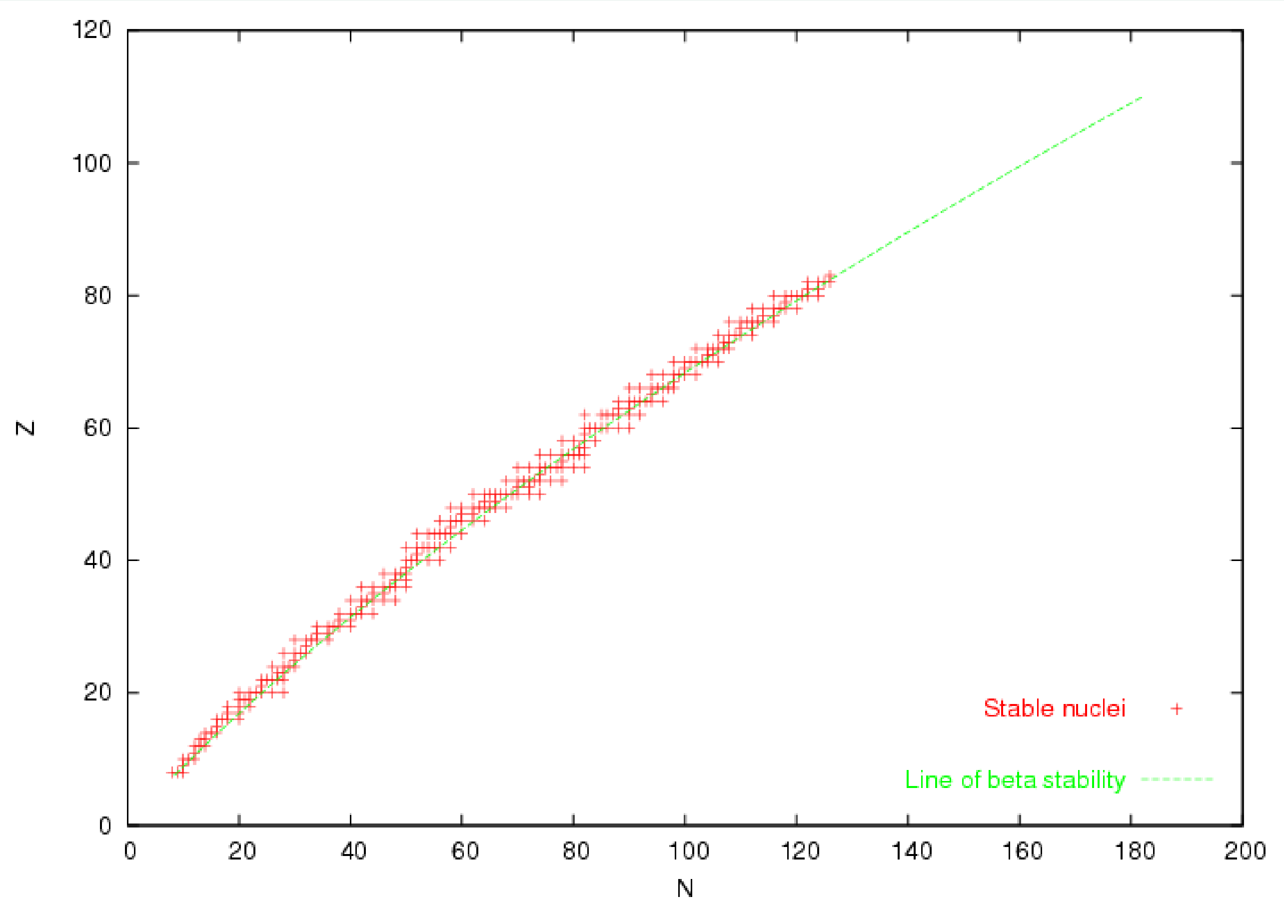


Fig. 2.2. Line of β stability for Weizsäcker formula.

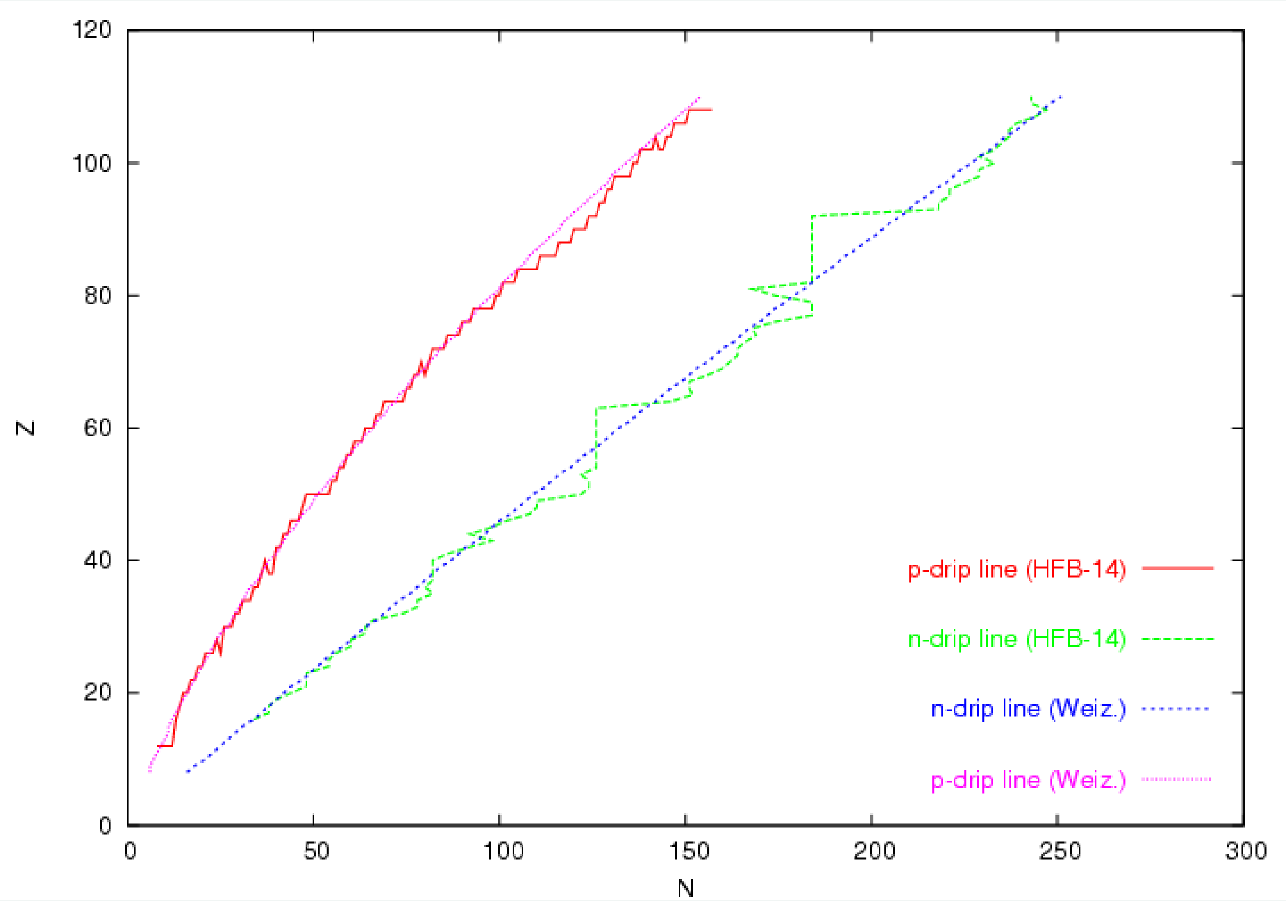


Fig. 2.3. Drip lines for Weizsäcker formula and HFB-14 model.

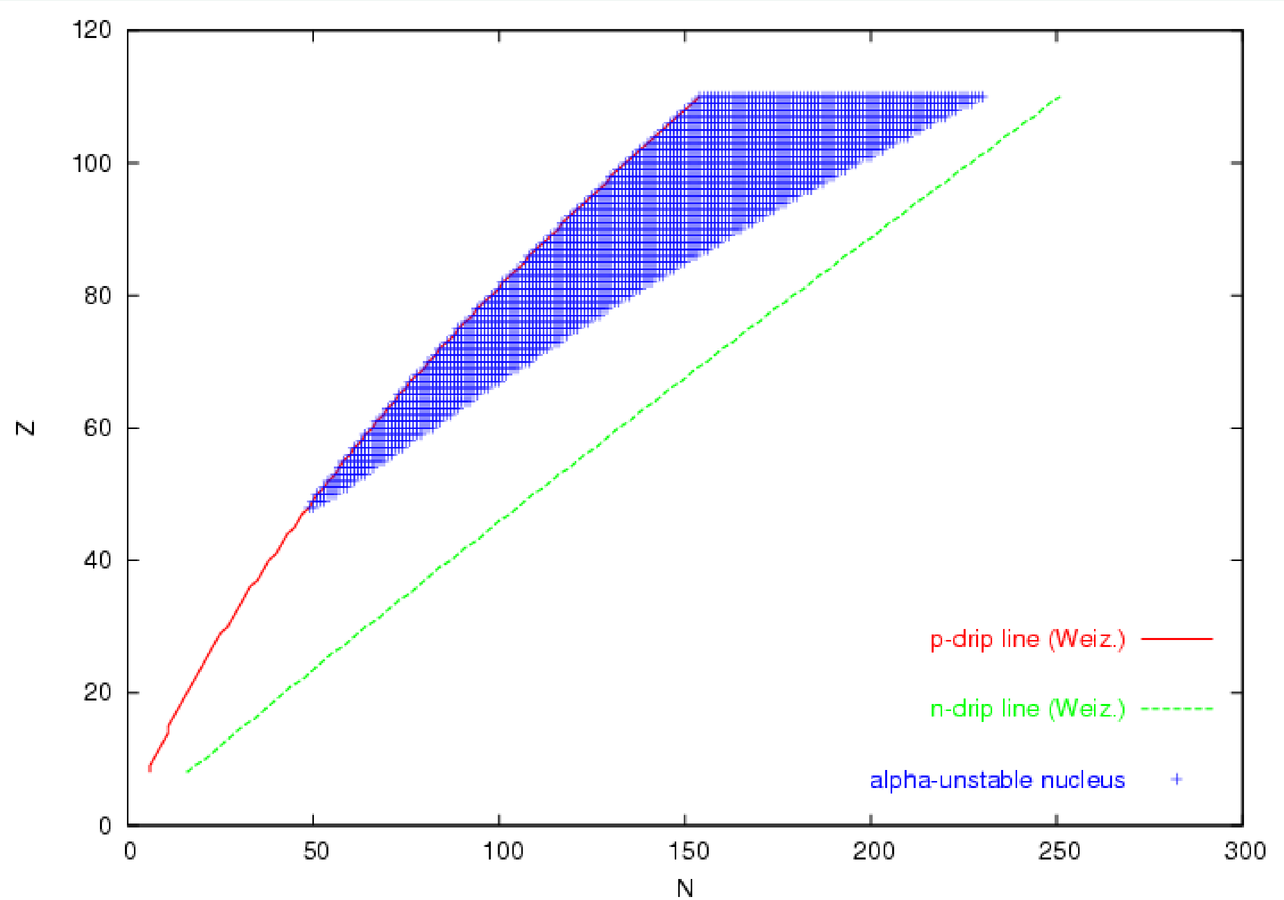


Fig. 2.4. α-unstable nuclei for Weizsäcker formula.

Home Page

Title Page

Contents

Page 27 of 109

Go Back

Full Screen

Close

Quit

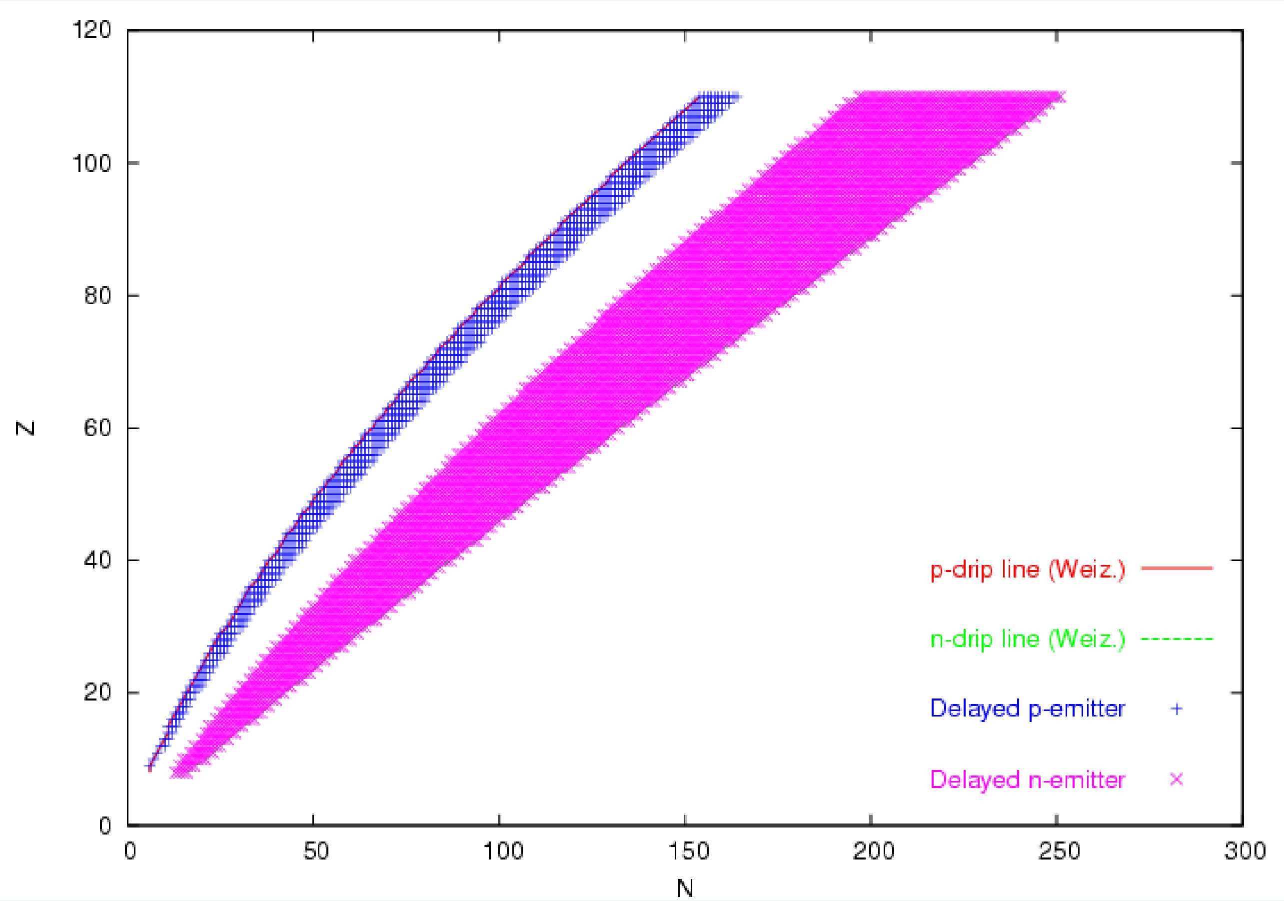


Fig. 2.5. Beta-delayed nucleon emitters for Weizsäcker formula.

Large A limit of Weizsäcker formula

$$e \equiv \frac{E}{A} = a_{vol} + a_{sf} A^{-1/3} + \frac{3e^2}{20r_0} A^{2/3}(1-I)^2 + (a_{sym} + a_{ss} A^{-1/3}) I^2$$

where $I = \frac{N-Z}{A}$.

Because of Coulomb term (non-saturating) this diverges unless $I = 1$, i.e., pure neutron system. So set $I = 1$:

$$e \sim a_{vol} + a_{sym} \quad ,$$

which is $\simeq +10.6$ MeV.

So large neutron systems are unbound?

But what about neutron stars?

- **They must be bound by gravity!**

So let's rederive the Weizsäcker formula, the way we did in kindergarten, except that this time we include gravity.

REMEMBER

Gravity is formally identical to Coulomb (but attractive): inverse-square and therefore non-saturating

$$E_G = \frac{3G\mathcal{M}^2}{5R} = \frac{3GM^2}{5r_0}A^{5/3}$$

$$e = a_{vol} + a_{sf}A^{-1/3} + \frac{3}{5r_0}\left\{\frac{e^2}{4}(1-I)^2 - GM^2\right\}A^{2/3} + (a_{sym} + a_{ss}A^{-1/3})I^2$$

For large A Coulomb repulsion dominates, unless pure neutron system. So set $I = 1$ again.

$$e \sim a_{vol} + a_{sym} - \frac{3GM^2}{5r_0} A^{2/3}$$

As A increases gravitational attraction becomes more and more important, and eventually will bind the system

$$e < 0$$

for

$$A > \left\{ \frac{5r_0}{3GM^2} (a_{vol} + a_{sym}) \right\}^{3/2} \approx 0.79 \times 10^{56}$$

$$A_{n.s.} \approx 1.6 \times 10^{57}$$

So Weizsäcker, modified for Newtonian gravity, gives us neutron stars to within a factor of 20:

neutron star is a giant nucleus.

Actually, our estimate for $A_{n.s.}$ is really a lower limit: minimum value for gravitational binding of star. Now sophisticated models of neutron stars also show minimum mass of around 0.1 $\mathcal{M}_\odot$, i.e.,

$$A_{n.s.}^{min} \approx 1.0 \times 10^{56}$$

below which the star is unstable (see, for example, Haensel *et al.* (2002), and references cited therein).

So the Weizsäcker estimate looks even better.

But don't get too excited:

1) Neutron stars are not pure neutron matter – there is some β-decay to p – e pairs

2) Central density $\rho_c \approx 4\rho_0$. So muons, and maybe even free quarks at center.

3) Must be treated in general relativity.

Nevertheless, there is something to learn from this:

Consider a binary pair of neutron stars, one of which is much lighter than the other. The lighter star will lose mass to the bigger star, and when its mass falls below the critical minimum mass there is a consensus that it will blow up.

Our analysis shows that it is the symmetry energy that blows the star up when the gravitational binding becomes inadequate.

Infinite nuclear matter (INM)

Hypothetical system, large-A limit of nuclei with electric charge switched off.

Beloved by nuclear theoreticians because of its *relative* simplicity: translational invariance.

Properties can be inferred from Weizsäcker formula:

$$e = a_{vol} + a_{sym} I^2 \quad \text{where } I = \frac{N-Z}{A}$$

$$\rho_0 = 1/(\tfrac{4\pi}{3} r_0^3) \qquad\qquad (\text{for } I = 0)$$

3. The fundamentalist's approach

i.e., the nuclear many-body problem

the basic problem of nuclear theory

$$H\Psi = E\Psi$$

where

$$H = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i>j} V_{ij} + \sum_{i>j>k} V_{ijk}$$

V_{ij} – fitted to N-N scattering and d

V_{ijk} – fitted to t, h, and (in principle) $N-d$ scattering

Also accept guidance from meson theory or QCD.

Solution of this Schrödinger equation very difficult because of

a) Strong short-range repulsion

b) Tensor coupling $^3S_1 - ^3D_1$

Infinite nuclear matter (INM): simplest many-body system

50 years after the first calculations of Brueckner fairly satisfactory results are being obtained with the v_{18} Argonne N-N force and various N-N-N forces:

Akmal *et al.* (1998): variational methods

Zuo *et al.* (2002a, b): Brueckner-Bethe-Goldstone methods

Note the importance of N-N-N forces for correct saturation.

Success of INM calculations a triumph for nuclear theory.

For astrophysics main interest lies in being able to calculate pure neutron matter ($\mathrm{I} = 1$) as a function of density.

Note that the Schrödinger equation that is solved, and the entire theory, is non-relativistic.

There is also a fully relativistic ("Dirac-Brueckner") theory, which claims to dispense with the need for N-N-N term, but this has been contested (Zuo *et al.* (2002a).

Finite nuclei

Above methods cannot give anything like the accuracy required for astrophysics.

Most promising approach is Green's function Monte Carlo method, but at present can't go beyond ^{12}C (see Barrett *et al.* (2003) for a review).

So the fundamentalist, or *ab initio*, approach really doesn't meet the needs of astrophysicists (except for neutron matter).

We are forced back to a semi-empirical approach.

Two possibilities for viable semi-empirical mass models:

either

simplify the many-body problem – keep Ψ

Hartree-Fock models
Relativistic mean-field method

or

refine the Weizsäcker formula – no Ψ

Macroscopic-microscopic models

4. Hartree-Fock-Bogoliubov model

Exact many-body problem

$$H\Psi = E\Psi$$

where

$$H = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i>j} V_{ij} + \sum_{i>j>k} V_{ijk}$$

Since we can't solve this Schrödinger equation with anything like the required accuracy we try to solve an easier one:

accept guidance from success of the shell model

Shell-model Hamiltonian is

$$H_0 = \sum_{i=1}^{A} h(x_i)$$

– each term is function only of coordinates of nucleon i. Solution is product

$$\Phi(x_1, x_2, \ldots, x_A) = \prod_{i=1}^{A} \phi_i(x_i) \quad ,$$

where

$$h(x_i)\phi_i(x_i) = \epsilon_i \phi_i(x_i) \quad .$$

Then

$$H_0\Phi = E_0\Phi \quad ,$$

where

$$E_0 = \sum_{i=1}^{A} \epsilon_i$$

antisymmetrization of Φ: product replaced by Slater determinant

$$\Phi = \det\{\phi_i(x_i)\}$$

If no antisymmetrization, i.e., for

$$\Phi(x_1, x_2, \ldots, x_A) = \prod_{i=1}^{A} \phi_i(x_i) \quad ,$$

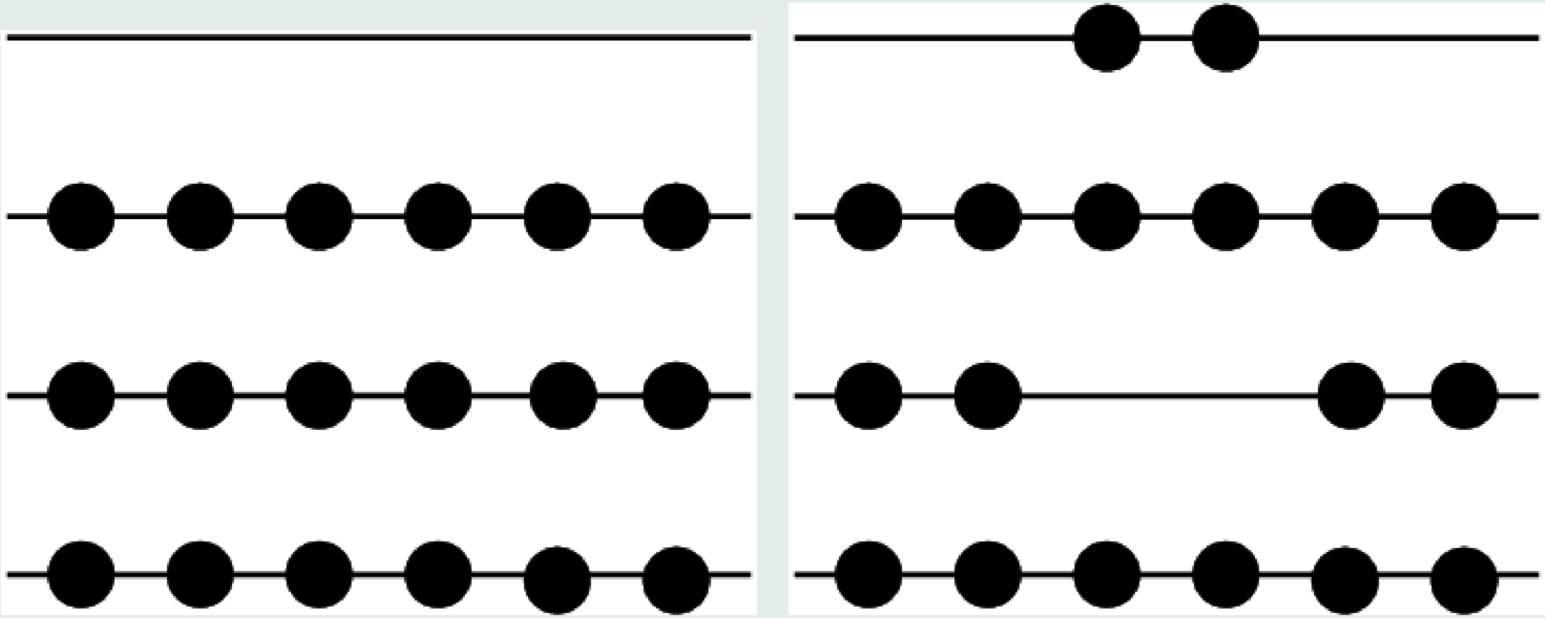
no correlations:

$$P(x_1, x_2) = P(x_1)P(x_2)$$

independent-particle motion

Pauli-principle correlations, but why no correlations associated with known strong short-range repulsion?

Understanding success of shell model was one of the big problems of nuclear physics in the 1950s.



Weisskopf: Pauli principle suppresses correlations associated with short-range repulsion.

Shell-model wavefunction Φ is valid *over a large fraction of nuclear volume.*

Hartree-Fock:

variational method using shell-model functions as trial functions:

$$E =< \Phi|H|\Phi >$$

where

$$\Phi = \det\{\phi_i(x_i)\}$$

Minimize E w.r.t. arbitrary $\delta\phi_i$

But what is H?

If we take the real Hamiltonian

$$H = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i>j} V_{ij} + \sum_{i>j>k} V_{ijk}$$

we will be in trouble.

Must modify Hamiltonian to take account of short-range correlations in wavefunction.

$$H^{eff} = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i>j} v_{ij}^{eff}$$

Ultimately, we might hope to deduce v_{ij}^{eff} from real forces, but that is just the many-body problem for a finite nucleus.

Solution to that problem (at least with required accuracy) lies in the distant future, and we want a mass model **NOW**.

So back to the semi-empirical approach:

take a suitable form of force and fit its parameters to the mass data, just like Weizsäcker did.

Only the non-relativistic approach has been developed to the required degree of accuracy. The method of the Relativistic Mean Field is promising, but at present is not sufficiently accurate.

Skyrme force 10 parameters

$$
\begin{aligned}
v_{ij} = & \ t_0(1 + x_0 P_\sigma)\delta(\mathbf{r}_{ij}) \\
& + t_1(1 + x_1 P_\sigma)\frac{1}{2\hbar^2}\{p_{ij}^2 \delta(\mathbf{r}_{ij}) + h.c.\} \\
& + t_2(1 + x_2 P_\sigma)\frac{1}{\hbar^2}\mathbf{p}_{ij}.\delta(\mathbf{r}_{ij})\mathbf{p}_{ij} \\
& + \frac{1}{6} t_3(1 + x_3 P_\sigma)\rho^\alpha \delta(\mathbf{r}_{ij}) \\
& + \frac{i}{\hbar^2} W_0(\boldsymbol{\sigma_i} + \boldsymbol{\sigma_j}).\mathbf{p}_{ij} \times \delta(\mathbf{r}_{ij})\mathbf{p}_{ij}
\end{aligned}
$$

This is the choice for the HFB mass models of the B-M group: see, for example, Samyn *et al.* (2004); also Lunney *et al.* (2003).

Implementation of pure HF

$$E = < \Phi | H^{eff} | \Phi >$$

where

$$\Phi = \det\{\phi_i\}$$

Variational principle

$$\frac{\delta E}{\delta \phi_i} = 0$$

for all ϕ_i

Leads to **HF equation** for each s.p. function ϕ

$$\left\{-\boldsymbol{\nabla}\cdot\frac{\hbar^2}{2M^*(\mathbf{r})}\boldsymbol{\nabla}+U(\mathbf{r})-i\mathbf{W}(\mathbf{r})\cdot\boldsymbol{\nabla}\times\boldsymbol{\sigma}\right\}\phi_i=\epsilon_i\phi_i$$

M^*, U, and W all depend on densities and thus on solutions ϕ.

Thus this s.p. Schrödinger equation has to be solved by successive reiterations until self-consistency is achieved.

Pairing

We observe that:

- even-even nuclei energetically favoured
  – see Weizsäcker formula.
- ground state of e-e nuclei is always $J = 0$.

We infer that:

energetically favourable for **like** valence nucleons to pair off to zero net ang. momentum.

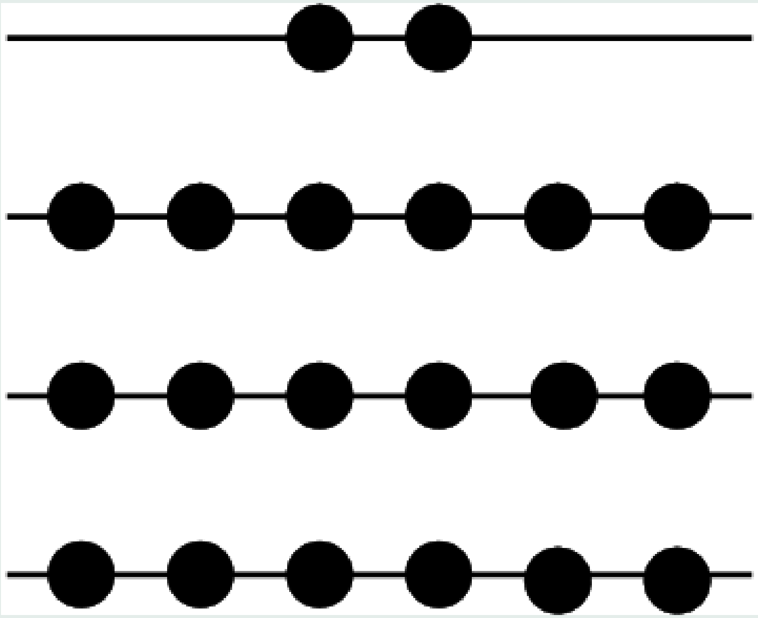
This is a correlation - cannot be accounted for within framework of pure HF.

Another problem:

In pure HF only doubly magic nuclei are spherical – it is pairing of like valence nucleons that keeps nuclei spherical, until sudden collapse (phase transition) to deformed shape close as mid-shell is approached.

How do pairing correlations arise?

What has happened to the Pauli-principle argument that accounts for validity of shell model?



Pauli principle no longer blocks scattering of *valence* nucleons.

Also interaction through coupling of two nucleons to surface phonon.

Hartree-Fock-Bogoliubov method:

introduces pairing correlations into variational function
– pairing and mean field treated on same footing.

Choice of pairing force in B-M collaboration:

$$v_{pair}(\boldsymbol{r}_{ij}) = V_{\pi q}\delta(\boldsymbol{r}_{ij})$$

BCS approximation

much simpler: HF and pairing decoupled, with pairing calculation done at the end of each HF iteration
– but not as reliable as HFB for neutron-rich nuclei

Wigner terms

If Skyrme and pairing forces are only ingredients then serious underbinding (≈ 2 MeV) for $N = Z$.

Two possible sources:

i) n-p $T = 0$ pairing. Attractive, strongly peaked at $N = Z$.

ii) Wigner supermultiplet theory. In real nucleus isospin T conserved (approximately).
Ground state: $T = |T_z| = |N - Z|$.
Wigner (1937): there should be an energy term $T(T + 1)$ - positive. In g. s. we have

$$T(T + 1) = (N - Z)^2 + |N - Z|$$

HF misses this, but $(N - Z)^2$ gets absorbed into the fitted force. However, $|N - Z|$ gives rise to sharp cusp that cannot be so absorbed. Thus such a term has to be added to HFB energy.

In the B-M collaboration we represent the two together by

$$E_W = V_W \exp\left\{-\lambda\left(\frac{N-Z}{A}\right)^2\right\}$$
$$+V'_W|N-Z|\exp\left\{-\left(\frac{A}{A_0}\right)^2\right\}$$

Isospin is a good quantum number only for light nuclei, so we put in exponential damping w. r. t. A in second term.

Fits always give $A_0 \approx 30$.

First term is more important.

Miscellania

- Rotational correction

Total angular momentum is not conserved in non-spherical self-consistent field. For g.s. we have $J = 0$ for even-even nuclei. Thus we have to subtract spurious rotational energy

$$E_{rot} = \frac{<\hat{J}^2>}{2\mathcal{I}}$$

where $\mathcal{I}$ is moment of inertia. In the B-M collaboration this contains two parameters that are fitted to masses.

- Vibrational correction

So far we have assumed that *shape* of self-consistent field is time-independent, although we allow deformed fields to rotate.

But this is unduly restrictive: vibrations. Effect is to *lower* g.s. energy - extra degree of freedom in variational function.

In models HFB-1 to HFB-13 we neglected this effect, without any serious consequence to masses – all nuclei are affected, and thus the effect is absorbed into the force on fitting to data.

However, with this procedure, i.e., without any *explicit* vibrational correction, we find that we underestimate height of high barriers, which always lie at high deformation. Now vibrational correction is known to become smaller at high deformations, which means that we were subtracting too much vibrational energy at large deformations.

Model HFB-14: 3-parameter phenomenological term that compensates for the vibrational over-correction at large deformations. See Goriely *et al.* (2007).

- Odd nuclei

In the models of the B-M collaboration we make some special approximations for these nuclei.

HF states for odd nucleons are not eigenstates of the time-reversal operator. In principle we should project out states of good time-reversal properties, which lowers the energy.

We do not do this, and compensate for the lost binding in odd nuclei by making the pairing force stronger in these nuclei than in even-even nuclei.

- Neutron matter

Beginning with model HFB-9 of the B-M collaboration, we impose a fit not only to the mass data, but also to the properties of neutron matter, as calculated from realistic N-N and N-N-N forces.

This leads to a slight deterioration in the quality of the fit to the mass data, but should improve the reliability of the mass predictions for highly neutron-rich nuclei.

Moreover, such forces are well adapted to the calculation of the EOS of the inner crust of neutron stars with the HFB method (or approximations thereto):

in addition to well representing the highly neutron-rich environment, the mass fit takes into account

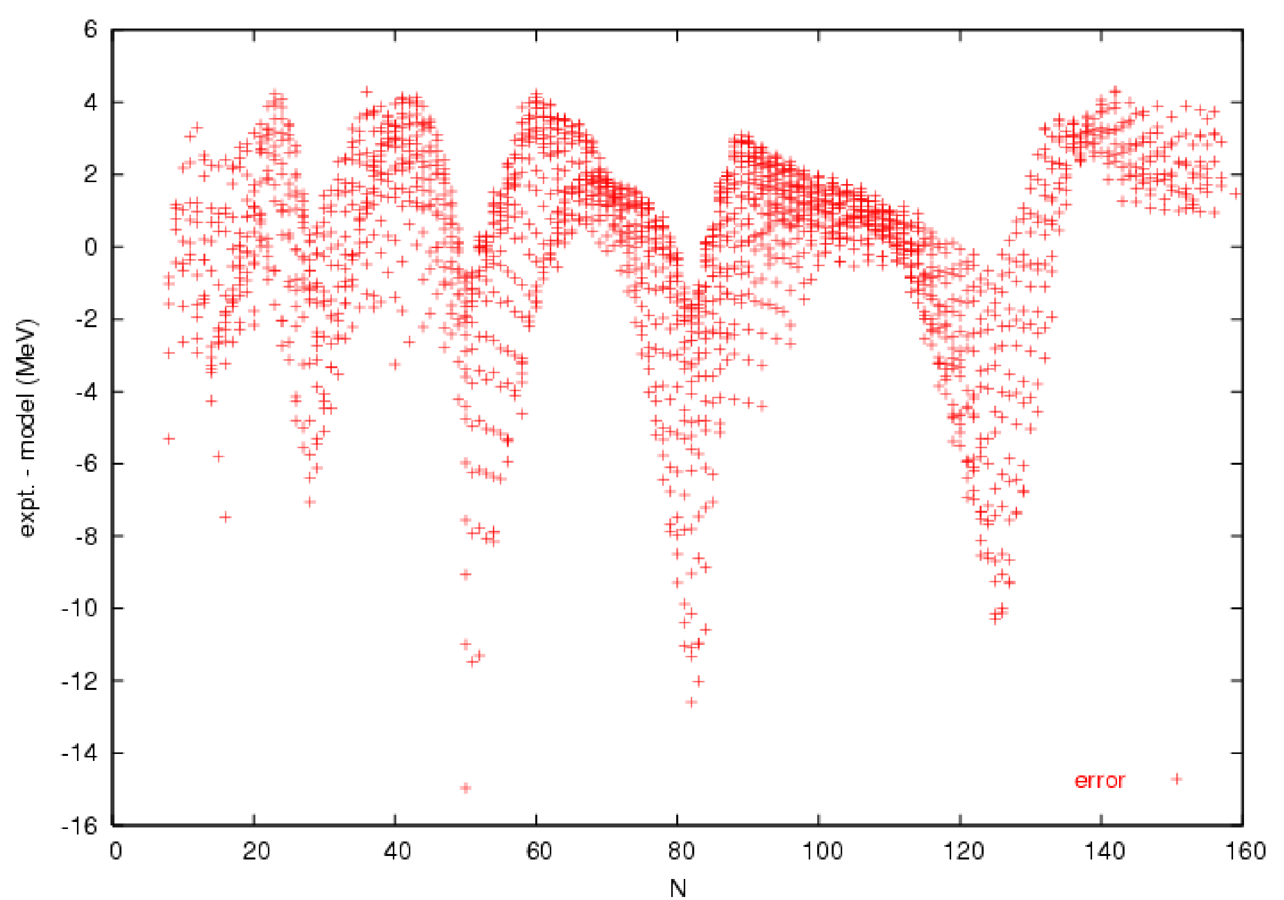
i) presence of protons
ii) inhomogeneities

5. Macroscopic-microscopic models: the FRDM and FRLDM

Recall Weizsäcker formula

$$E = a_{vol}A + a_{sf}A^{2/3} + \frac{3e^2}{5r_0}Z^2A^{-1/3} + \left(a_{sym}A + a_{ss}A^{2/3}\right)I^2 + \Delta_n + \Delta_p$$

Most obvious defect is lack of shell corrections.


6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
expt. - model (MeV)
0
20
40
60
80
100
120
140
160
N
error

Finite-Range Droplet Model

–preferred model of experimentalists when presenting new mass measurements

Möller *et al.* (1995)

But this same paper also presents the

Finite-Range Liquid-Drop Model

FRDM is more sophisticated – better fit to masses

but has serious problems for barriers

$$E = E_{mac} + E_{mic}$$

E_{mac}: refined version of Weizsäcker's liquid drop

E_{mic}: shell + pairing + Wigner terms

Total energy E minimized wrt deformations.

FRDM and FRLDM differ in macro. part; identical micro. parts (determined in FRDM fit).

Finite-Range Liquid-Drop Model – macro. term

$$E = a_{vol}A + a_1 B_1 A^{2/3} + \frac{3e^2}{5r_0} B_3 Z^2 A^{-1/3} + \left(a_{sym}A + a_{ss}B_1 A^{2/3}\right) I^2 + \cdots$$

B_1 and B_3 intended to take care of deformations.

N. B. $a_1 \neq a_{sf}$

Surface energy is manifestation of *finite range* of forces.

Deformation dependence of surface taken into account by folding finite-range force over nuclear volume:

$$B_1 = \frac{A^{-2/3}}{8\pi^2 r_0^2 a^4} \int \int \left(2 - \frac{|\boldsymbol{r} - \boldsymbol{r}'|}{a}\right) \frac{\exp(-|\boldsymbol{r} - \boldsymbol{r}'|/a)}{|\boldsymbol{r} - \boldsymbol{r}'|/a} d^3\boldsymbol{r}\, d^3\boldsymbol{r}'$$

- force is difference of a Yukawa and an exponential term.

Likewise, Coulomb energy for arbitrary shape determined by folding Coulomb force over nuclear volume.

$$B_3 = \frac{15\, A^{-5/3}}{32\pi^2 r_0^5} \int\int \frac{d^3\boldsymbol{r} d^3\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|} \times \left[1 - \left(1 + \frac{|\boldsymbol{r}-\boldsymbol{r}'|}{2a_{den}}\right) \exp(-|\boldsymbol{r}-\boldsymbol{r}'|/a_{den})\right]$$

a_{den} represents diffusivity of nuclear surface

Finite-Range Droplet Model – macro. term

Replacement of liquid-drop by so-called **droplet** model

Myers and Swiatecki (1969, 1974)
Treiner *et al.* (1986)
Möller *et al.* (1995)

Retain the basic idea of the Weizsäcker liquid drop:

$$E_{mac} = E_{vol} + E_{sf} + E_{coul}$$

– but much more complicated.

Assume spherical shape at first.

Droplet is compressible: can be squeezed by surface tension and dilated by Coulomb repulsion. This is first new degree of freedom introduced by droplet model.

$$\epsilon = (\rho_0 - \rho)/3\rho_0,$$

ρ_0 equilibrium density of symmetric INM – this is density appearing in Weizsäcker model.

$$\begin{aligned} E_{vol}/A &\equiv e_\infty(\rho,\delta) \\ &= a_{vol} + \frac{1}{2}K_{vol}\epsilon^2 + \left(a_{sym} - L\epsilon\right)\delta^2 + \ldots \end{aligned}$$

$$\delta = (\rho_n - \rho_p)/\rho$$

$$\rho_{eq} = \rho_0 \left\{1 - (3L/K_{vol})\delta^2\right\} \quad .$$

All these densities assumed to be uniform throughout bulk of nucleus

$$\rho_{n,p} \equiv \rho_{n,p}^{bulk}$$

But densities on surface, ρ_n^s, etc., are allowed to be different,

$$\delta \equiv (\rho_n - \rho_p)/\rho \neq I \equiv \frac{N-Z}{A}$$

Droplet model treats all departures from uniformity as surface effects

Surface

neglect asymmetry effects at first

$$E_{sf} = 4\pi\, R^2 \sigma$$

But

$$(4\pi/3)\rho\, R^3 = A$$

and

$$\begin{aligned} \rho &= \rho_0(1-3\epsilon) \\ &= \frac{3}{4\pi\, r_0^3}(1-3\epsilon) \end{aligned}$$

Then

$$\begin{aligned} E_{sf} &= 4\pi\, r_0^2\,(1-3\epsilon)^{-2/3}\sigma\, A^{2/3} \\ &= (1-3\epsilon)^{-2/3} a_{sf} A^{2/3} \end{aligned}$$

Surface-symmetry effects:

possible dependence of E_{sf} on neutron excess I.

Shown implicitly by Myers and Swiatecki (1969), and explicitly by Treiner and Krivine (1986), that such a dependence can arise only if a neutron skin is formed, i.e., different equivalent sharp radii R_n and R_p for n and p, respectively

$$(4\pi/3)\rho_n R_n^3 = N$$

$$(4\pi/3)\rho_p R_p^3 = Z$$

Then

$$R_{n,p} \approx r_0 A^{1/3}\{1 + \epsilon \pm \frac{1}{3}(I - \delta) + \ldots\}$$

and neutron-skin thickness is

$$\tau \equiv R_n - R_p = \frac{2}{3} r_0 (I - \delta) A^{1/3} + \ldots$$

Droplet model allows neutron and proton surfaces to separate, i.e., permits formation of neutron skin. This is the second new degree of freedom introduced by droplet model.

Because of charge symmetry take dependence of E_{sf} on τ to be quadratic:

$$\begin{aligned} E_{sf} &= 4\pi R^2 \left\{ \sigma + \frac{Q}{4\pi r_0^2} \left(\frac{\tau}{r_0} \right)^2 \right\} \\ &\approx (1+2\epsilon) a_{sf} A^{2/3} + \frac{4}{9} Q (I-\delta)^2 A^{4/3} \end{aligned}$$

Q: surface-stiffness coefficient

Take now for Coulomb energy

$$E_{coul} = \frac{3}{5}\frac{e^2 Z^2}{R_p}$$

where

$$R_p \approx r_0 A^{1/3}\{1 + \epsilon - \frac{1}{3}(I - \delta) + \ldots\}$$

Minimize

$$E_{mac} = E_{vol} + E_{sf} + E_{coul}$$

w.r.t. δ and ϵ. We find

$$\delta = \frac{I + (9e^2/40r_0 Q)Z^2 A^{-5/3}}{1 + (9a_{sym}/4Q)A^{-1/3}}$$

and

$$\epsilon = \frac{-2a_{sf}A^{-1/3} + L\delta^2 + (3e^2/5r_0)Z^2 A^{-4/3}}{K_{vol}}$$

Substitute these values of δ and ϵ into expressions for E_{vol}, E_{sf} and E_{coul}:

$$
\begin{aligned}
E_{mac} = & \left(a_{vol} + a_{sym}\delta^2 - \frac{1}{2}K_{vol}\epsilon^2\right)A \\
& + \left(a_{sf} + \frac{9a_{sym}^2}{4Q}\delta^2\right)A^{2/3} \\
& + \frac{3e^2}{5r_0}Z^2A^{-1/3} - \frac{9e^4}{400r_0^2Q}Z^4A^{-2}
\end{aligned}
$$

holds only for equilibrium

Extract from Eq. (40) of Möller *et al.* (1995)

$E_{\mathrm{mac}}(Z, N, \mathrm{shape}) =$

$M_{\mathrm{H}} Z + M_{\mathrm{n}} N$	mass excesses of Z hydrogen atoms and N neutrons
$+ \left(-a_1 + J\bar{\delta}^2 - \frac{1}{2} K \bar{\epsilon}^2\right) A$	volume energy
$+ \left(a_2 B_1 + \frac{9}{4} \frac{J^2}{Q} \bar{\delta}^2 \frac{B_s^2}{B_1}\right) A^{2/3}$	surface energy
$+ a_3 A^{1/3} B_k$	curvature energy
$+ a_0 A^0$	A^0 energy
$+ c_1 \frac{Z^2}{A^{1/3}} B_3$	Coulomb energy
$- c_2 Z^2 A^{1/3} B_r$	volume redistribution energy
$- c_4 \frac{Z^{4/3}}{A^{1/3}}$	Coulomb exchange correction
$- c_5 Z^2 \frac{B_w B_s}{B_1}$	surface redistribution energy
$+ f_0 \frac{Z^2}{A}$	proton form-factor correction to the Coulomb energy
$- c_a (N - Z)$	charge-asymmetry energy

Exponential compressibility term

$$\epsilon = \frac{-2a_{sf}A^{-1/3} + L\delta^2 + (3e^2/5r_0)Z^2A^{-4/3}}{K_{vol}}$$

If we neglect asymmetry and Coulomb effects density rises monotonically as A decreases – natural consequence of surface tension.

But HF and TF calculations all show that density goes through a maximum for A around 60

$$E_{mac} = E_{vol} + E_{sf} + E_{coul} - CA\exp(-\gamma A^{1/3})\epsilon$$

Expression for ϵ is modified,

$$\epsilon = \frac{C\exp(-\gamma A^{1/3}) - 2a_{sf}A^{-1/3} + L\delta^2 + (3e^2/5r_0)Z^2A^{-4/3}}{K_{vol}},$$

but new term does not appear explicitly in E_{mac} at equilibrium

Deformations

As in FRLDM most terms multiplied by deformation-dependent $B-$factors

– but not the exponential compressibility term.

That is why the model cannot be used for large deformations, and in particular for fission.

(Some other problematical terms also.)

Such problems do not arise with Hartree-Fock, or even in its semi-classical approximations.

Microscopic Corrections

Derived for FRDM, carried over into FRLDM.

Microscopic term 1: shell corrections

Strutinsky theorem:

$$E = E_{mac} + E_{sc} \quad ,$$

where

$$E_{sc} = \sum_i n_i \epsilon_i - \widetilde{\sum_i n_i \epsilon_i} \quad .$$

ϵ_i: s.p. energies

n_i: occupation probabilities

second term: smoothed version of first

For s.p. energies need to have a s.p. field U that is related, in the interest of self-consistency, to macro. term

$$U = V_1 + V_{s.o.} + V_{coul}$$

where

$$V_1(\boldsymbol{r}) = -\frac{V_0^q}{4\pi a_{pot}^3} \int \frac{\exp(-|\boldsymbol{r} - \boldsymbol{r'}|/a_{pot})}{|\boldsymbol{r} - \boldsymbol{r'}|/a_{pot}} d^3\boldsymbol{r'}$$

Requirement of consistency between macro. and micro. parts is only partially satisfied.

Also

$$V_{s.o.}(\boldsymbol{r}, \boldsymbol{p}) = -\lambda^q \frac{\hbar}{4M^2c^2} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} V_1(\boldsymbol{r}) \times \boldsymbol{p}$$

Implementation of Strutinsky theorem

$$E_{sc} = \sum_i n_i \epsilon_i - \widetilde{\sum_i n_i \epsilon_i}$$

How to smooth?

$$\sum_i n_i \epsilon_i = \int_{-\infty}^{\infty} \epsilon g(\epsilon)\, d\epsilon$$

where we have introduced spectral function

$$g(\epsilon) = \sum_i n_i \delta(\epsilon - \epsilon_i)$$

Then

$$\widetilde{\sum_i n_i \epsilon_i} = \int_{-\infty}^{\infty} \epsilon \tilde{g}(\epsilon)\, d\epsilon$$

$$\delta(\epsilon - \epsilon_i) \rightarrow \frac{1}{\gamma\sqrt{\pi}} \exp\left\{-(\epsilon - \epsilon_i)^2/\gamma^2\right\}$$

"plateau condition":

results should be independent of smoothing parameter γ

not always satisfied

Microscopic term 2: Pairing corrections

- Constant-G scheme (“seniority” force)
- BCS approximation
- Lipkin-Nogami procedure for approximate number conservation

Microscopic term 3: **Wigner correction**

Only a term linear in T term is considered,

$$E_W = \frac{V_W}{A}\left(|N - Z| + \delta\right)$$

where $\delta = 1$ if N and Z are both odd and equal.

No term representing $n - p$ $T = 0$ pairing.

6. Comparison of models

Rms and mean (expt. - model) deviations between data and predictions for various models. The first pair of lines refers to all the 2149 measured masses M of nuclei with Z and $N \geq 8$ given in the 2003 AME, the second pair to the masses M_{nr} of the subset of 185 neutron-rich nuclei with $S_n \leq 5.0$ MeV, and the third pair to the 782 measured charge radii given in the compilation of Angeli (2004).
HFB-8: Samyn *et al.* (2004) - no neutron-matter constraint
HFB-14: Goriely *et al.* 2007 - neutron-matter constraint
DZ = Duflo and Zuker (1995), a model that parametrizes multipoles of an implicit force: intermediate between macro. and micro., but more unified than macro-micro methods.

	FRDM	FRLDM	HFB-8	HFB-14	DZ
$\sigma(M)$ [MeV]	0.656	0.769	0.635	0.729	0.360
$\bar{\epsilon}(M)$ [MeV]	0.058	-0.403	0.009	-0.057	0.009
$\sigma(M_{nr})$ [MeV]	0.910	0.955	0.838	0.833	0.527
$\bar{\epsilon}(M_{nr})$ [MeV]	0.047	-0.078	-0.025	0.261	0.126
$\sigma(R_c)$ [fm]	0.0545	0.159	0.0275	0.0309	-
$\bar{\epsilon}(R_c)$ [fm]	-0.0366	-0.151	0.0025	-0.0117	-

Number of model parameters

DZ (1)	FRDM (2)	HFB-14 (3)
28	19	21

1) Duflo and Zuker (1995).

2) Estimate of Lunney *et al.* (2003).

3) +3 parameters for large-deformation vibrational correction, which are fitted to fission barriers.

Fission barriers for HFB-14

Data: RIPL-2 compilation (2006): www-nds.iaea.org/RIPL-2/

	σ (MeV)	$\bar{\epsilon}$ (MeV)*
Set 1	1.31	-0.72
Set 2	0.67	-0.36

* expt. - model

Set 1: complete RIPL-2 data set of 77 primary barriers, $80 \leq Z \leq 96$.

Set 2: subset of all the 52 primary barriers lower than 13.5 MeV (higher barriers of less astrophysical interest).

Performance on new data

HFB-14 was fitted to latest data (2149 nuclei of 2003 AME) so no checks possible.

DZ fitted to 1995 AME - 1964 nuclei:
$\sigma = 0.346$ MeV (0.360 MeV for 2003 AME)
- only a slight deterioration.

FRDM fitted to 1989 "midstream" AME - 1654 nuclei:
$\sigma = 0.681$ MeV * (0.656 MeV for 2003 AME)
- FRDM actually improves with age!

Improvement lies on p-rich side where most of new data lie.

* Möller *et al.* quote a "model" error.

All these models agree closely in the known region.

But what happens when we extrapolate to the neutron drip line?

Fig. 6.1

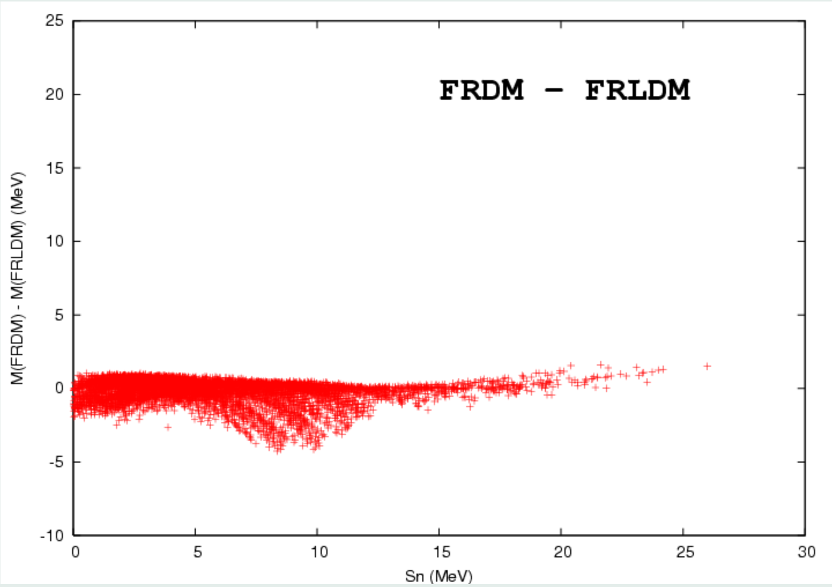


Fig. 6.2

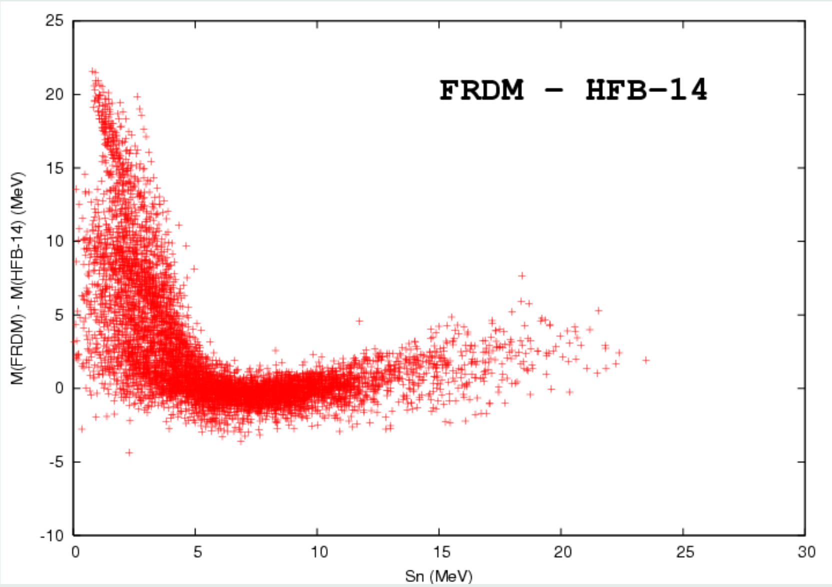
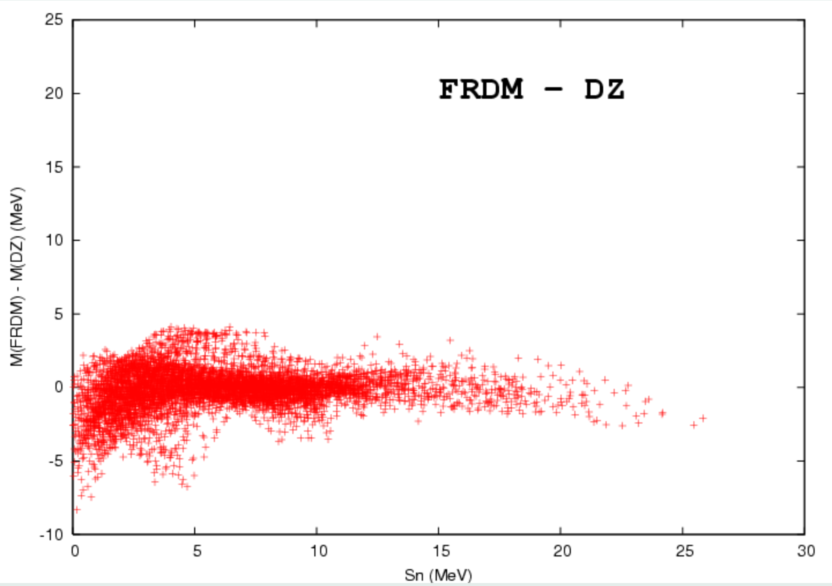


Fig. 6.3



Largest divergence is between FRDM and HFB-14

latter more strongly bound at n-drip line

–neutron skin is softer.

Difference reduced by extra term in FRDM surface energy:

$$E_{sf} = 4\pi R^2 \left\{ \sigma + \frac{Q}{4\pi r_0^2}\left(\frac{\tau}{r_0}\right)^2 + \frac{Q'}{4\pi r_0^2}\left(\frac{\tau}{r_0}\right)^4 \right\}$$

Dutta *et al.* (1986).

Could be unphysical constraint implicit in Skyrme force, but other mean-field models are similar to HFB-14 in this respect: see Fig. 11b of Lunney *et al.* (2003).

Comparison of FRDM and HFB-14 predictions for M, S_n and Q_β of highly neutron-rich nuclei with $S_n < 4.0$ MeV. We show rms and mean (FRDM - HFB-14) differences (MeV).

	M	S_n	Q_β
σ	8.22	0.75	1.12
$\bar{\epsilon}$	6.30	-0.32	0.79

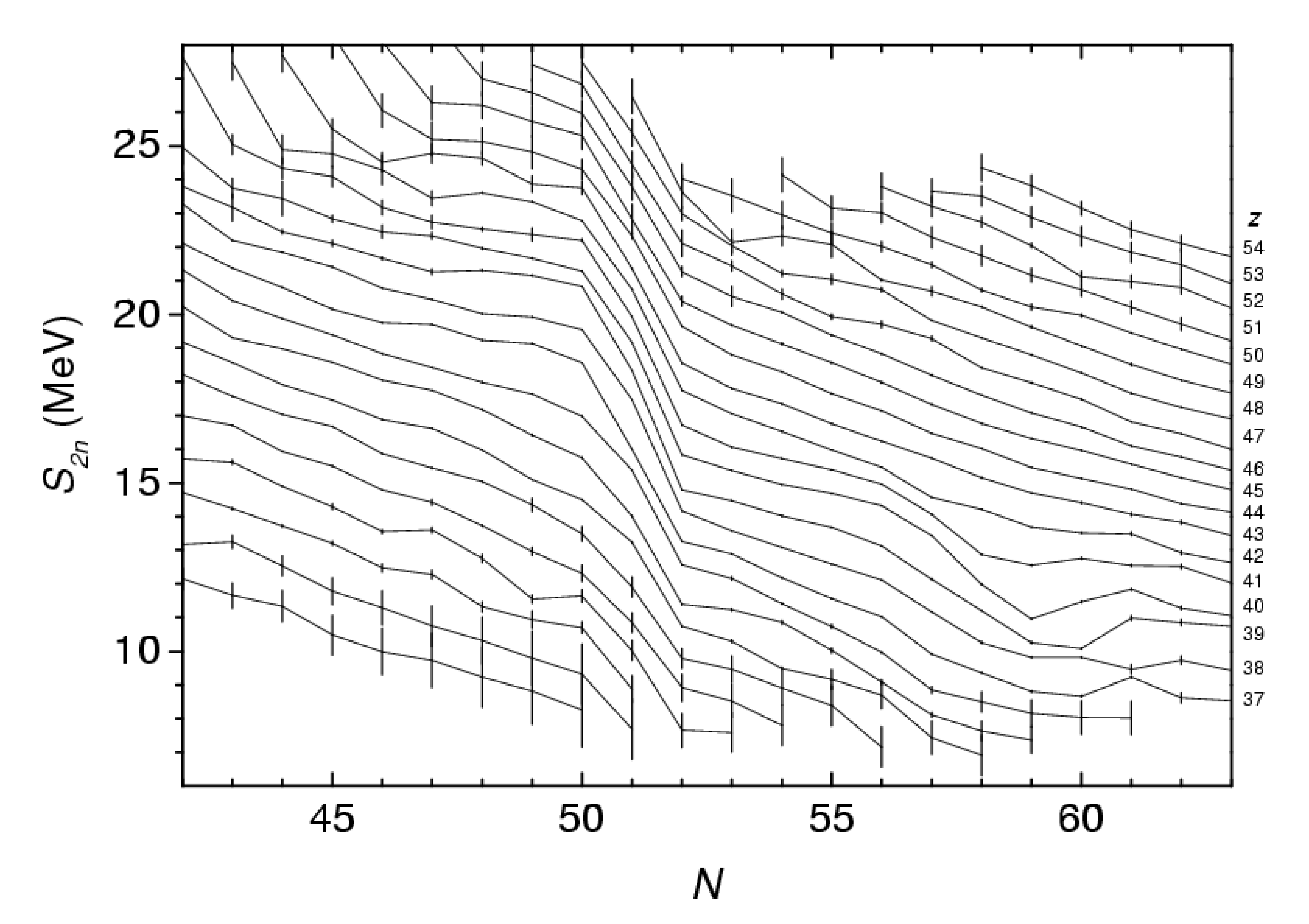


Fig. 1.1.Two-neutron separation energy S_{2n} of several elements in the range $Z \sim 30$-50, as a function of neutron number N.

Measure of discontinuity in S_{2n} at magic neutron numbers N_0:

Shell gap

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

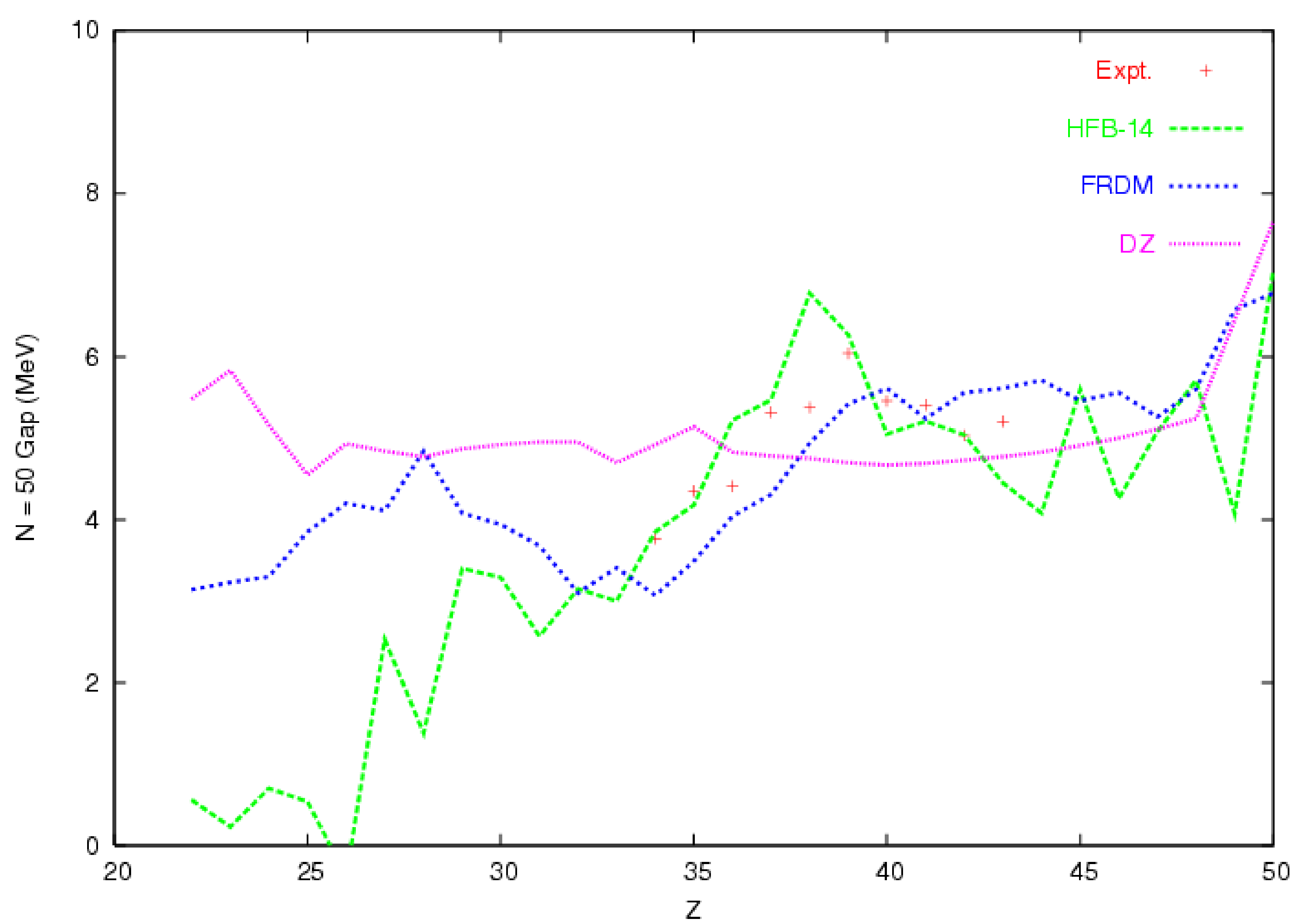


Fig. 6.4. $N_0 = 50$ gaps

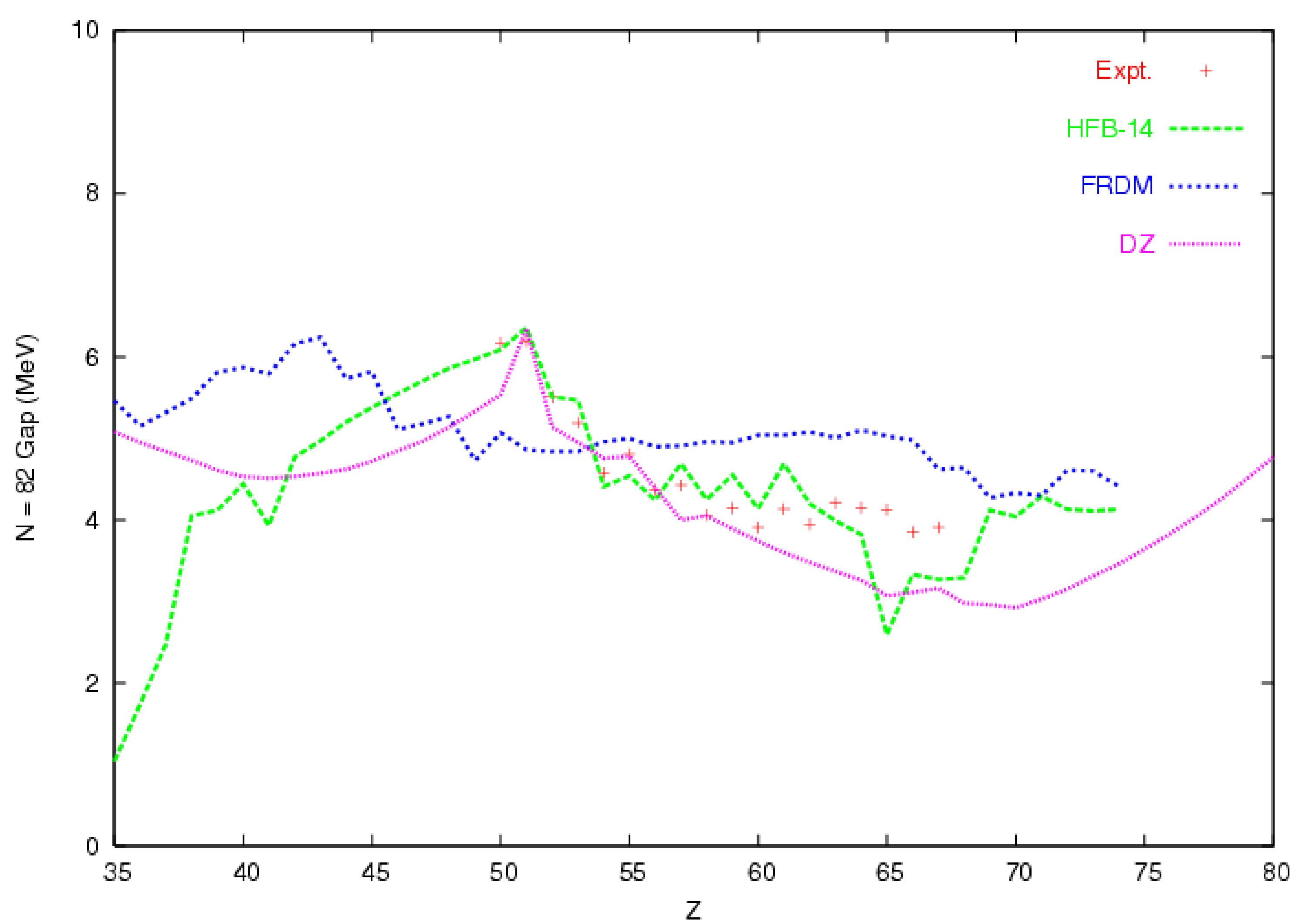


Fig. 6.5. $N_0 = 82$ gaps

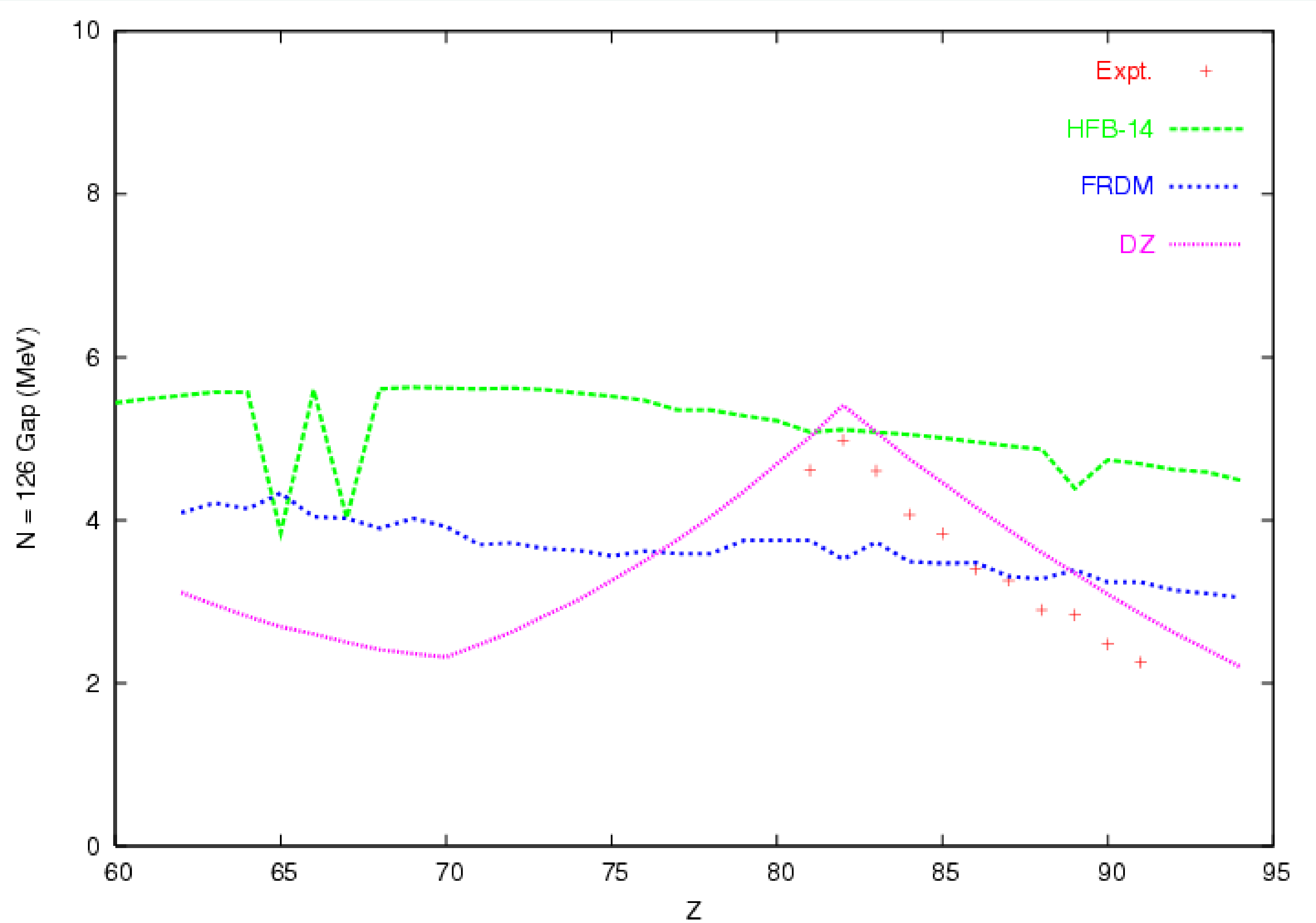


Fig. 6.6. $N_0 = 126$ gaps

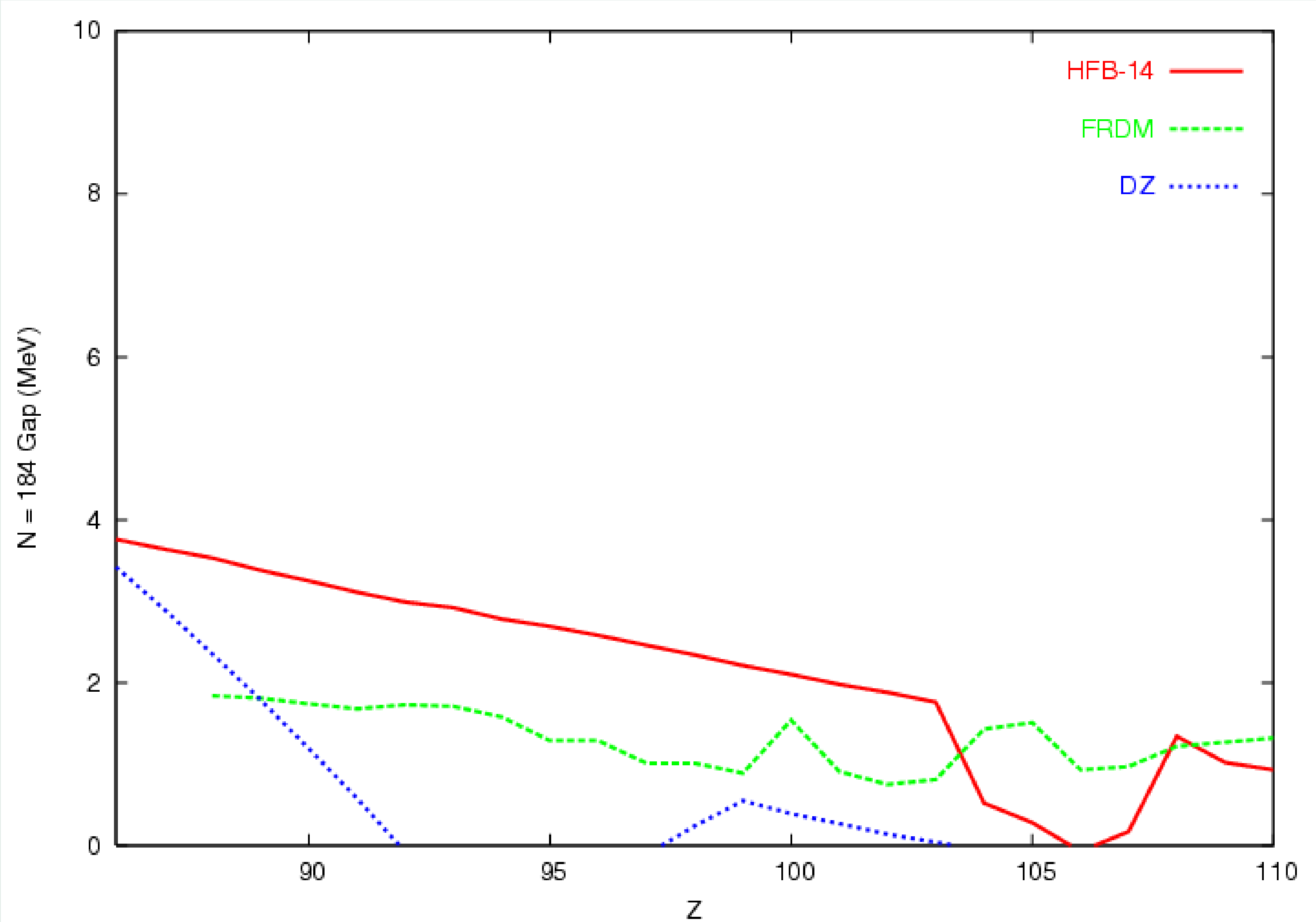


Fig. 6.7. $N_0 = 184$ gaps

Shell gaps tell us:

- Vital need for more data.
- No model works very well.

7. Conclusions

Present situation

Of the three models DZ, FRDM and HFB-14, none can be used with total confidence

– if possible, r-process calculations should be performed with all three models.

Future directions

Duflo-Zuker Even if it is possible to improve DZ (and it is already very good), it should be remembered that it can be used only for masses, and cannot be extended to other quantities of astrophysical interest.

Macro-micro. This approach generalizes the simple but extremely fruitful Weizsäcker mass formula, but the failure of the FRDM at large deformations and the need to resort to the older FRLDM for fission suggests that further developments along these lines might be difficult.

HFB This is the path to follow in the future, where investment of effort is most likely to lead to progress

– remember, it is only five years since the publication of the first HFB model, and more than seventy since the Weizsäcker mass formula was published!

But plenty of room for improvement on HFB-14

Following improvements are possible – and needed:

- Correct treatment of odd nuclei.
- More realistic pairing force.
- Correct treatment of continuum.
- More microscopic collective corrections.
- Microscopic treatment of Wigner terms.
- Higher-order terms in the Skyrme force.
- Replace Skyrme forces by finite-range effective forces.

Many of these improvements have already been realized, mainly through the efforts of the Oak Ridge-Warsaw group and their many collaborators. Hope to see them incorporated in future mass models.

HFB mass models can easily be extended to the calculation of other quantities of astrophysical importance: fission, level-density formulas, EOS, beta-decay strength functions, etc.

Moreover, this is the channel through which we may ultimately hope to relate the properties of finite nuclei with the basic nucleonic forces –

the fundamental problem of nuclear physics.

Home Page

Title Page

Contents

◀◀ ▶▶

◀ ▶

Go Back

Full Screen

Close

Quit

Bibliography

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