Hartree-Fock-Bogoliubov Mass Models

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PLAN

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1. Motivation

1995: "finite-range droplet model" of Möller, Nix, Myers and Swiatecki (macro-micro approach):

Excellent data fit: $\sigma = 0.669$ MeV (1654 nuclei).

After this successful climax to 60 years work is there anything left to be done with mass models?

There is considerable interest in constructing a mass model that is as microscopic as possible.

The drive here is partly ideological: the ultimate objective of nuclear theory must surely be to derive masses, and all other nuclear properties, from basic nucleonic forces, i.e., realistic forces determined by two- and three-nucleon data, with guidance from QCD, meson theory, etc.

- However, our own primary motivation is much more practical.

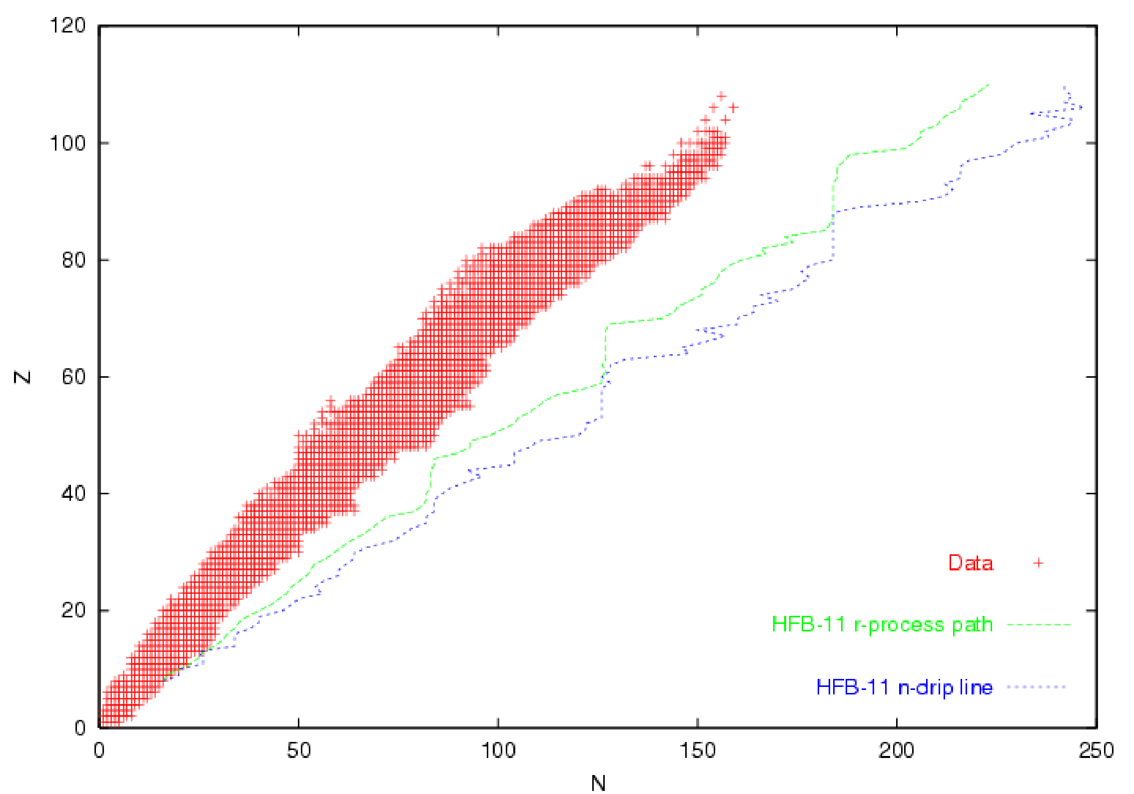
Astrophysical interest

A. r-process of nucleosynthesis

• Evolution of r-process depends on masses (among other quantities) of intermediate nuclei that are so neutron-rich that there is no hope of measuring them in the foreseeable future.

Position of r-path depends on neutron-separation energy S_n.

Rate of evolution along r-path depends on beta-decay energy Q_β.



- Need reliable mass models to extrapolate from the data out to the neutron drip line.

- For reliability mass model must not only fit data but be as theoretically sound as possible.

- If we had a complete nuclear theory and were able to derive masses, along with all other nuclear properties, from realistic nucleonic forces there would be no problem: provided we were absolutely sure of the forces, and of the many-body calculational methods, we could have total confidence in all our calculated masses. Some progress along these lines has been made, notably at Argonne, but so far limited to $A = 12$.

- In the meantime we should, in pursuing this ideal, try to make calculations as microscopic as possible.

- Best that can be done so far is Hartree-Fock-Bogoliubov (HFB) method with Skyrme forces. The force parameters are fitted to the mass data, exactly as with the original Weizsäcker semi-empirical formula.

CAVEAT EMPTOR

Skyrme forces are *effective* forces, and their relation to realistic forces is somewhat tenuous. Thus there is no guarantee that the extrapolations based on such mass models will be more reliable than those based on macro-micro approach. But the Skyrme HFB method is an essential first step on the way to the ultimate theory.

B. Extrapolation beyond the neutron drip line

Forces fitted in HFB to masses well adapted to calculating the EOS of neutron-star matter.

2. HFB model

Skyrme force

$$\begin{aligned} v_{ij} = {} & t_0(1 + x_0 P_\sigma)\delta(\mathbf{r}_{ij}) \\ & + t_1(1 + x_1 P_\sigma)\frac{1}{2\hbar^2}\{p_{ij}^2 \delta(\mathbf{r}_{ij}) + h.c.\} \\ & + t_2(1 + x_2 P_\sigma)\frac{1}{\hbar^2}\mathbf{p}_{ij}.\delta(\mathbf{r}_{ij})\mathbf{p}_{ij} \\ & + \frac{1}{6}t_3(1 + x_3 P_\sigma)\rho^\alpha \delta(\mathbf{r}_{ij}) \\ *** \quad & + \frac{1}{2\hbar^2}t_4(1 + x_4 P_\sigma)\{p_{ij}^2 \rho(\mathbf{r}_i)^\beta \delta(\mathbf{r}_{ij}) + h.c.\} \\ & + \frac{i}{\hbar^2}W_0(\boldsymbol{\sigma_i} + \boldsymbol{\sigma_j}).\mathbf{p}_{ij} \times \delta(\mathbf{r}_{ij})\mathbf{p}_{ij} \end{aligned} \quad (1)$$

*** non-conventional "t_4"

Pairing force

$$v_{pair}(\boldsymbol{r}_{ij}) = V_{\pi q}\left[1 - \eta\left(\frac{\rho}{\rho_0}\right)^{\sigma}\right]\delta(\boldsymbol{r}_{ij})$$

cutoff: $E_F - \varepsilon_\Lambda \leq \varepsilon_i \leq E_F + \varepsilon_\Lambda$

Generalized Wigner term for nuclei with $N \simeq Z$

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

Details of code

- HFB equations solved by expansion on oscillator basis.

  Spherical code: 13 to 25 major shells for each l

  Deformed code: Basis truncated at $21\hbar\omega$

- Axial symmetry
- Left-right symmetry (relaxed in fission code)

- Approximate projection of states of good angular momentum

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

where

$$\mathcal{I} = \frac{1}{b}\mathcal{I}_{cr} \coth(c|\beta_2|) \quad ,$$

in which I_{cr} is cranking moment of inertia, and parameters b and c are fitted to masses of highly deformed nuclei and shape isomers.

- Vibrational states are neglected.

Framework is one of time-independent *shape* of mean field.

Neglected correlation energy will have to be absorbed into Skyrme or pairing forces. If pairing is fitted to even-odd mass differences then open-shell nuclei always underbound with conventional Skyrme force. That is, without t_4 term Skyrme force cannot absorb this correlation energy, so pairing becomes excessively strong - stronger than required by even-odd differences.

- "Staggered pairing".

Mass fits require that even-odd differences be well reproduced: pairing stronger in odd states than even states.

- Odd nuclei.

We adopt "blocking", with "filling approximation": unpaired nucleon is put with equal probability in each of the degenerate available states. However, one should allow mean field to break time-reversal symmetry, and then project out states of good time-reversal properties. Our failure to do this leads to a loss of some binding in odd nuclei, which is compensated in the mass fits by allowing pairing to "stagger" - this is second role of staggering.

- Data from 2003 Atomic Mass Evaluation

  Audi, Wapstra, Thibault, Nucl. Phys. **A729** (2003) 337.

Take all 2149 measured masses for $Z, N \geq 8$.

3. Résumé of main published results.

a) Feasibility of HFB mass models.

Best fit so far is parameter set BSk8 (mass table HFB-8):

$$\sigma = 0.635 \text{ MeV}.$$

This is slightly better than FRDM, but this situation would probably be reversed if FRDM were fitted to new data that we have included.

Complete mass table, HFB-8, constructed from one drip line to the other, with $8 \leq Z \leq 110$.

b) Effective mass.

For best force, BSk8, isoscalar effective mass at $\rho = \rho_0$ is

$$M_s^* = 0.8M$$

• This value has been imposed, since traditionally it is the preferred "realistic" nuclear-matter value, and we want to calculate EOS of neutron-star matter with our forces.

• If we did not constrain M_s^* a still better fit would be found with $M_s^*/M \simeq 1$. This corrsponds simply to the well known fact that in mean-field calculations this value of M_s^* gives best fit to s.p. energies near the Fermi surface.

• However, the improvement would not be dramatic, and we have found that excellent fits can be found over an appreciable range of M_s^*, i.e., without optimizing fit to s.p. levels, by adjusting pairing cutoff.

- To understand this result refer to Strutinsky theorem

$$E \simeq \tilde{E} + \sum_i \epsilon_i \, \delta n_i$$

where $\delta\, n_i = n_i - \tilde{n}_i$.

- We now favour for the “realistic” nuclear-matter value

$$M_s^* = 0.92M$$

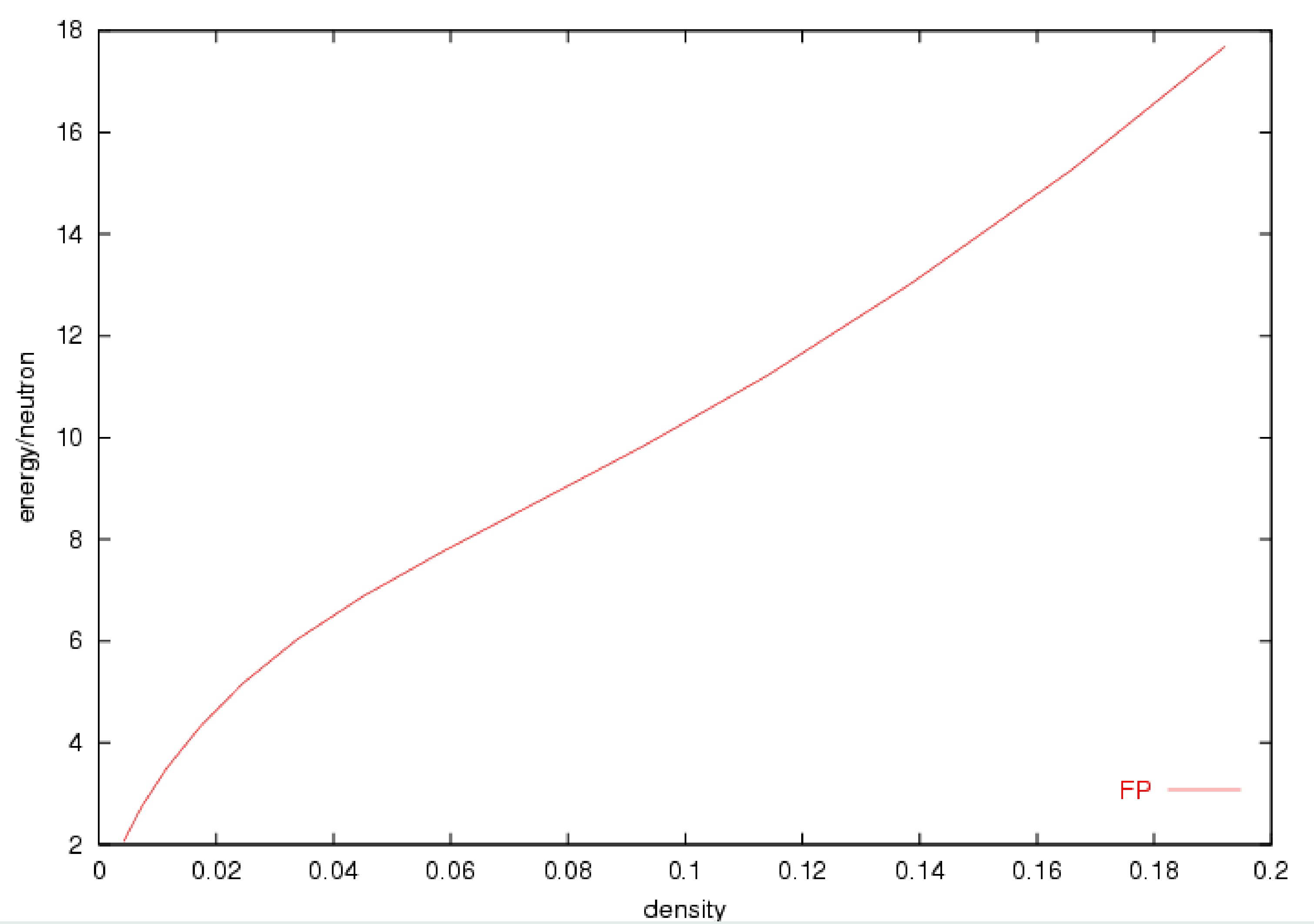
as given by “extended HF-Brueckner” calculations of nuclear matter by Zuo *et al.* This is better established theoretically than old value of $M_s^* = 0.8M$, and leads to better masses and s.p. energies.

c) Neutron-matter constraint and the EOS of neutron-star matter.

BSk8 gives excellent fit to data, but how reliable are extrapolations to neutron-rich nuclei?

fit pure neutron matter

- this can be reliably calculated from realistic two- and three-nucleon forces, e.g., Friedman and Pandharipande (1981) - FP.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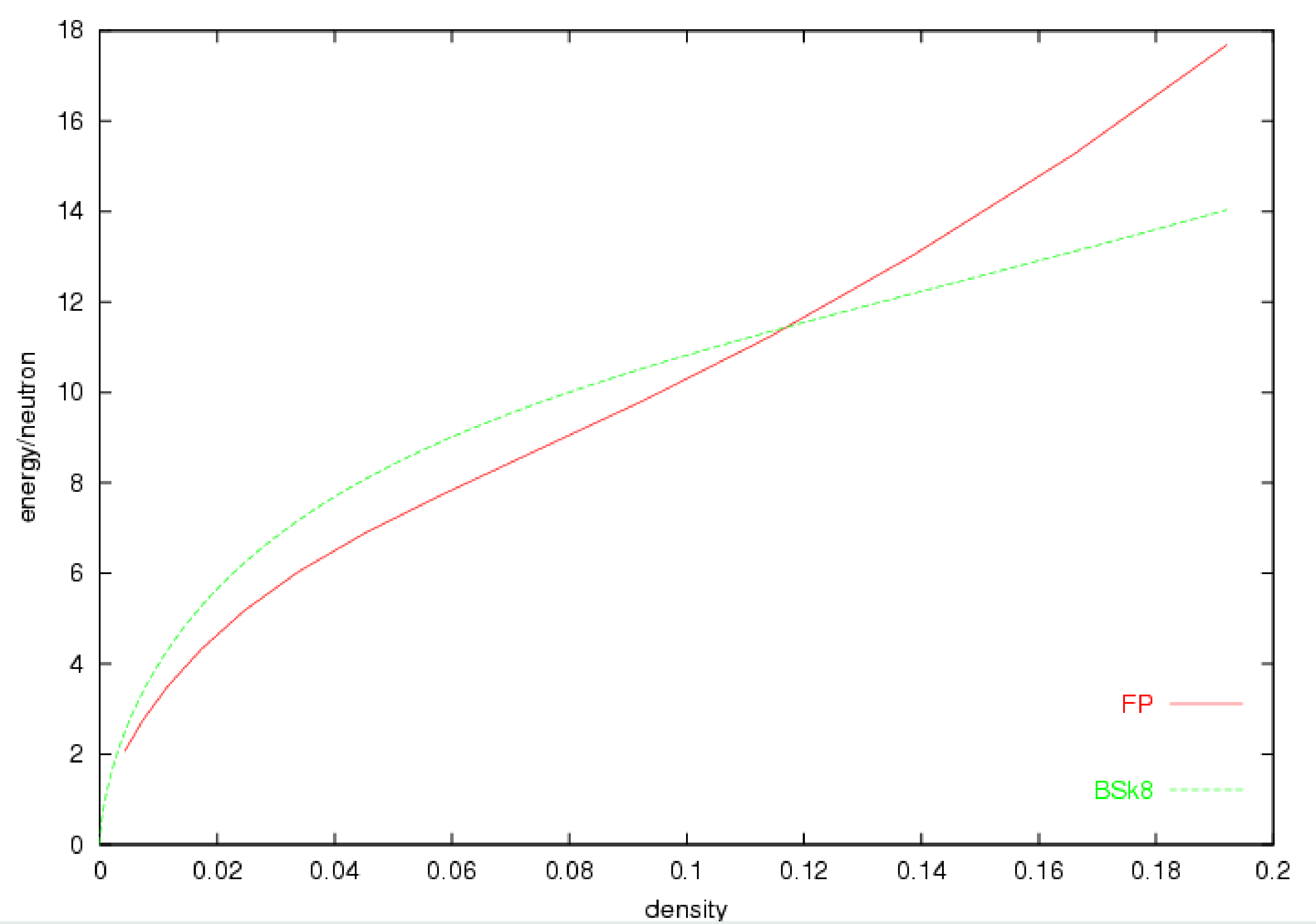
energy/neutron
density
FP

A force that fits the masses and satisfies this condition will be highly suitable not only for extrapolation to the neutron-rich nuclei involved in the r-process but also for extrapolating still further, beyond both the r-process path and the n-drip line, out to neutron-star matter.

Role of mass fit for EOS is two-fold:

ties down $T = 0$ force - neutron star contains some protons

ties down surface properties - crust of neutron star inhomogeneous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0.18
0.2
density
FP
BSk8

- **Situation is actually worse than we have shown here for BSk8:**

neutron matter collapses at sub-nuclear densities if mass fit is completely optimized.

- Crucial factor here is *symmetry coefficient* J:

energy/nucleon of nuclear matter

$$e = a_v + J\left(\frac{N-Z}{A}\right)^2 + \cdots$$

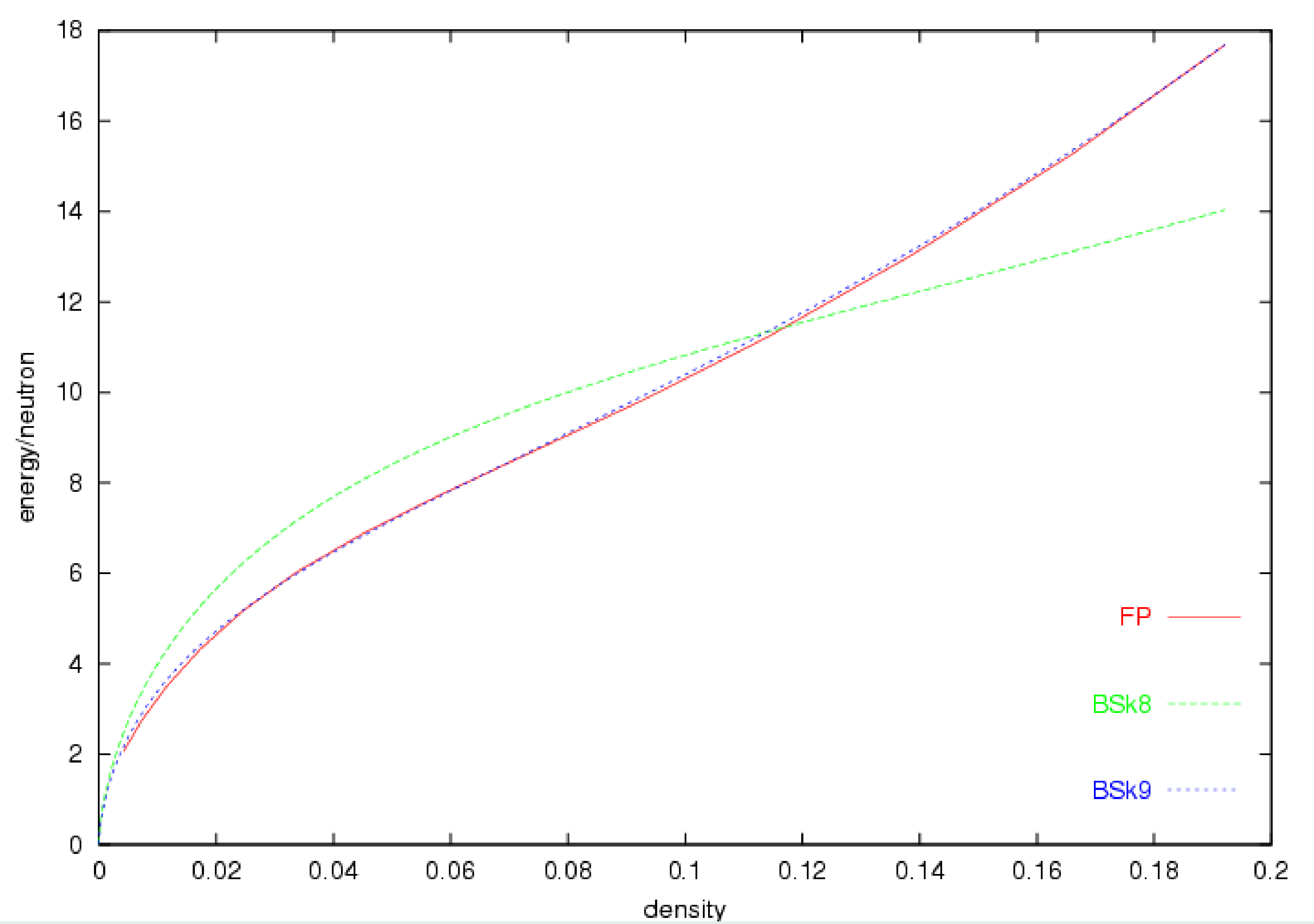
In a completely free fit of masses $J \simeq 27.5$ MeV.
We stopped the collapse in BSk8 by imposing $J = 28.0$ MeV.

- **This shows how to get a good fit to FP neutron-matter curve:**

increase J still further

Fit BSk9 achieved by imposing

$$J = \mathbf{30.0\ MeV}$$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FP
BSk8
BSk9

Rms (σ) and mean ($\bar{\epsilon}$) deviations between data and predictions for parameter sets BSk8 and BSk9. The first pair of lines refers to all the 2149 measured absolute masses M, the second pair to the absolute masses M_{nr} of the subset of 185 neutron-rich nuclei with $S_n \leq$ 5.0 MeV, the third pair to the neutron separation energies S_n (1988 measured values), the fourth pair to beta-decay energies Q_β (1868 measured values), and the last pair to charge radii (782 measured values).

	BSk8	BSk9
$\sigma(M)$ [MeV]	0.635	0.733
$\bar{\epsilon}(M)$ [MeV]	0.009	0.025
$\sigma(M_{nr})$ [MeV]	0.838	0.840
$\bar{\epsilon}(M_{nr})$ [MeV]	-0.025	0.169
$\sigma(S_n)$ [MeV]	0.564	0.589
$\bar{\epsilon}(S_n)$ [MeV]	0.013	0.007
$\sigma(Q_\beta)$ [MeV]	0.704	0.721
$\bar{\epsilon}(Q_\beta)$ [MeV]	-0.027	-0.009
$\sigma(r_c)$ [fm]	0.0275	0.0271
$\bar{\epsilon}(r_c)$ [fm]	0.0025	-0.0049

- **So imposing neutron-matter constraint has led to a slight deterioration in the quality of the mass fit.**

- **This shows a fundamental limitation in the conventional form of Skyrme force, as used here.**

- **However, for the n-rich nuclei there is virtually no loss in quality of fit.**

- **In any case, for r-process what counts is not the absolute masses but rather the neutron-separation energy S_n and the beta-decay energy Q_β. In this crucial respect virtually no deterioration.**

- **So *a priori* we should have equal confidence in extrapolating the two out to the r-process path.**

- **But do the two mass models give similar extrapolations out to the neutron drip line?**

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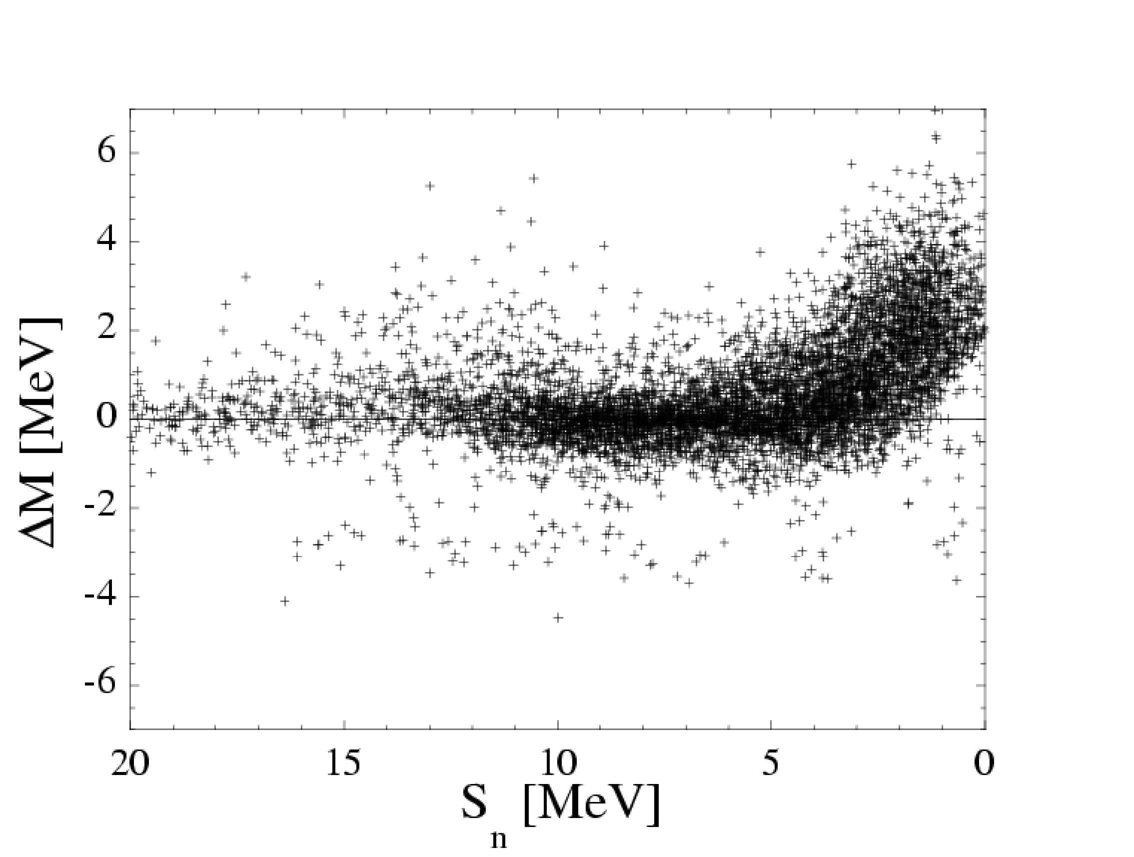


Significant differences between BSk8 and BSk9 as neutron drip line is approached: higher J leads to lower masses.

• **But what counts for the r-process is S_n and Q_β.**

Rms and mean differences (in MeV) between the BSk8 and BSk9 models for the S_n and Q_β of 1639 neutron-rich nuclei ($Z \geq 26; 4$ MeV $\geq S_n \geq 0.5$ MeV). (Mean differences correspond to BSk8 - BSk9.)

	S_n	Q_β
σ	0.560	0.774
$\bar{\epsilon}$	-0.084	0.255

• **Differences between two models for extrapolation comparable to errors with which each model fits the data.**

• **Thus as far as r-process predictions are concerned BSk8 and BSk9 extrapolations are very similar.**

Extrapolation beyond neutron-drip line: EOS of neutron-star matter

Even if BSk8 and BSk9 are equivalent for the r-process, BSk9 more appropriate for neutron-star EOS - fit to neutron matter.

Recognize three distinct regions in neutron star:

- Outer crust.

$$\rho < 1.2 \times 10^{-3}\rho_0 \simeq 1.8 \times 10^{-4}\ \mathrm{fm}^{-3}$$

This is "sub-drip" region, i.e., inside neutron drip line.

- Inner crust.

$$1.2 \times 10^{-3}\rho_0 \leq \rho \leq 0.7\rho_0$$

n-p clusters in neutron gas
n bubbles in n-p liquid

- Homogeneous core

$$\rho \geq 0.7\rho_0 \simeq 0.1\ \mathrm{fm}^{-3}$$

- Outer crust.

Since we are dealing with nuclei that are inside neutron drip line (although highly neutron rich), distribution depends only on differences between neighbouring nuclei, i.e., on S_n and Q_β.

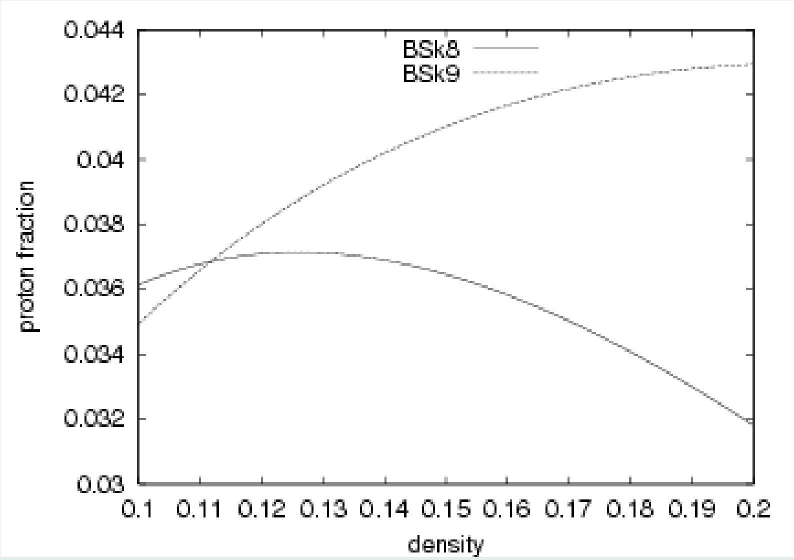
So no essential difference between BSk8 and BSk9, i.e, insensitive to neutron-matter constraint.

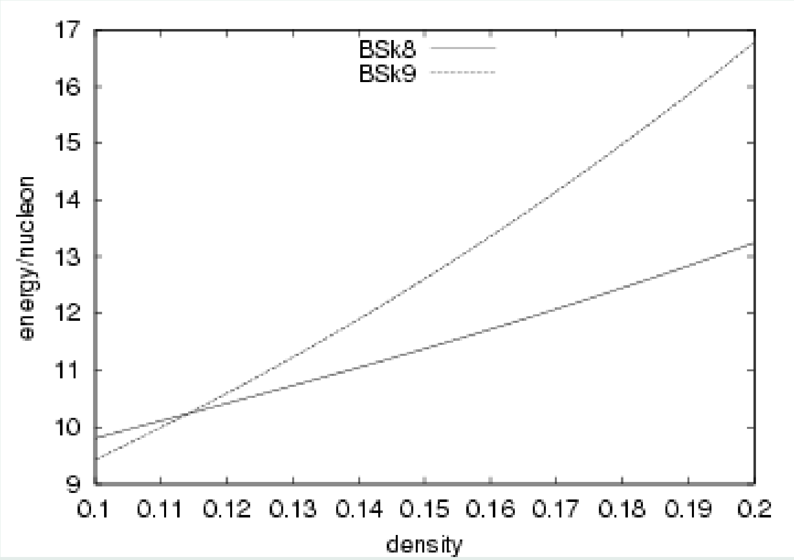
- Homogeneous core.

Imposing neutron-matter constraint will certainly have implications for homogeneous core of neutron star.

Note that core is not pure neutron matter, but rather is β-equilibrated, i.e., $e - p$ pairs.

Increase of J between BSk8 and BSk9 leads to a considerable increase in number of $e - p$ pairs.





Of course, for homogeneous core we can use EOS calculated with realistic forces.

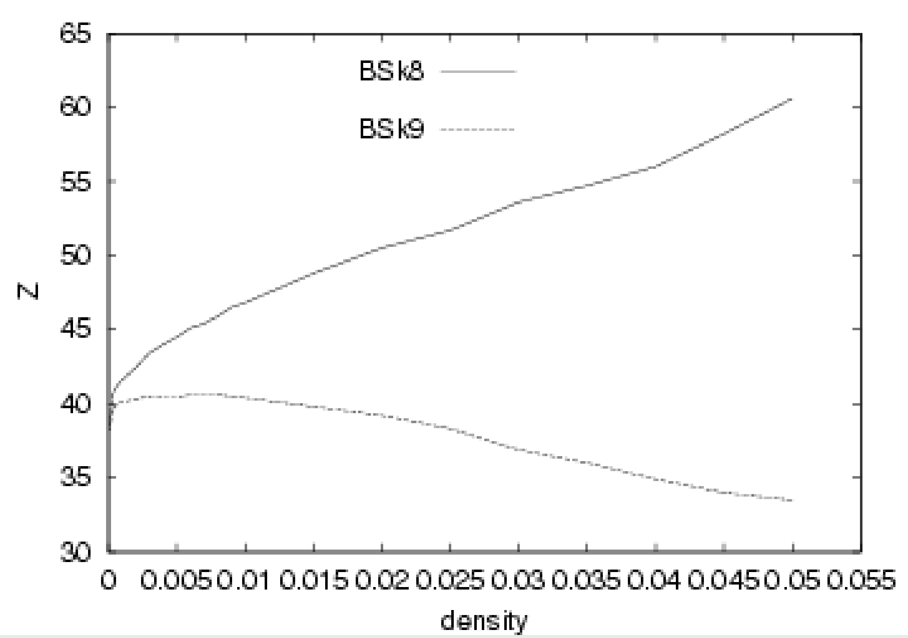
- Inner Crust.

Calculations:

Wigner-Seitz model; 4th-order Extended Thomas-Fermi

Onsi et al. Phys. Rev. C **55** 3139 (1997)

Calculate optimal cell composition at each density ($T = 0$).



- **Optimal value of Z depends critically on J, i.e., on neutron-matter constraint.**

4. Current projects.

a) t_4 Skyrme term and the pairing problem.

Statement of pairing problem:

• If pairing is fitted to even-odd mass differences then open-shell nuclei always underbound with conventional Skyrme force. That is, there is some residual correlation energy, presumably quadrupole, that cannot be absorbed into Skyrme force. Thus, since we fit pairing to absolute masses, pairing becomes excessively strong, in the sense that it is stronger than required by even-odd mass differences.

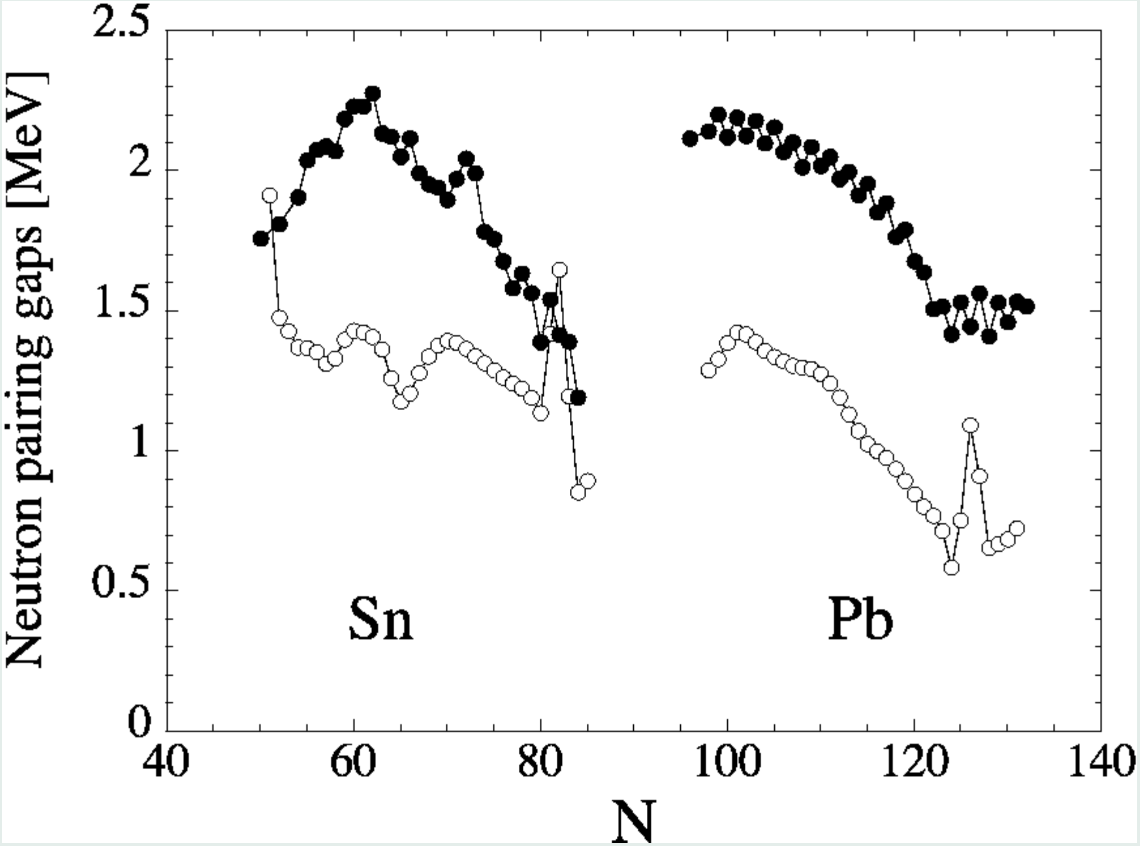
Problem of excessive pairing can be put on quantitative basis:

- compare even-odd mass difference ($\Delta^{(5)}$) with intrinsic average ("spectral") gap

$$\langle uv\Delta\rangle = \frac{\sum_i f_i u_i v_i \Delta_i}{\sum_i f_i u_i v_i}$$

Minimal pairing strength corresponds to these being roughly equal.

Not the case for BSk9 (or any of previous forces)



- because a part of the quadrupole correlation energy has been absorbed by pairing rather than by Skyrme.

Problems for fission barriers and level densities.

- **There is no fundamental reason why a suitable generalization of the Skyrme force should not absorb the residual correlation energy, rather than leaving it to the pairing force.**

After all, even conventional Skyrme force absorbs all the correlation energy associated with the strong short-range repulsion of the real $N - N$ force.

Adding t_4 term to Skyrme force does the trick.

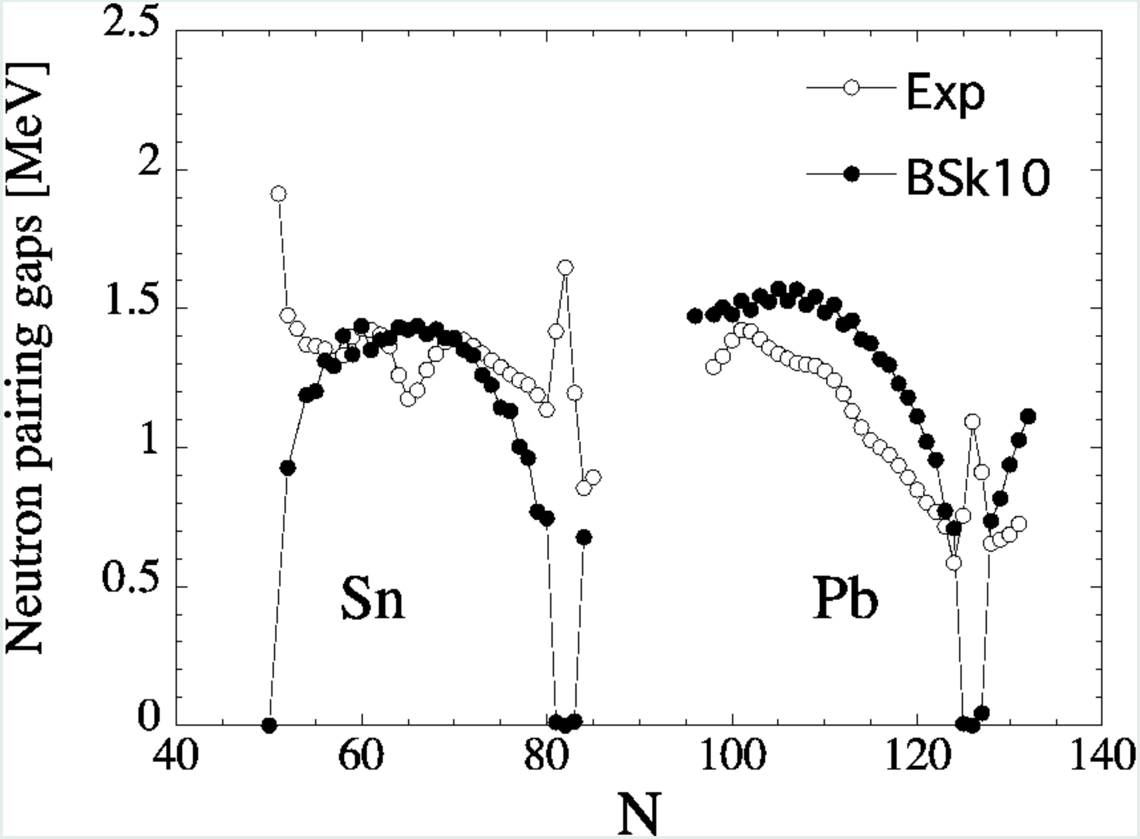
$$\frac{1}{2\hbar^2}t_4(1 + x_4P_\sigma)\{p_{ij}^2\rho(\mathbf{r}_i)^\beta\delta(\mathbf{r}_{ij}) + h.c.\}$$

(Three extra parameters)

New force : BSk10

Very similar to BSk9 - fit to masses and neutron matter.

BUT pairing properties much better



b) Bulgac-Yu renormalization of pairing.

- **Bulgac-Yu renormalization: main features.**

a) For use with δ-function pairing force, which always requires a cutoff.

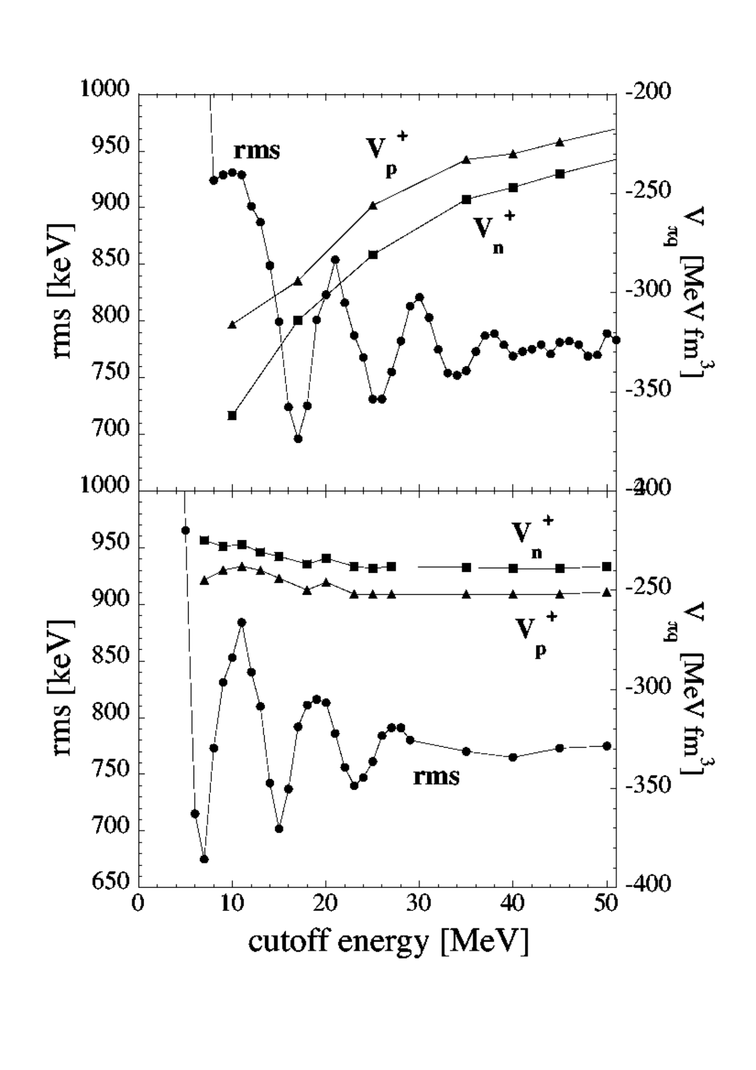
b) Aims to make results independent of choice of cutoff energy.

c) With cutoff defined by

$$\varepsilon_i \leq E_F + \varepsilon_\Lambda \quad ,$$

Bulgac and Yu found that energy becomes independent of ε_i for $\varepsilon_\Lambda \geq 25$ MeV.

Set of 657 (quasi-)spherical nuclei.



- Confirm BY result that energies independent of ε_Λ for $\varepsilon_\Lambda \geq 25$ MeV.

- With BY can reduce cutoff from 17 to 7 MeV, whence enormous time savings.

- Better fits also.

- Force BSk10 (t_4) incorporates BY schema, but with ε_Λ at its BY value of 25 MeV.

- BY was NOT the reason why we were able to weaken pairing in BSk10: t_4 term is necessary and sufficient.

Have now produced a new t_4 force, BSk11.
Very similar to BSk10, except $\varepsilon_\Lambda = 7$ MeV.

c) Coulomb correlations.

A. Bulgac and V. R. Shaginyan, Nucl. Phys. A601 (1996) 103,

Phys. Lett. B469 (1999) 1.

Coulomb-correlation energy comparable in magnitude but opposite in sign to Coulomb-exchange energy. Thus it can be taken into account simply by dropping the exchange term.

Force BSk12

Refit force BSk11 without Coulomb-exchange term. Fit to masses is actually slightly better, but extrapolations out to neutron drip line diverge.

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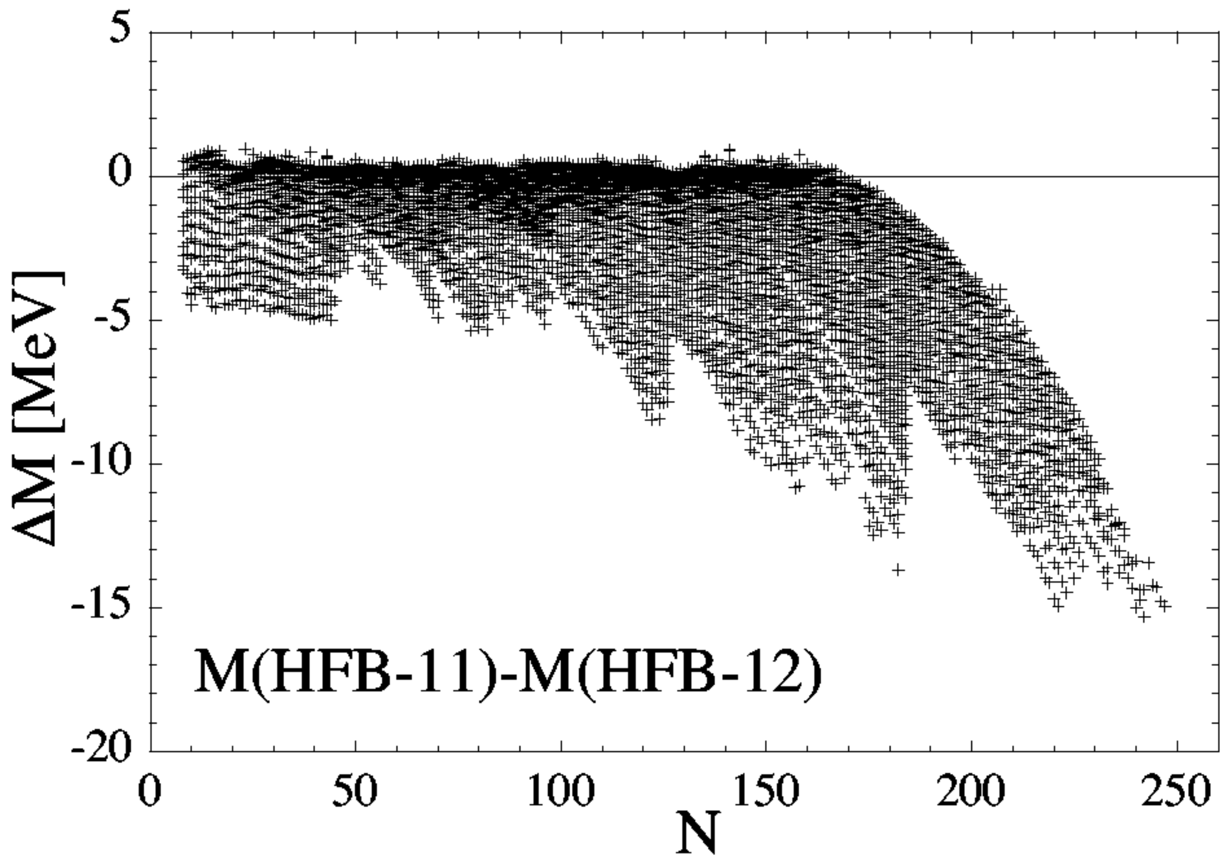

• **But again, what counts for the r-process is S_n and Q_β.**

Rms and mean differences (in MeV) between the BSk11 and BSk12 models for the S_n and Q_β of 2182 neutron-rich nuclei ($Z \geq 26; 4$ MeV $\geq S_n \geq 0.5$ MeV). (Mean differences correspond to BSk11 - BSk12.)

	S_n	Q_β
σ	0.266	0.593
$\bar{\epsilon}$	0.198	-0.545

• Dropping Coulomb exchange has no significant effect on S_n (and negligible effect on position of neutron drip line).

• Dropping Coulomb exchange systematically increases Q_β of n-rich nuclei by around 0.5 MeV. This is probably below the threshold of significance, given all the other uncertainties.

5. Concluding remarks.

- Mass models based on the Skyrme-HFB method are now quite feasible, with high quality fits to the mass data, and to neutron matter.

- Some flexibility on M_s^*. Best overall fit to masses and s.p. energies for $M_s^* = 0.92M$; this value is also theoretically acceptable.

- Bulgac-Yu scheme permits lower pairing cutoff and thus considerable reduction in computer time.

- For astrophysical purposes can probably forget about Coulomb correlations.

- With t_4 term residual correlation energy is absorbed into Skyrme force, whence pairing strength can be reduced to the minimal value required by even-odd differences.

- Tables constructed for $N, Z \geq 8$ from one drip line to the other.

- Can be extrapolated *beyond* the drip line to give EOS of neutron-star matter; important to fit to theoretical neutron-matter energy curve.

- Note that our model(s) are not yet completely microscopic: Wigner term.

- Will want to go beyond Skyrme + δ-function pairing to get closer to "real" forces.