Hartree-Fock Mass Formulas and the r-Process

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Relevence of Mass Formula to r-Process

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

S_n neutron separation energy

determines position of r-process path for given physical conditions (at least in canonical model)

Q_β beta-decay energy

necessary for β-decay rates, which determine relative elemental abundances along r-path

NB Determination of β-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

[MM]

droplet

(refinement of liquid-drop model)

shell effects (Strutinsky)

pairing effects (BCS)

Shell Corrections

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

$$\left(-\frac{\hbar^2}{2M}\nabla^2 + \hat{v}\right)\varphi_i = \varepsilon_i \varphi_i$$

Strutinsky Theorem

$$E_{tot} = E_{mac} + \sum_i \varepsilon_i - \widetilde{\sum_i} \varepsilon_i$$

$\widetilde{\sum} \varepsilon_i$ - 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

Finite-Range Droplet Model (FRDM)

Möller, Nix, Myers, and Swiatecki
ADNDT 59 185 (1995)

1654 masses fitted

$$\sigma_{rms} = 0.669 \text{ MeV}$$

Excellent fit to data

- but how reliable are extrapolations?

1. No unambiguous choice of $\tilde{U}$

   - how to relate it to macro. term?

2. Strutinsky smoothing procedures very ambiguous at n-drip 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

HFBCS-1

S. Goriely, F. Tondeur, J.M. Pearson

ADNDT 77, 311 (2001)

Skyrme force - conventional 10 param.

$$v_{ij} = t_0(1+x_0P_\sigma)\delta(\mathbf{r}_{ij}) + t_1(1+x_1P_\sigma)\frac{1}{2\hbar^2}\{p_{ij}^2\delta(\mathbf{r}_{ij}) + h.c.\}$$
$$+t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\mathbf{p}_{ij}.\delta(\mathbf{r}_{ij})\mathbf{p}_{ij} + \frac{1}{6}t_3(1+x_3P_\sigma)\rho^\gamma\delta(\mathbf{r}_{ij})$$
$$+\frac{i}{\hbar^2}W_0(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j).\mathbf{p}_{ij}\times\delta(\mathbf{r}_{ij})\mathbf{p}_{ij}$$

many Skyrme forces already on market S3, SkM*, SkP, Sly n, ... but this is first time that essentially all mass data are fitted.

Pairing term 4 param.

$$v_{pair} = V^{\pm}_{\pi q} \, \delta(r_{ij})$$

treated in BCS approx.

Wigner term 2 param.

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

T=0 pairing?

Combinations of Skyrme params. corresponding to M_S^* and M_V^* (isoscalar and isovector effective masses) constrained such that

$$M_S^* = M_V^*$$

$\therefore$ 15 degrees of freedom

Fit to Audi-Wapstra (1995)

1768 nuclei with $Z, N \geq 8$

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

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

$\sigma(S_n) = 0.489$ MeV

$\sigma(Q_\beta) = 0.614$ MeV

Charge radii : 523 measured values

rms error = 0.024 fm

Quadrupole deformation parameter β_2

274 measured values

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 Bogolyubov

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new mass formula

Samyn et al. Nucl. Phys. **A700** 142 (2002)

Same form of Skyrme + pairing forces

Same pairing cutoff $(=\hbar\omega)$

With original force MSk7 (force of HFBCS-1) quality of data fit deteriorates in HFB.

$\therefore$ new fit : force BSk1

$\sigma(1768) = 0.740$ MeV

(0.718 MeV before)

Extrapolation to neutron-drip line

$$| M(\text{HFB-1}) - M(\text{HFBCS-1}) | < 2 \text{ MeV}$$

- usually much smaller.

Also shifts in S_n and Q_β very small

e.g., shell gaps at magic neutron numbers.

This suggests that BCS might be sufficient - for masses

(Radii of nuclei at neutron-drip 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-1 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 δ-function pairing force there will be a divergence if no cutoff)

See how HFB-1 can be improved

Wigner Energy

originally had

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

now write

$$E_W = V_W \exp\left\{-\lambda \left(\frac{N-Z}{A}\right)^2\right\}$$ T = 0 pairing ?

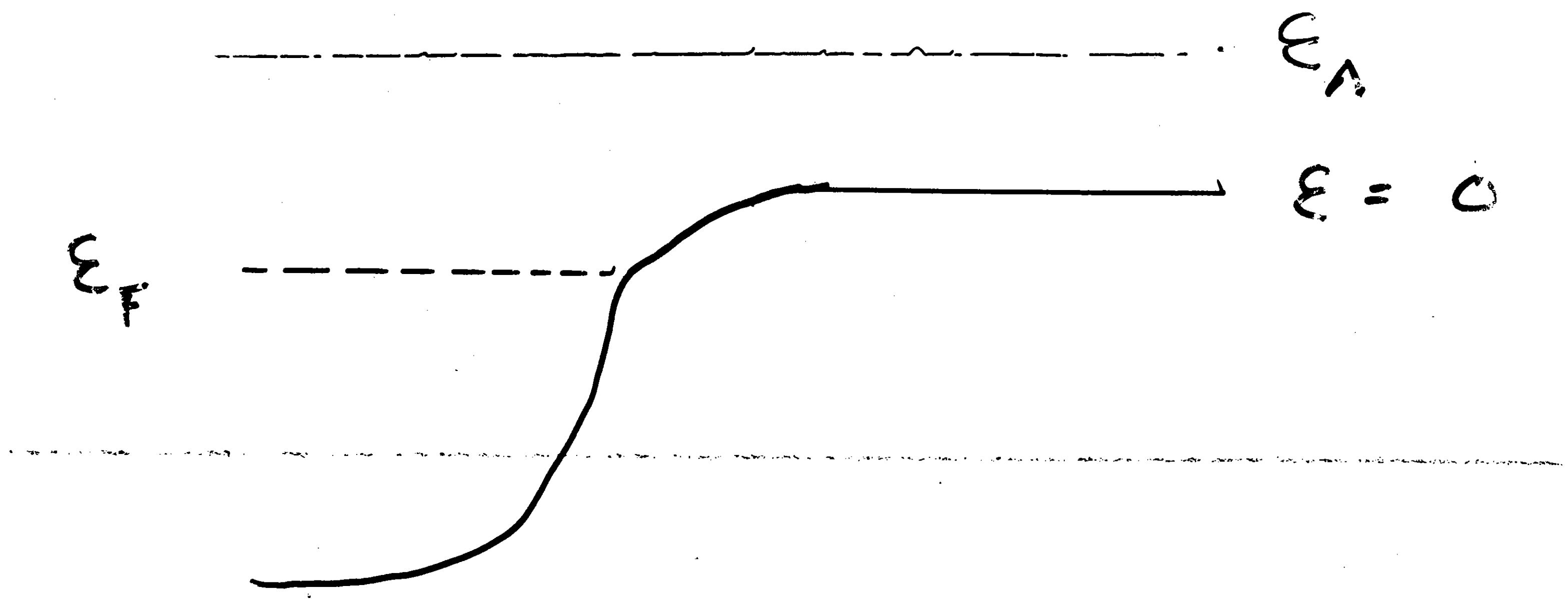
$$+ \underbrace{V_W' \, |N-Z| \exp\left(-\frac{A}{A_0}\right)^2}$$

SU(4) spin-isospin symmetry ?

- confined to light nuclei :

best fit with $A_0 = 20$

Pairing Cutoff



HFBCS-1, HFB-1

$$\varepsilon_\Lambda = \hbar\omega = 41\,A^{-1/3}\ \mathrm{MeV}$$

Alternative scenario

ε_Λ specified w.r.t. ε_F

We optimized both models

Latter scenario favoured

$$\varepsilon_\Lambda = \varepsilon_F + 15 \text{ MeV}$$

HFB-1'

Fit to 1995 data improves by 0.051 MeV

Extrapolation 0.172 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. σ denotes rms error, ϵ denotes mean error; all errors in MeV.

	1995 data	(1768 nuclei)	new data	(382 nuclei)
	σ	ϵ	σ	ϵ
FRDM	0.678	0.023	0.655	0.247
HFBCS-1	0.718	0.102	1.115	0.494
HFB-1	0.740	0.040	1.123	0.510
HFB-1′	0.651	-0.039	0.857	0.470

N.B.

We have adopted very simple parametrizations for pairing cutoff. More elaborate parametrizations, e.g., different treatment of n and p, may lead to better fits — and may be required by ~~f~~ 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!

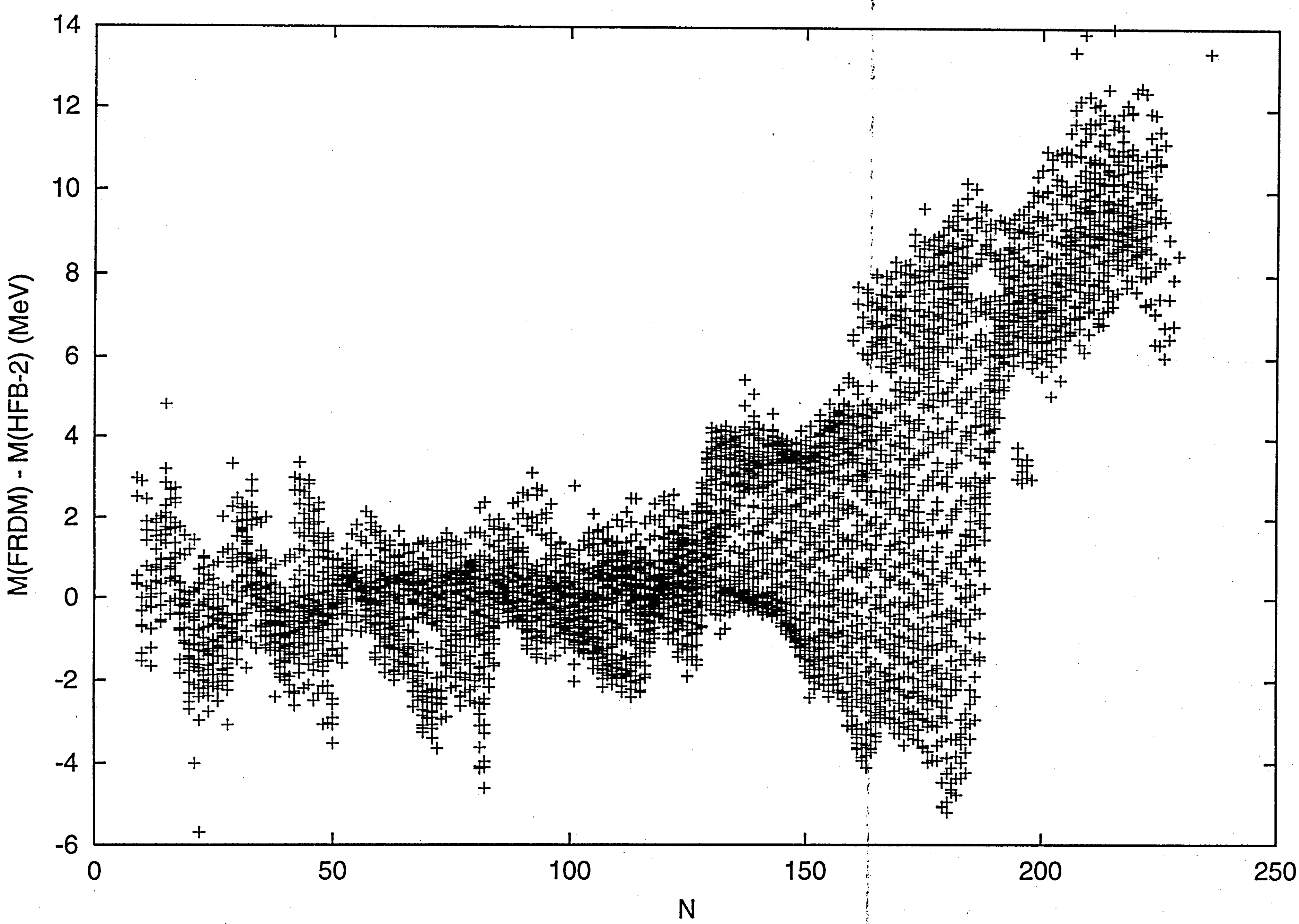
So make a fit to complete new data set of 2135 nuclei with this new model, i.e. new Wigner term --- cutoff prescription

new mass formula HFB-2

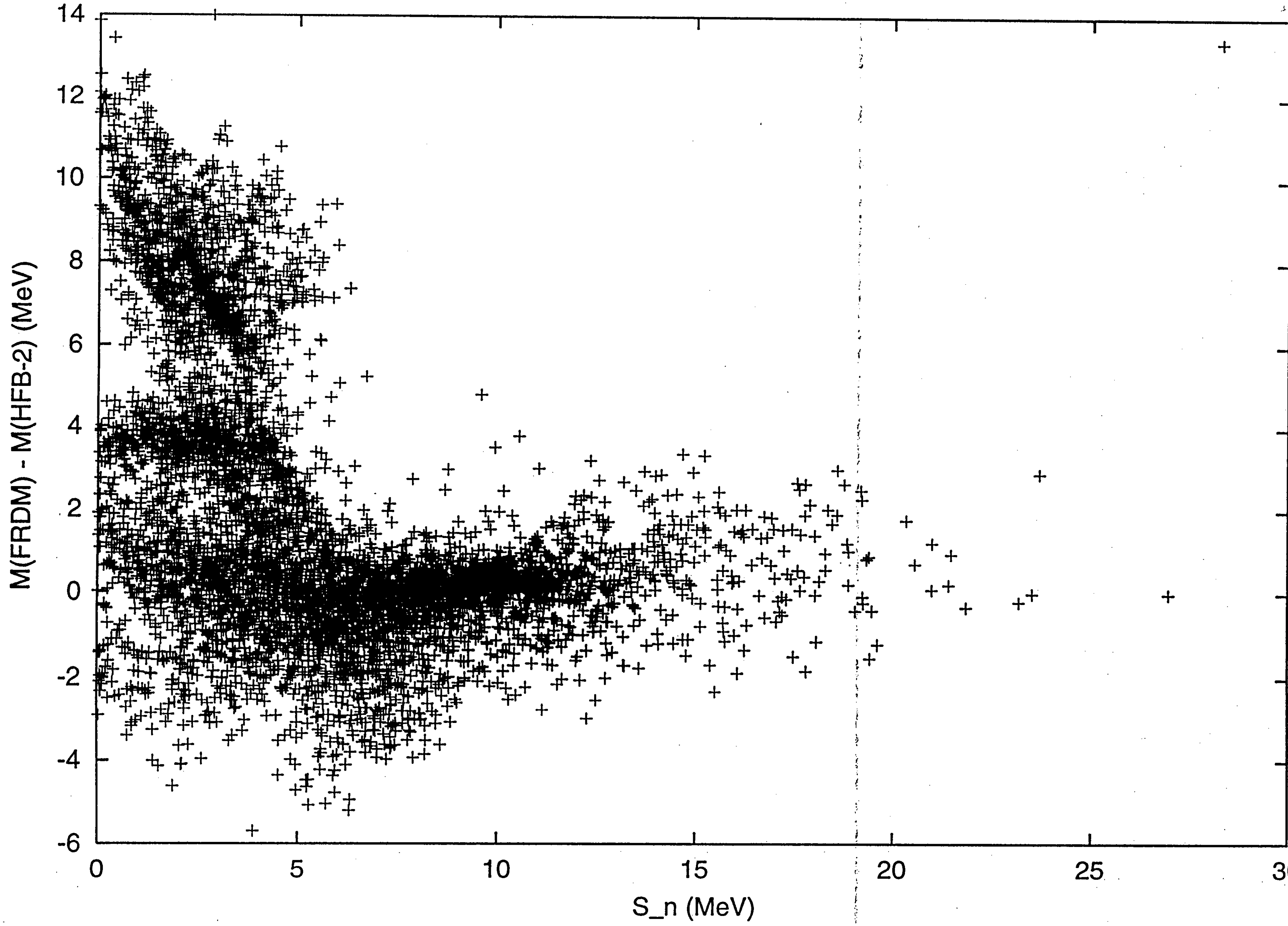
	2001 data	(2135 nuclei)	new data	(382 nuclei)
	σ	ϵ	σ	ϵ
FRDM	0.676	0.072	0.655	0.247
HFB-2	0.674	0.000	0.769	0.377

N.B.

FRDM fitted to only 1654 masses (~1993). So if refitted to new data it would almost certainly out-perform HFB-2



M(FRDM) - M(HFB-2) (MeV)
14
12
10
8
6
4
2
0
-2
-4
-6
0
50
100
150
200
250
N



M(FRDM) - M(HFB-2) (MeV)
14
12
10
8
6
4
2
0
-2
-4
-6
0
5
10
15
20
25
30
S_n (MeV)

Of particular interest to r-process

magic neutron-shell gap

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

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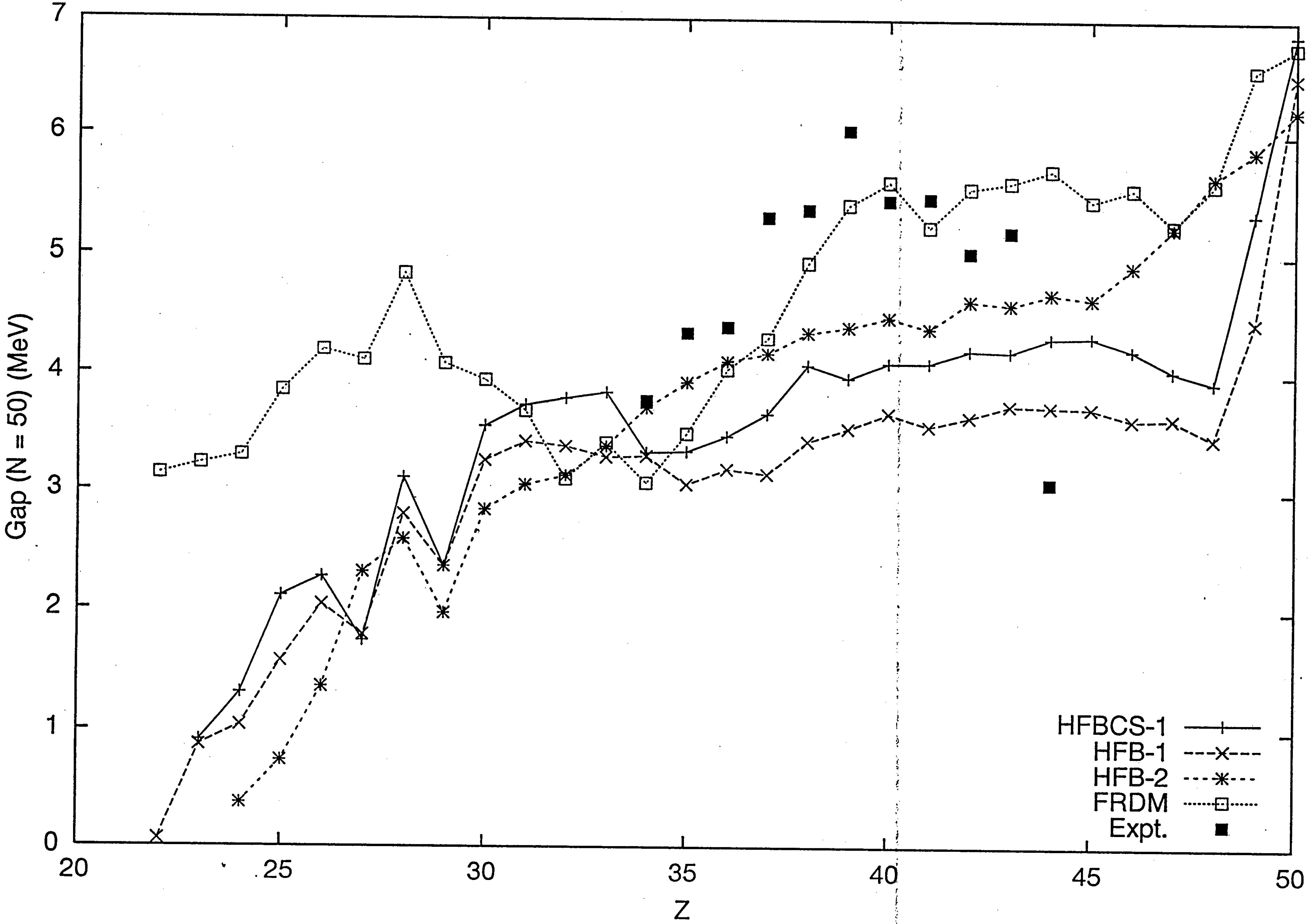
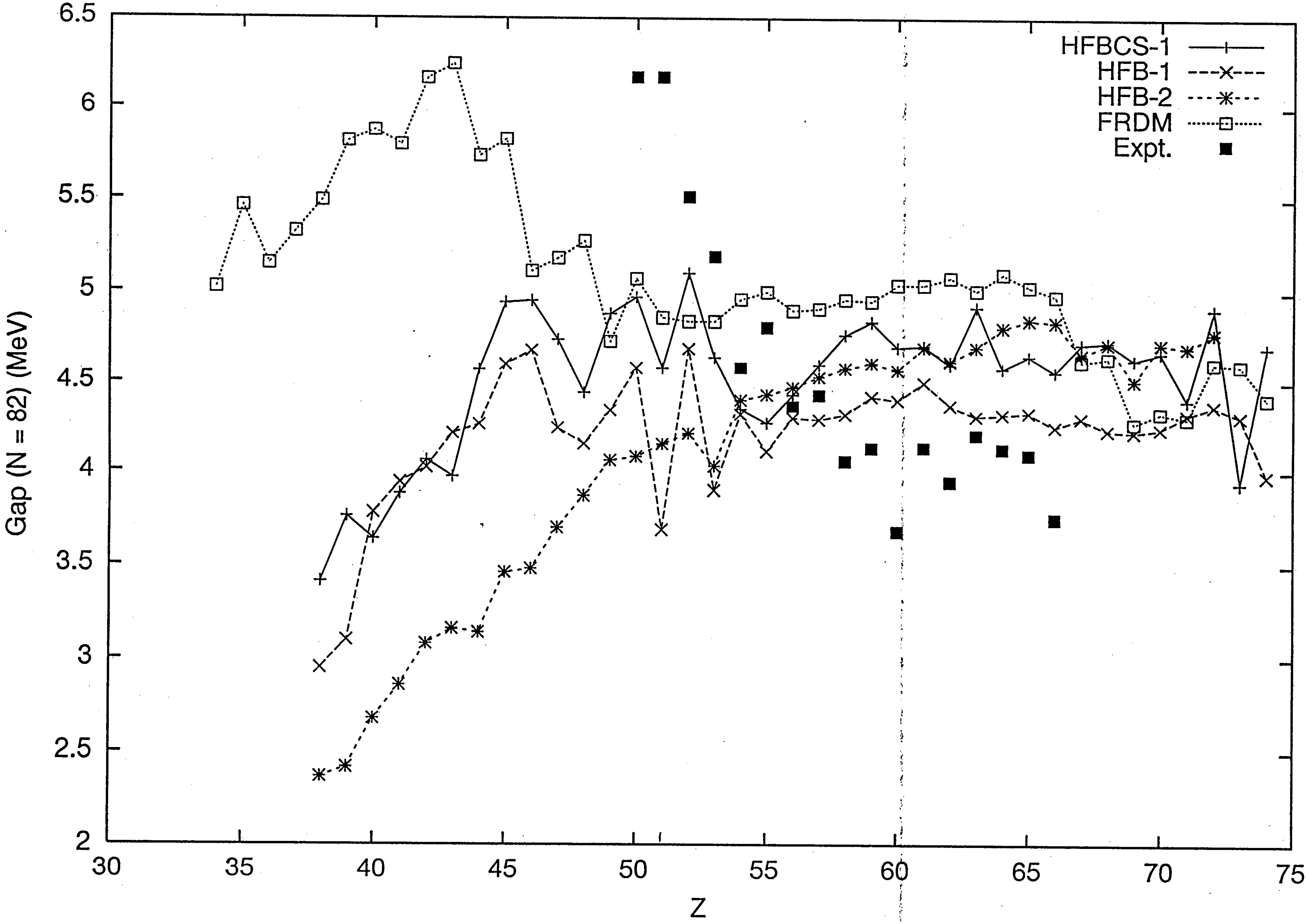
possibility of gap quenching

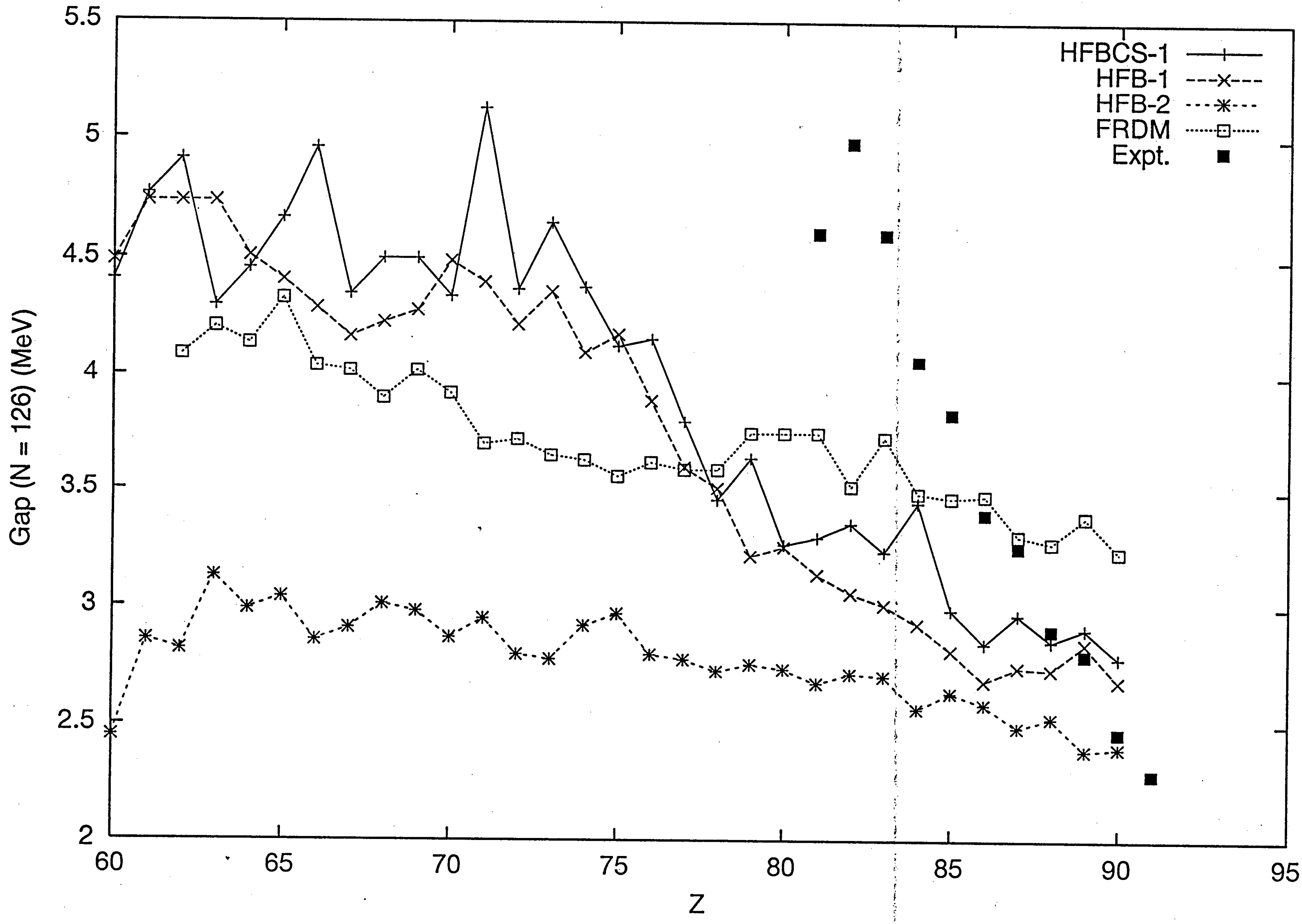
as n-drip line is approached,

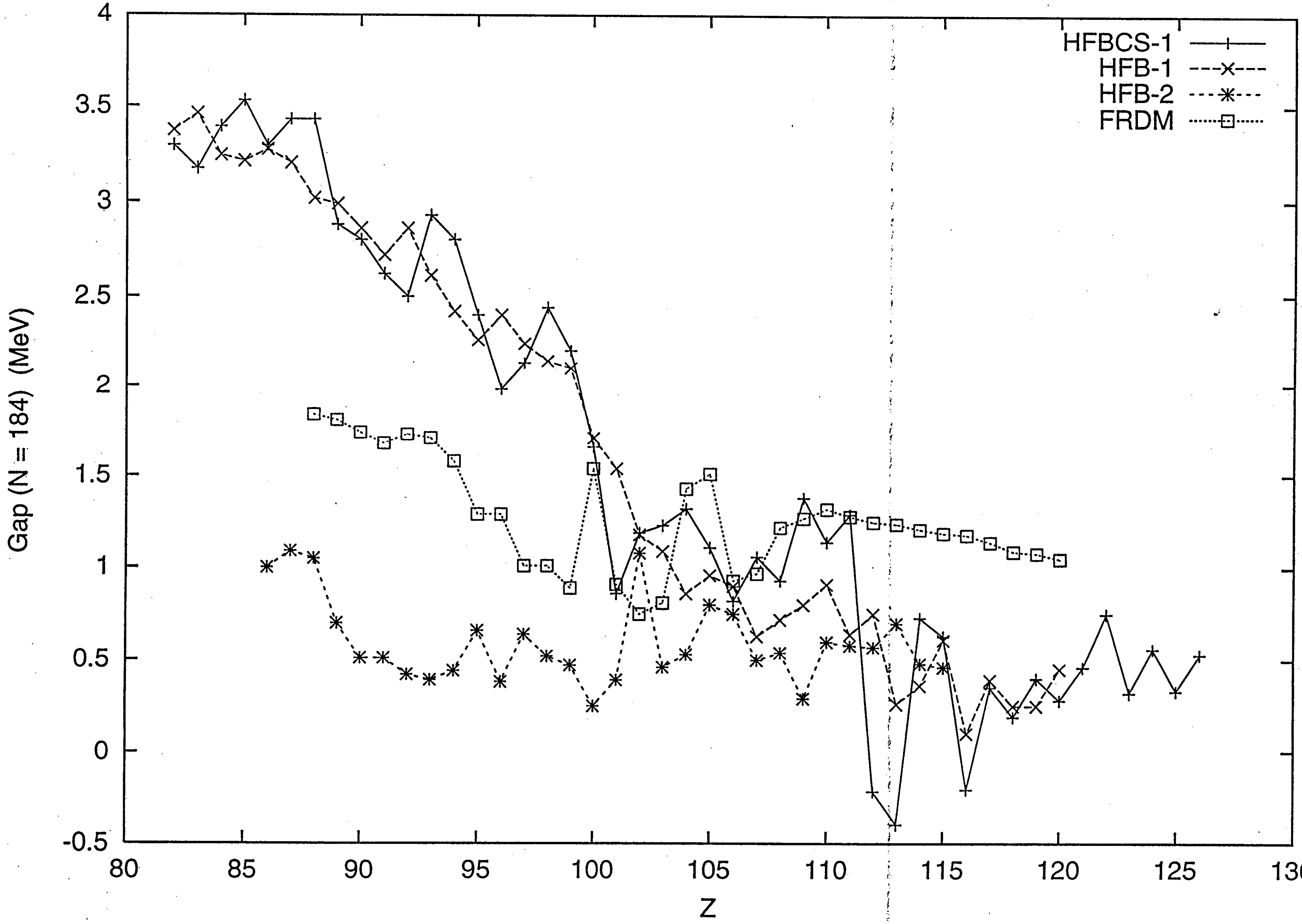
i.e., as protons are removed for

the given N_0


Gap (N = 50) (MeV)
0
1
2
3
4
5
6
7
20
25
30
35
40
45
50
Z
HFBCS-1
HFB-1
HFB-2
FRDM
Expt.


HFBCS-1
HFB-1
HFB-2
FRDM
Expt.
Gap (N = 82) (MeV)
Z
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
30
35
40
45
50
55
60
65
70
75


HFBCS-1
HFB-1
HFB-2
FRDM
Expt.
Gap (N = 126) (MeV)
Z
5.5
5
4.5
4
3.5
3
2.5
2
60
65
70
75
80
85
90
95



HFBCS-1
HFB-1
HFB-2
FRDM
Gap (N = 184) (MeV)
Z
4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
80
85
90
95
100
105
110
115
120
125
130

HFBCS-1 and HFB-1 quite similar

but HFB-2 follows distinct trend

$\Rightarrow$ Quenching depends on pairing cutoff

Treatment of pairing in FRDM

parametrization of pairing gap

$$\tilde{\Delta}_{n\text{-pair}} \propto \frac{1}{N^{1/3}}$$

$$\hat{\Delta}_{p\text{-pair}} \propto \frac{1}{Z^{1/3}}$$

Symmetry Coefficient of INM

INM : Infinite nuclear matter

Weizsäcker mass formula

$$\frac{E}{A} = a_{vol} + a_{sf} A^{-1/3} + a_c \frac{Z^2}{A^{4/3}} + a_{sym} \left(\frac{N-Z}{A}\right)^2$$

All Skyrme-HF mass formulas lead to

$$a_{sym} \simeq 28 \text{ MeV}$$

FRDM $\Rightarrow$ 32 - 35 MeV

Very important to have an independent determination of a_{sym}

if $a_{sym} > 29$ MeV, say, then

bad news for Skyrme forces

- would have to turn to

finite-range forces -

very much more complicated

Theory:

Calc^n of INM with Argonne v_{14} force

$a_{sym} = 28{\cdot}7$ MeV

Zuo et al

Phys. Rev. C 60 024605 (1999)

Experiment

mass-independent measurement required

neutron-skin thickness

$$\theta_n = R_n - R_p$$

measurement of R_n is difficult

old measurement of scattering of protons

^{208}Pb : $\theta_n = 0.14 \pm 0.04$ fm

Hoffmann et al. Phys. Rev. C 21 1488 (1980)

$$\Rightarrow \quad a_{sym} = 29 \pm 2 \text{ MeV}$$

- 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.