3rd CNS International Summer School (CISS04)

Towards the Universal Nuclear Energy Density Functional

(August 17-20, 2004)

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- Introduction
- Basic concepts, general strategy, burning questions
- Mean-field theory
  - Hartree-Fock (-Bogoliubov)
  - Spontaneous Symmetry Breaking
  - Deformed Mean Fields
  - Pairing
- Density functional theory
  - Introduction to DFT and LDA
  - Nuclear Energy Density Functional
- Nuclear fields
  - Energy, shell effects
  - Densities, radii
- Beyond Mean Field (correlation terms)
  - Generator Coordinate Method
  - Random Phase Approximation
- Summary & Perspectives

Literature

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第三回国際サマースクール

CISS04
The 3rd CNS International Summer School

August 17–20, 2004
Center for Nuclear Study (CNS), Wako Campus
University of Tokyo

TOPICS TO BE COVERED INCLUDE:
Nuclear mean field theory
No core shell model
Shell evolution in unstable nuclei
Spin-isospin excitations in nuclei
Gamma-ray spectroscopy of unstable nuclei
Penta-quark state

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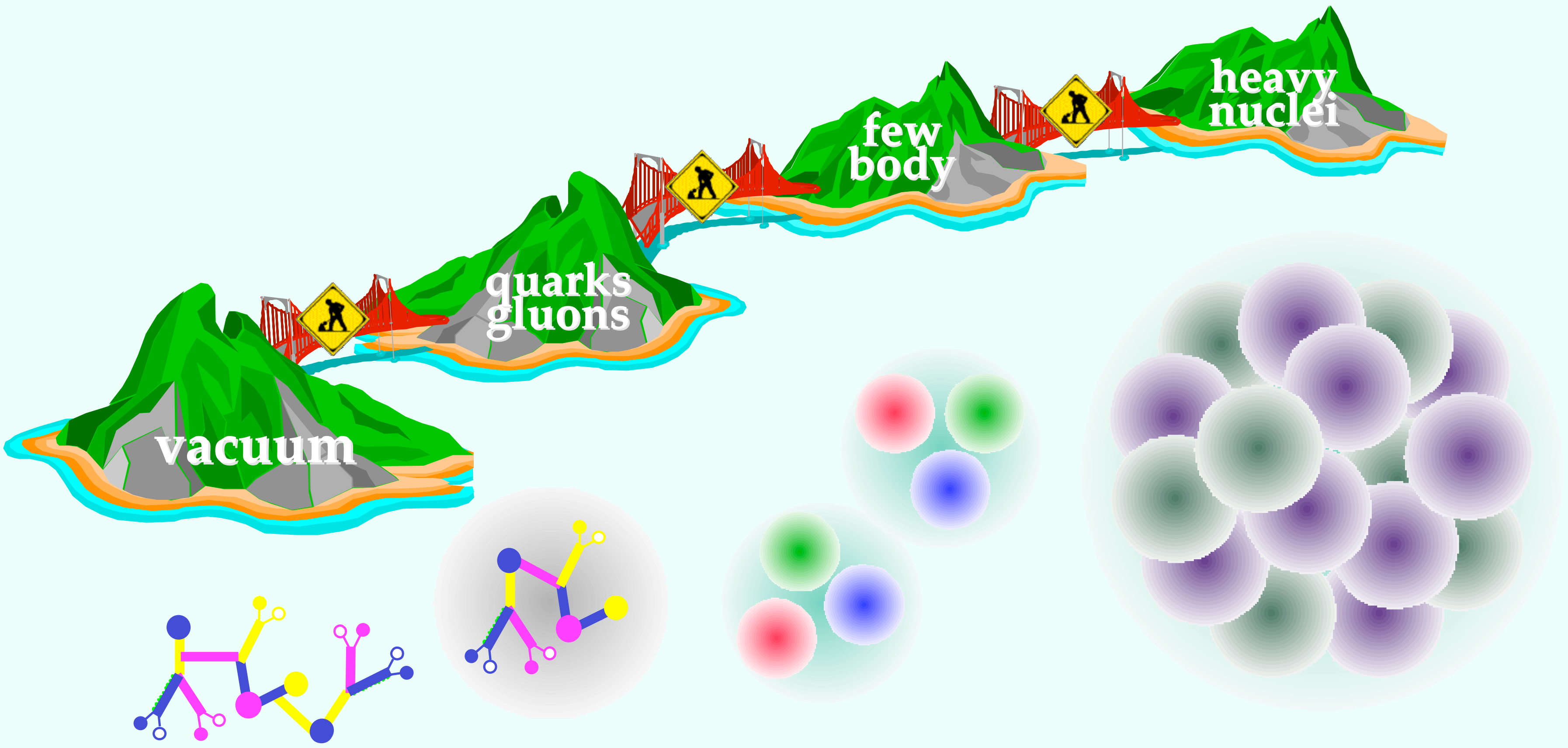
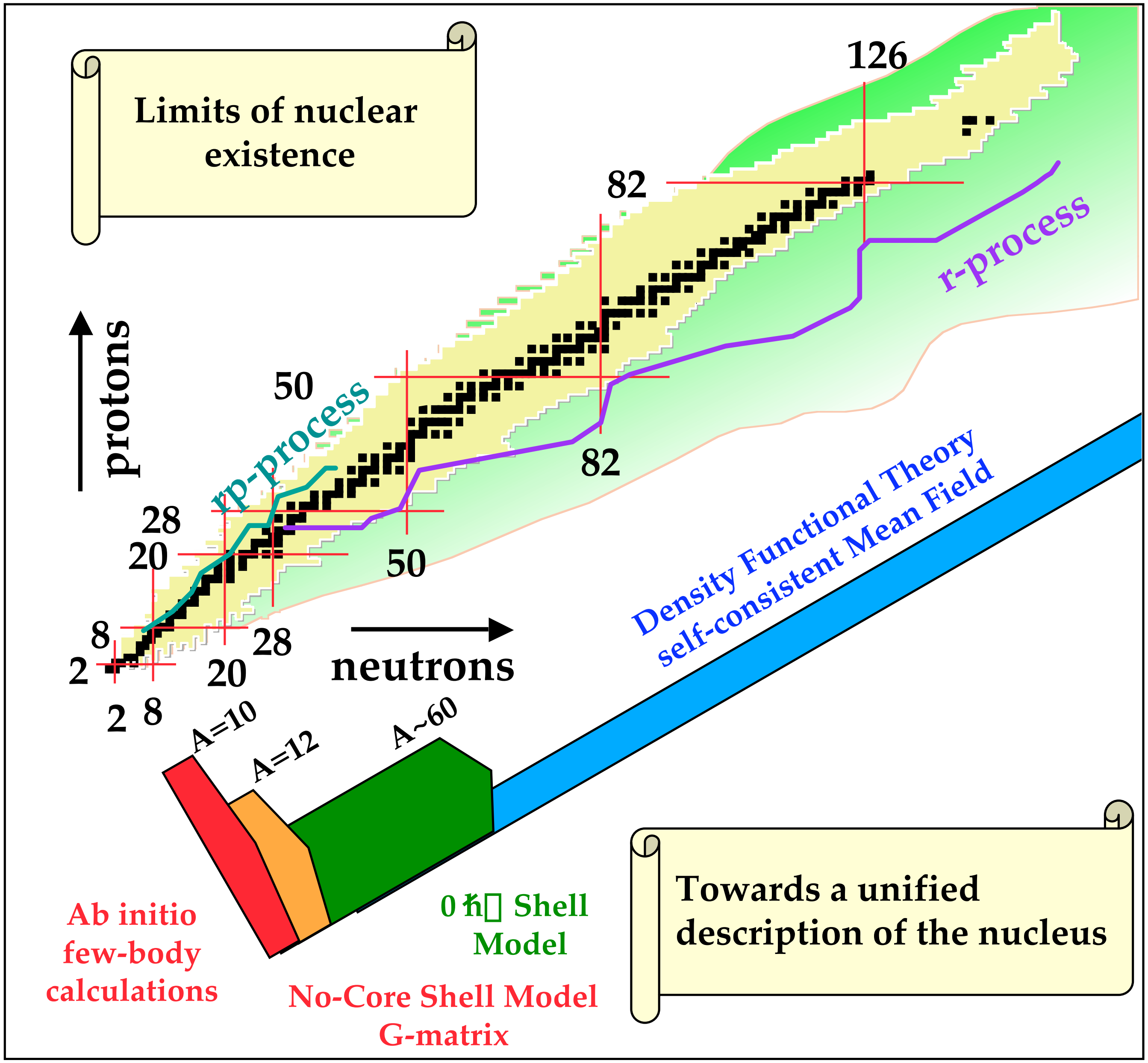


quark-gluon plasma
QCD

nucleon
QCD

few body systems
free NN force

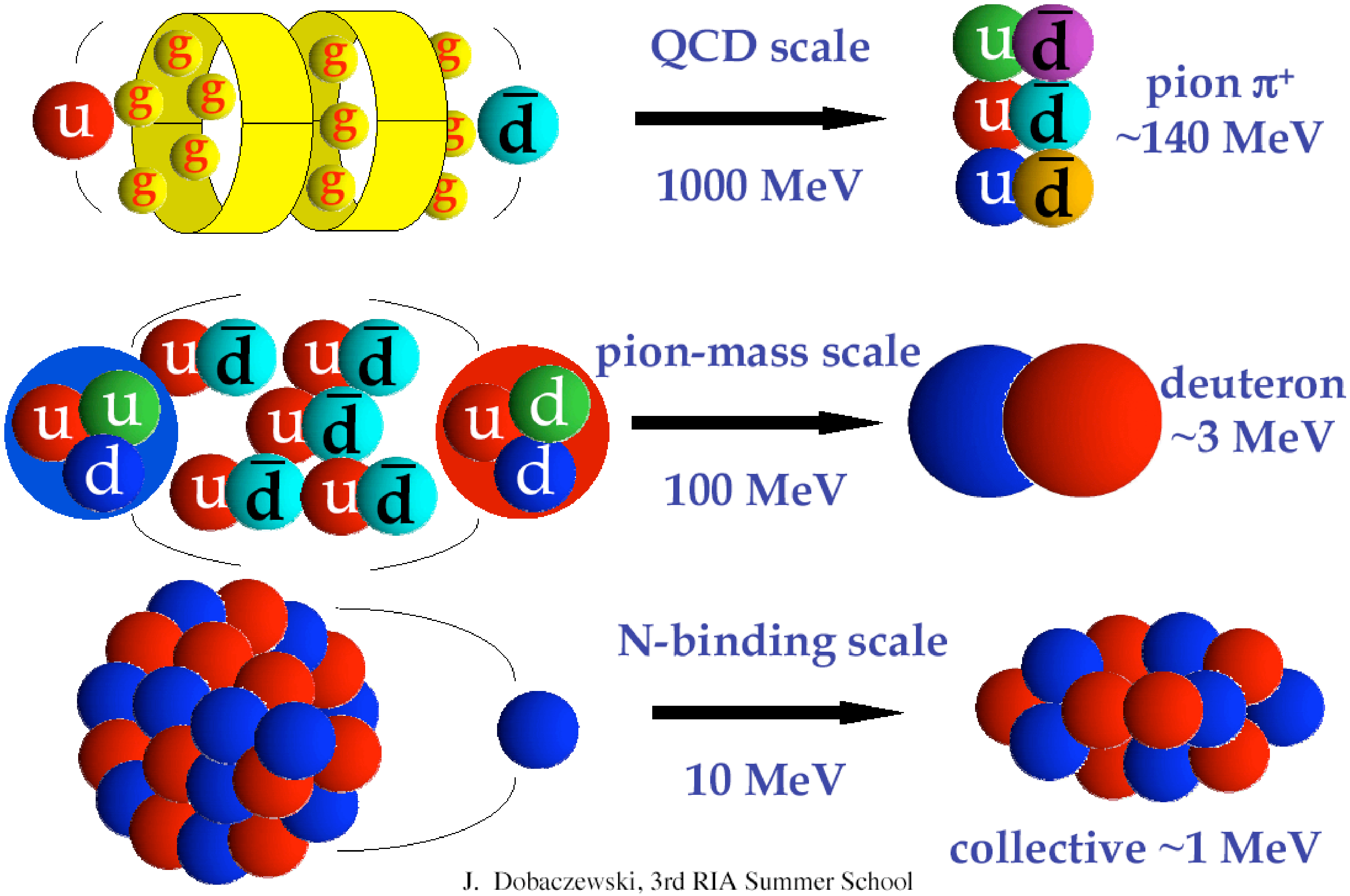
many body systems
effective NN force



Limits of nuclear existence

Towards a unified description of the nucleus

Energy Scales in Nuclear Physics



QCD scale

1000 MeV

pion π^+
~140 MeV

pion-mass scale

100 MeV

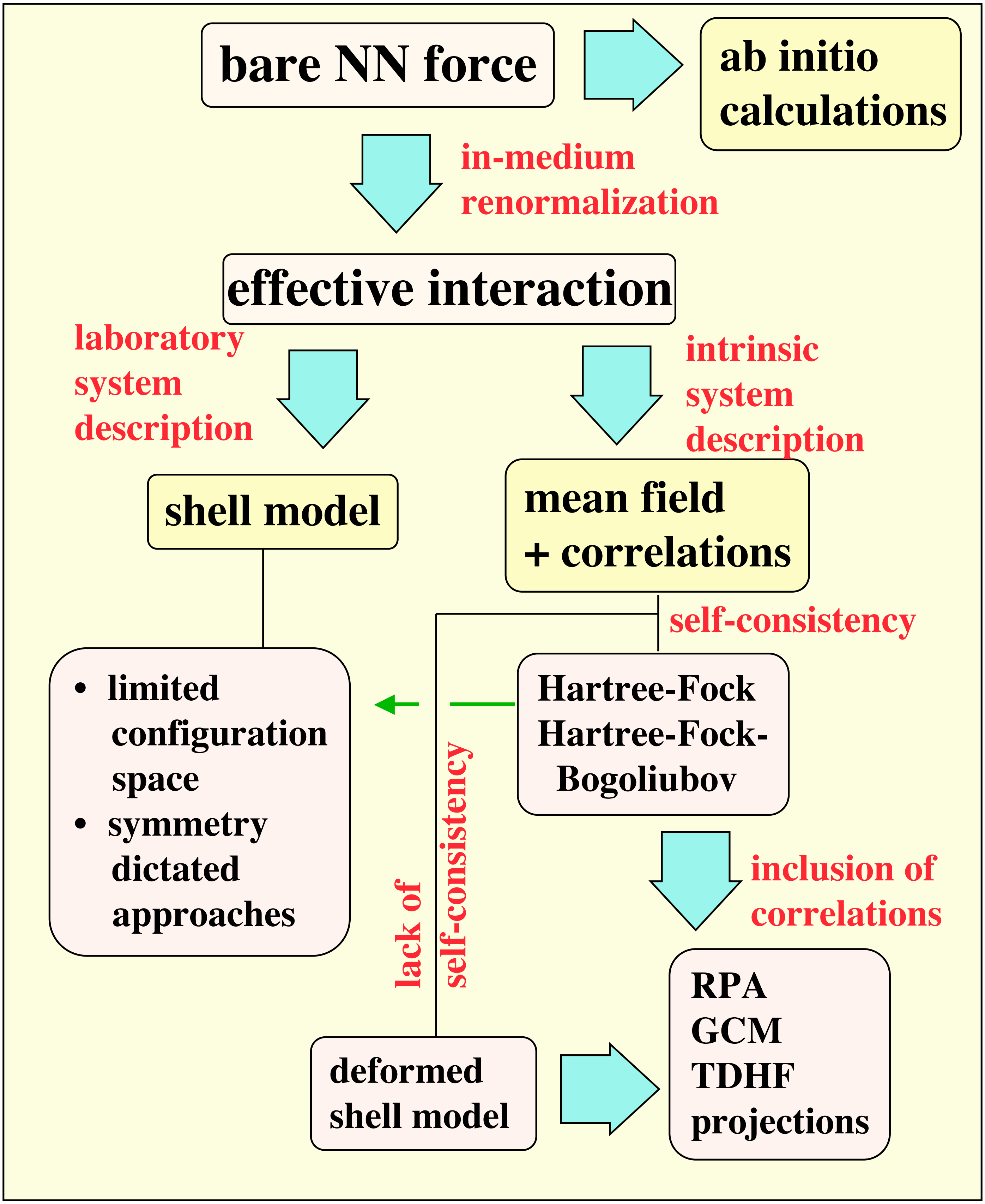
deuteron
~3 MeV

N-binding scale

10 MeV

collective ~1 MeV

The Nuclear Many-Body Problem



bare NN force

ab initio calculations

in-medium renormalization

effective interaction

laboratory system description

intrinsic system description

shell model

mean field
+ correlations

self-consistency

- limited configuration space
- symmetry dictated approaches

Hartree-Fock
Hartree-Fock-Bogoliubov

lack of self-consistency

inclusion of correlations

deformed shell model

RPA
GCM
TDHF
projections

Hartree Fock

(a brief summary)

A. Two-body (density-dependent) interaction (or the energy density functional)

$$\hat{H} = \sum_{ij} t_{ij} c_i^+ c_j + \tfrac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} c_i^+ c_j^+ c_l c_k$$

B. Variational principle:

$$\delta E[\Psi] = 0; \quad E[\Psi] = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}; \quad E[\Psi] > E_0$$

C. Trial wave functions: particle-number conserving product states

$$|\Psi\rangle = \prod_{\nu=1}^{A} a_\nu^+ |0\rangle; \quad h_{HF} |\nu\rangle = \varepsilon_\nu |\nu\rangle$$

$$a_\nu^+ = \sum_i D_{i\nu} c_i^+; \quad D^+ D = D D^+ = 1$$

known basis (e.g., h.o. basis)

...or one can explicitly use the Thouless theorem:

$$|\Psi\rangle = \frac{1}{\sqrt{\langle \tilde{Z} | \tilde{Z} \rangle}} |\tilde{Z}\rangle, \quad |\tilde{Z}\rangle = \exp\left(\sum_{ph} \tilde{Z}^*_{ph} a_p^+ a_h \right) a_1^+ a_2^+ \ldots a_A^+ |0\rangle$$

Density matrix:

$$\rho_{ij} \equiv \langle\Phi|c_j^+ c_i|\Phi\rangle = \sum_{\nu=1}^{A} D_{i\nu} D_{j\nu}^*$$

$$Tr(\hat\rho) = A; \quad \hat\rho^2 = \hat\rho \Leftrightarrow \hat\rho(1-\hat\rho) = 0$$

Eigenvalues of ρ are the occupation quantum numbers:

$$n_\nu = \begin{cases} 1 \text{ for } \nu \le A \\ 0 \text{ for } \nu > A \end{cases}$$

Consider a small variation $\delta\rho$:

$$(\hat\rho + \delta\hat\rho)^2 = \hat\rho + \delta\hat\rho$$

$$\Rightarrow \quad \hat\rho\,\delta\hat\rho\,\hat\rho = 0$$

$\delta\rho$ has only matrix elements in the ph channel!

occupied (holes) empty (particles)

$$\hat\rho = \left(\begin{array}{ccccc|cccc}
1 & 0 & & & & & & & \\
0 & 1 & & & & & & & \\
 & & \ddots & & & & 0 & & \\
 & & & 1 & 0 & & & & \\
 & & & 0 & 1 & & & & \\
\hline
 & & & & & 0 & & & \\
 & & & & & & 0 & & \\
 & & 0 & & & & & \ddots & \\
 & & & & & & & & 0 \\
\end{array}\right)$$

1 A A+1

$$E_{HF}\left(\hat{\rho}\right) = Tr\left(t\hat{\rho}\right) + \tfrac{1}{2}Tr_1 Tr_1\left(\hat{\rho}\bar{v}\hat{\rho}\right)$$

$$\delta E_{HF} = E_{HF}\left(\hat{\rho}+\delta\hat{\rho}\right) - E_{HF}\left(\hat{\rho}\right) = 0$$

$$\delta E_{HF} = \sum_{ij} h_{ij}\delta\rho_{ij} = 0, \quad h_{ij} \equiv \frac{\partial E_{HF}\left(\hat{\rho}\right)}{\partial\rho_{ji}} = t_{ij} + \Gamma_{ij}$$

h=0 in the ph channel!

HF hamiltonian does not couple particle and hole states!

Self-consistent HF field:

$$\Gamma_{ij} \equiv \sum_{kl} \bar{v}_{ikjl}\rho_{kl} + \left\langle \Phi \left| \frac{\partial\bar{v}}{\partial\rho_{ji}} \right| \Phi \right\rangle$$

Rearrangement potential (results from the density dependence of v)

Hartree-Fock equations

$$\left[h,\hat{\rho}\right]=\left[t+\Gamma(\hat{\rho}),\hat{\rho}\right]=0 \Rightarrow \sum_j h_{ij}\left(D,D^*\right)D_{j\mu}=\varepsilon_\mu D_{i\mu}$$

ρ and *h* can be diagonalized simultaneously

Non-linear Hermitian eigenvalue problem

Deformed shell model energy

Absent in the deformed shell model

$$E_{HF}=\sum_{\mu=1}^{A}\varepsilon_\mu-\tfrac{1}{2}\sum_{\mu\nu=1}^{A}\bar{v}_{\mu\nu\mu\nu}-\tfrac{1}{2}\sum_{\mu=1}^{A}\left\langle\Phi\left|\frac{\partial\bar{v}}{\partial\rho_\mu}\right|\Phi\right\rangle=$$

$$=\tfrac{1}{2}\sum_{\mu=1}^{A}\left[t_{\mu\mu}+\varepsilon_\mu-\left\langle\Phi\left|\frac{\partial\bar{v}}{\partial\rho_\mu}\right|\Phi\right\rangle\right]$$

Hartree Fock stability condition

HF minimum should correspond to the positive second derivative of the energy.

$$\square = \square^{(0)} + \square^{(1)} + \square^{(2)} + \ldots \quad \left(\square^{(0)} >> \square^{(1)} >> \square^{(2)} >> \ldots\right)$$

$$\square^2 = \square \quad \Rightarrow \quad \boxed{\begin{aligned} \square^{(1)} &= \left[\left[\square^{(1)},\square^{(0)}\right],\square^{(0)}\right] \\ \square^{(2)} &= \left[\left[\square^{(2)},\square^{(0)}\right],\square^{(0)}\right] + \frac{1}{2}\left[\left[\square^{(1)},\square^{(0)}\right],\square^{(1)}\right] \end{aligned}}$$

This implies that independent variations are only in the ph channel (pp and hh matrix elements of $\square^{(1)}$ and $\square^{(2)}$ vanish)

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \ldots$$

$$E^{(0)} = \mathrm{Tr}\left(T\square^{(0)}\right) + \frac{1}{2}\mathrm{Tr}\left(\square^{(0)}\square^{(0)}\right)$$

$$E^{(1)} = \mathrm{Tr}\left(\left[h^{(0)},\square^{(0)}\right]\left[\square^{(0)},\square^{(1)}\right]\right)$$

$$E^{(2)} = \mathrm{Tr}\left(\left[h^{(0)},\square^{(0)}\right]\left[\square^{(0)},\square^{(21)}\right]\right)$$

$$+ \frac{1}{2}\mathrm{Tr}\left(\square^{(1)}\left[\left[h^{(0)},\square^{(1)}\right] + \left[\square^{(1)},\square^{(0)}\right],\square^{(0)}\right]\right)$$

$$E^{(1)} = 0$$

$$E^{(2)} = \frac{1}{2}\left(\square^{(1)}\middle|M^{(0)}\middle|\square^{(1)}\right) > 0$$

$$M^{(0)}\square^{(1)} = \left[\left[h^{(0)},\square^{(1)}\right] + \left[\square^{(1)},\square^{(0)}\right],\square^{(0)}\right]$$

The HF stability matrix
(must be positively defined)

Relativistic mean field theory

RMF: Walecka, Ann. Phys. 83 (1974) 491

$$
\begin{aligned}
L = \bar\psi\left[i\gamma^\mu\partial_\mu - M\right]\psi &+ \tfrac{1}{2}\partial_\mu\sigma\partial^\mu\sigma - U(\sigma) - g_\sigma\bar\psi\sigma\psi \\
&-\tfrac{1}{4}H_{\mu\nu}H^{\mu\nu} + \tfrac{1}{2}m_\omega^2\omega_\mu\omega^\mu - g_\omega\bar\psi\gamma_\mu\psi\omega^\mu \\
&-\tfrac{1}{4}G^a_{\mu\nu}G^{a\mu\nu} + \tfrac{1}{2}m_\rho^2\rho^a_\mu\rho^{a\mu} - g_\rho\bar\psi\gamma_\mu\tau^a\psi\rho^{\mu a} \\
&-\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} - e\bar\psi\gamma_\mu\frac{(1-\tau_3)}{2}\psi A^\mu
\end{aligned}
$$

ψ - SU(2) baryon field of mass M, $\sigma, \omega_\mu, \rho^a_\mu$ - mesonic fields with masses $m_\sigma, m_\omega, m_\rho$

A_μ - photon field, $H_{\mu\nu}, G^a_{\mu\nu}, F_{\mu\nu}$ - field tensors for the vector fields

$g_\sigma, g_\omega, g_\rho$ - meson - NN coupling constants

$U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_3\sigma^3 + \frac{1}{4}g_4\sigma^4$ - nonlinear (NL) σ - potential.

The stationary Dirac equation for baryons

$$\left[-i\vec\alpha\cdot\vec\nabla + \beta M^*(\vec r) + V(\vec r)\right]\psi_i(\vec r) = \varepsilon_i\psi_i(\vec r)$$

$$M^*(\vec r) = M + g_\sigma\sigma(\vec r), \qquad V(\vec r) = g_\omega\omega^0(\vec r) + g_\rho\tau_3\rho_3^0(\vec r) + e\frac{1-\tau_3}{2}A^0(\vec r)$$

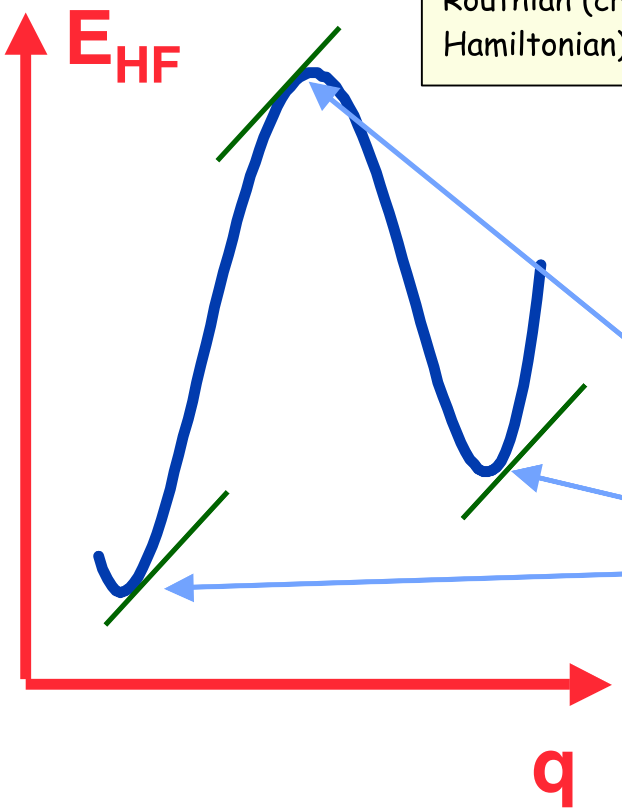
The spatial currents vanish if spherical symmetry imposed. Charge conservation guarantees that only the third component of ρ survives. The mesonic field are found by solving the Klein-Gordon equations. The photon field is found by solving the Poisson equation. For example:

$$\left(-\Delta + m_\rho^2\right)\rho_3^0(r) = g_\rho\rho_3(r), \qquad \rho_3(r) = \sum_{i=1}^{A}\bar\psi_i(r)\tau_3\gamma^0\psi_i(r)$$

Constrained Hartree-Fock

Often, we are interested not only in the local HF minima but also in the whole potential energy surface (PES)

$$\delta\langle\Phi|\hat{H}|\Phi\rangle = 0 \quad \text{at a fixed value of} \quad q = \langle\Phi|\hat{Q}|\Phi\rangle$$



Routhian (cranked Hamiltonian)

$$\hat{H}' = \hat{H} - \lambda\hat{Q}$$

$$\delta\langle\Phi|\hat{H}'|\Phi\rangle = 0$$

$$\lambda = \frac{dE}{dq}$$

Collective coordinate

- ❑ Several ways of solving the CHF equations (linear constraint, quadratic constraint, gradient method)
- ❑ Usually: many-dimensional surfaces
- ❑ Static picture - fluctuations are not included!

Self-consistent HF symmetries

$$\left[\hat{H}, S\right] = 0 \;\Rightarrow\; S\Gamma[\hat{\rho}]S^{+} = \Gamma\left[S\hat{\rho}S^{+}\right]$$

$$\Rightarrow\; Sh[\tilde{\rho}]S^{+} = h\left[S\tilde{\rho}S^{+}\right]$$

If $\hat{\rho}_{(i)}$ has a certain symmetry then $\hat{\rho}_{(i+1)}$ has the same symmetry.

- If a certain symmetry for the solution is expected, one can start with an initial density which has this symmetry
- If one starts with a certain symmetry, one will always stay within this symmetry (if the deepest minimum is deformed, one will never get to it starting with a spherically symmetric density matrix)
- The above discussion can be generalized to density dependent interactions satisfying the condition:

$$SV[\hat{\rho}]S^{-1} = V\left[S\hat{\rho}S^{-1}\right]$$

If there is a solution with a (spontaneously) broken symmetry S...

$$S\hat{\rho}S^{+} = \hat{\rho}_1 \neq \hat{\rho}$$

$$\Downarrow$$

$$h(\hat{\rho}_1) = Sh(\hat{\rho})S^{+}$$

$$\Downarrow$$

$$\left[h(\hat{\rho}_1),\hat{\rho}_1\right] = S\left[h(\hat{\rho}),\hat{\rho}\right]S^{+} = 0$$

...then every transformed (rotated) state is also a solution of the HF equations!

Goldstone Theorem

$$\hat{\rho}_1 = S\hat{\rho}S^{+} \qquad \Rightarrow \qquad M^{(0)}\hat{\rho}_1 = 0$$

If a symmetry is broken, there appears a zero-energy mode (Goldstone boson!)

Nuclear deformation: spontaneous symmetry breaking

Molecular physics: Jahn-Teller effect 1937

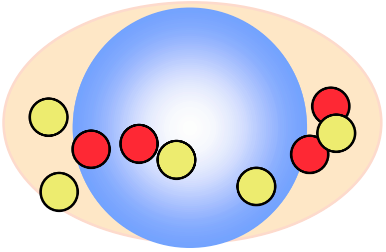
Any configuration of atoms or ions (except a linear chain) can develop a stable symmetry-breaking deformation provided the coupling between degenerate electronic excitations and collective molecular vibrations is strong.

Nuclear physics: Bohr-Mottelson 1952-53

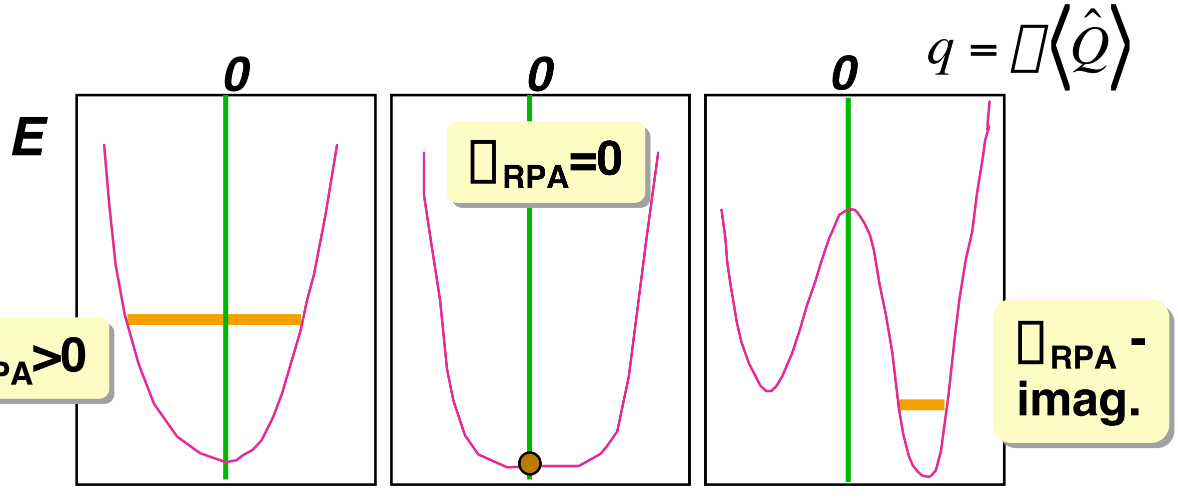
Any nuclear configuration can develop a stable symmetry-breaking deformation provided the coupling between degenerate single-nucleonic excitations and collective nuclear modes is strong.

The unified model. Particle vibration coupling

$$V_{\text{int}} = \square\square(r)\sum_{\square\square} \square_{\square\square} Y_{\square\square}(\square)$$



Symmetry breaking



$□_{RPA}>0$

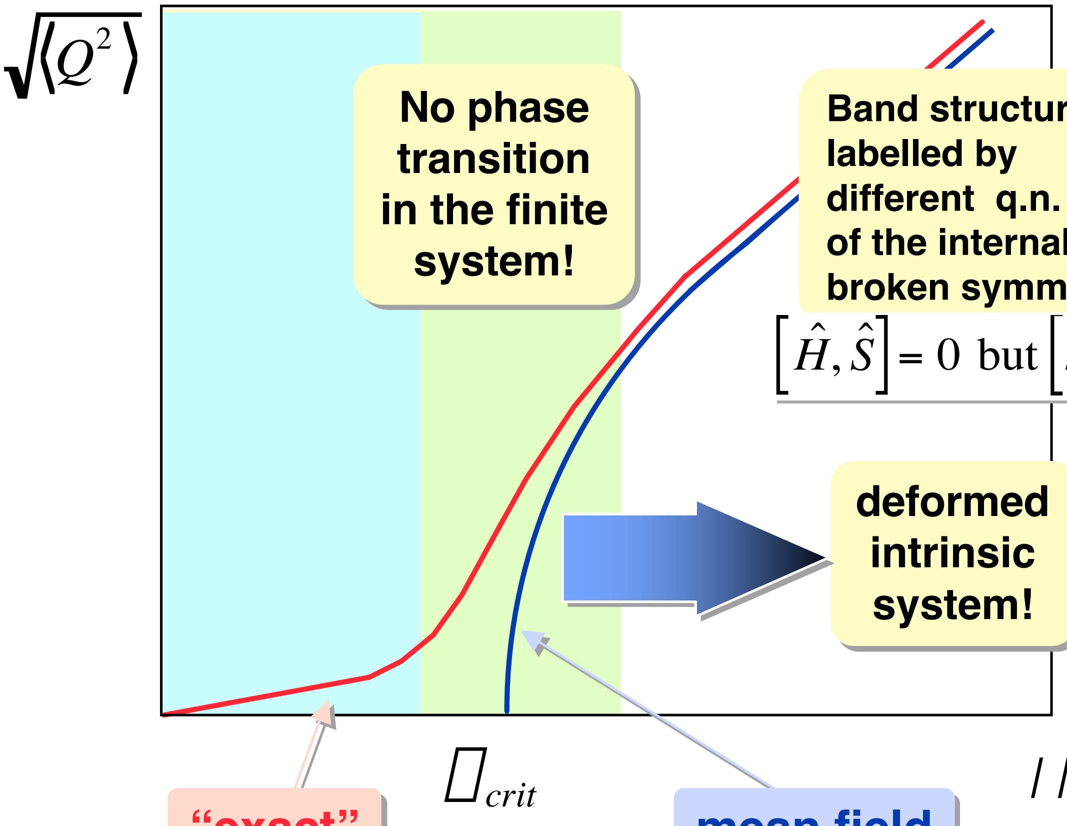
$□_{RPA}=0$

$□_{RPA}$ - imag.

Vibrator (weak coupling)

Soft (interm. coupling)

Rotor (strong coupling)



No phase transition in the finite system!

Band structures labelled by different q.n. of the internally broken symmetries

$$\left[\hat{H},\hat{S}\right]=0 \text{ but } \left[\hat{h},\hat{S}\right]\neq 0$$

deformed intrinsic system!

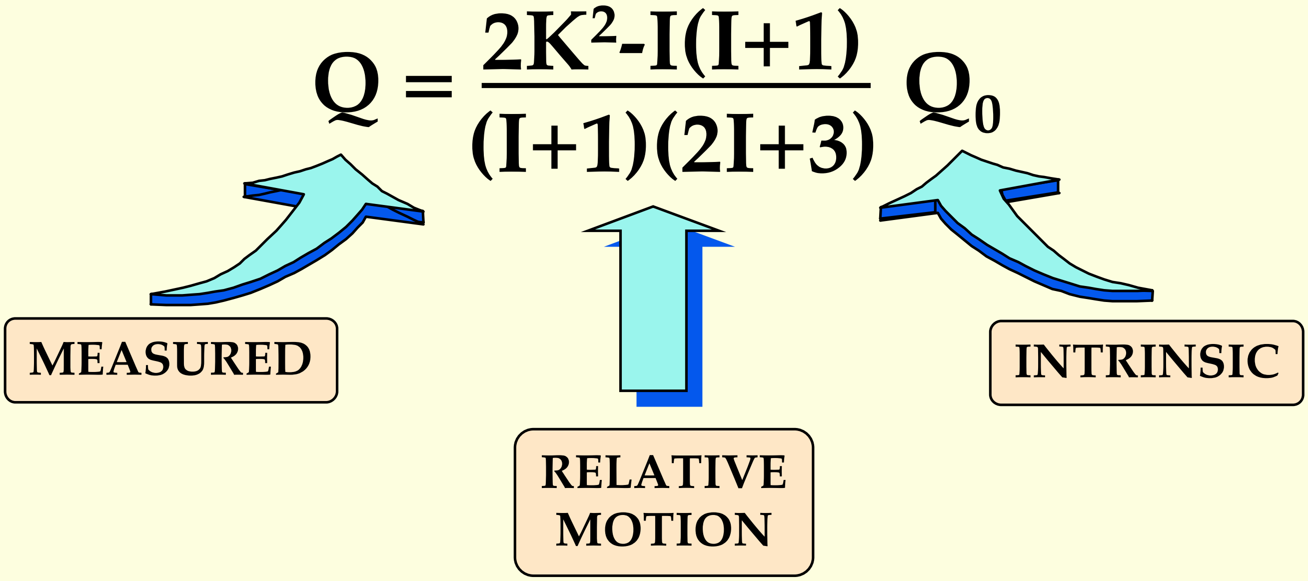
"exact"

mean field

Nuclear deformations, examples

- Isoscalar shape deformations
  - Even-L I^2 (K) - broken
  - All-L I^2, □ - broken
- Isovector shape deformations
  - L=1   (intrinsic dipole moments)
  - L=2, K=1   (scissors modes)
- Pair deformations
  - J=0, T=1   N - broken
  - J=1, T=0   T, N - broken
- Odd-T modes, spin modes
  - orientation angles

Laboratory frame and intrinsic frame



$$Q = \frac{2K^2 - I(I+1)}{(I+1)(2I+3)} Q_0$$

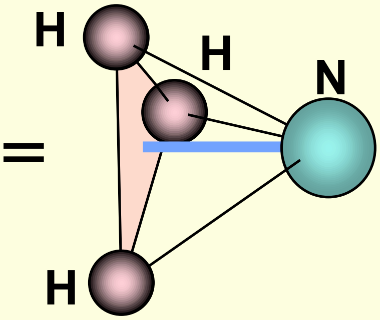
MEASURED

RELATIVE MOTION

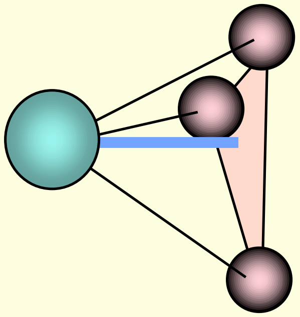
INTRINSIC

Q=0 for I=K=0, independently of Q_0 !

$|R\rangle =$

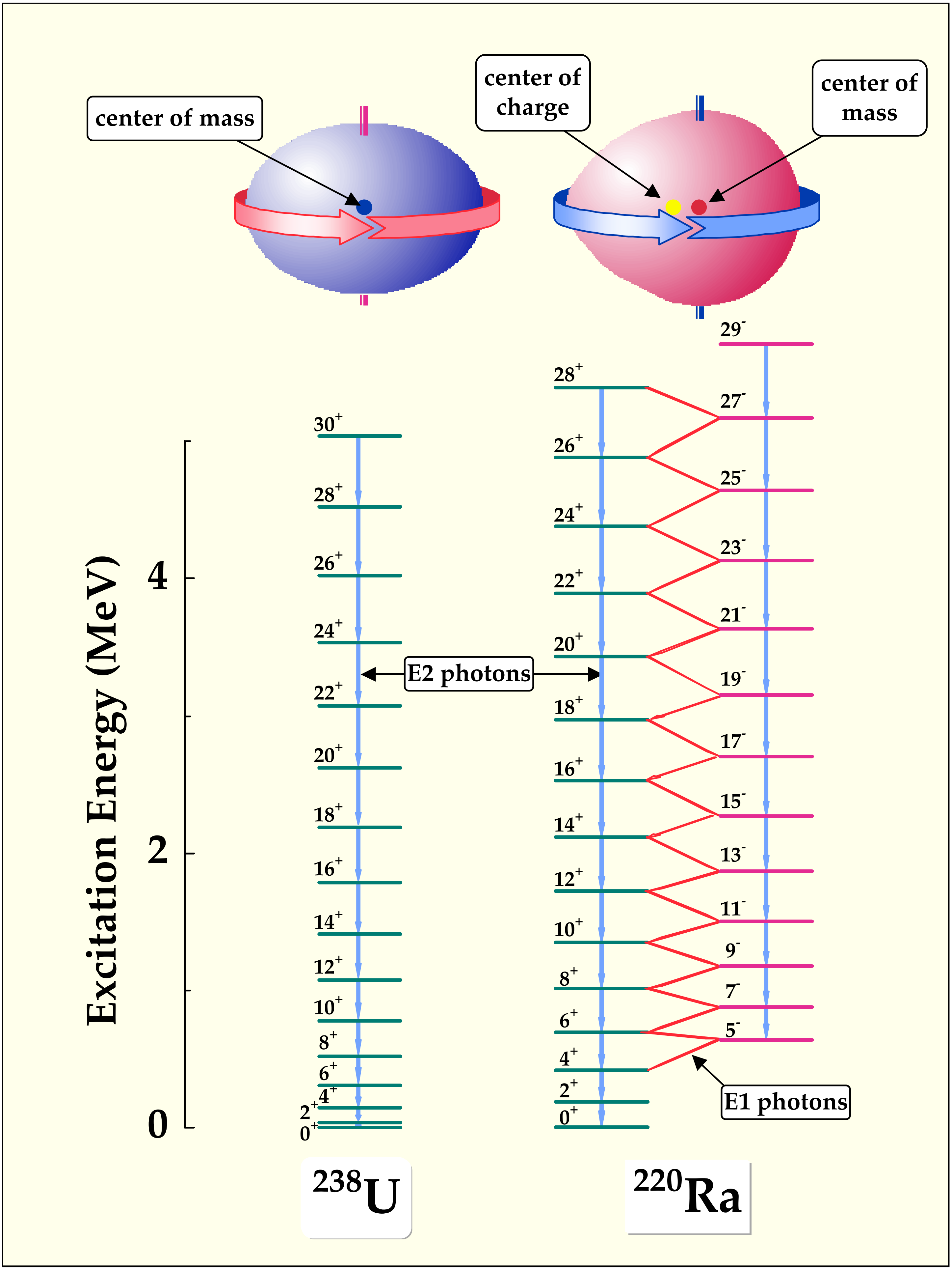


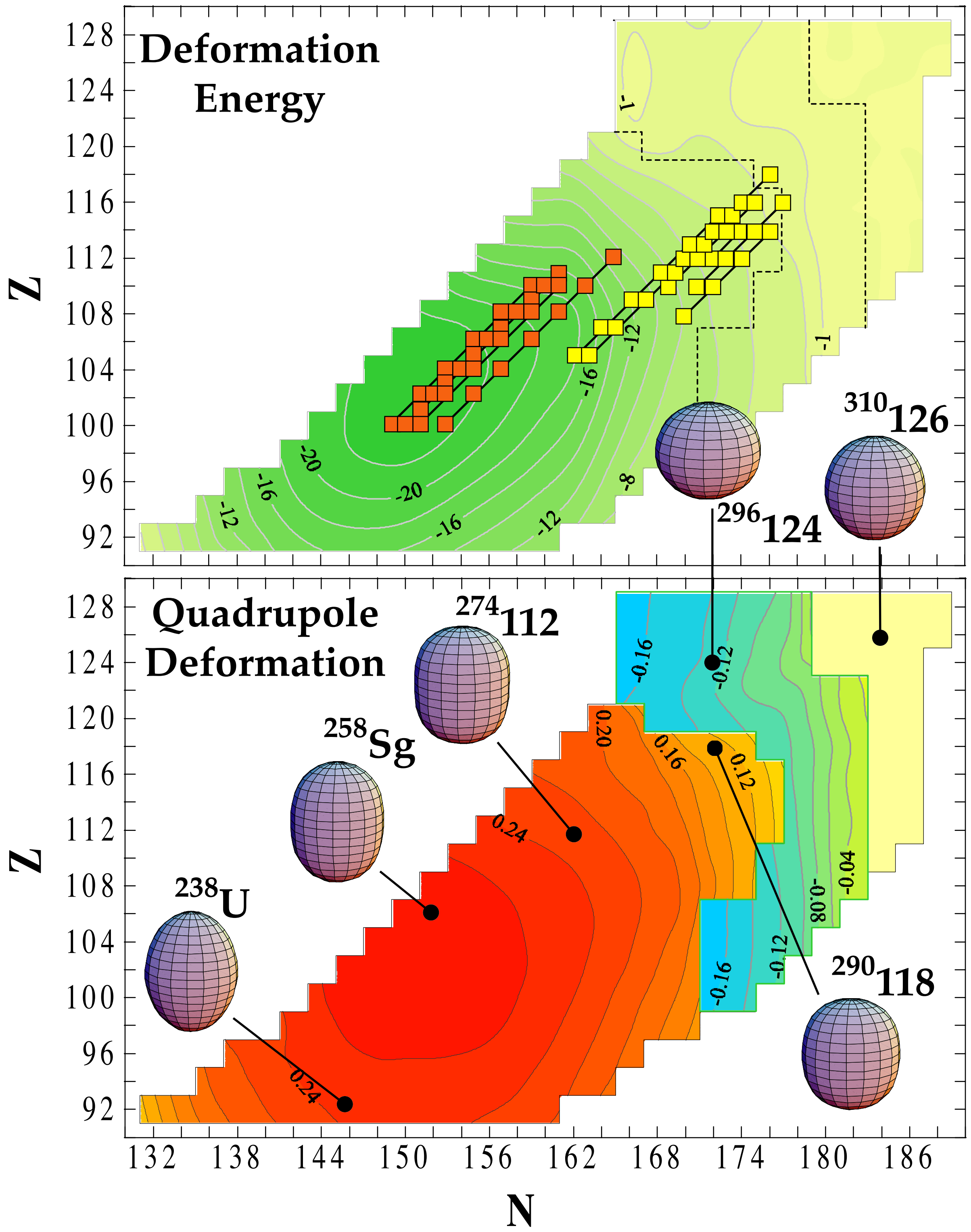
$|L\rangle =$



$$\hat{P}|L\rangle = |R\rangle \qquad |\square_{\square}\rangle = \frac{1}{\sqrt{2}}\left(1 + \square\hat{P}\right)|L\rangle$$

$\langle\square_{\square}|\vec{D}|\square_{\square}\rangle = 0$ **but** $\langle L|\vec{D}|L\rangle \neq 0$


center of mass
center of charge
center of mass
Excitation Energy (MeV)
0
2
4
30+
28+
26+
24+
22+
20+
18+
16+
14+
12+
10+
8+
6+
4+
2+
0+
E2 photons
28+
26+
24+
22+
20+
18+
16+
14+
12+
10+
8+
6+
4+
2+
0+
29-
27-
25-
23-
21-
19-
17-
15-
13-
11-
9-
7-
5-
E1 photons
238U
220Ra



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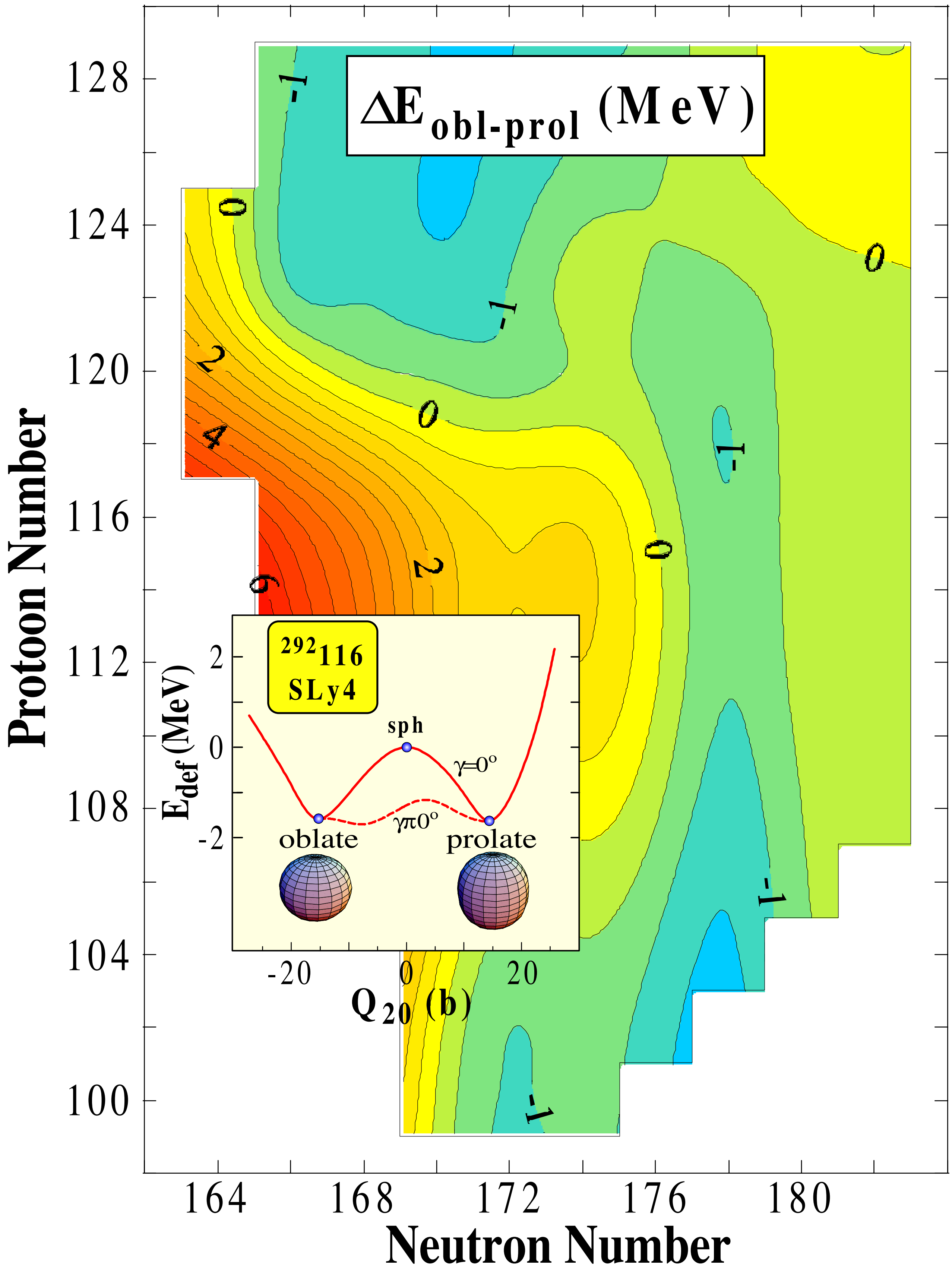
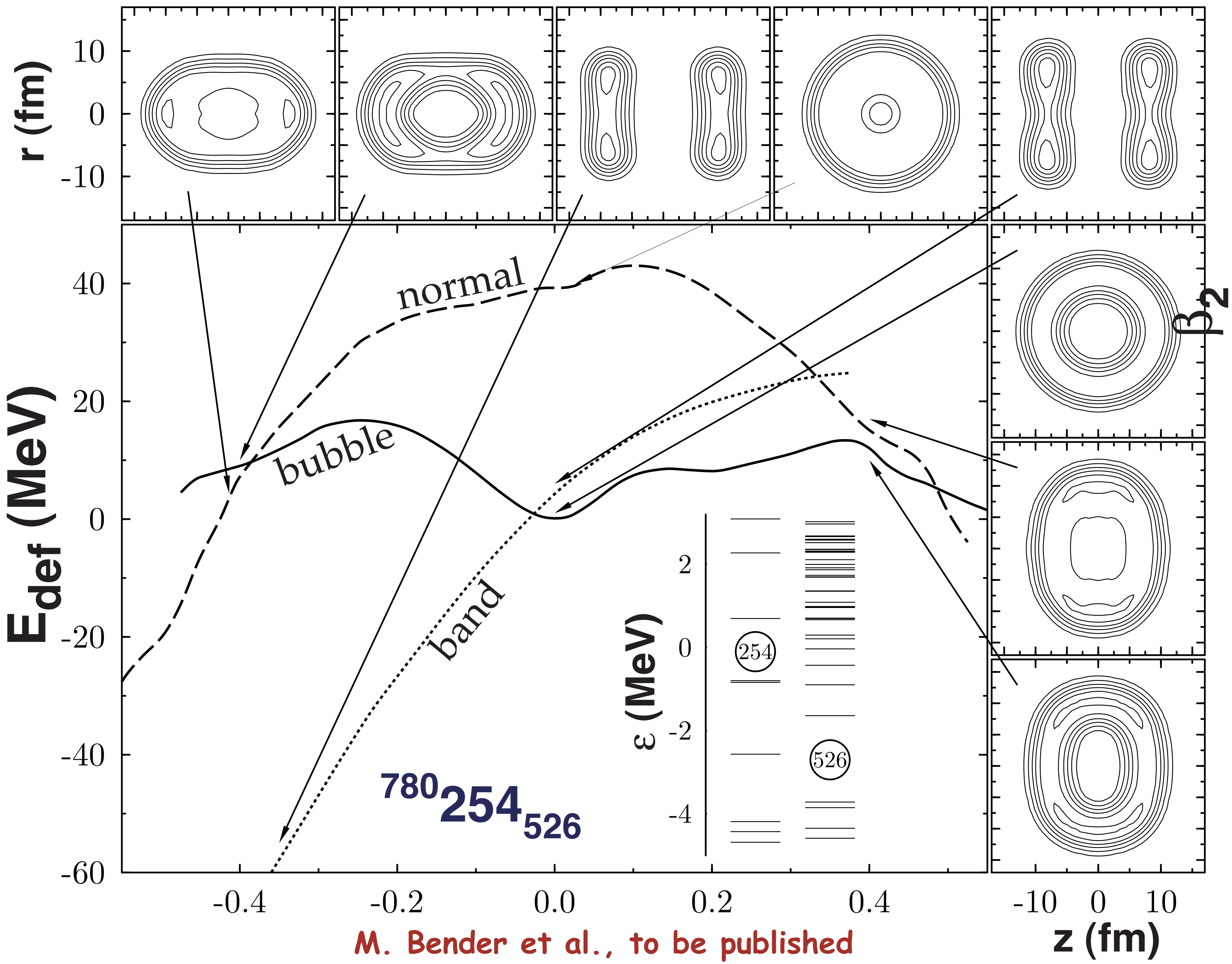
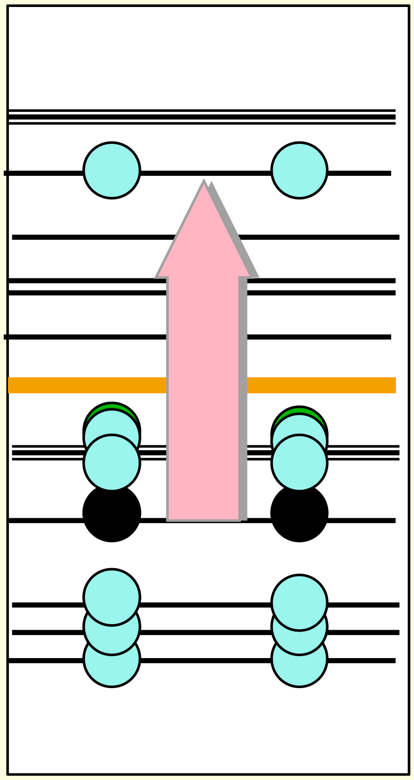




M. Bender et al., to be published

Independent quasiparticle approach



ε_F

$$\alpha_k^+ = u_k c_k^+ - v_k c_{\bar{k}}$$

$$\alpha_{\bar{k}}^+ = u_k c_{\bar{k}}^+ + v_k c_k$$

Bogoliubov-Valatin Transformation

$$\text{phase convention:}\quad u_{\bar{k}} = u_k > 0,\qquad v_k = -v_{\bar{k}} > 0$$

$$\{\alpha_k, \alpha_j\} = 0, \quad \{\alpha_k^+, \alpha_j^+\} = 0,$$

$$\{\alpha_k, \alpha_j^+\} = \delta_{ij} \Rightarrow u_k^2 + v_k^2 = 1$$

$$|0\rangle = |BCS\rangle = \prod_{k>0} \left(u_k + v_k c_k^+ c_{\bar{k}}^+\right)|-\rangle$$

BCS wave function is the quasiparticle vacuum!

$$\alpha_k|0\rangle = 0$$

$$|0\rangle \propto \exp\left(A^+\right)|-\rangle = \sum_{n=0} \tfrac{1}{n!}\left(A^+\right)^n|-\rangle$$

$$A^+ = \sum_{k>0} \frac{u_k}{v_k} c_k^+ c_{\bar{k}}^+$$

BCS function is a superposition of different number of pairs

- **Important ground-state correlations are included**
- **BCS wave function does not have a sharp particle number (an intrinsic wave function!)**

Hartree-Fock-Bogoliubov

A. Two-body (density-dependent) interaction:

$$\hat{H} = \sum_{ij} t_{ij} c_i^+ c_j + \tfrac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} c_i^+ c_j^+ c_l c_k$$

B. Variational principle:

$$\delta E[\Psi] = 0; \quad E[\Psi] = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}; \quad E[\Psi] > E_0$$

C. Trial wave functions: product states

$$\alpha_K^+ = \sum_i \left(u_{iK} c_i^+ + v_{iK} c_i \right)$$

general Bogoliubov transformation

$$|\Phi\rangle = \prod_K \alpha_K |0\rangle; \quad \alpha_K |\Phi\rangle = 0$$

HFB wave function is the quasuparticle vacuum

- HFB - quasiparticles incorporated into the HF formalism
- HFB wave function - the most general product wave function consisting of independently moving quasiparticles (in HF: particles)
- Selfconsistent description of coupling between p-h an p-p channels

HFB - density matrix and pairing tensor

HFB density matrix

HFB pairing tensor

$$\rho_{ij} \equiv \langle \Phi | c_j^+ c_i | \Phi \rangle, \quad \kappa_{ij} \equiv \langle \Phi | c_j c_i | \Phi \rangle$$

$$\hat{\rho} = v^* v^T, \quad \hat{\kappa} = v^* u^T$$

$$\hat{\rho}^2 - \hat{\rho} = -\hat{\kappa}\hat{\kappa}^+, \quad \hat{\rho}\hat{\kappa} = \hat{\kappa}\hat{\rho}^*$$

$$\hat{\mathcal{R}} = \begin{pmatrix} \hat{\rho} & \hat{\kappa} \\ -\hat{\kappa}^* & 1 - \hat{\rho}^* \end{pmatrix}, \quad \hat{\mathcal{R}}^2 = \hat{\mathcal{R}}$$

$$\hat{\mathcal{R}} \begin{pmatrix} u_K \\ v_K \end{pmatrix} = 0, \quad \hat{\mathcal{R}} \begin{pmatrix} v_K^* \\ u_K^* \end{pmatrix} = \begin{pmatrix} v_K^* \\ u_K^* \end{pmatrix}$$

Generalized density matrix

Eigenvalues are 0 or 1 (thus defining occupations of quasiparticle states)

$$\hat{H}(c^+, c) \to \hat{H}(\alpha^+, \alpha) = E_0 + \hat{H}_{20} + \hat{H}_{11} + \hat{H}_{\text{int}}$$

Independent quasiparticle Hamiltonian (H_{HFB})

Quasiparticle interaction

$$\left[\hat{H}, \hat{N}\right] = 0, \quad \text{but} \quad \left[\hat{H}_{HFB}, \hat{N}\right] \neq 0$$

However, we require that $\left\langle \hat{N} \right\rangle = N \Rightarrow \hat{H}' = \hat{H} - \lambda \hat{N}$

HFB equations

$$\hat{K} = \begin{pmatrix} \hat{h} \square \square & \hat{\square} \\ \square \square \hat{\square}^{*} & \square \hat{h}^{*} + \square \end{pmatrix}$$

HFB Hamiltonian

$$h_{ij} = t_{ij} + \square_{ij}$$

HF Hamiltonian

$$\square_{ij} = \underset{kl}{\square} \bar{v}_{iljk} \square_{kl}$$

Selfconsistent HF field

$$\square_{ij} = \tfrac{1}{2} \underset{kl}{\square} \bar{v}_{ijkl} \square_{kl}$$

Selfconsistent pair field

HFB equations

$$\begin{pmatrix} \hat{h} \square \square & \hat{\square} \\ \square \square \hat{\square}^{*} & \square \hat{h}^{*} + \square \end{pmatrix} \begin{pmatrix} u_K \\ v_K \end{pmatrix} = E_K \begin{pmatrix} u_K \\ v_K \end{pmatrix}$$

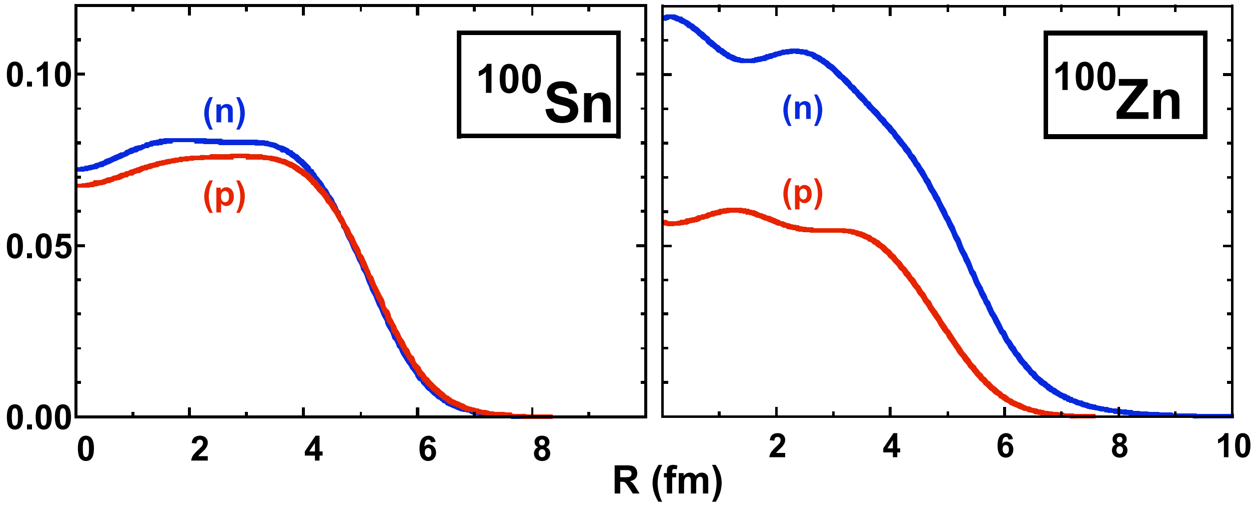
$$\left[\hat{K}, \hat{\ }\right] = 0$$

Complicated eigenvalue problem

- HFB equations treat p-h and p-p on the same footing
- □ is a state-dependent field. In general, it depends on density and has a kinetic term
- The generalized density matrix and the HFB Hamiltonian can be diagonalized simultaneously
- Fermi level determined from the particle number equation
- Often it is convenien to express the HFB equations in the canonical basis

MEAN-FIELD APPROACH

Towards Nuclear Energy Density Functional



Modern Mean-Field Theory ≡ Energy Density Functional

$\square$, $\square$, $\overset{\square}{J}$, $\overset{\square}{j}$, $\overset{\square}{T}$, $\overset{\square}{s}$, $\overset{\square}{F}$,

+ pairing densities!

mean field □ one-body densities

zero range □ local densities

finite range □ non-local densities

- Hohenberg-Kohn
- Kohn-Sham
- Negele-Vautherin
- Landau-Migdal
- Nilsson-Strutinsky

What are the main goals we want to achieve?

1. Find a universal energy density functional which correctly describes:
   a) static ground-state properties of all bound nuclei,
   b) infinite nuclear and neutron matter,
   c) rotational properties,
   d) low-energy vibrations,
   e) small-amplitude vibrations,
   f) large-amplitude adiabatic properties (fission),

2. Find limits of applicability of the energy density functional approach:
   a) explicit symmetry restoration,
   b) configuration mixing,
   c) two-body effects and correlations,
   d) non-local effects,
   e) energy, density, spin, isospin, and mass limits,

3. Find derivation and/or motivation from first principles.

Thomas Fermi Energy Density Functional
(early atomic applications)

The ground state energy of electrons is given by **the energy density functional:**

$$E_{TF}\left[\rho(\vec{r})\right] = T_{TF}\left[\rho(\vec{r})\right] + E_{C}\left[\rho(\vec{r})\right]$$

$$T_{TF}\left[\rho(\vec{r})\right] = \frac{\hbar^2}{2m}\frac{3}{5}\left(3\pi^2\right)^{2/3}\int \rho(\vec{r})^{5/3} d^3r$$

kinetic energy of non-interacting electron gas

$$\int \rho(\vec{r}) d^3r = n$$

particle-number constraint

$$E_C\left[\rho(\vec{r})\right] = \int\int \rho(\vec{r})\rho(\vec{r}\,')\frac{e^2}{\left|\vec{r} - \vec{r}\,'\right|} d^3r d^3r'$$

$$+ E_{C,nucl}\left[\rho(\vec{r})\right]$$

electrostatic (Coulomb) energy

- Instead of the many-body wave function described by (3+1)*n* variables, one focuses on the one-body density, which is a function of *(x,y,z)*
- Describes bulk effects (shell effects ignored)
- Exchange-correlation energy is ignored

- Can be extended in terms of a systematic semiclassical $\hbar$ expansion of the Bloch density matrix (Wigner-Kirkwood expansion), see Brack and Bhaduri, "Semiclassical Physics" (Addison-Wesley Publ.), 1997

Density Functional Theory

(introduced for many-electron systems)

The Hohenberg-Kohn theorem states that the ground state electron density minimizes the energy functional:

$$E\left[\rho(\vec{r})\right] = F\left[\rho(\vec{r})\right] + \int \rho(\vec{r}) V_{ion}(\vec{r}) d^3r$$

an universal
functional

P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas",
Phys. Rev. **136**, B864 (1964)
M. Levy, Proc. Natl. Acad. Sci (USA) **76**, 6062 (1979)

The original HK proof applies to systems with nondegenerate ground states. It proceeds by *reductio ad absurdum,* using the variational principle. A more general proof was given by Levy.

- Assume that another functional *F'* with the ground state Ψ' gives rise to *the same density* ρ
- Unless *F'*-*F*=const, Ψ'≠Ψ since they satisfy different Schroedinger equations.

$$E' = \langle \Psi' | \hat{H}' | \Psi' \rangle < \langle \Psi | \hat{H}' | \Psi \rangle = E + F'[\rho] - F[\rho]$$

$$E = \langle \Psi | \hat{H} | \Psi \rangle < \langle \Psi' | \hat{H} | \Psi' \rangle = E' + F[\rho] - F'[\rho]$$

$$\Longrightarrow \quad E + E' < E + E'$$

- Thus *F* is (within a constant) a unique functional of ρ

- The minimum value of *E* is the ground state electronic energy
- Since *F* is a unique functional of the charge density, the energy is uniquely defined by ρ
- Electron density is the fundamental variable
- Calculations based on DFT are restricted to systems in their ground state
- proof of the Hohenberg-Kohn theorem is not constructive, hence the form of the universal functional *F* is not known

Since the density can unambiguously specify the potential, then contained within the charge density is the total information about the ground state of the system. Thus what was a **4N(3N)-variable problem** (where N is the number of electrons, each one having three Cartesian variables and electron spin) is reduced to the **four (three) variables** needed to define the charge density at a point.

The density determined via the variational equation

$$\frac{\delta}{\delta\rho(\vec{r})}\left[E[\rho(\vec{r})]-\mu\int d^3r\,\rho(\vec{r})\right]=0$$

exchange correlation energy

$$F[\rho(\vec{r})]=T_s[\rho(\vec{r})]+\frac{1}{2}\int\rho(\vec{r})V_H[\rho(\vec{r})]d^3r+E_{xc}[\rho(\vec{r})]$$

kinetic energy density

Hartree potential

- T_s represents that *part* of kinetic energy which corresponds to a system of independent particles with density ρ.
- The Hartree potential V_H is found self-consistently
- The exchange correlation energy contains the exchange part of the energy, plus all the contributions due to the correlations, coming from the fact that the exact wave function is not a Slater determinant. In particular, correlations coming from the total kinetic energy enter this term.
- T_s is not known explicitly for many-fermion systems. One can approximate it with the ETF expression, but the semiclassical functional cannot describe quantum shell effects!

Density Functional Theory

Kohn-Sham equations

W. Kohn and L.J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," Phys. Rev. **140**, A1133 (1965)

$$\rho(\vec{r}) \equiv \sum_i n_i |\varphi(\vec{r})|^2$$

$$T[\rho(\vec{r})] = \frac{\hbar^2}{2m} \sum_i n_i \int |\vec{\nabla} \varphi_i(\vec{r})|^2 d^3 r$$

- Takes into account shell effects
- The link between *T* and ρ is indirect, via the orbitals φ
- The occupations n determine the electronic configuration

Orbitals φ form a complete set. The occupations *n* are given by the Pauli principle (e.g., *n*=2 or 0). The variation of the functional can be done through variations of individual s.p. trial functions with a constrtaint on their norms. It almost looks like HF, but $\langle \Phi | \hat{H} | \Phi \rangle$ is replaced by *E[ρ]*.

$$\left\{ \hat{T} + V_{KS}(\vec{r}) \right\} \varphi_i(\vec{r}) = E_i \varphi_i(\vec{r})$$

Kohn-Sham equation

$$V_{KS}(\vec{r}) = V_H[\rho(\vec{r})] + V_{xc}[\rho(\vec{r})]$$

Kohn-Sham potential (local!)

$$V_{xc}[\rho(\vec{r})] = \frac{\delta}{\delta \rho(\vec{r})} E_{xc}(\rho)$$

has to be evaluated approximately

Local Density Approximation (LDA) for the exchange+correlation potential:

- One performs many-body calculations for an infinite system with a constant density ρ
- The resulting energy per particle is used to extract the xc-part of the energy, $e_{xc}(\rho)$, which is a function of ρ
- The LDA of a finite system with variable density $\rho(r)$ consists in assuming the local xc-density to be that of the corresponding infinite system with density $\rho = \rho(r)$:

$$E_{xc}^{LDA}[\rho] = \int \rho(\vec{r}) e_{xc}[\rho(\vec{r})] d^3 r$$

- The formalism can be extended to take spin degrees of freedom, by introducing spin-up and spin-down densities ('Local Spin Density' formalism, LSD or LSDA)

In regions **where the charge density is slowly varying**, the exchange correlation energy at that point can be considered the same as that for a locally uniform electron gas of the same charge density. Interestingly, the LDA even works reasonably well in systems where the charge density is rapidly varying. In order to move beyond the LDA, the addition of gradient corrections to incorporate longer range gradient effects is necessary.

The LDA is often used in nuclear physics (Brueckner et al., Negele). It states that the G-matrix at any place in a finite nucleus is the same as that for nuclear matter at the same density, so that locally one can calculate G-matrix as in nuclear matter calculation.

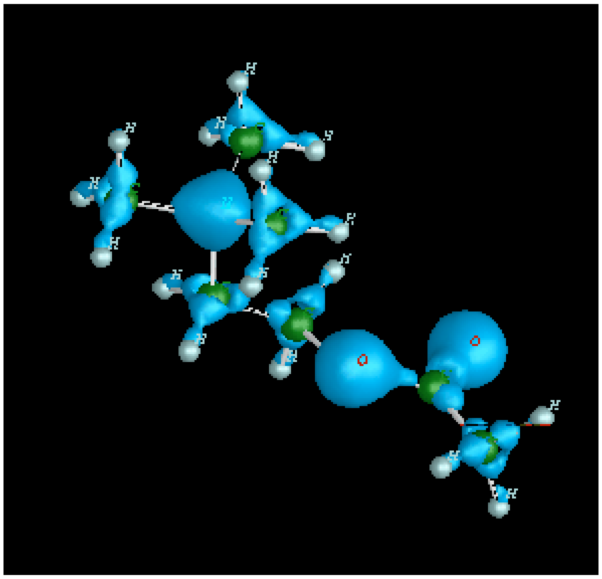
The exchange+correlation potential
(an example)

$$e_{xc} = \begin{cases} \square\left(1 + \square_1\sqrt{r_s} + \square_2 r_s\right)^{\square 1} & \text{for } r_s \geq 1 \\ B + \left(A + Cr_s\right)\ln r_s + Dr_s & \text{for } r_s < 1 \end{cases}$$

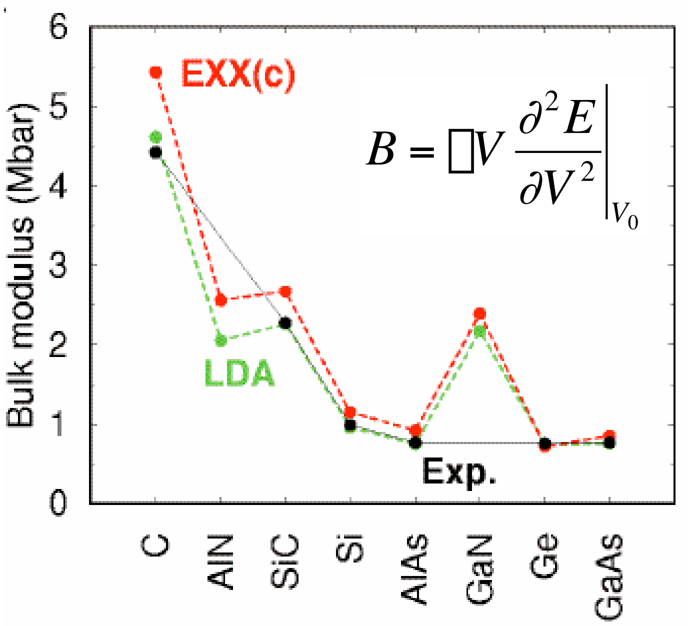
$$r_s = \left(\frac{4\square\square}{3}\right)^{\square 1/3}$$

Wigner-Seitz radius

The parameters in the above expression depend on the spin polarization; they are obtained by means of extrapolation between calculated values for fully-polarized and non-polarized cases. Calculations were carried out using the quantum Monte Carlo method. (See, e.g., J. P. Perdew and A. Zunger, Phys. Rev. B **23** , 5048 (1981).)



The calculated minimum energy conformation of acetylcholine showing electron density isosurface (from http://www.tcm.phy.cam.ac.uk/~mds21/report/node30.html)



The calculated bulk moduli (from http://www.physics.ohio-state.edu/~aulbur/dft/bdft5.html)

Nuclear Densities as Composite Fields

Let us first consider unpaired systems. The basic building blocks of the nuclear energy density functional are densities and currents. Let us denote: $\vec{x} \equiv (\vec{r},\sigma,\tau)$

The single-particle density matrix:

$$\rho(\vec{x},\vec{x}\,') = \langle \Psi | a^+(\vec{x}\,') a(\vec{x}) | \Psi \rangle = \boxed{\sum_k n_k \phi_k^*(\vec{x}\,')\phi_k(\vec{x})}$$ **natural orbitals**

$$= \frac{1}{4}\left\{\left[\rho_{00}(\vec{r},\vec{r}\,')\delta_{\sigma\sigma'} + \vec{s}_{00}(\vec{r},\vec{r}\,')\cdot\vec{\sigma}_{\sigma'\sigma}\right]\delta_{\tau\tau'}\right.$$ **isoscalar**

$$\left. + \sum_{t=-1}^{+1}\left[\rho_{1t}(\vec{r},\vec{r}\,')\delta_{\sigma\sigma'} + \vec{s}_{1t}(\vec{r},\vec{r}\,')\cdot\vec{\sigma}_{\sigma'\sigma}\right]\left(\vec{\tau}_{\tau\tau'}\right)_t\right\}$$ **isovector**

$$\vec{\sigma}_{\sigma'\sigma} = \langle\sigma'|\vec{\sigma}|\sigma\rangle, \quad \vec{\tau}_{\tau'\tau} = \langle\tau'|\vec{\tau}|\tau\rangle$$

Often, one can consider pure neutron and proton states. In such a case, only t=0 components of the isovector densities contribute and the second index can be disregarded. This gives the following local densities and currents:

matter

$$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau}\rho(\vec{r}\sigma\tau,\vec{r}\sigma\tau)$$ **isoscalar (T=0) density** $(\rho_0 = \rho_n + \rho_p)$

$$\rho_1(\vec{r}) = \rho_1(\vec{r},\vec{r}) = \sum_{\sigma\tau}\rho(\vec{r}\sigma\tau,\vec{r}\sigma\tau)\tau$$ **isovector (T=1) density** $(\rho_1 = \rho_n - \rho_p)$

spin

$$\vec{s}_0(\vec{r}) = \sum_{\sigma\sigma'\tau}\rho(\vec{r}\sigma\tau,\vec{r}\sigma'\tau)\vec{\sigma}_{\sigma'\sigma}$$ **isoscalar spin density**

$$\vec{s}_1(\vec{r}) = \sum_{\sigma\sigma'\tau}\rho(\vec{r}\sigma\tau,\vec{r}\sigma'\tau)\vec{\sigma}_{\sigma'\sigma}\tau$$ **isovector spin density**

momentum

$$\vec{j}_T(\vec{r}) = \frac{i}{2}\left(\vec{\nabla}' - \vec{\nabla}\right)\rho_T(\vec{r},\vec{r}\,')\Big|_{\vec{r}\,'=\vec{r}}$$ **current density**

spin-momentum

$$\vec{J}_T(\vec{r}) = \frac{i}{2}\left(\vec{\nabla}' - \vec{\nabla}\right) \otimes \vec{s}_T(\vec{r},\vec{r}\,')\Big|_{\vec{r}\,'=\vec{r}}$$ **spin-current tensor density**

kinetic

$$\tau_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\rho_T(\vec{r},\vec{r}\,')\Big|_{\vec{r}\,'=\vec{r}}$$ **kinetic density**

$$\vec{\mathbf{T}}_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\,\vec{s}_T(\vec{r},\vec{r}\,')\Big|_{\vec{r}\,'=\vec{r}}$$ **kinetic spin density**

$$\mathbf{F}_T(\vec{r}) = \frac{1}{2}\left[\vec{\nabla} \otimes \vec{\nabla}' + \vec{\nabla}' \otimes \vec{\nabla}\right]\vec{s}_T(\vec{r},\vec{r}\,')\Big|_{\vec{r}\,'=\vec{r}}$$ **kinetic tensor density**

The spin-current tensor density is usually replaced by the spin-orbit current:

$$\vec{J}_T = \sum_{ijk} \epsilon_{ijk} \left(\overleftrightarrow{J}_T\right)_{jk} \vec{e}_i$$

In the **relativistic treatment**, one has to deal with four-component Dirac spinor wave functions. Consequently, there are 16 independent bilinear covariants:

$$\bar{\psi}(\vec{r})\,\Gamma\,\psi(\vec{r})$$

This gives the following local densities:

$\Gamma^{s} = 1$ **scalar density**

$\Gamma^{v}_{\mu} = \gamma_{\mu}$ **vector density**

$\Gamma^{t}_{\mu\nu} = (i/2)\left(\gamma_{\mu}\gamma_{\nu} - \gamma_{\nu}\gamma_{\mu}\right)$ **tensor density**

$\Gamma^{p} = \gamma_{5}$ **pseudoscalar density**

$\Gamma^{a}_{\mu} = \gamma_{\mu}\gamma_{5}$ **axial density**

(which have isoscalar and isovector components.) In most applications, only three densities are required:

$\rho_{v0}(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau, \vec{r}\sigma'\tau)\left(\gamma_{0}\right)_{\sigma'\sigma}$ **isoscalar vector density**

$\rho_{v1}(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau, \vec{r}\sigma'\tau)\left(\gamma_{0}\right)_{\sigma'\sigma}\tau$ **isovector vector density**

$\rho_{0}(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau, \vec{r}\sigma'\tau)$ **isoscalar scalar density**

The sums run over four spinor components. Usually, states from the Dirac sea are neglected (no-sea approximation).

Justification of the Skyrme functional

For simplicity, consider non-local, but velocity-independent interaction (and let us disregard for a moment spin and isospin degrees of freedom):

$$V\left(\vec{r}_1,\vec{r}_2;\vec{r}_1{}',\vec{r}_2{}'\right)$$

The corresponding HF interaction energy contains both direct term and exchange term:

$$E_{\text{int}} = \frac{1}{2}\int d^3r_1\, d^3r_2\, d^3r_1'\, d^3r_2'\, V\left(\vec{r}_1,\vec{r}_2;\vec{r}_1{}',\vec{r}_2{}'\right)\times$$
$$\left[\rho\left(\vec{r}_1,\vec{r}_1{}'\right)\rho\left(\vec{r}_2,\vec{r}_2{}'\right)-\rho\left(\vec{r}_2,\vec{r}_1{}'\right)\rho\left(\vec{r}_1,\vec{r}_2{}'\right)\right]$$

Let us now consider **a local gauge transformation** of the HF wave function:

$$\left|\Phi'\right\rangle = \exp\left(i\sum_{j=1}^{A}\phi\left(\vec{r}_j\right)\right)\left|\Phi\right\rangle$$

where ϕ is a **real** function. The corresponding density matrix reads:

$$\rho'\left(\vec{r},\vec{r}\,'\right) = \exp\left\{i\left[\phi\left(\vec{r}\right)-\phi\left(\vec{r}\,'\right)\right]\right\}\rho\left(\vec{r},\vec{r}\,'\right)$$

In general, the interaction energy is not invariant with respect to such transformation. However, it is invariant for **local interactions**:

$$V\left(\vec{r}_1,\vec{r}_2;\vec{r}_1{}',\vec{r}_2{}'\right) = \delta\left(\vec{r}_1-\vec{r}_1{}'\right)\delta\left(\vec{r}_2-\vec{r}_2{}'\right)V\left(\vec{r}_1,\vec{r}_2\right)$$

Indeed:

$$E_{\text{int}} = \frac{1}{2}\int d^3r_1\, d^3r_2\, V\left(\vec{r}_1,\vec{r}_2\right)\times$$
$$\left[\rho\left(\vec{r}_1\right)\rho\left(\vec{r}_2\right)-\rho\left(\vec{r}_2,\vec{r}_1\right)\rho\left(\vec{r}_1,\vec{r}_2\right)\right] = E_{\text{int}}'$$

see J. Dobaczewski and J. Dudek, Phys. Rev. C52, 1827 (1995)

The local densities transform as follows:

$$\rho' = \rho$$

$$\tau' = \tau + 2\vec{j}\cdot\vec{\nabla}\phi + \rho\left(\vec{\nabla}\phi\right)^2$$

$$\vec{s}' = \vec{s}$$

$$\vec{j}' = \vec{j} + \rho\vec{\nabla}\phi$$

$$\vec{T}' = \vec{T} + \overleftrightarrow{J}\vec{\nabla}\phi + \vec{s}\left(\vec{\nabla}\phi\right)^2$$

$$\overleftrightarrow{J}' = \overleftrightarrow{J} + \vec{\nabla}\phi \otimes \vec{s}$$

Now it is easy to check that the following combinations of local densities are gauge invariant:

$$\rho_T\tau_T - j_T^2$$

$$\vec{s}_T\cdot\vec{T}_T - \overleftrightarrow{J}_T^2$$

$$\rho_T\vec{\nabla}\cdot\vec{J}_T + \vec{s}_T\cdot\left(\vec{\nabla}\times\vec{j}_T\right)$$

The transformation relations for j and τ make it possible to interpret φ in terms of a velocity field:

$$\vec{v} = \frac{\hbar}{m}\vec{\nabla}\phi \qquad \left(\vec{\nabla}\times\vec{v} = 0\right)$$

Gauge transformation is irrotational

The Galilean invariance is a **special case** of the local gauge invariance:

constant linear momentum of the boost transformation

$$\phi\left(\vec{r}\right) = \frac{\vec{p}\cdot\vec{r}}{\hbar}$$

Here, the potential energy is invariant while the kinetic energy acquires a term

$$\Delta E_{kin} = \frac{\vec{p}^{\,2}}{2m}A$$

Translational energy of the boosted system

Invariance under local gauge transformations suggests that the functional can be written as:

$$\mathcal{H}_T(\vec r) = C_T^\rho \rho_T^2 + C_T^s s_T^2 + C_T^{\Delta\rho}\rho_T\Delta\rho_T + C_T^{\Delta s}\vec s_T\cdot\Delta\vec s_T$$
$$+ C_T^\tau\left(\rho_T\tau_T - j_T^2\right) + C_T^T\left(\vec s_T\cdot\vec T_T - \vec J_T^2\right) + C_T^{\nabla J}\left[\rho_T\nabla\cdot\vec J_T + \vec s_T\cdot\left(\nabla\times\vec j_T\right)\right]$$

$$E_{tot} = \int\left[\frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\vec r) + \mathcal{H}_1(\vec r)\right]d^3r$$

Total ground-state HF energy

Another motivation… Let us consider a local two-body interaction $V(\vec r - \vec r')$
The HF interaction energy is:

$$E_{\text{int}} = \frac{1}{2}\int d^3r\,d^3r'\,V(\vec r - \vec r')\left[\rho(\vec r)\rho(\vec r') - \rho(\vec r,\vec r')\rho(\vec r',\vec r)\right]$$

In practice, the density matrix is strongly peaked around r=r' (cf. TF expression!). Therefore, one can expand it around the mid-point:

$$\rho(\vec r,\vec r') \approx \rho(\vec q)i\vec s\cdot\vec j(\vec q) + \frac{1}{2}s^2\left[\tau(\vec q) - \frac{1}{4}\Delta_{\vec q}\,\rho(\vec q)\right], \quad \vec q = \frac{\vec r + \vec r'}{2}, \quad \vec s = \vec r - \vec r'$$

$$\left|\rho(\vec r,\vec r')\right|^2 \approx \rho^2(\vec q) - s^2\left[\rho(\vec q)\tau(\vec q) - \vec j^{\,2}(\vec q) - \frac{1}{4}\rho(\vec q)\Delta_{\vec q}\,\rho(\vec q)\right]$$

The corresponding **local exchange energy-density functional** is:

$$E_{ex} = \frac{1}{2}\int\left[V_0\rho^2 + V_2\left(\rho\tau - \vec j^{\,2} - \frac{1}{4}\rho\Delta\rho\right)\right]d^3r$$

$$V_n = \int d^3s\,V(\vec s)\,\vec s^{\,n}$$

The direct term is already written in terms of the local density. Still, for symmetry, it can be expanded around q, and the result is:

$$E_{dir} = \frac{1}{2}\int\left[V_0\rho^2 + \frac{1}{2}V_2\,\rho\Delta\rho\right]d^3r$$

The actual two-body effective interaction is the $\mathcal{T}$ matrix in the nuclear medium. In principle, it can be determined from microscopic BHF calculations. The matrix is density-dependent and nonlocal. The potential energy becomes:

$$E_{pot} = \frac{1}{2}\int d^3x\,d^3x'\,d^3y\,d^3y'\,\rho(\vec{x},\vec{x}')\,\mathcal{T}(\vec{x},\vec{x}';\vec{y},\vec{y}')\,\rho(\vec{y},\vec{y}')$$

The Skyrme functional was justified in such a way in, e.g.,

- Negele and Vautherin, Phys. Rev. **C5**, 1472 (1972); Phys. Rev. **C11**, 1031 (1975)
- Campi and Bouyssy, Phys. Lett. **73B**, 263 (1978)

However, the parameters derived in such a way do not reproduce the nuclear bulk properties precisely enough. Hence, the density matrix expansion should be used as a guiding principle, but the ectual parameters should be adjusted phenomenologically.

Many insights can also be obtained from the effective field theory, see Puglia, Bhattacharyya, Furnstahl, Nucl.Phys. **A723**, 145 (2003)

One can relate the Skyrme functional to the zero-range momentum-dependent two-body force (Skyrme 1956, 1959)

$$\left.\begin{aligned} V_{Sk}(1,2) = {} & t_0\left(1+x_0\hat{P}_\sigma\right)\delta(\vec{r}_{12}) \\ & + \frac{1}{2}t_1\left(1+x_1\hat{P}_\sigma\right)\left[\hat{k}^{+2}\delta(\vec{r}_{12})+\delta(\vec{r}_{12})\hat{k}^2\right] \\ & + \frac{1}{2}t_2\left(1+x_2\hat{P}_\sigma\right)\left[\hat{k}^{+}\delta(\vec{r}_{12})\hat{k}\;\right] \end{aligned}\right\}$$

zero-range limit of a finite-range force up to second order in derivatives (finite range = momentum dependence!)

$$+\,iW_0(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{k}^{+}\times\delta(\vec{r}_{12})\hat{k}$$

two-body spin-orbit

$$+\,\frac{1}{6}t_3\left(1+x_3\hat{P}_\sigma\right)\delta(\vec{r}_{12})\,\rho^{\alpha}\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)$$

density dependent term (3-body,…)

$$\hat{P}_\sigma = \frac{1}{2}\left(1+\vec{\sigma}_1\cdot\vec{\sigma}_2\right),\quad \hat{k} = \frac{1}{2i}\left(\vec{\nabla}_1-\vec{\nabla}_2\right)$$

For N=Z even-even nuclei (and σ=1), one gets:

$$\mathcal{H}(\vec{r}) = \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^3 + \frac{1}{16}(3t_1+5t_2)\rho\tau$$
$$+\frac{1}{64}(9t_1-5t_2)(\vec{\nabla}\rho)^2 - \frac{3}{4}W_0\rho\vec{\nabla}\vec{J} + \frac{1}{32}(t_1-t_2)\vec{J}^2$$

The binding energy per particle in the infinite homogenous symmetric nuclear matter is

$$\frac{E_0}{A} = \frac{\mathcal{H}}{\rho} = \frac{3}{5}\frac{\hbar^2}{2m}k_F^2 + \frac{3}{8}t_0\rho + \frac{1}{16}t_3\rho^2 + \frac{3}{80}(3t_1+5t_2)\rho k_F^2, \quad \rho = \frac{2}{3\pi^2}k_F^3$$

$$\frac{\partial}{\partial\rho}\left(\frac{E_0}{A}\right)\Bigg|_{\rho=\rho_0} = 0$$ the saturation property

$$K = k_F^2\frac{\partial^2}{\partial k_F^2}\left(\frac{E_0}{A}\right)\Bigg|_{\rho=\rho_0}$$ the incompressibility coefficient

However, the Skyrme functional does not have to be related to an effective two-body force!

Actually, many currently used nuclear energy functionals are not related to a force.

$$h_{Sk}\left[\rho(\vec{r})\right] = \frac{\delta E_{Sk}(\rho)}{\delta\rho(\vec{r})}$$ contains the ‘rearrangement’ terms

Construction of the functional

E. Perlinska, S.G. Rohozinski, J. Dobaczewski, and W. Nazarewicz
Phys. Rev. C 69, 014316 (2004)

Density distributions of matter, spin, and current cand be used as fields defining new degrees of freedom that describe the nucleus a a composite particle.

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau_0(\boldsymbol{r}) + \sum_{t=0,1}\left(\overset{\text{p-h density}}{\chi_t(\boldsymbol{r})} + \overset{\text{p-p density}}{\breve{\chi}_t(\boldsymbol{r})}\right),$$

Most general, second order expansion in densities and their derivatives

The coupling terms depend on density (=higher-order contact terms which represent high-energy phenomena that are not explicitely important in the nuclear scale)

$$\begin{aligned}
\chi_0(\boldsymbol{r}) &= C_0^\rho\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^\tau\rho_0\tau_0 + C_0^{J0}J_0^2 + C_0^{J1}\boldsymbol{J}_0^2 + C_0^{J2}\underline{\mathsf{J}}_0^2 + C_0^{\nabla J}\rho_0\boldsymbol{\nabla}\cdot\boldsymbol{J}_0 \\
&+ C_0^s\boldsymbol{s}_0^2 + C_0^{\Delta s}\boldsymbol{s}_0\cdot\Delta\boldsymbol{s}_0 + C_0^T\boldsymbol{s}_0\cdot\boldsymbol{T}_0 + C_0^j\boldsymbol{j}_0^2 + C_0^{\nabla j}\boldsymbol{s}_0\cdot(\boldsymbol{\nabla}\times\boldsymbol{j}_0) + C_0^{\nabla s}(\boldsymbol{\nabla}\cdot\boldsymbol{s}_0)^2 + C_0^F\boldsymbol{s}_0\cdot\boldsymbol{F}_0, \\
\chi_1(\boldsymbol{r}) &= C_1^\rho\vec{\rho}^{\,2} + C_1^{\Delta\rho}\vec{\rho}\circ\Delta\vec{\rho} + C_1^\tau\vec{\rho}\circ\vec{\tau} + C_1^{J0}\vec{J}^2 + C_1^{J1}\vec{\boldsymbol{J}}^2 + C_1^{J2}\vec{\underline{\mathsf{J}}}^2 + C_1^{\nabla J}\vec{\rho}\circ\boldsymbol{\nabla}\cdot\vec{\boldsymbol{J}} \\
&+ C_1^s\vec{\boldsymbol{s}}^2 + C_1^{\Delta s}\vec{\boldsymbol{s}}\cdot\circ\Delta\vec{\boldsymbol{s}} + C_1^T\vec{\boldsymbol{s}}\cdot\circ\vec{\boldsymbol{T}} + C_1^j\vec{\boldsymbol{\jmath}}^{\,2} + C_1^{\nabla j}\vec{\boldsymbol{s}}\cdot\circ(\boldsymbol{\nabla}\times\vec{\boldsymbol{\jmath}}) + C_1^{\nabla s}(\boldsymbol{\nabla}\cdot\vec{\boldsymbol{s}})^2 + C_1^F\vec{\boldsymbol{s}}\cdot\circ\vec{\boldsymbol{F}}, \\
\breve{\chi}_0(\boldsymbol{r}) &= \breve{C}_0^s|\breve{\boldsymbol{s}}_0|^2 + \breve{C}_0^{\Delta s}\Re(\breve{\boldsymbol{s}}_0^*\cdot\Delta\breve{\boldsymbol{s}}_0) + \breve{C}_0^T\Re(\breve{\boldsymbol{s}}_0^*\cdot\breve{\boldsymbol{T}}_0) \\
&+ \breve{C}_0^j|\breve{\boldsymbol{j}}_0|^2 + \breve{C}_0^{\nabla j}\Re(\breve{\boldsymbol{s}}_0^*\cdot(\boldsymbol{\nabla}\times\breve{\boldsymbol{j}}_0)) + \breve{C}_0^{\nabla s}|\boldsymbol{\nabla}\cdot\breve{\boldsymbol{s}}_0|^2 + \breve{C}_0^F\Re(\breve{\boldsymbol{s}}_0^*\cdot\breve{\boldsymbol{F}}_0), \\
\breve{\chi}_1(\boldsymbol{r}) &= \breve{C}_1^\rho|\vec{\breve{\rho}}|^2 + \breve{C}_1^{\Delta\rho}\Re(\vec{\breve{\rho}}^{\,*}\circ\Delta\vec{\breve{\rho}}) + \breve{C}_1^\tau\Re(\vec{\breve{\rho}}^{\,*}\circ\vec{\breve{\tau}}) \\
&+ \breve{C}_1^{J0}|\vec{\breve{J}}|^2 + \breve{C}_1^{J1}|\vec{\breve{\boldsymbol{J}}}|^2 + \breve{C}_1^{J2}|\vec{\breve{\underline{\mathsf{J}}}}|^2 + \breve{C}_1^{\nabla J}\Re(\vec{\breve{\rho}}^{\,*}\circ\boldsymbol{\nabla}\cdot\vec{\breve{\boldsymbol{J}}}).
\end{aligned}$$

Not all terms are equally important! Some probe specific observables!

Example: pairing mean field

$$\begin{aligned}
\breve{h}_0(\boldsymbol{r};s',s) &= \breve{\boldsymbol{\Sigma}}_0\cdot\hat{\boldsymbol{\sigma}}_{s's} + \tfrac{1}{2i}\left\{\boldsymbol{\nabla}\cdot\breve{\boldsymbol{I}}_0\delta_{s's} + \breve{\boldsymbol{I}}_0\delta_{s's}\cdot\boldsymbol{\nabla}\right\} - \boldsymbol{\nabla}\cdot[\breve{\mathsf{C}}_0\cdot\hat{\boldsymbol{\sigma}}_{s's}]\boldsymbol{\nabla} - \boldsymbol{\nabla}\cdot\breve{\mathsf{D}}_0\,\hat{\boldsymbol{\sigma}}_{s's}\cdot\boldsymbol{\nabla}, \\
\vec{\breve{h}}(\boldsymbol{r};s',s) &= \vec{\breve{U}}(\boldsymbol{r})\delta_{s's} + \tfrac{1}{2i}\left\{\boldsymbol{\nabla}\cdot[\vec{\breve{\mathsf{B}}}(\boldsymbol{r})\cdot\hat{\boldsymbol{\sigma}}_{s's}] + [\vec{\breve{\mathsf{B}}}(\boldsymbol{r})\cdot\hat{\boldsymbol{\sigma}}_{s's}]\cdot\boldsymbol{\nabla}\right\} - \boldsymbol{\nabla}\cdot\vec{\breve{\mathsf{M}}}\delta_{s's}\boldsymbol{\nabla}.
\end{aligned}$$

Nuclear DFT, Local Density Approximation (2)

E. Perlinska, S.G. Rohozinski, J. Dobaczewski, and W. Nazarewicz
Phys. Rev. C 69, 014316 (2004)

Symmetries!

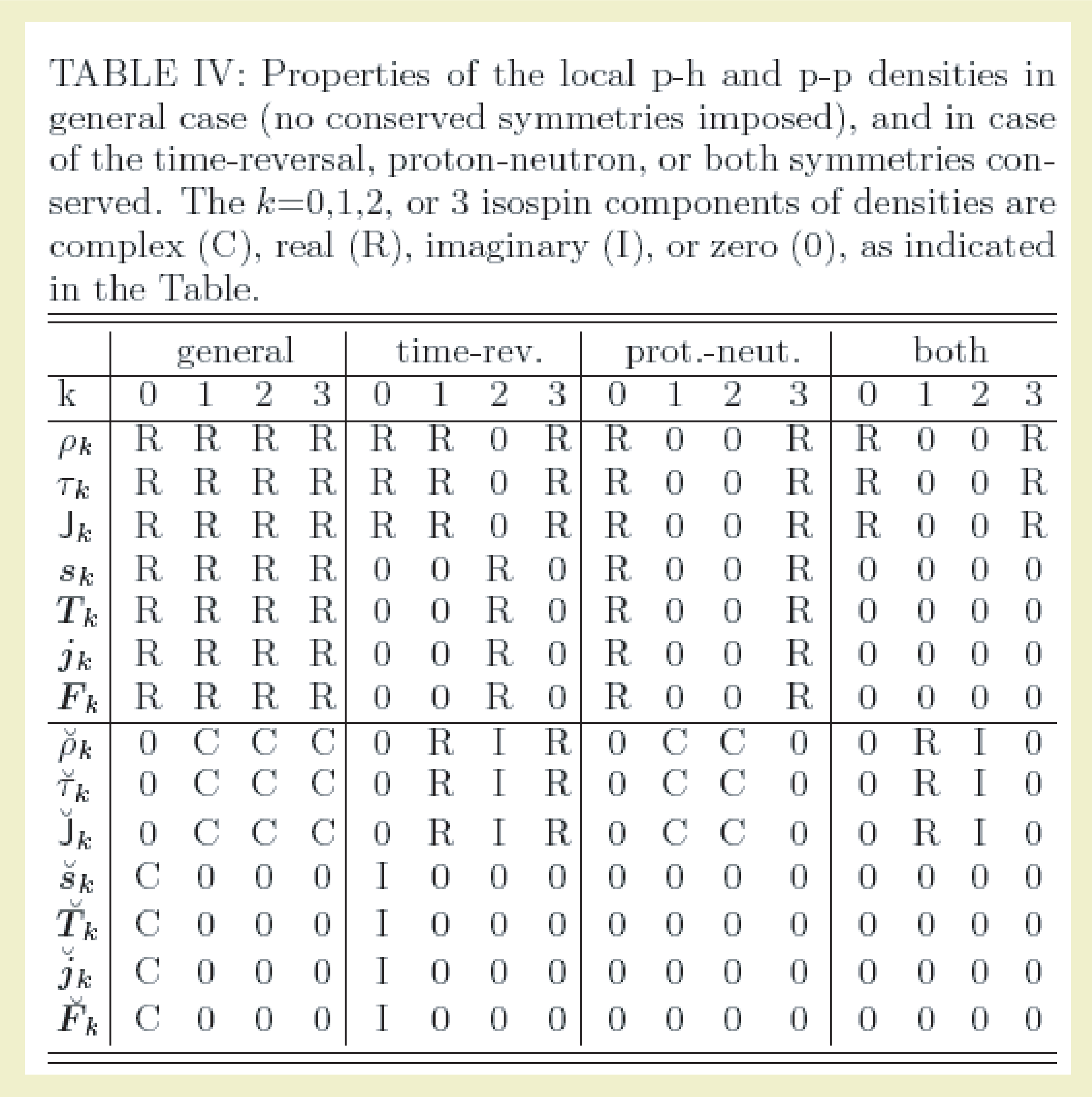


TABLE IV: Properties of the local p-h and p-p densities in general case (no conserved symmetries imposed), and in case of the time-reversal, proton-neutron, or both symmetries conserved. The k=0,1,2, or 3 isospin components of densities are complex (C), real (R), imaginary (I), or zero (0), as indicated in the Table.

	general				time-rev.				prot.-neut.				both			
k	0	1	2	3	0	1	2	3	0	1	2	3	0	1	2	3
ρ_k	R	R	R	R	R	R	0	R	R	0	0	R	R	0	0	R
τ_k	R	R	R	R	R	R	0	R	R	0	0	R	R	0	0	R
J_k	R	R	R	R	R	R	0	R	R	0	0	R	R	0	0	R
$\boldsymbol{s}_k$	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
$\boldsymbol{T}_k$	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
$\boldsymbol{j}_k$	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
$\boldsymbol{F}_k$	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
$\breve{\rho}_k$	0	C	C	C	0	R	I	R	0	C	C	0	0	R	I	0
$\breve{\tau}_k$	0	C	C	C	0	R	I	R	0	C	C	0	0	R	I	0
$\breve{\mathsf{J}}_k$	0	C	C	C	0	R	I	R	0	C	C	0	0	R	I	0
$\breve{\boldsymbol{s}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0
$\breve{\boldsymbol{T}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0
$\breve{\boldsymbol{j}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0
$\breve{\boldsymbol{F}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0

Relativistic mean field functionals

- The depth of the mean-field potential (~50 MeV) is the result of the cancellation between a long-range attractive scalar field and a short-range repulsive vector field
- The strong spin-orbit interaction emerges naturally
- Saturation properties of nuclear matter are explained
- The many-body state is a product wave function built on four-component Dirac spinors.
- The motion of the nucleons is governed by the Dirac equation
- Zero-range forces (point coupling models) and finite-range interactions are used
    - ❖In point-coupling approaches, single-particle potentials are functions of relativistic densities
    - ❖In finite-range models, the effective interaction is introduced through Klein-Gordon equations for the **meson fields**, which are coupled to the Dirac equation for the nucleons. Nucleon densities act as source terms in the KG equations, and mesonic fields enter the Dirac equations.

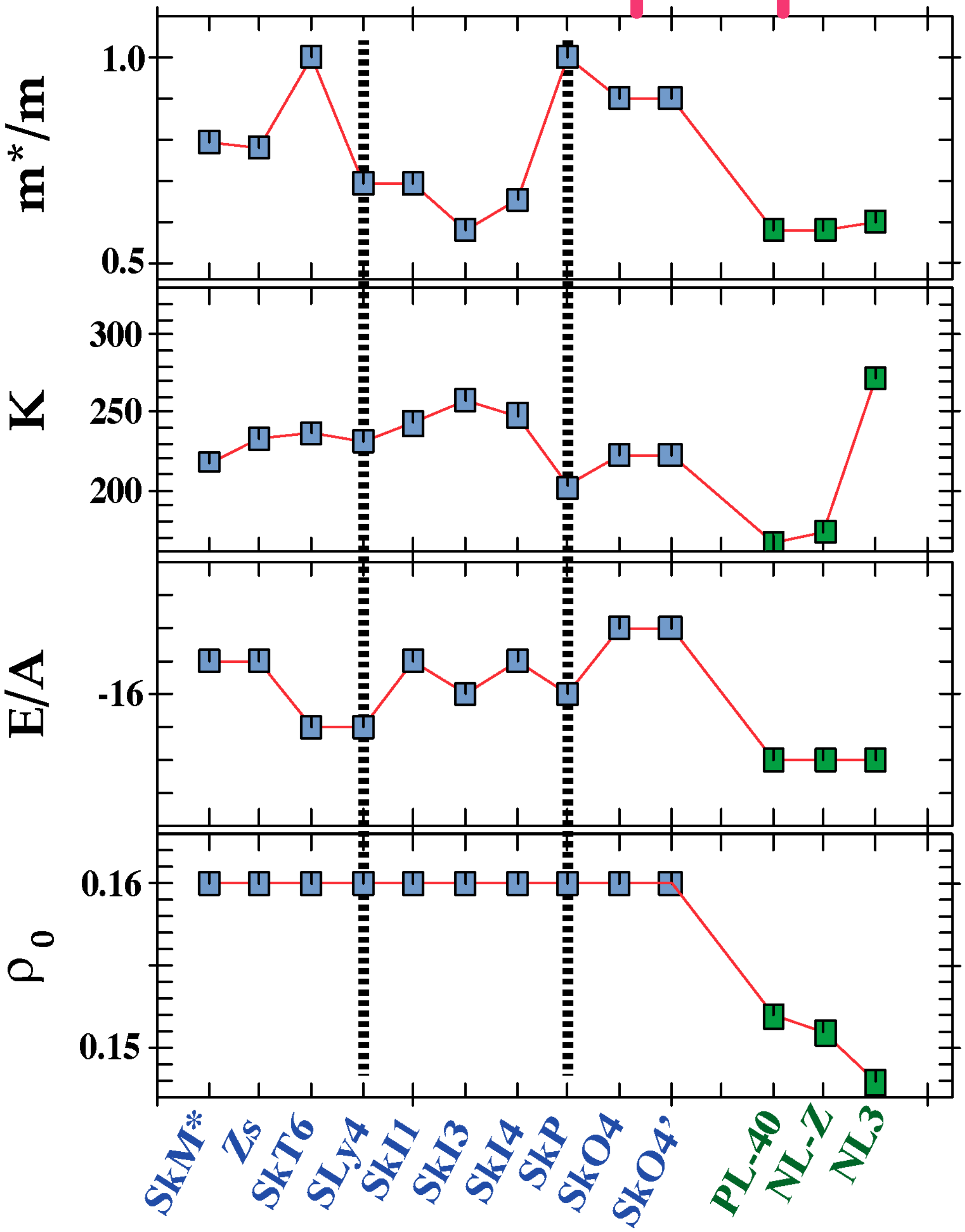
Serot and Walecka, Adv. Nucl. Phys. **16**, 1 (1986); Ring, Prog. Part. Nucl. Phys. **37**, 193 (1996).

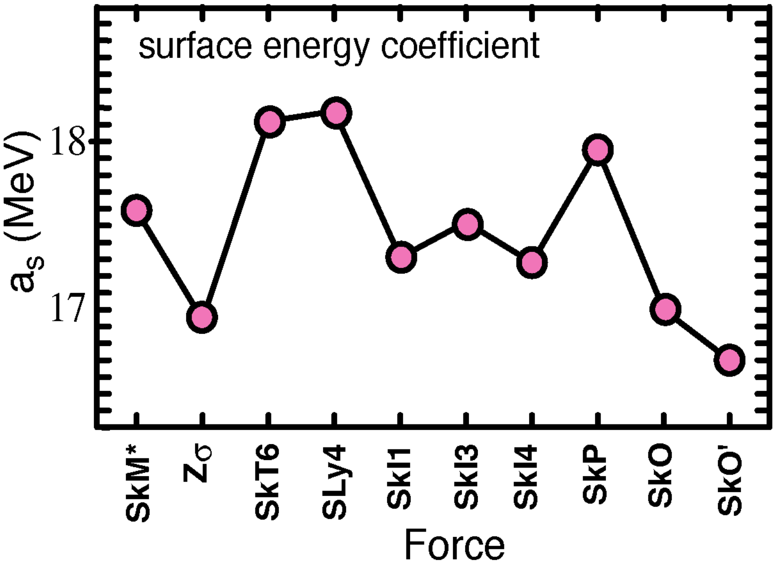
The basic mesons of the RMF:

- σ-field, $J^{\pi}=0^{+}$, T=0; medium-range attraction
- ω-field, $J^{\pi}=1^{-}$, T=0; short-range repulsion
- ρ-field, $J^{\pi}=1^{-}$, T=1; responsible for the isospin channel

The pion is absent; it has $J^{\pi}=0^{-}$, T=1, hence it cannot contribute on the Hartree level (the associate fields violate parity and time reversal)

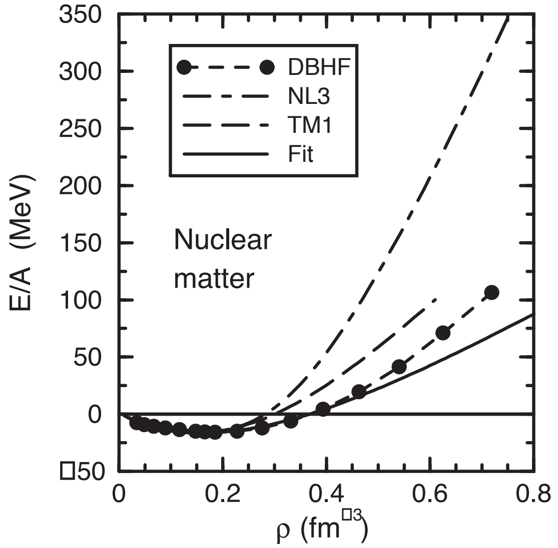
Nuclear matter properties...



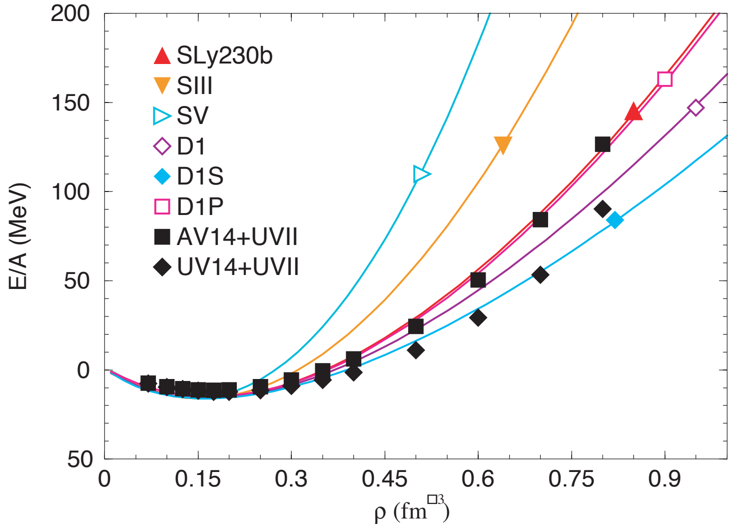


P.-G. Reinhard et al.
Phys. Rev. C 60, 014316
(1999)

EOS and effective forces

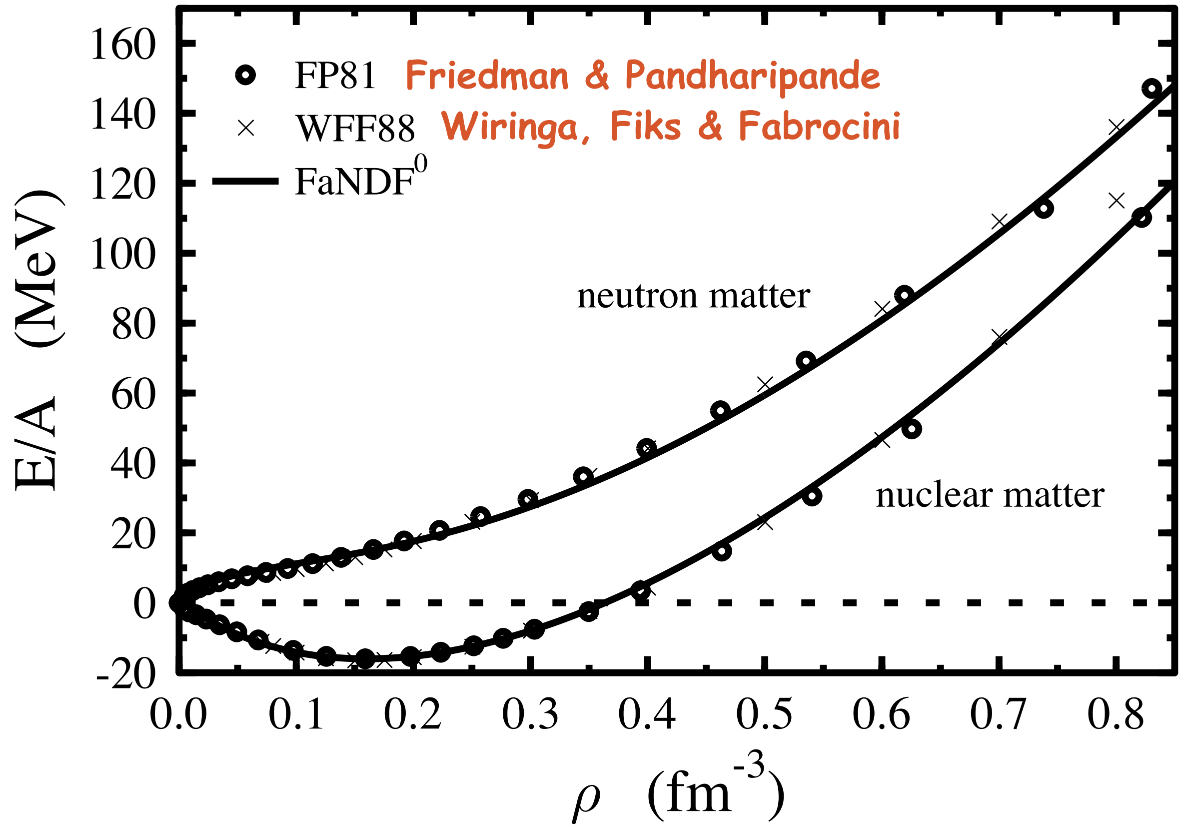


Centelles et al., Brijuni2001



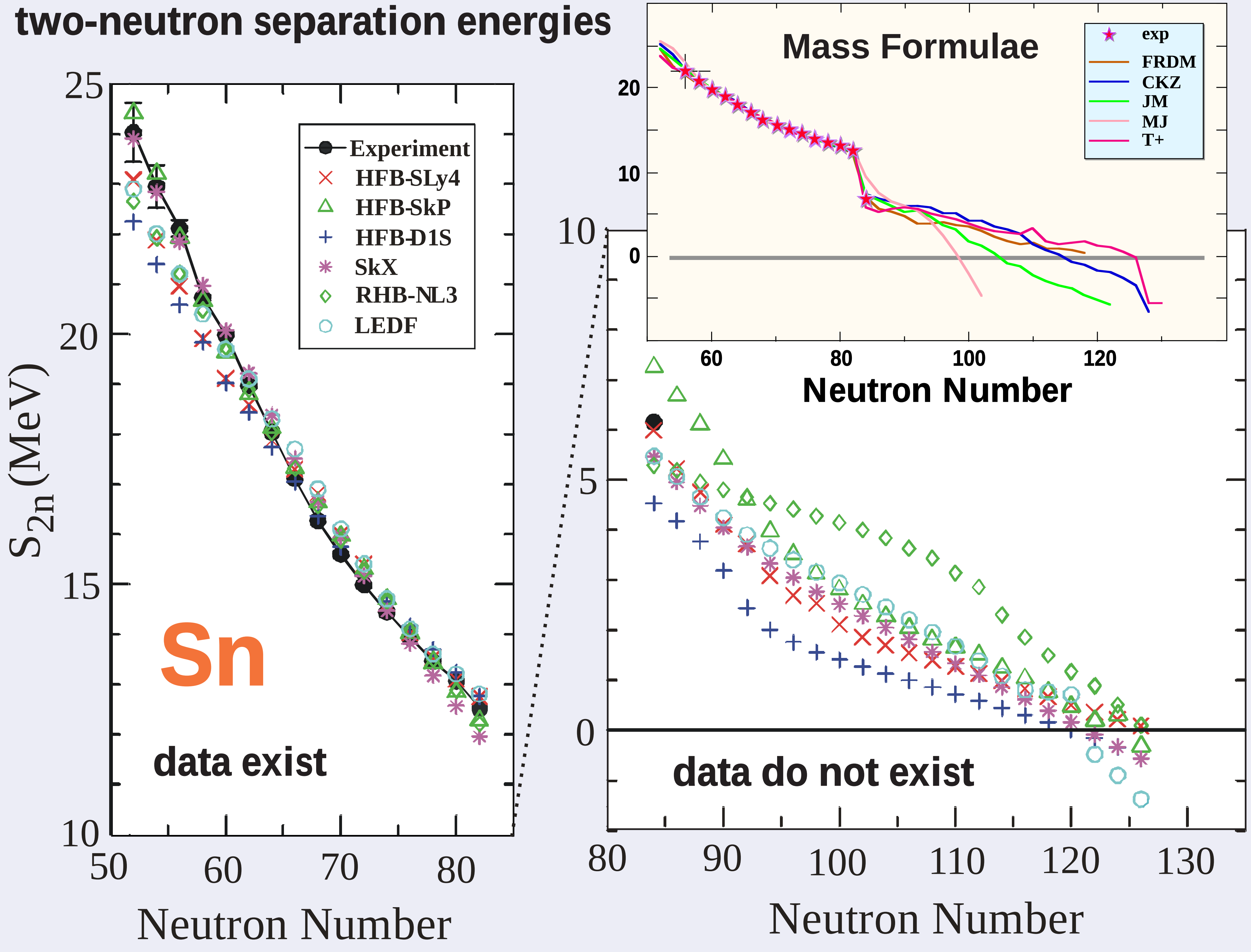
Margureon et al., Brijuni2001

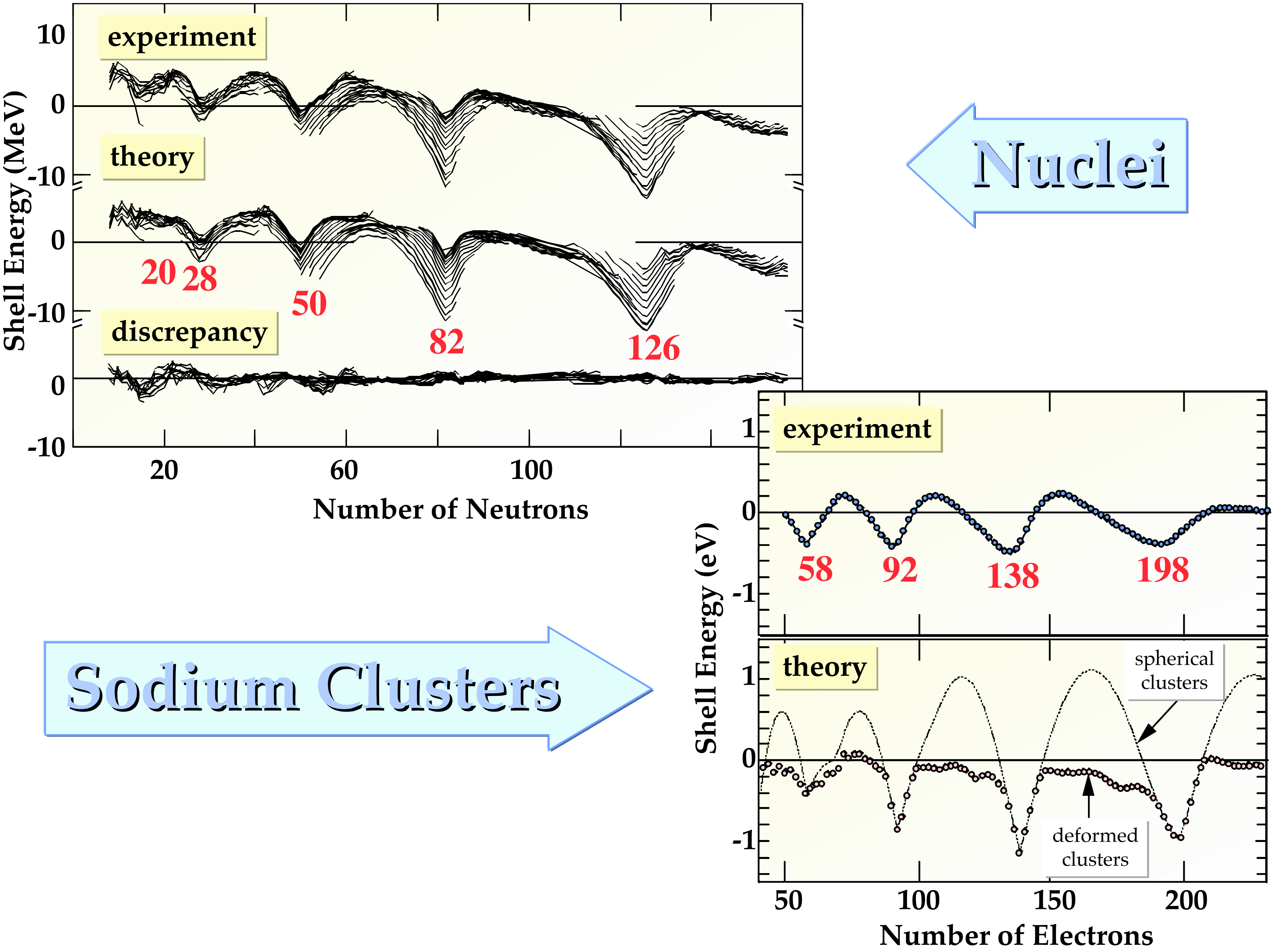
Fayans & Zawisha, nucl-th/0009034



see also Akmal, Pandharipande, Ravenhall, Phys. Rev. C58, 1804 (1998)

two-neutron separation energies



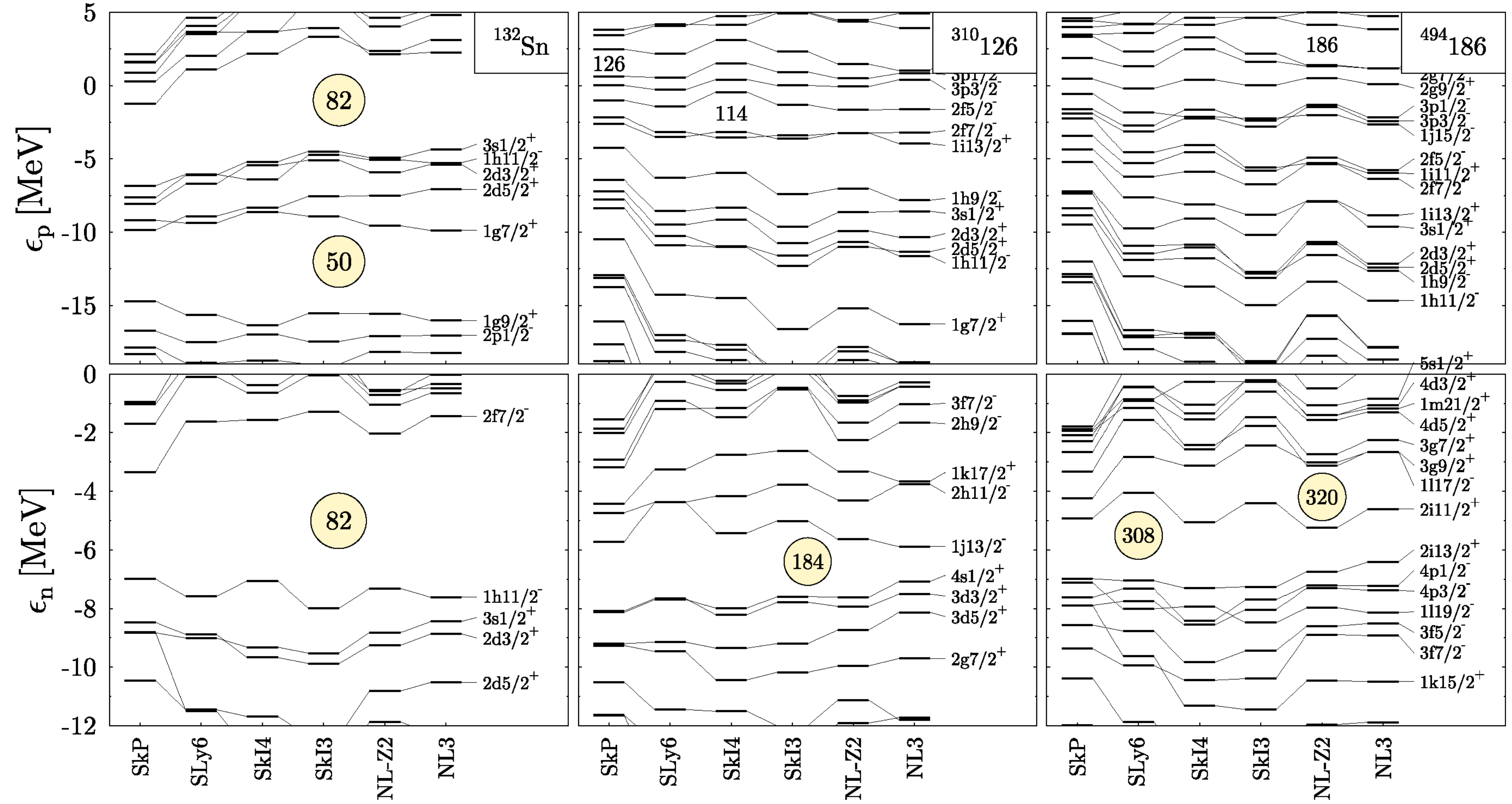


Nuclei

Sodium Clusters

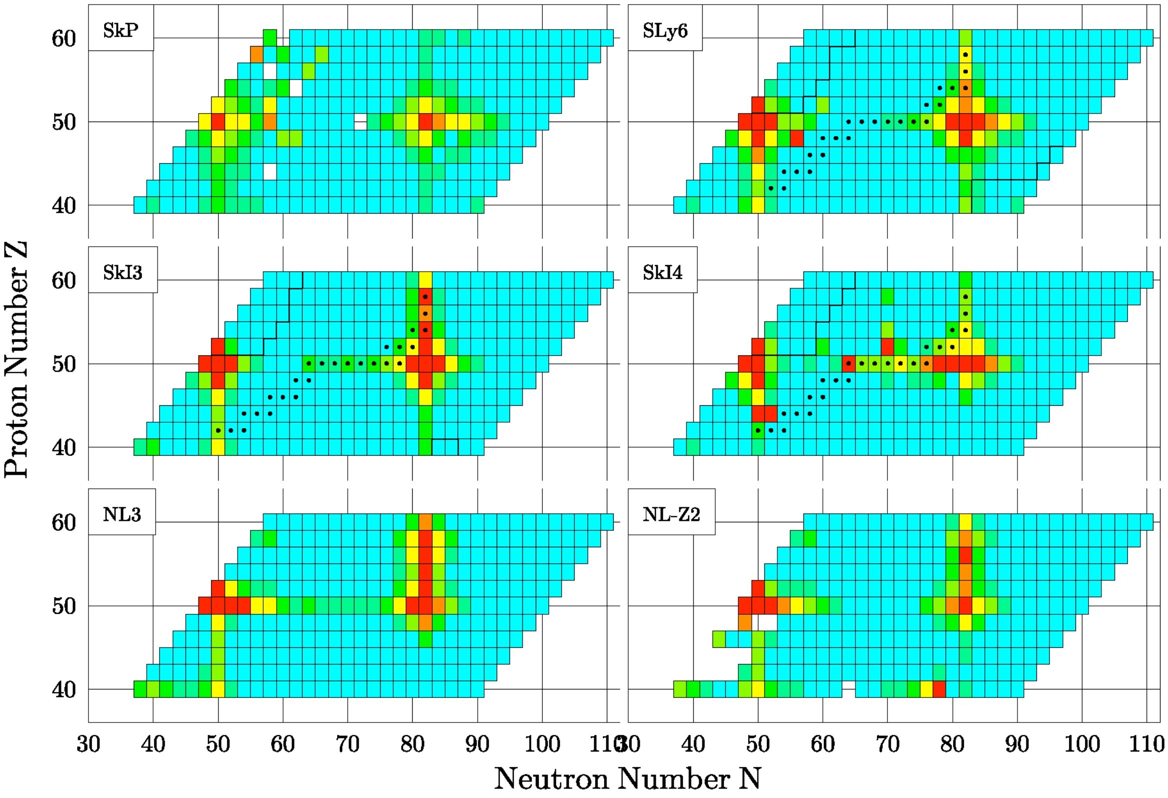
Shell structure in normal, superheavy, and hyperheavy nuclei

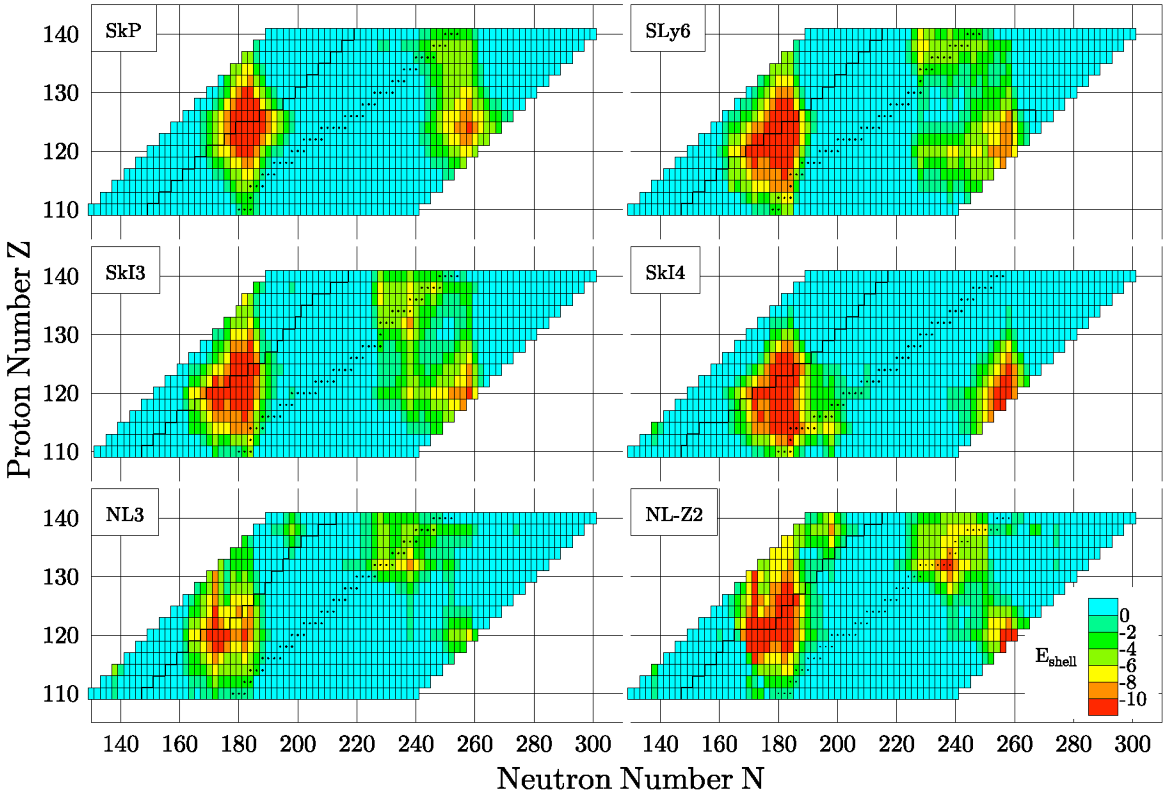
^{132}Sn $\quad$ ^{310}126 $\quad$ ^{494}186



M.Bender, W.Nazarewicz, and P.-G.Reinhard, Phys. Lett. B515, 42 (2001)

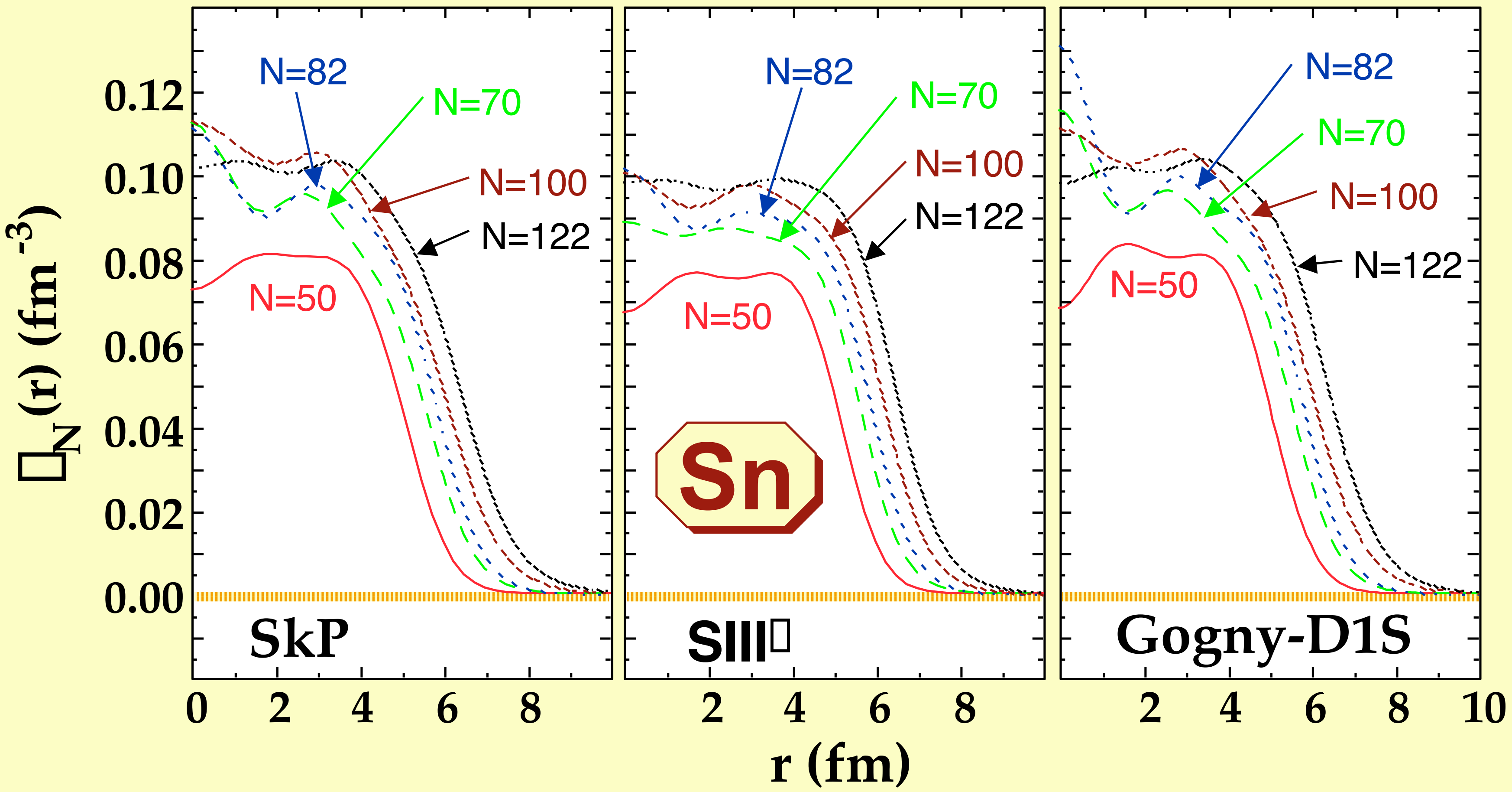
Shell structure in normal, superheavy, and hyperheavy nuclei





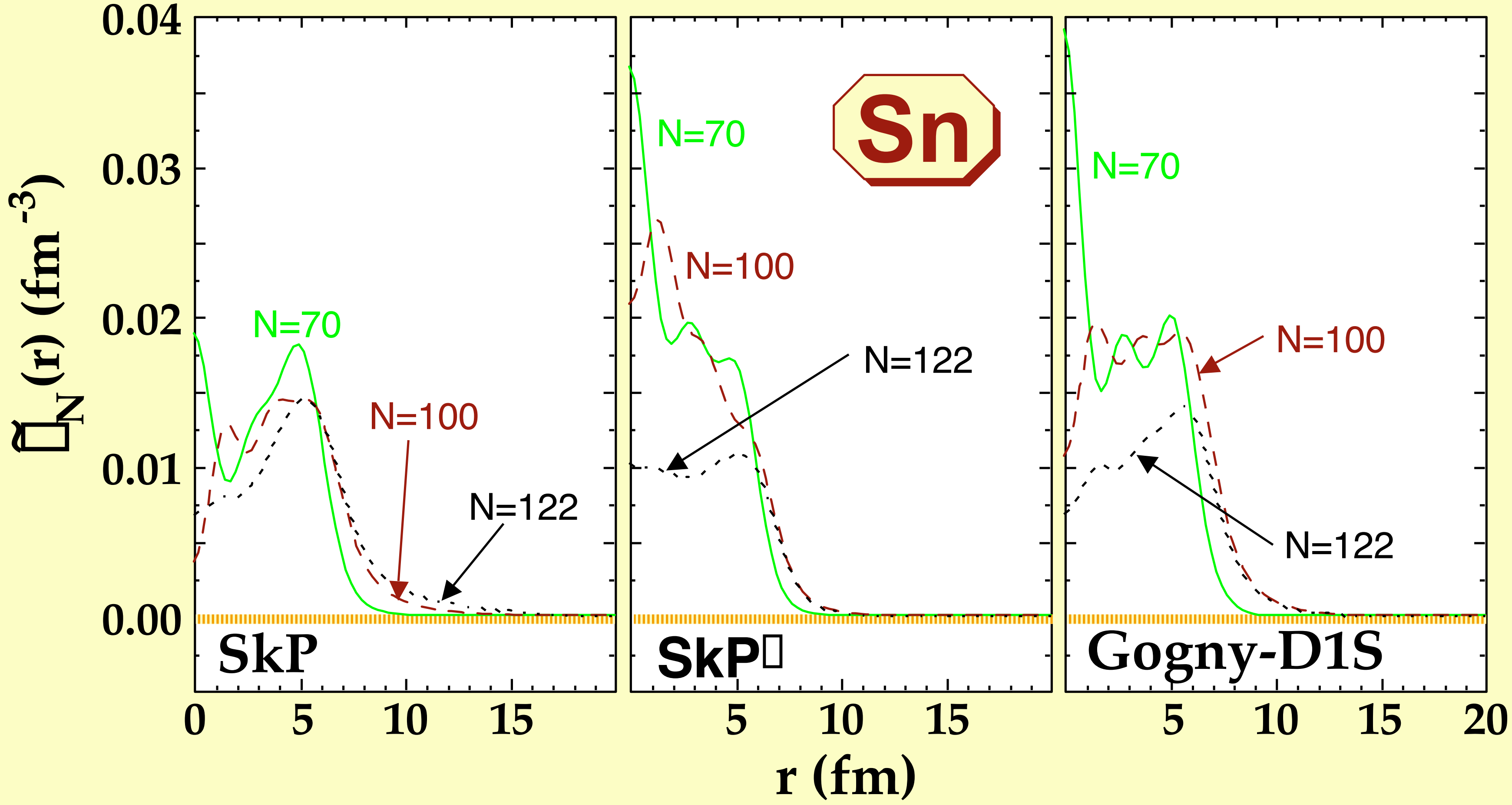
M.Bender, W.Nazarewicz, and P.-G.Reinhard, Phys. Lett. B515, 42 (2001)

HFB: Nuclear density



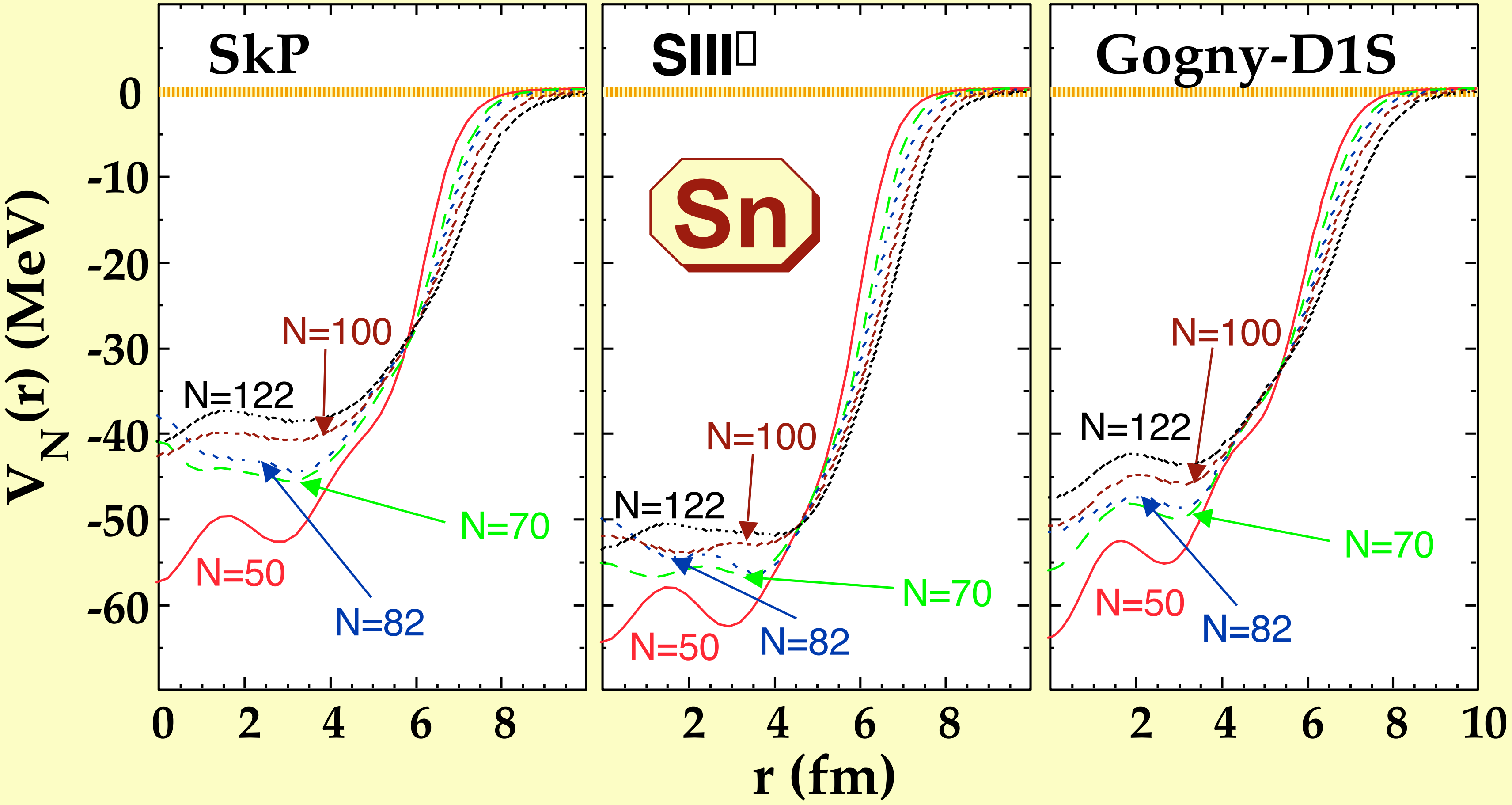
Phys. Rev. C53, 2809 (1996)

HFB: Pairing density



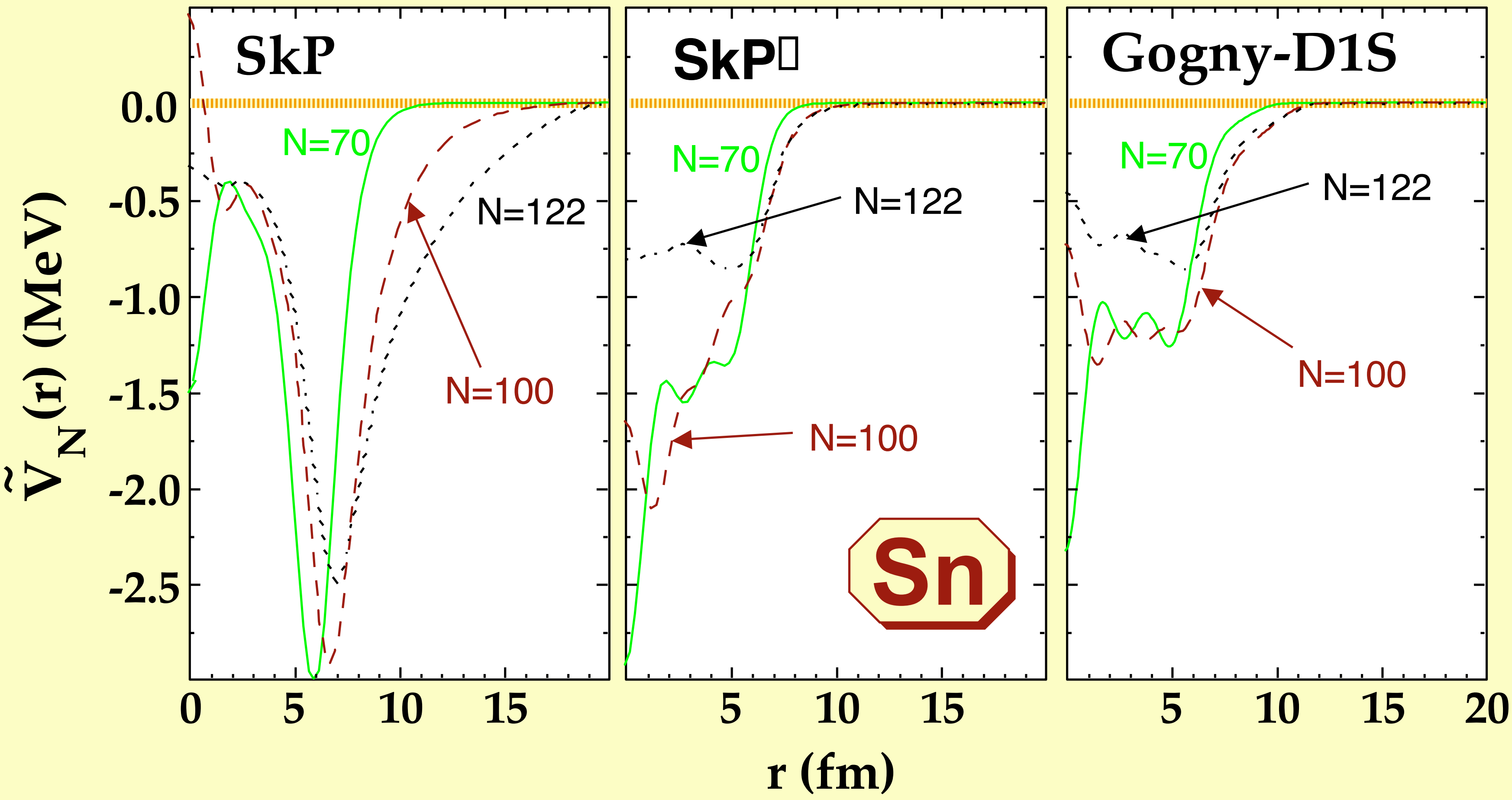
Phys. Rev. C53, 2809 (1996)

HFB: Average potential



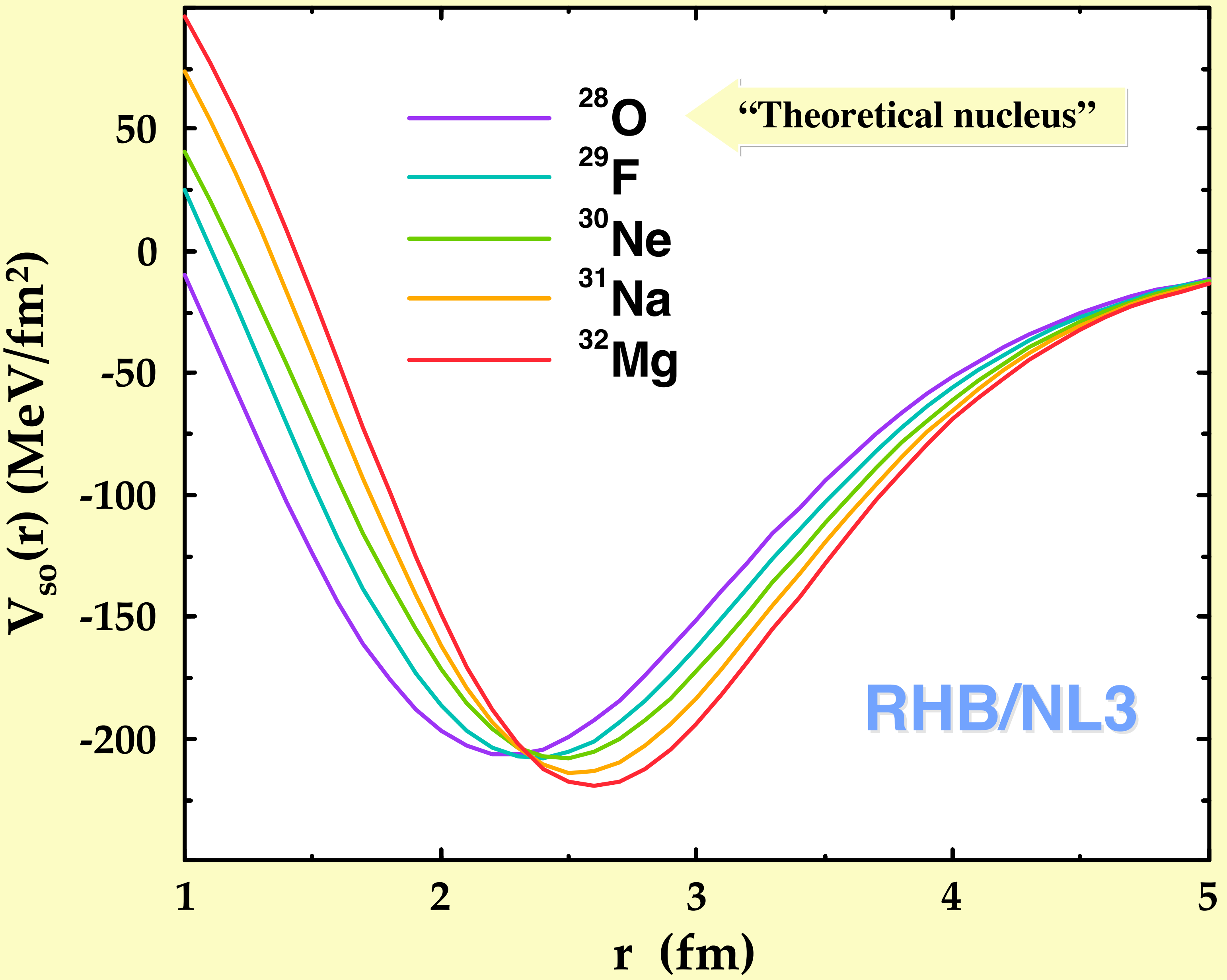
Phys. Rev. C53, 2809 (1996)

HFB: Average pairing potential



Phys. Rev. C53, 2809 (1996)

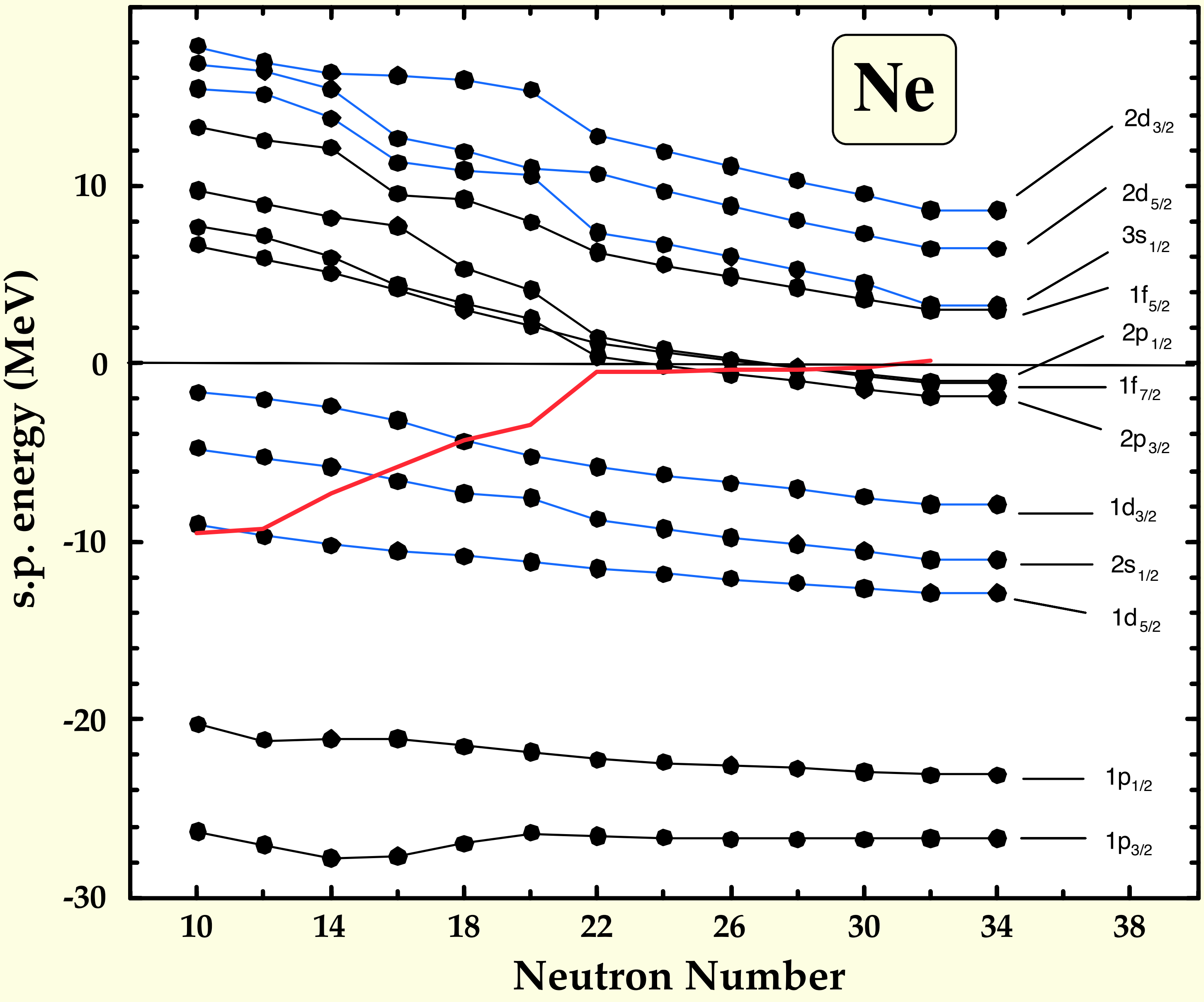
Lalazissis et al., Phys. Lett. B 418, 7 (1998)



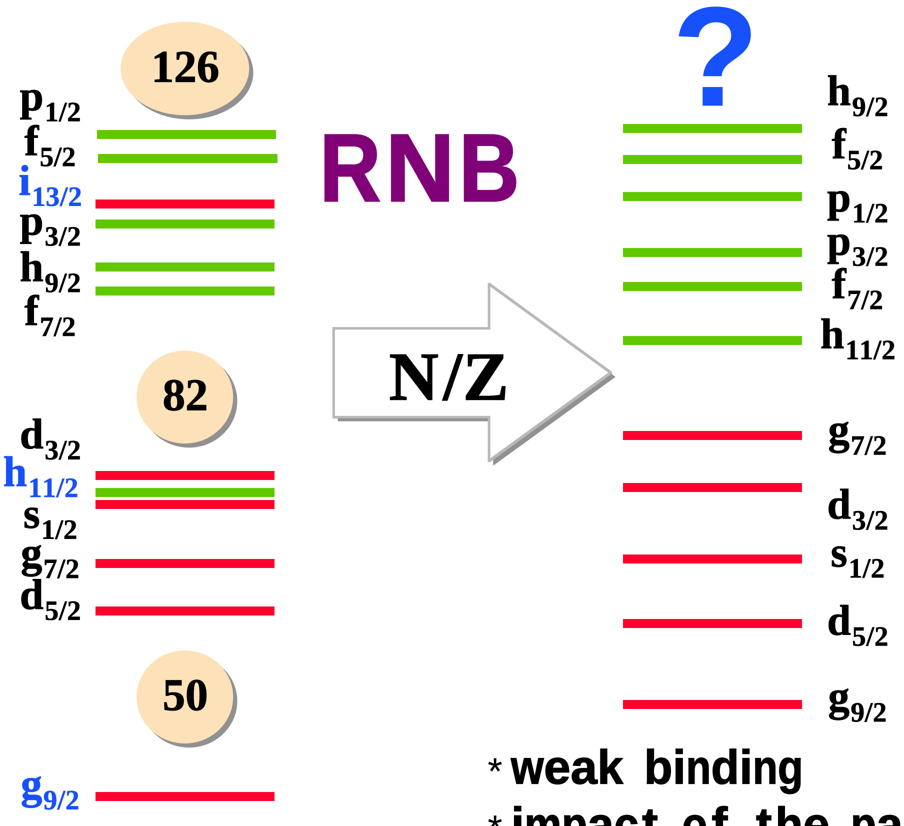
“Theoretical nucleus”

Pöschl et al., RHFB in coordinate space

Phys. Rev. Lett. 79, 3841 (1997)

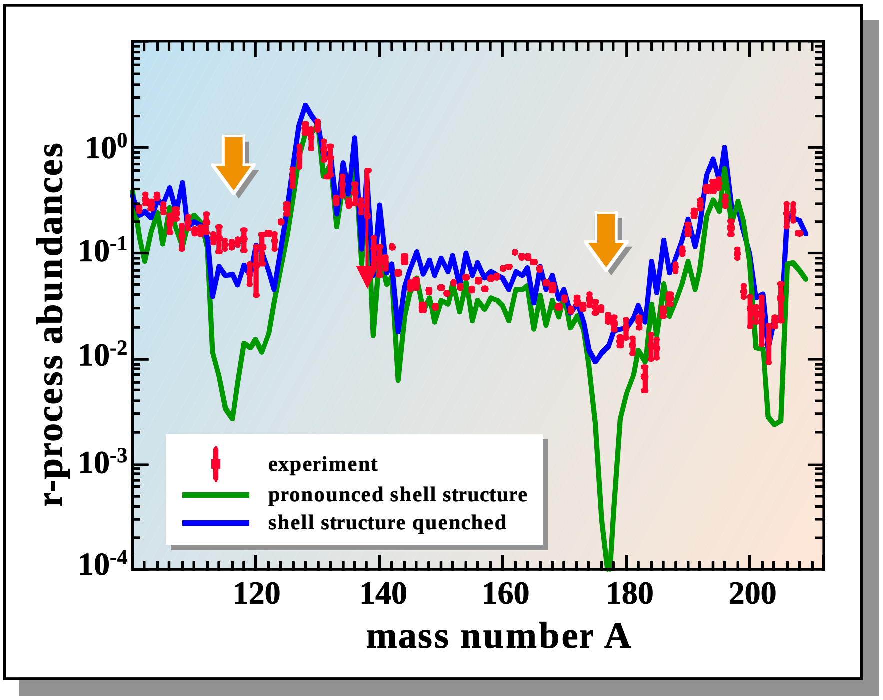


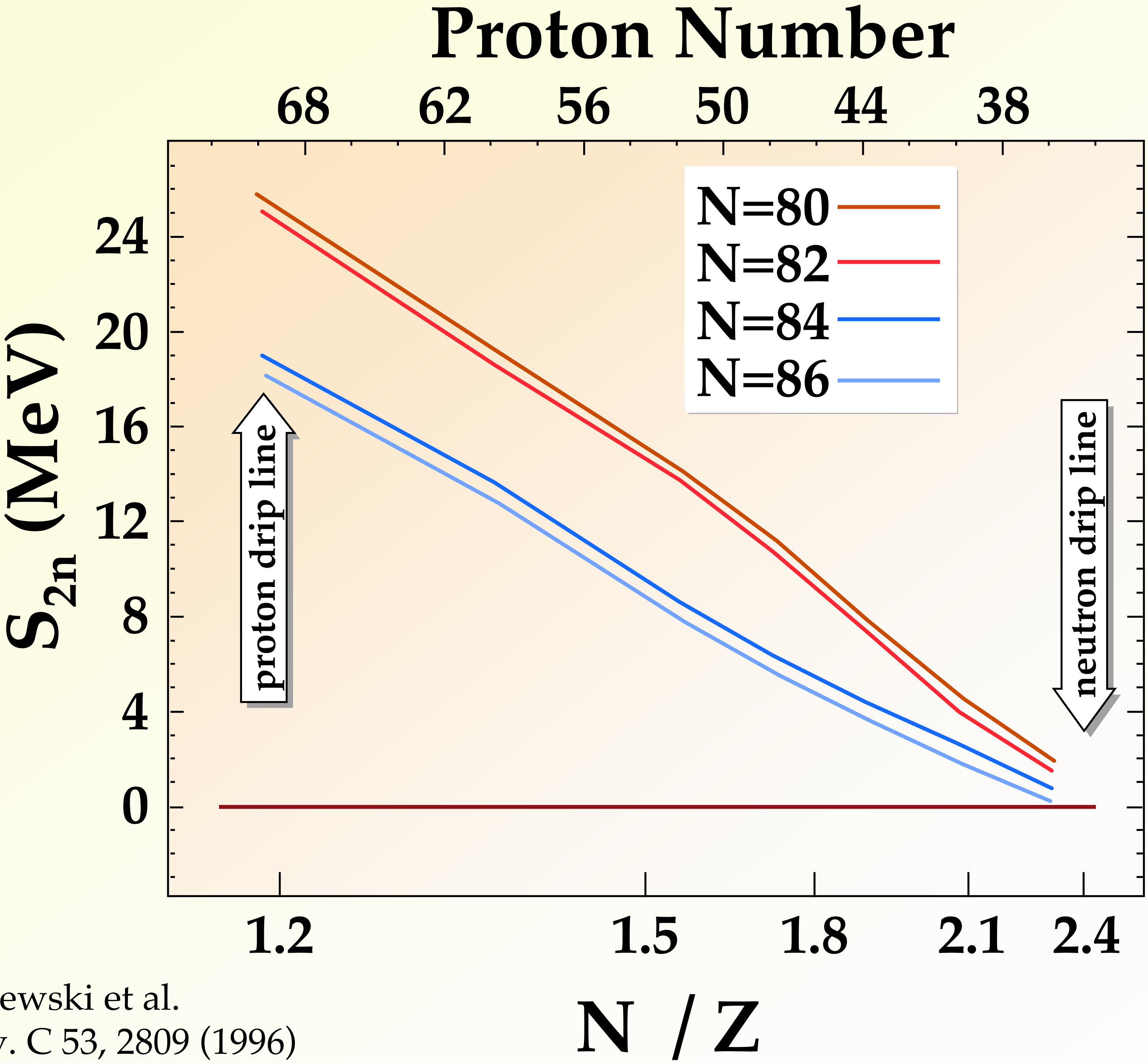
New shell model



- * weak binding
- * impact of the particle continuum
- * collective skin modes
- * clustering in the skin

Emergence of new shells
Quenching of the old shells
Independent-particle motion
less pronounced...

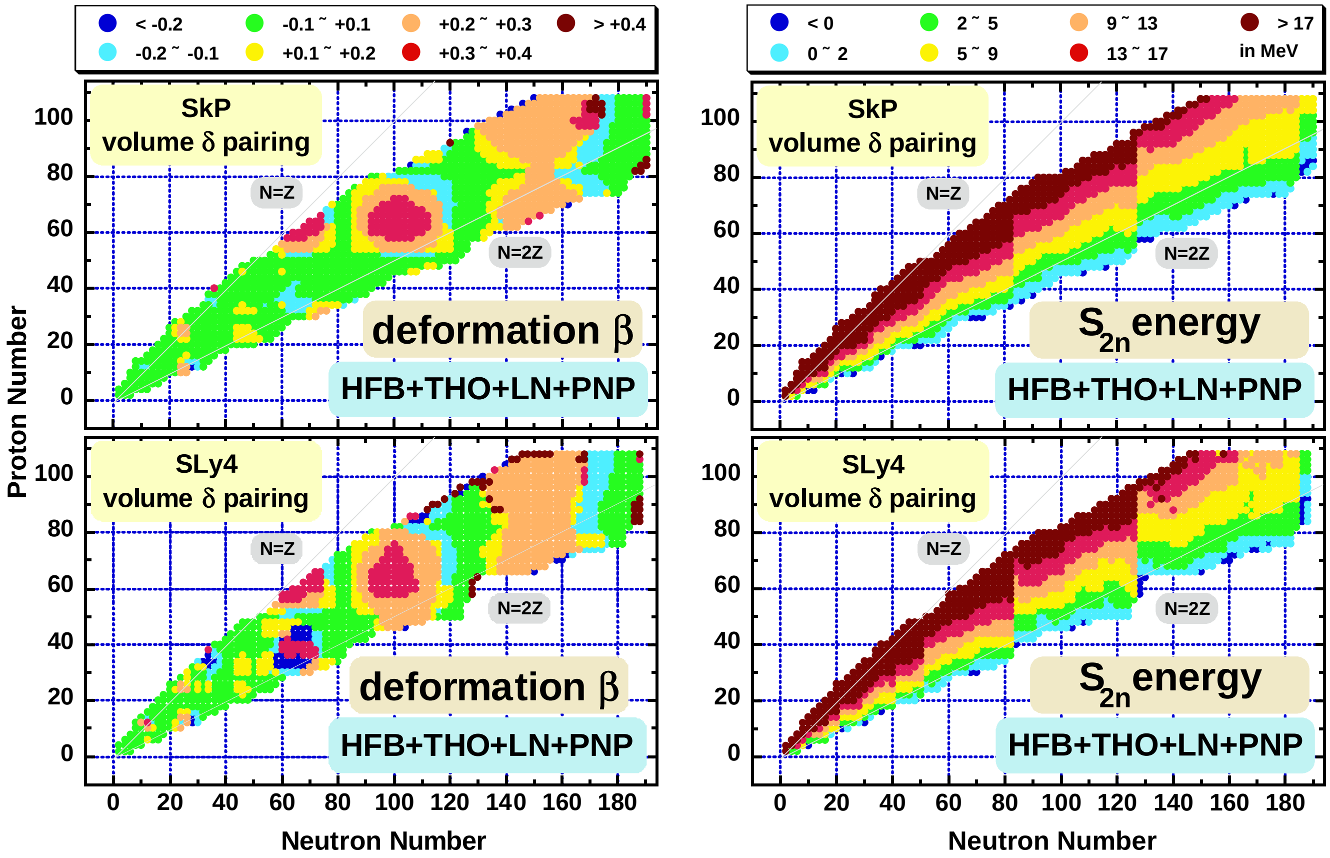




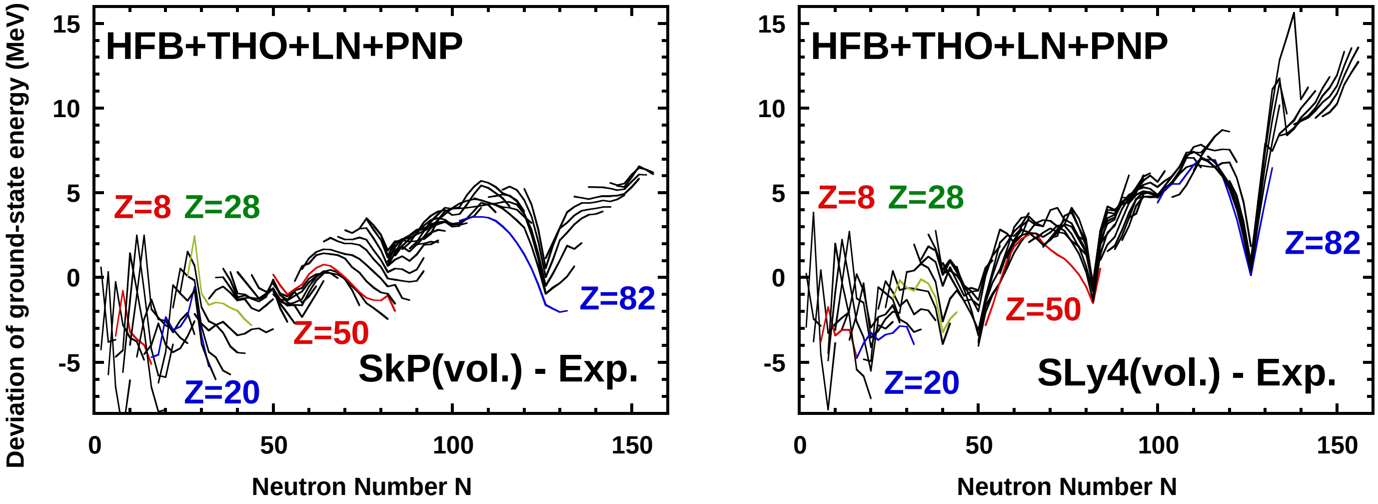
J. Dobaczewski et al.
Phys. Rev. C 53, 2809 (1996)

Microscopic Mass Table

M.V. Stoitsov et al., nucl-th/0406075
J. Dobaczewski et al., nucl-th/040407

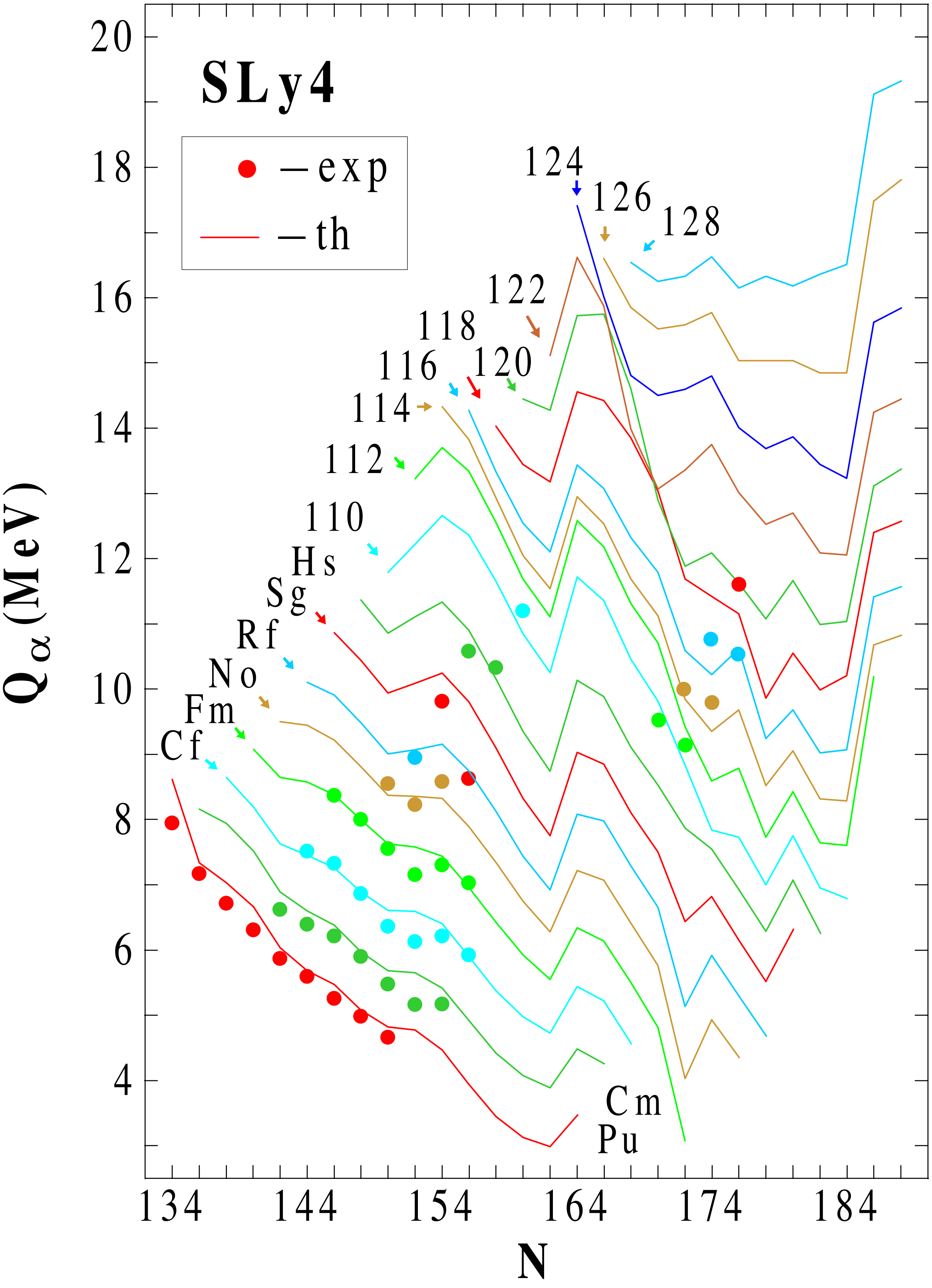


Deviation from experiment

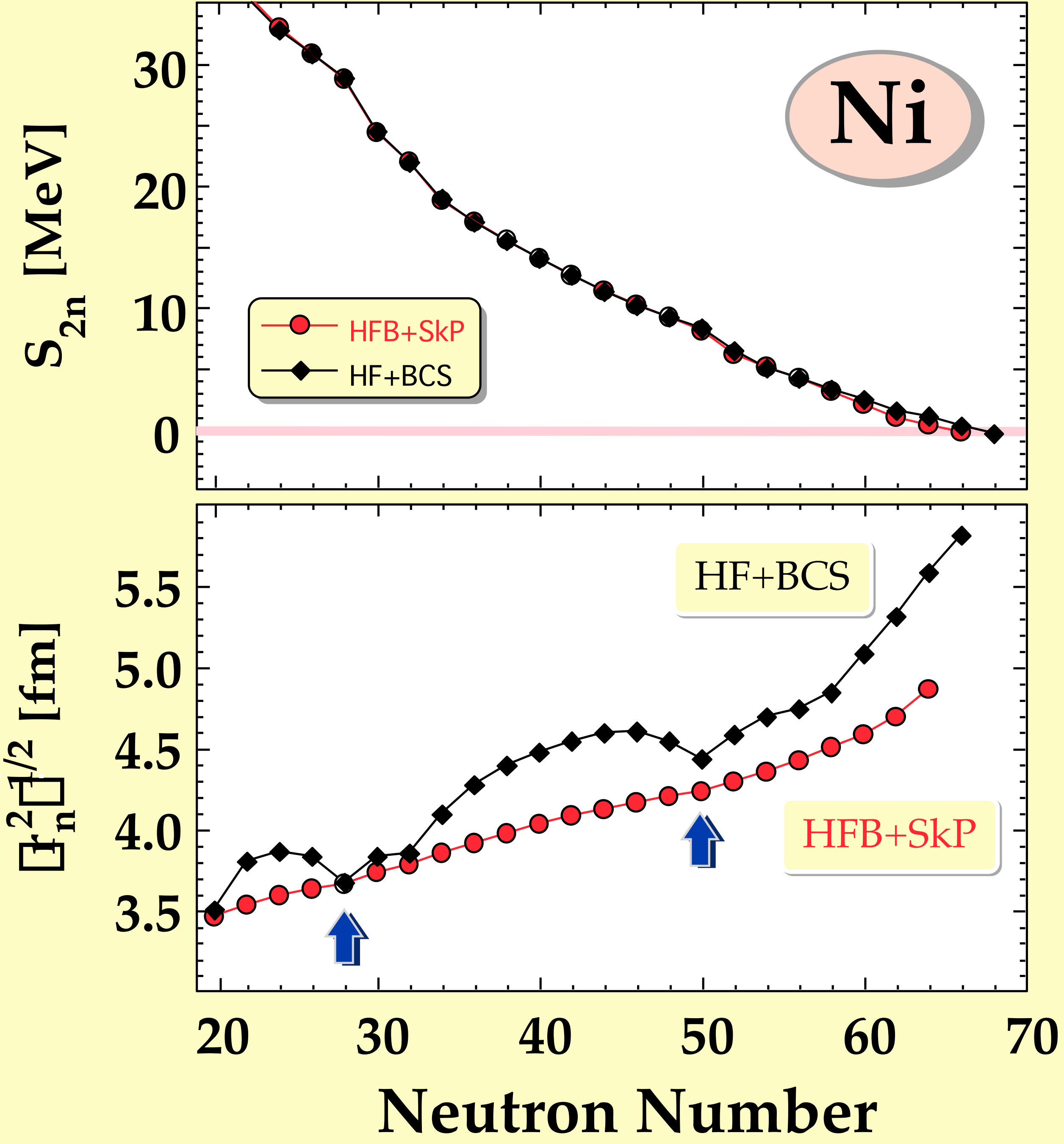


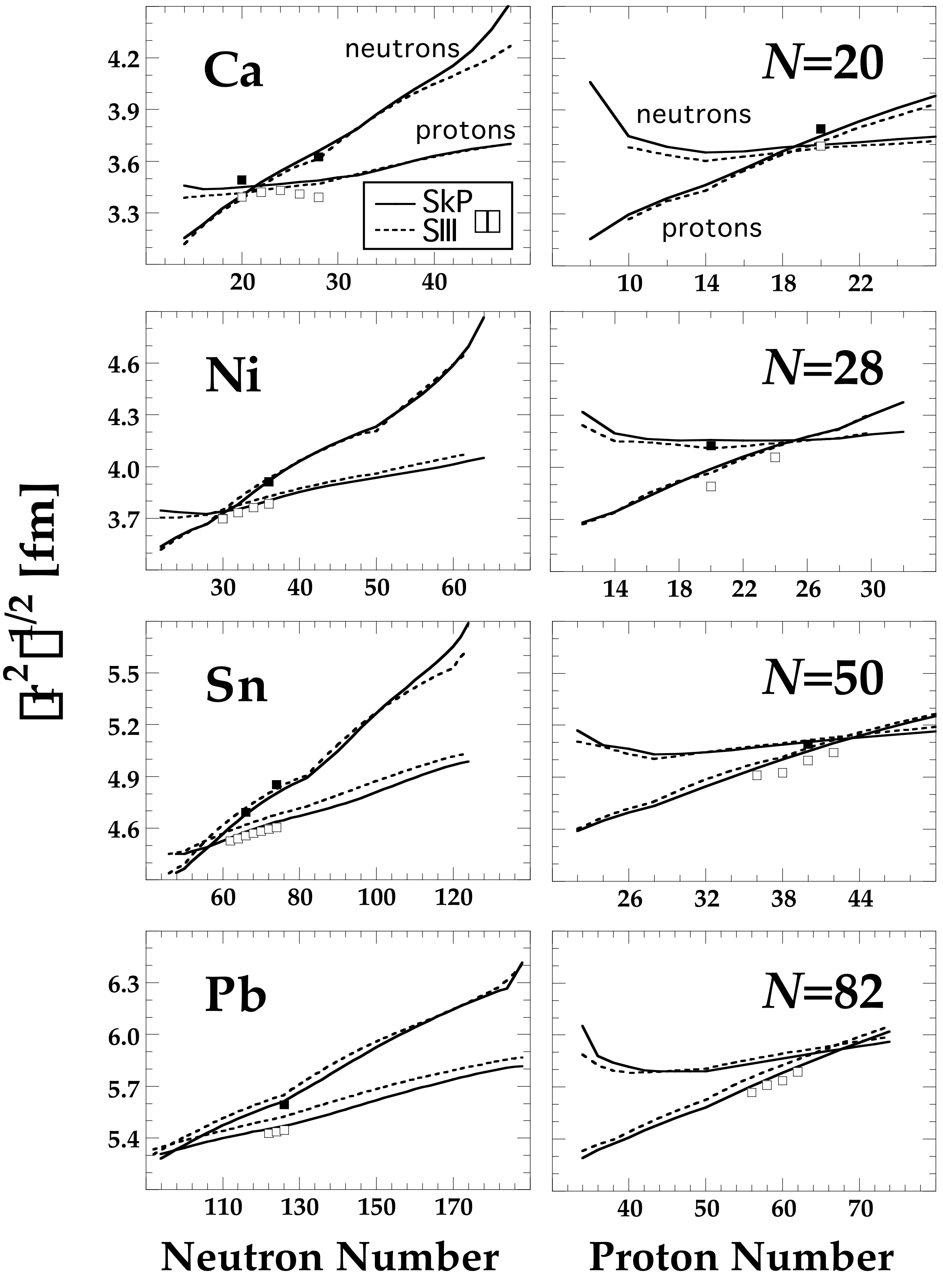
G. Audi, A.H. Wapstra, and C. Thibault, Nucl. Phys. A729 (2003) 337

S. Cwiok, P.H. Heenen, W. Nazarewicz



J. Dobaczewski, W. Nazarewicz, and T. Werner
Z. Phys. A 354, 27 (1996)

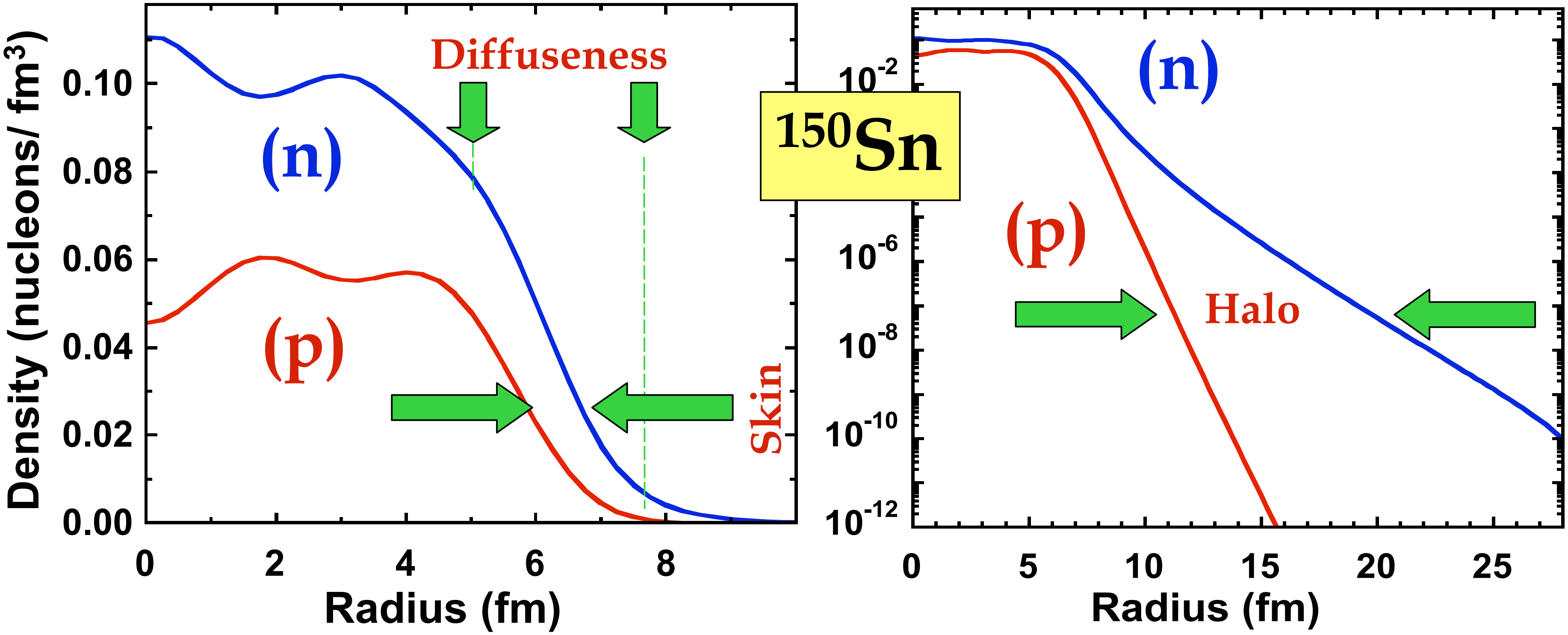




Ca
neutrons
protons
SkP
SIII
4.2
3.9
3.6
3.3
20
30
40
N=20
neutrons
protons
3.9
3.6
3.3
3.0
10
14
18
22
Ni
4.6
4.3
4.0
3.7
30
40
50
60
N=28
4.1
3.8
3.5
3.2
14
18
22
26
30
Sn
5.5
5.2
4.9
4.6
60
80
100
120
N=50
4.7
4.4
4.1
3.8
26
32
38
44
Pb
6.3
6.0
5.7
5.4
110
130
150
170
N=82
5.4
5.1
4.8
4.5
40
50
60
70
⟨r²⟩^1/2 [fm]
Neutron Number
Proton Number

Neutron & proton density distributions

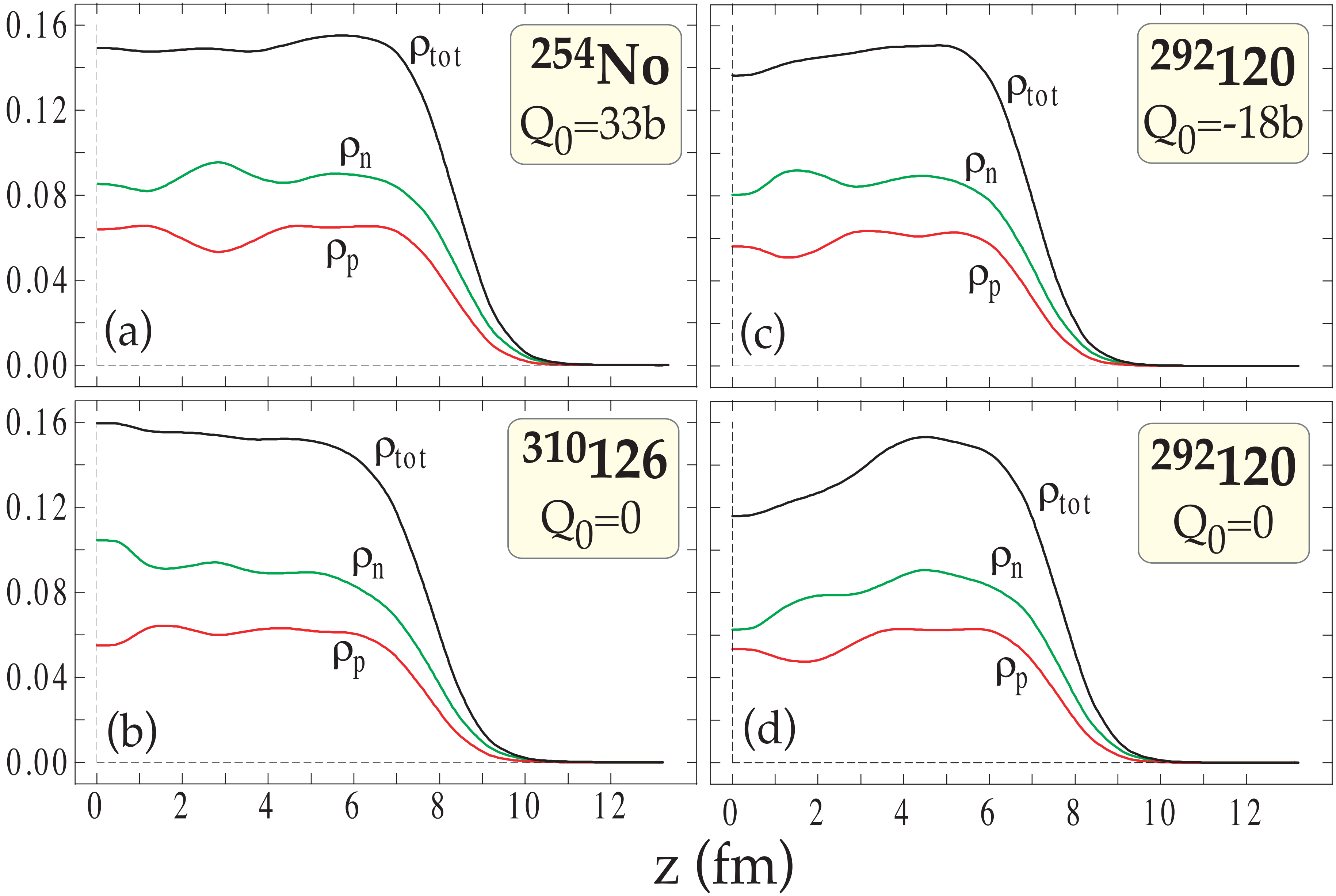
HFB+SkP, J. Dobaczewski et al., Phys. Rev. C 53, 2809 (1996)



Volume (bulk) effect

Binding-energy effect

S. Cwiok, P.H. Heenen, W. Nazarewicz



Helm model

R.H. Helm, Phys. Rev. 104, 1466 (1956)

How to characterize nucleonic density?

$$R_{\mathrm{rms}} \equiv \sqrt{\langle r^2 \rangle} = \sqrt{\frac{\int d^3\mathbf{r}\, r^2 \rho(\mathbf{r})}{\int d^3\mathbf{r}\, \rho(\mathbf{r})}}$$

$$F(\mathbf{q}) \equiv \int e^{i\mathbf{q}\mathbf{r}} \rho(\mathbf{r}) d^3\mathbf{r}$$

form factor

$$F(q) = \int j_0(qr)\rho(r) r^2 dr$$

spherical shape

In the Helm model, nucleonic density is approximated by a convolution of a sharp-surface density with radius R_0 with the Gaussian profile:

$$\rho^{(\mathrm{H})}(\mathbf{r}) = \int d^3\mathbf{r}'\, f_{\mathrm{G}}(\mathbf{r}-\mathbf{r}')\rho_0 \Theta(R_0 - |\mathbf{r}'|)$$

diffraction radius

$$f_{\mathrm{G}}(r) = \frac{1}{(2\pi)^{3/2}\sigma^3} e^{-\frac{r^2}{2\sigma^2}}$$

surface thickness

$$\rho_0 = \frac{3N}{4\pi R_0^3}$$

Helm model (cont.)

$$F^{(\mathrm{H})}(q) = \frac{3}{R_0 q} j_1(qR_0) e^{-\frac{\sigma^2 q^2}{2}}$$

The first zero of $F^{H}(q)$ is uniquely related to the radius parameter R_0

$$R_0 = 4.49341/q_1$$

first zero of F(q)

$$\sigma^2 = \frac{2}{q_m^2} \ln \frac{3R_0^2 j_1(q_m R_0)}{R_0 q_m F(q_m)}$$

first maximum of F(q)

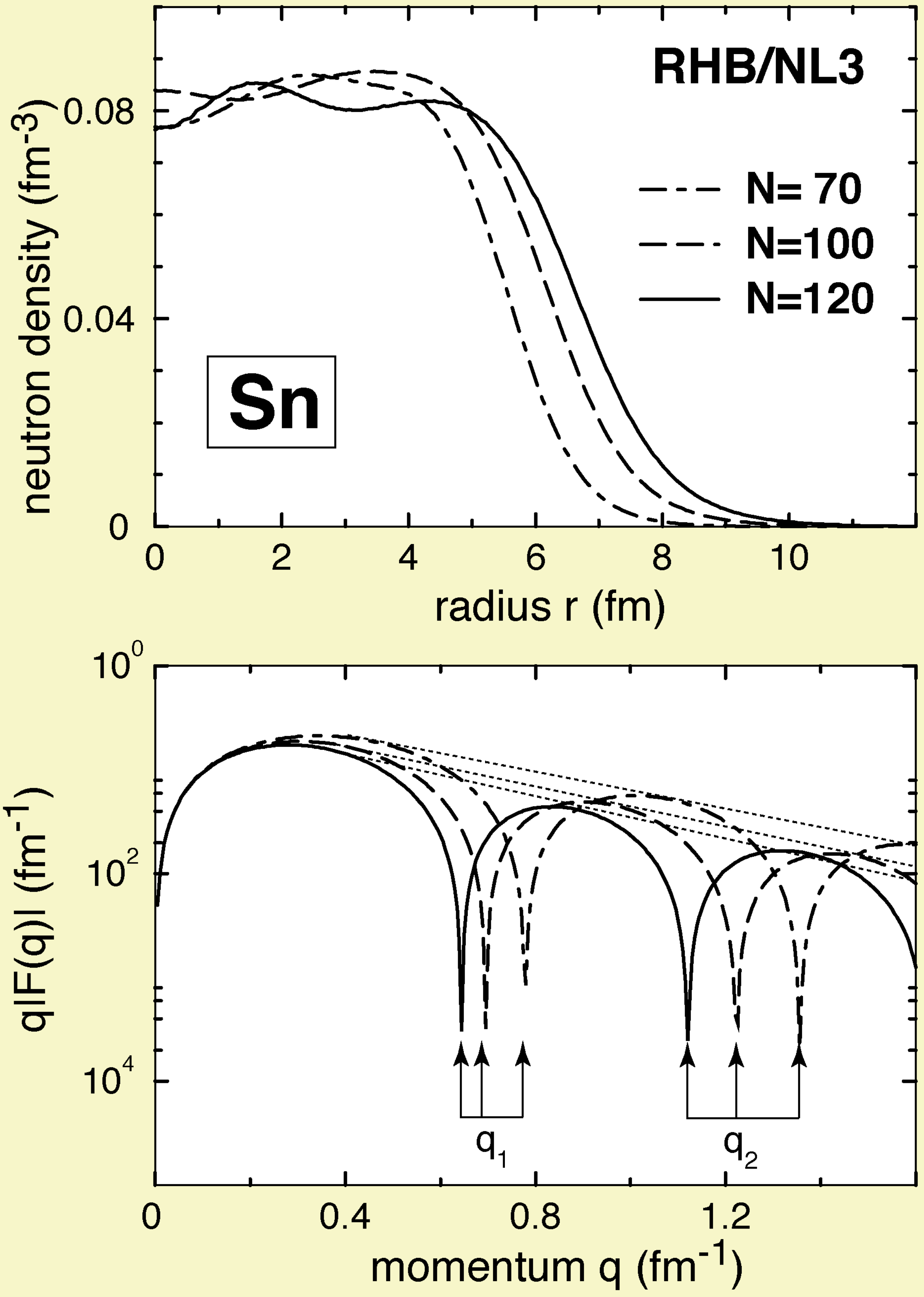
$$R_{\mathrm{rms}}^{(\mathrm{H})} = \sqrt{\tfrac{3}{5}\left(R_0^2 + 5\sigma^2\right)}$$

$$R_{\mathrm{geom}} = \sqrt{\tfrac{5}{3}} R_{\mathrm{rms}}$$

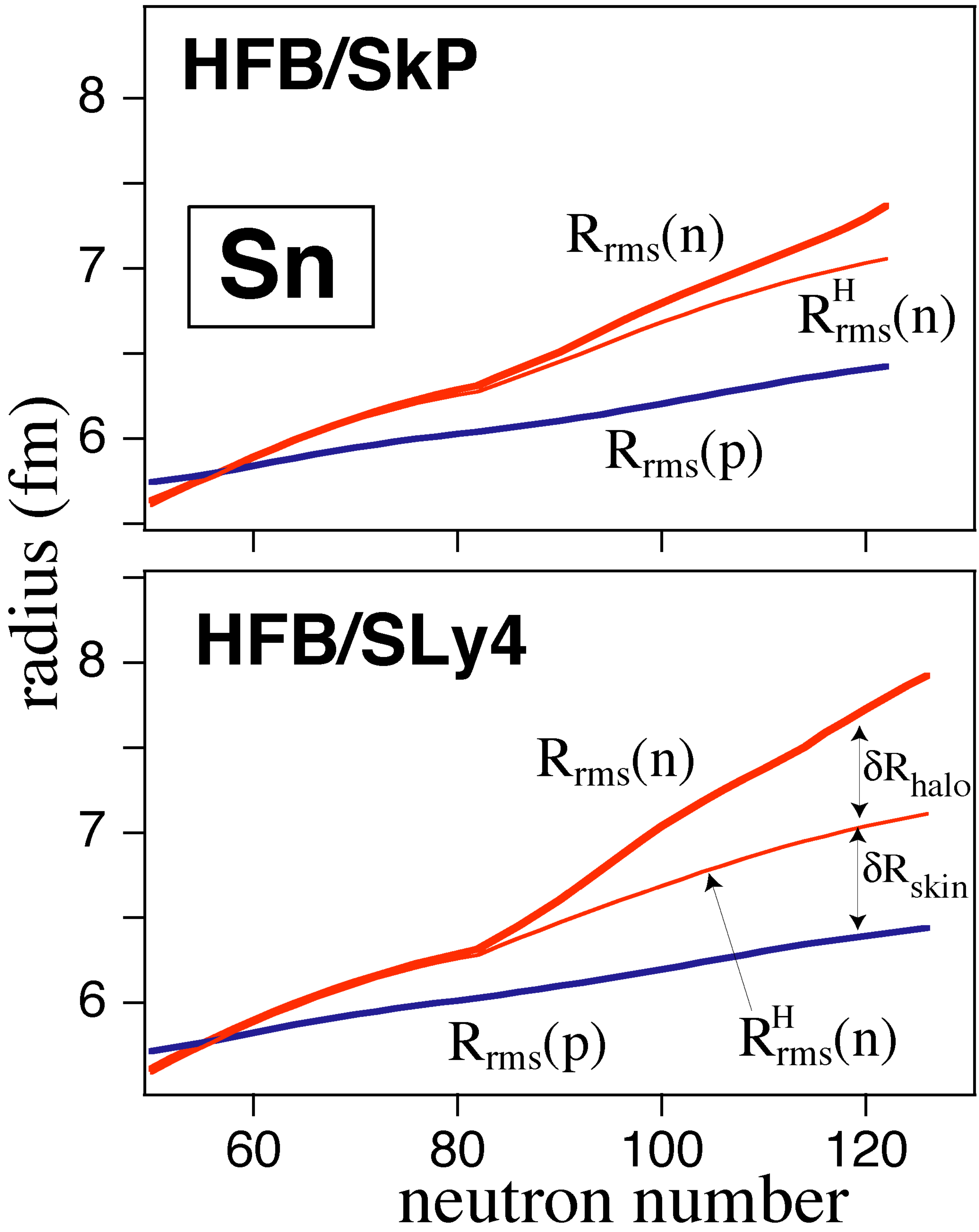
$$\boxed{\delta R_{\mathrm{halo}} \equiv R_{\mathrm{geom}} - R_{\mathrm{Helm}}}$$

$$R_{\mathrm{geom}}(\mathrm{p}) \approx R_{\mathrm{Helm}}(\mathrm{p})$$

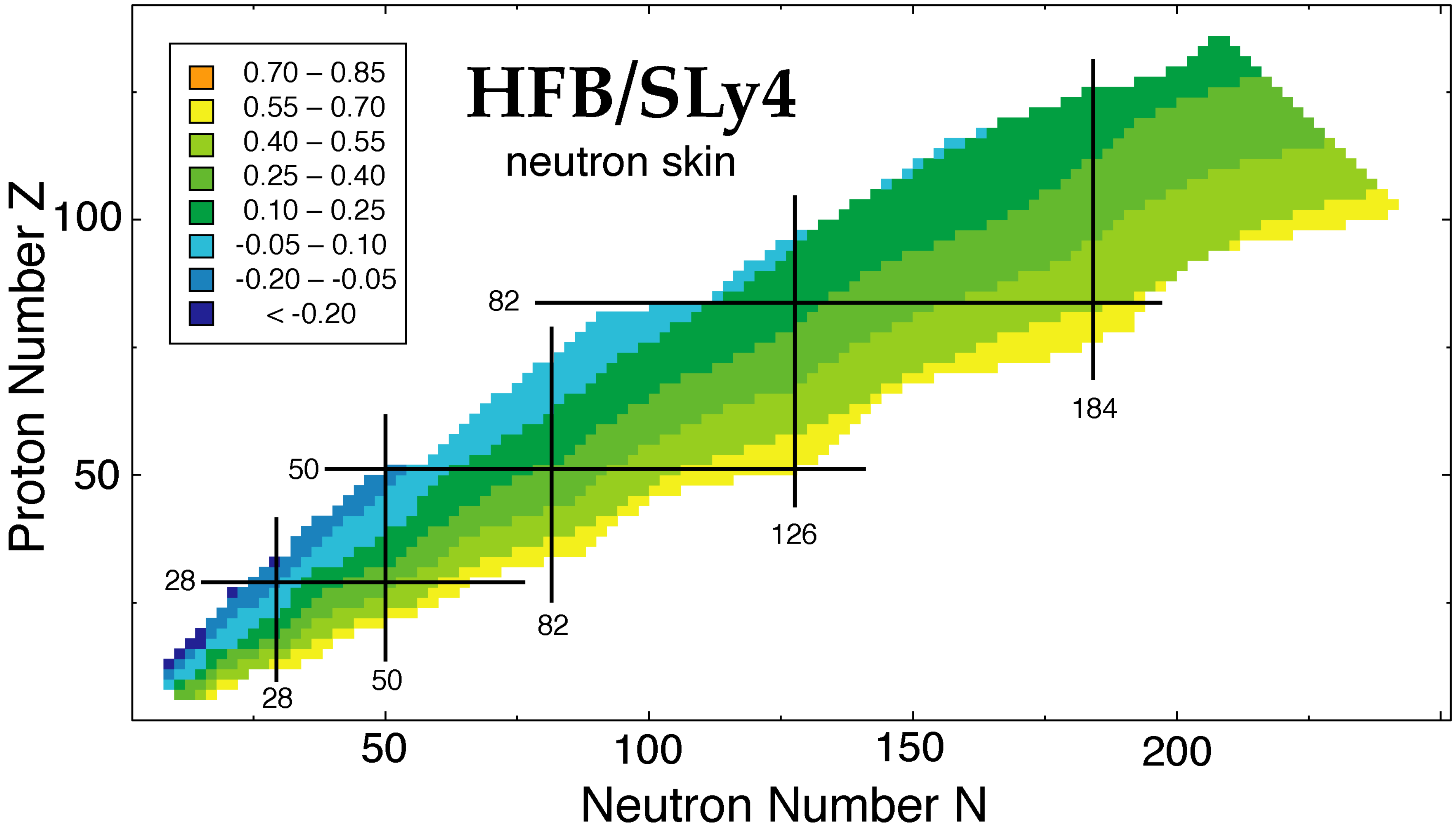
$$\boxed{\delta R_{\mathrm{skin}} \equiv R_{\mathrm{Helm}}(n) - R_{\mathrm{Helm}}(p)}$$



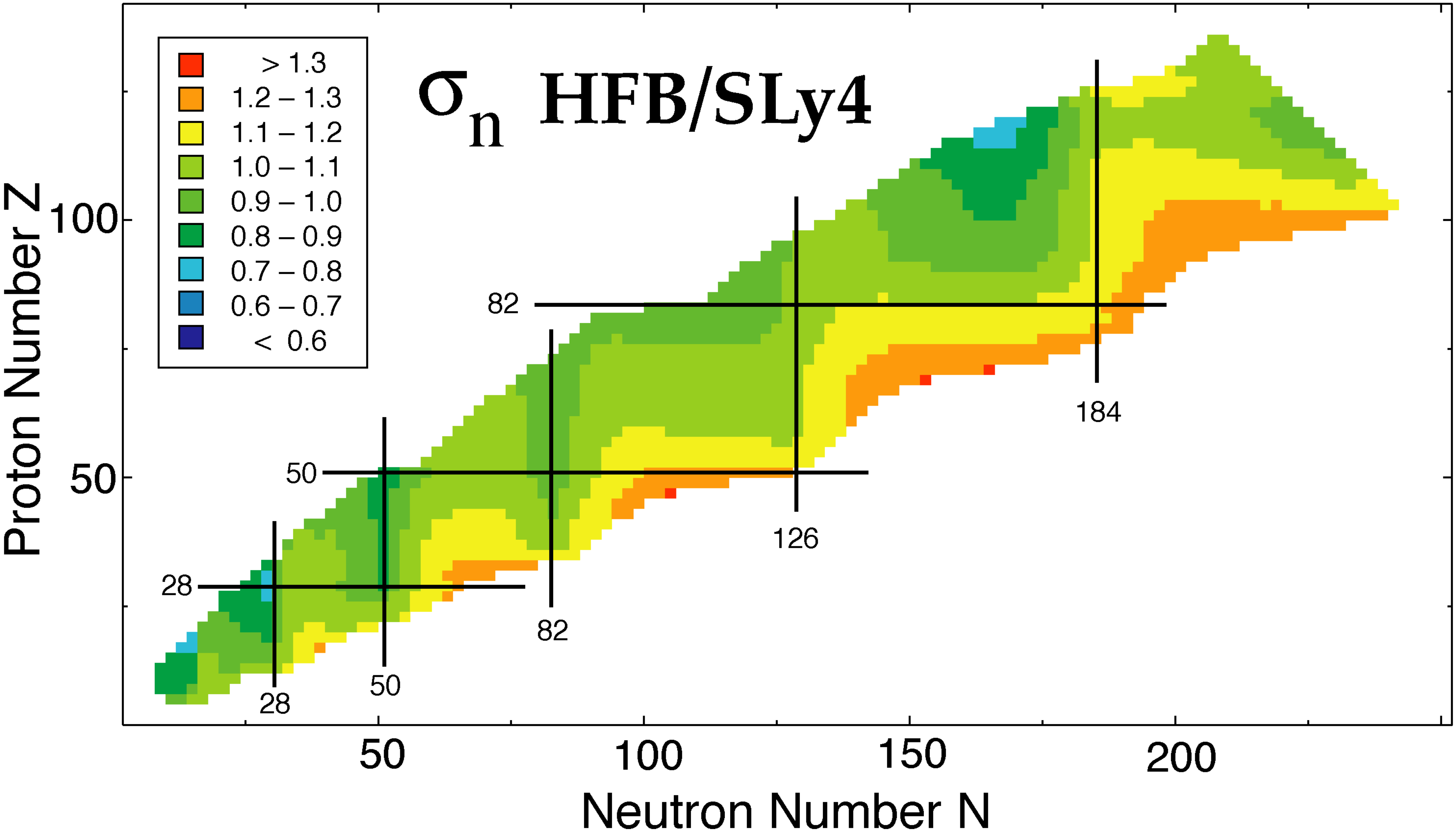
S. Mizutori et al., Phys. Rev. C 61, 044326 (2000)


HFB/SkP
Sn
$R_{rms}(n)$
$R^H_{rms}(n)$
$R_{rms}(p)$
HFB/SLy4
$R_{rms}(n)$
δR_{halo}
δR_{skin}
$R_{rms}(p)$
$R^H_{rms}(n)$
radius (fm)
6
7
8
60
80
100
120
neutron number

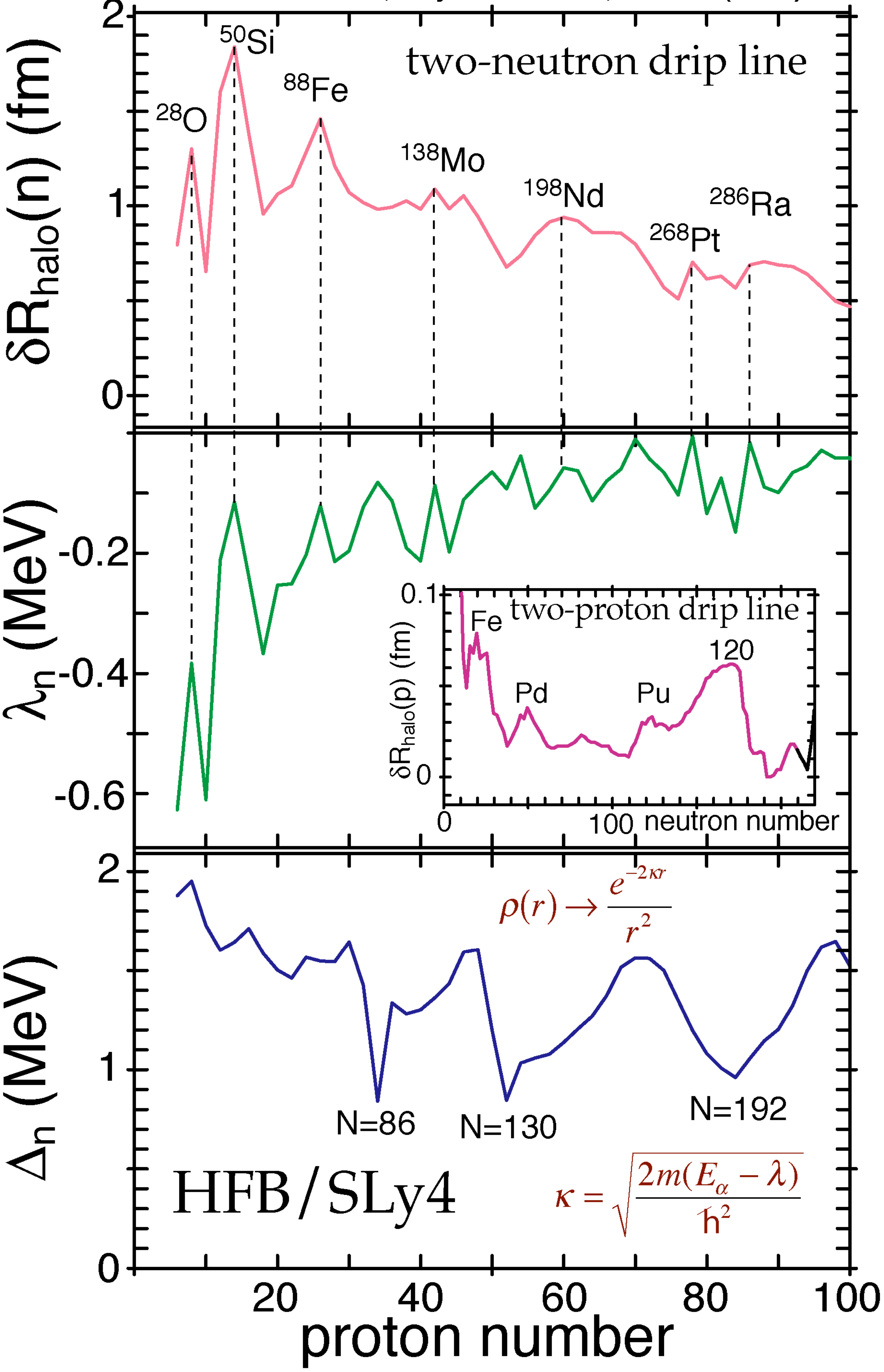
S. Mizutori et al., Phys. Rev. C61, 044326 (2000)



$$\delta R_{\rm skin} \equiv R_{\rm Helm}(n) - R_{\rm Helm}(p)$$

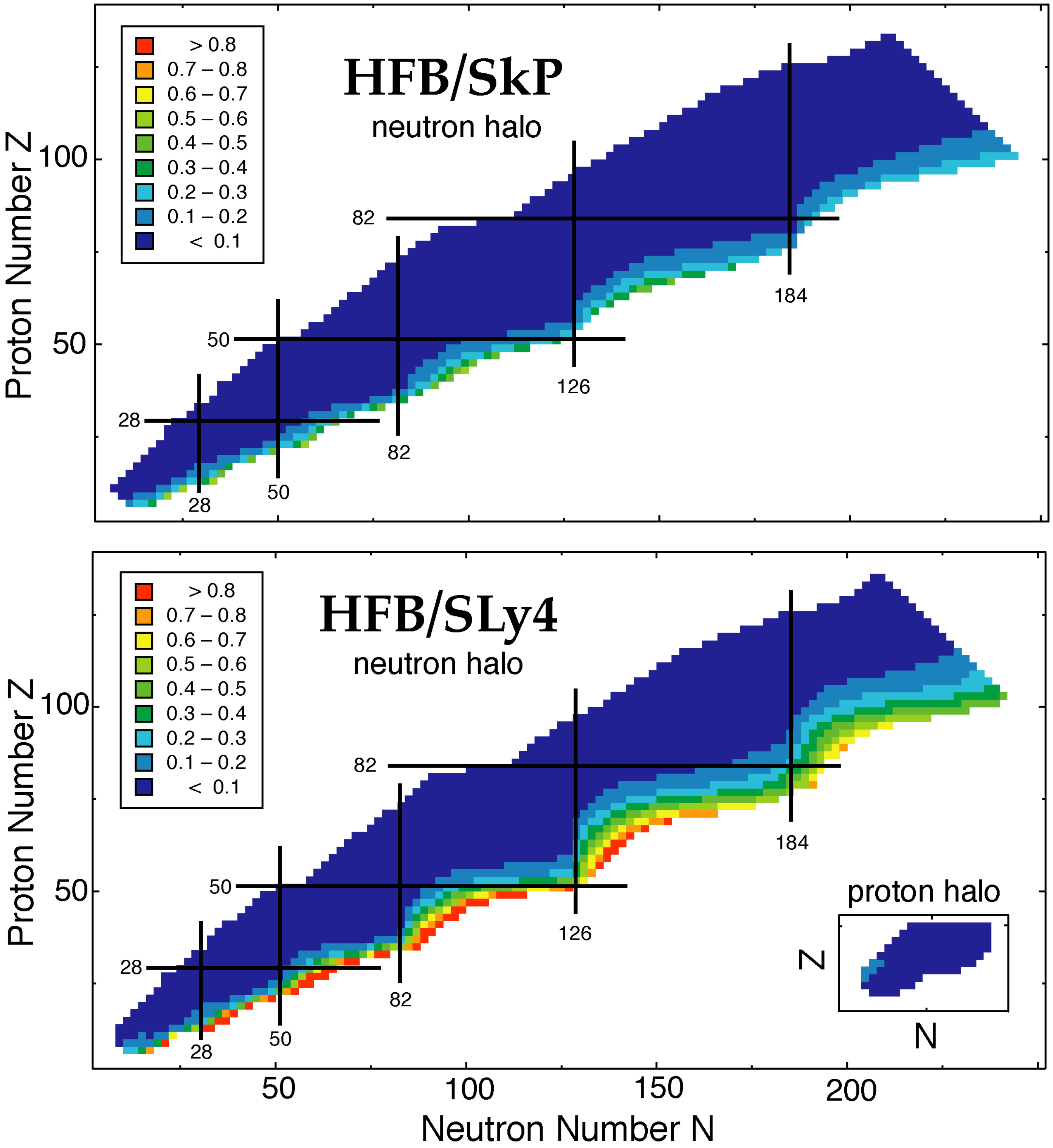

σ_n HFB/SLy4
> 1.3
1.2 – 1.3
1.1 – 1.2
1.0 – 1.1
0.9 – 1.0
0.8 – 0.9
0.7 – 0.8
0.6 – 0.7
< 0.6
28
50
82
126
184
28
50
82
Proton Number Z
100
50
Neutron Number N
50
100
150
200

S. Mizutori et al., Phys. Rev. C 61, 044326 (2000)

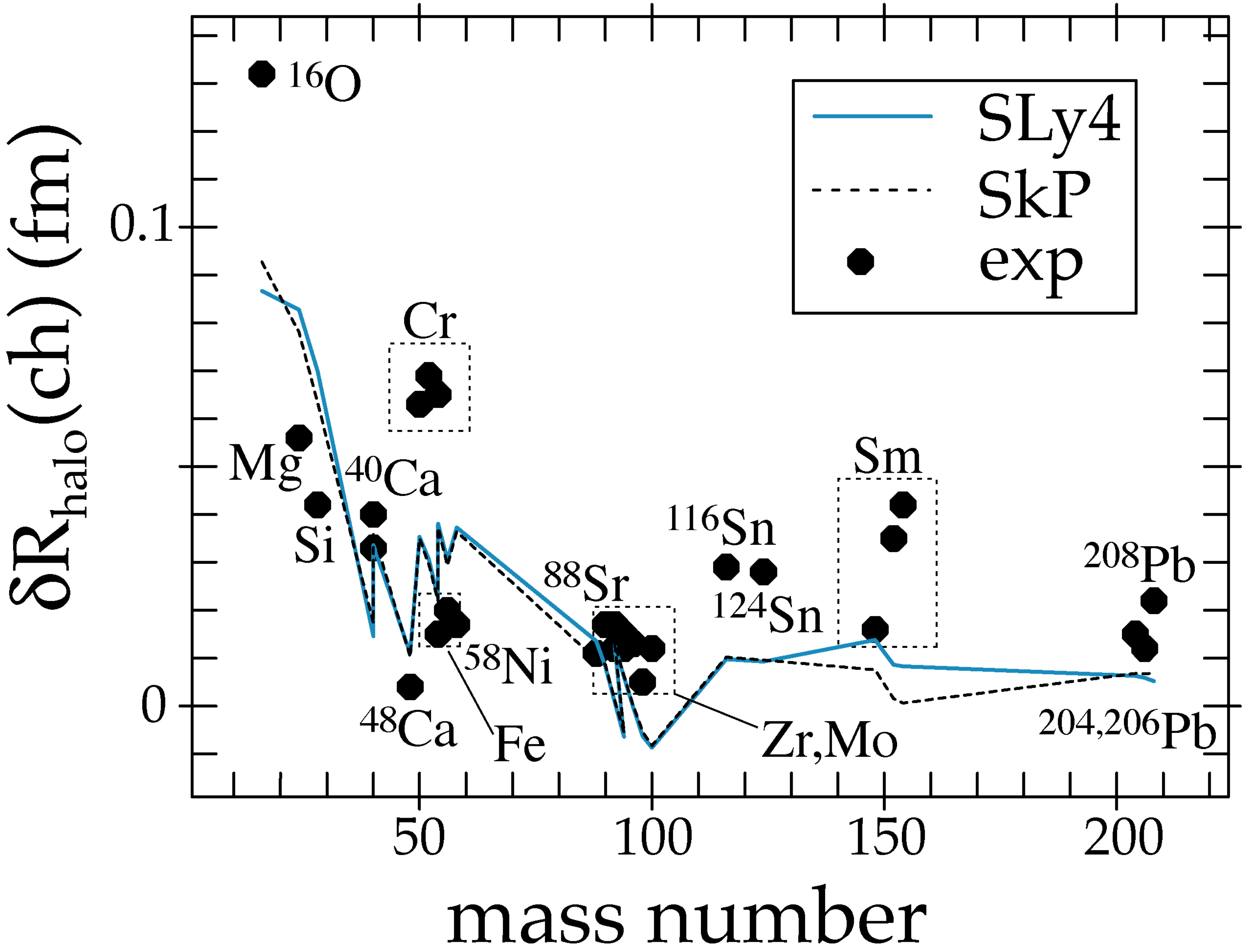


Neutron Halo

S. Mizutori et al., Phys. Rev. C61, 044326 (2000)



Halo is strongly influenced by pairing!



S. Mizutori et al., Phys. Rev. C61, 044326 (2000)

Generator Coordinate Method (GCM)

In molecules

$$\square(Q,x)=\underset{n}{\square}\square_n(Q,x)\square_n(Q)$$

In atomic nuclei

$$\square(x)=\underset{n}{\square}\square dQ\,\square_n(Q,x)f_n(Q)$$

$Q=\{Q_i\}\quad(i=1,2,\ldots F)$ - generator coordinates

$f_n(Q)$ - weight functions

$\square_{\mathrm{n}}(Q,x)$ - intrinsic (e.g. HFB) wave functions

$$\square\frac{\langle\square|\hat{H}|\square\rangle}{\langle\square|\square\rangle}=0$$

Variational principle leads to the Hill-Wheeler equation

$$\square dQ'\left\langle\square(Q)\middle|\hat{H}\middle|\square(Q')\right\rangle f(Q')=E\,\square dQ'\left\langle\square(Q)\middle|\square(Q')\right\rangle f(Q')$$

$\mathcal{H}(Q,Q')$

Hamiltonian kernel

$\mathcal{N}(Q,Q')$

Norm kernel

$$\mathcal{H}f=E\mathcal{N}f$$

Diagonalization of the Hamiltonian in the nonorthogonal “basis” of the generator states. The norm kernel cannot be inverted since it has zero eigenvalues!

Symmetric orthogonalization

$$\int dQ'\,\mathcal{N}(Q,Q')u_k(Q') = n_k u_k(Q)$$

- Since $\mathcal{N}$ is a norm, its eigenvalues are non-negative ($n_k \geq 0$)
- The functions u_k form a complete set in the space of weight functions f(Q)

$$\sum_k u_k(Q)u_k^*(Q') = \delta(Q-Q'); \quad \int dQ\,u_k^*(Q)u_{k'}(Q) = \delta_{kk'}$$

$$\mathcal{N} = \mathcal{N}^{1/2}\cdot\mathcal{N}^{1/2} \Longrightarrow \mathcal{N}^{1/2}(Q,Q') = \sum_k u_k(Q)\sqrt{n_k}\,u_k^*(Q')$$

$$\mathcal{N}^{1/2}\mathcal{H}\mathcal{N}^{1/2}g = Eg, \quad g = \mathcal{N}^{-1/2}f$$

- Again, we have to deal with zero eigenvalue states
- Fortunately, the corresponding states lead to GCM states f_0 with zero norm!

$$\langle\Psi|\Psi\rangle = \int dQ\,dQ'\,f_0^*(Q)\mathcal{N}(Q,Q')f_0(Q') = 0$$

- Consequently, we can restrict ourselves to states with $n_k > 0$.

Let us introduce the basis of **natural states**:

$$|k\rangle = \frac{1}{\sqrt{n_k}}\int u_k(Q)|\Phi(Q)\rangle dQ$$

- Those states are orthogonal
- They span a sub Hilbert space called **"collective" subspace** (the smallest Hilbert space containing all the generating states

$$P_C = \sum_{k,n_k\neq 0}|k\rangle\langle k| \Longrightarrow \sum_{k'}\langle k|\hat{H}|k'\rangle g_{k'} = Eg_k$$

$$|\square\rangle = \sum_{k,n_k \neq 0} g_k |k\rangle$$ **GCM eigenstates**

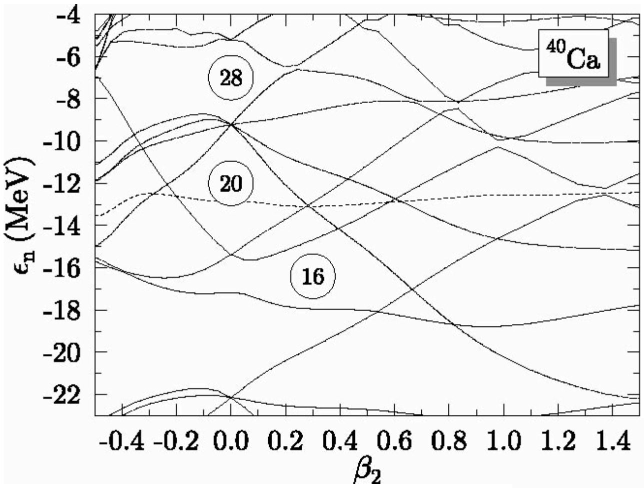
$$f(Q) = \sum_{k,n_k \neq 0} \frac{1}{\sqrt{n_k}} g_k u_k(Q)$$ **weight functions**

$$g(Q) = \sum_{k,n_k \neq 0} g_k u_k(Q)$$ **collective vawe functions**

$$\int |g(Q)|^2 dQ = \sum_k |g_k|^2 = 1, \quad \text{but} \quad \int |f(Q)|^2 dQ = \sum_k \frac{1}{n_k} |g_k|^2 \neq 1$$

- Microscopic
- Based on variational principle
- Allows for a coupling between intrinsic states
- Dynamics determined by the choice of Q's
- A useful point for further approximations (e.g., GOA, CSE, etc.)
- Transformation to the lab system still necessary, unless the Euler (or gauge) angles are taken as collective coordinates

An example: projected GCM+HF+BCS

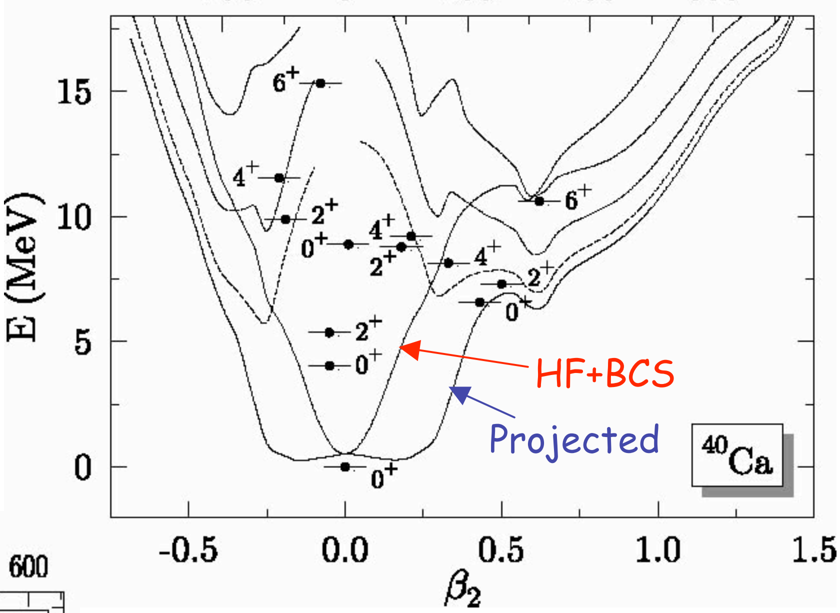


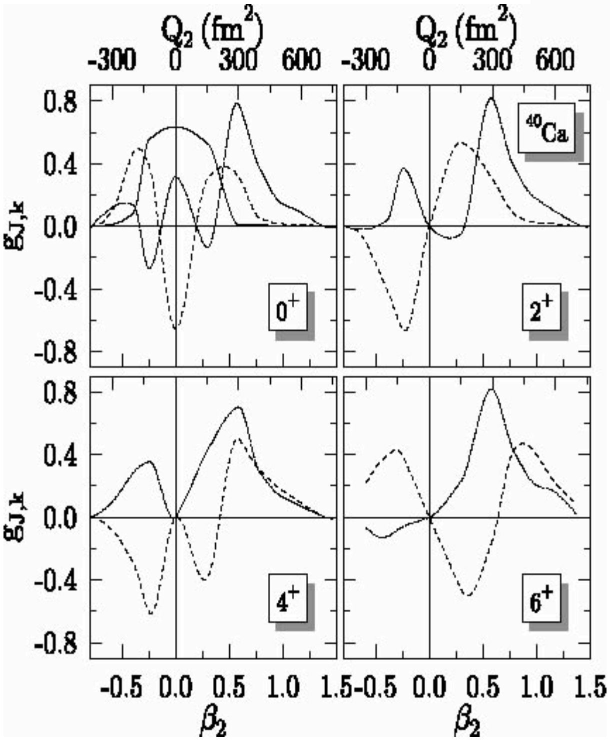
M. Bender ,H. Flocard ,P.-H. Heenen
nucl-th/0305021

Usual starting point: deformed mean fields

PESs and GCM eigenstates

$$\bar{\beta}_2 = \int \beta_2 \left| g_{J,k}(\beta_2) \right|^2 d\beta_2$$





Collective wave functions

———	ground state
·········	SD
- - - - -	ND

The Gaussian Overlap Approximation

$$q=\frac{Q+Q'}{2},\quad s=Q-Q'$$

$$\mathcal{N}(Q,Q')=\mathcal{N}\left(q+\frac{s}{2},q-\frac{s}{2}\right)=e^{-\frac{1}{2}\gamma(q)s^2}$$

For small values of s, one obtains:

$$\gamma(q)\approx\frac{1}{\hbar^2}\left(\langle q|\hat{P}^2|q\rangle-\langle q|\hat{P}|q\rangle^2\right)$$

$$\hat{P}=i\hbar\frac{\partial}{\partial q}$$

Collective momentum operator

If the fluctuation in collective momentum is large, one ends up with the Gaussian shape. (Well justified for heavy systems.)

$$\mathcal{H}_{coll}=-\frac{1}{\sqrt{\gamma}}\frac{\partial}{\partial q}\sqrt{\gamma}\frac{\hbar^2}{2M(q)}\frac{\partial}{\partial q}+V(q)$$

Collective Hamiltonian

$$M(q)$$

Collective mass (collective inertia)

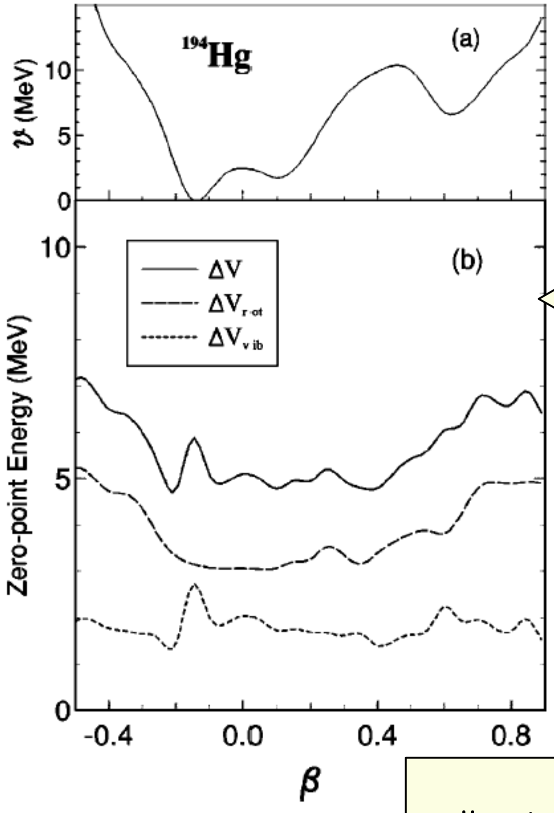
$$V(q)=\langle q|\hat{H}|q\rangle-\epsilon_{zpe}(q)$$

Collective potential

$$\epsilon_{zpe}(q)$$

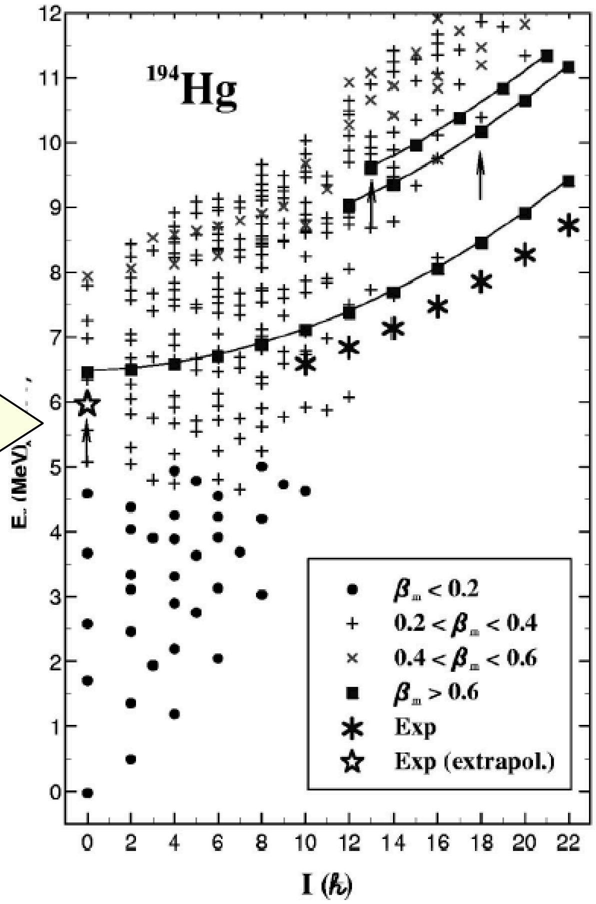
Zero-point energy

An example: GOA+HF(B) Gogny calculations

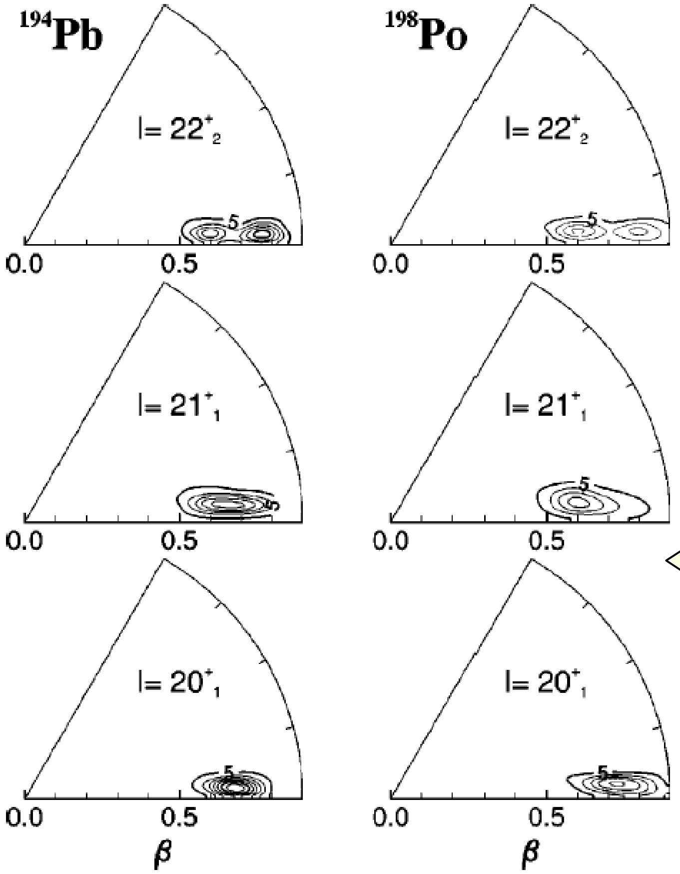


J. Libert, M. Girod, and J.-P. Delaroche
Phys. Rev. C **60** , 054301 (1999)

zero-point energy corrections



collective levels



collective wave functions

Random Phase Approximation

Small harmonic oscillations about the stationary mean-field ground state
Not based on a variational principle

$$\hat{H}|\nu\rangle = E_\nu|\nu\rangle$$

$$|\nu\rangle = \hat{Q}^+_\nu|\square\rangle \text{ and } \hat{Q}_\nu|0\rangle = 0$$

$$\left[\hat{H},\hat{Q}^+_\nu\right]|0\rangle = (E_\nu - E_0)\hat{Q}^+_\nu|0\rangle$$

A) Tamm-Dancoff approximation

$$|0\rangle = |HF\rangle, \quad \hat{Q}^+_\nu = \sum_{ph} C^\nu_{ph} a^+_p a_h$$

The TD phonon
is a p-h operator

$$\sum_{nj} \langle HF|\left[a^+_i a_m,\left[\hat{H},a^+_n a_j\right]\right]|HF\rangle C^\nu_{nj} = E^{TDA}_\nu C^\nu_{mi}$$

B) Random Phase approximation

$$|0\rangle = |RPA\rangle, \quad \hat{Q}^+_\nu = \sum_{ph} X^\nu_{ph} a^+_p a_h - \sum_{ph} Y^\nu_{ph} a^+_h a_p, \quad \hat{Q}_\nu|RPA\rangle = 0$$

RPA ground state contains correlations beyond HF
Usually, one assumes that the RPA state does not differ much from the HF state, at least when commutators are computed ("quasi-boson approximation")

$$\langle RPA|\left[a^+_i a_n,\left[\hat{H},Q^+_\nu\right]\right]|RPA\rangle = \hbar\omega_\nu\langle RPA|\left[a^+_i a_n,Q^+_\nu\right]|RPA\rangle$$

$$\langle RPA|\left[a^+_n a_i,\left[\hat{H},Q^+_\nu\right]\right]|RPA\rangle = \hbar\omega_\nu\langle RPA|\left[a^+_n a_i,Q^+_\nu\right]|RPA\rangle$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix} = \hbar\omega_{\nu}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix}$$

RPA equations

$$A_{nimj} = \langle HF|\left[a_i^+ a_n,\left[\hat{H},a_m^+ a_j\right]\right]|HF\rangle = (\varepsilon_n - \varepsilon_i)\delta_{mn}\delta_{ij} + \bar{v}_{njim}$$

$$B_{nimj} = \langle HF|\left[a_i^+ a_m,\left[\hat{H},a_j^+ a_n\right]\right]|HF\rangle = \bar{v}_{nmij}$$

$$\sum_{ph}\left(X_{ph}^{\nu}X_{ph}^{\nu'*} - Y_{ph}^{\nu}Y_{ph}^{\nu'*}\right) = \delta_{\nu\nu'}$$

Random Phase Approximation and symmetry breaking

$$\left[\rho^{(0)},\hat{P}\right] \neq 0, \quad \text{where } \rho^{(0)} \text{ is the HF density}$$

some ph matrix elements of P do not vanish!

$$\left[\hat{H},\hat{P}\right] = 0, \text{ where } \hat{P} \text{ is a one-body symmetry generator}$$

this implies that P is an exact but spurious solution of the RPA equation

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} P \\ -P^* \end{pmatrix} = 0$$

If calculations are carried out precisely, and the self-consistency is maintained, the spurious solutions separate out. They are orthogonal to other excitations, they lie at zero excitation energy, and they carry spurious strength.

Another way of deriving the RPA equations: the linear response theory

Here, the starting point is TDHF. We investigate the influence of an external, time-dependent field:

$$F(t) = Fe^{-i\omega t} + F^{+}e^{i\omega t}, \quad F(t) = \sum_{kl} f_{kl}(t)a_k^{+}a_l$$

F is a one-body operator; the field is weak

$$i\hbar\dot{\rho} = \left[h(\rho) + f(t), \rho\right]$$

TDHF equation

$$\rho^2 = \rho$$

we are dealing with a time-dependent Slater determinant

$$\rho(t) = \rho^{(0)} + \delta\rho(t), \quad \delta\rho(t) = \rho^{(1)}e^{-i\omega t} + \rho^{(1)+}e^{i\omega t}$$

$$\left[\begin{pmatrix} A & B \\ B^{*} & A^{*} \end{pmatrix} - \hbar\omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]\begin{pmatrix} \rho^{(1)ph} \\ \rho^{(1)hp} \end{pmatrix} = -\begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix}$$

$$A_{nimj} = (\varepsilon_n - \varepsilon_i)\delta_{mn}\delta_{ij} + \frac{\partial h_{ni}}{\partial \rho_{mj}}$$

$$B_{nimj} = \frac{\partial h_{ni}}{\partial \rho_{jm}}$$

$$\tilde{v}_{psqr} = \frac{\partial h_{pq}}{\partial \rho_{rs}} = \frac{\partial^2 E}{\partial \rho_{pq}\partial \rho_{rs}}$$

Also valid for density-dependent forces and density functionals!

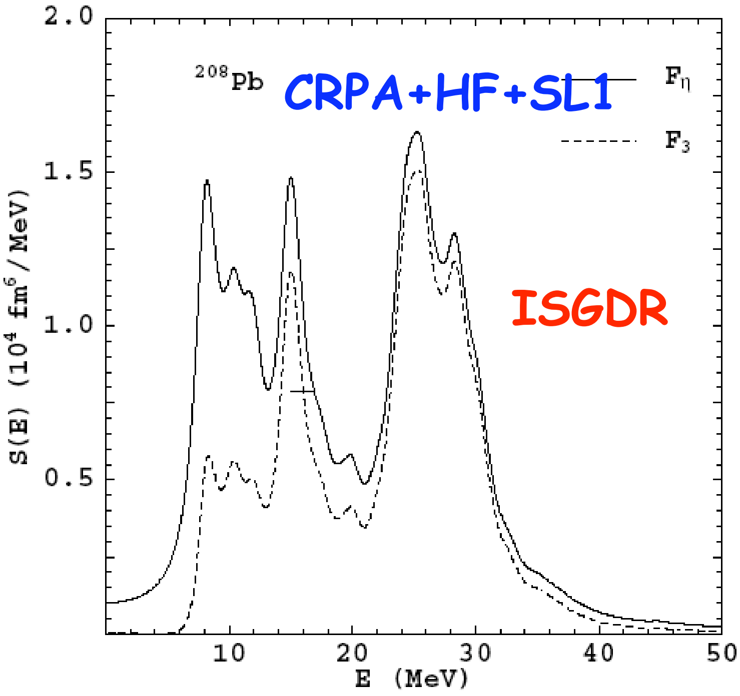
A nice connection with the HF theory: the average nuclear potential oscillates around the stationary value. In the limit of small external force, we obtain the normal modes of the system. Hence RPA is the small amplitude limit of the TDHF!

Inclusion of pairing: Q(uasiparticle)RPA
Inclusion of continuum: C(ontinuum)RPA

RPA calculations: examples

S. Shlomo ,A.I. Sanzhur
Phys.Rev. C65, 044310 (2002)

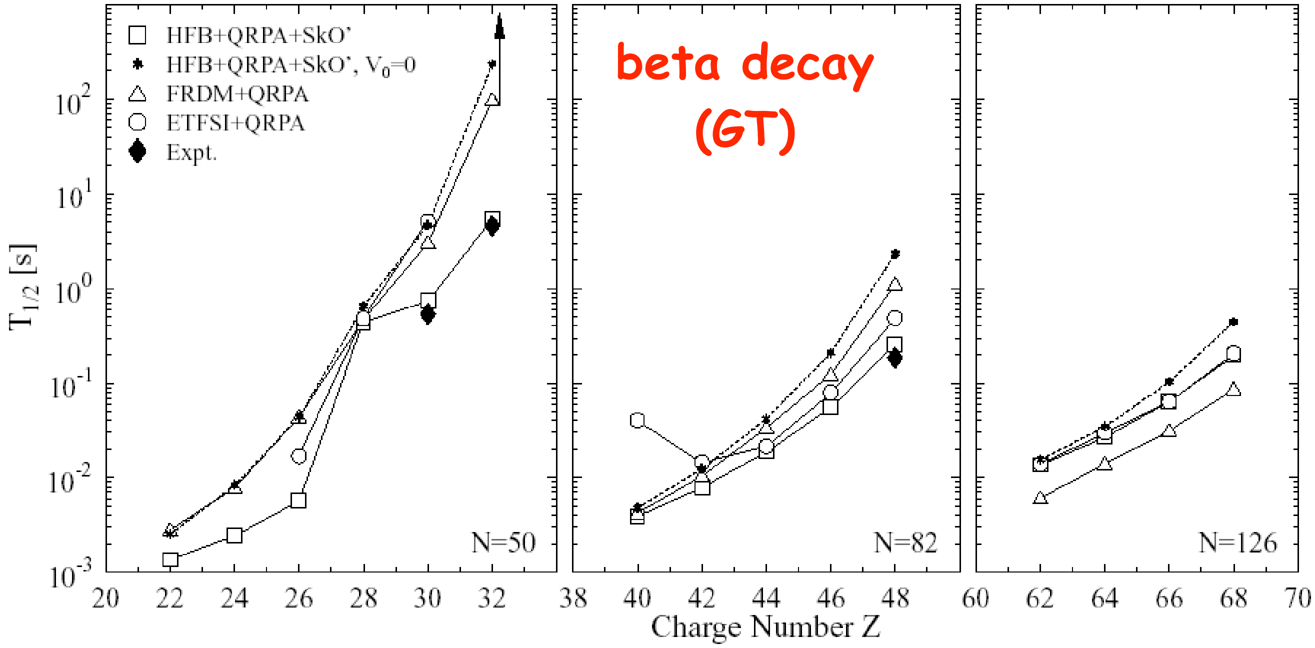
Agrawal, Shlomo , Sanzhur
Phys.Rev. C67, 034314 (2003)



CRPA+HF+SL1

ISGDR

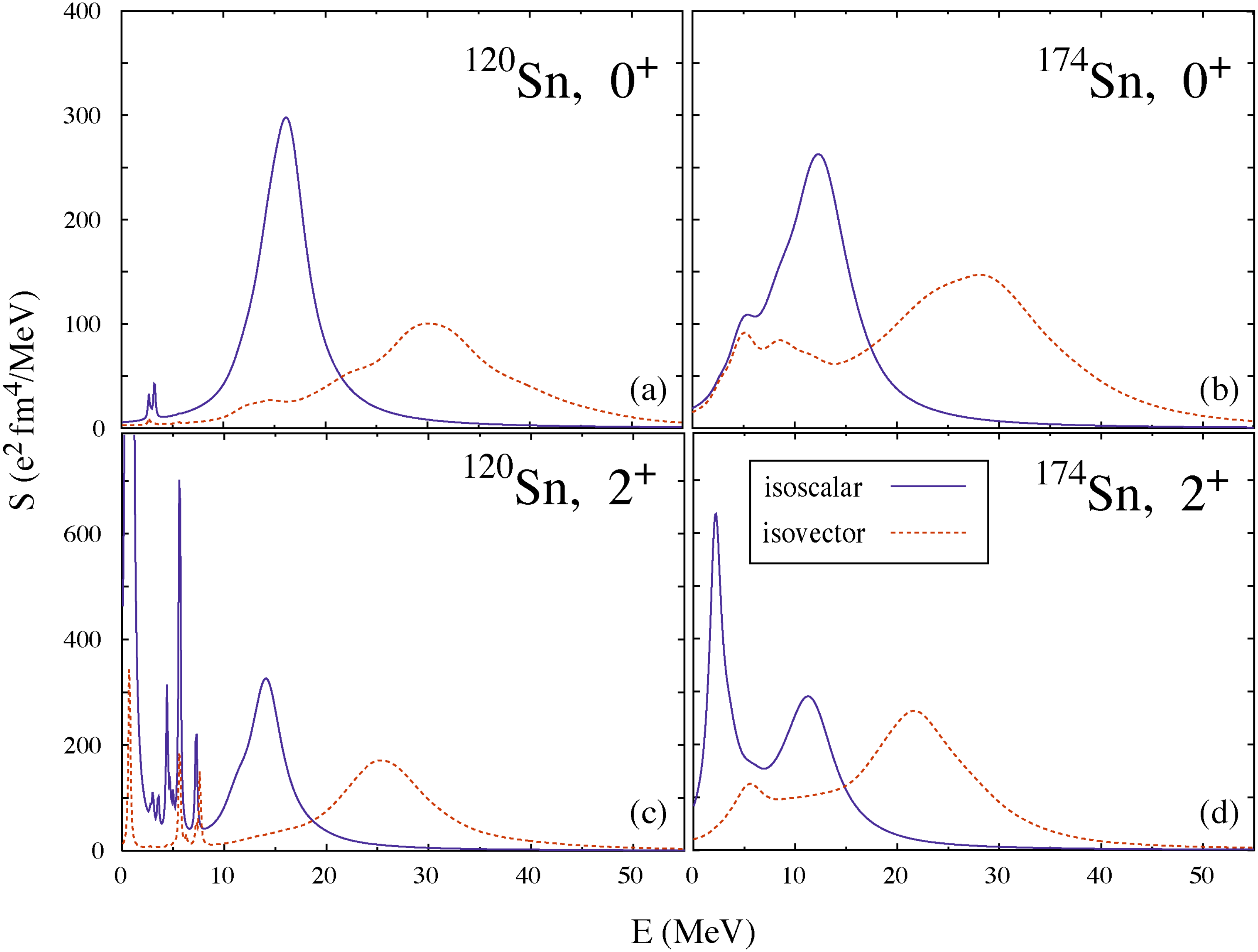
QRPA+HFB+SkO'



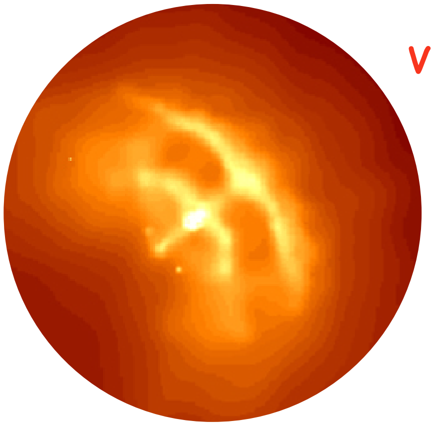
beta decay
(GT)

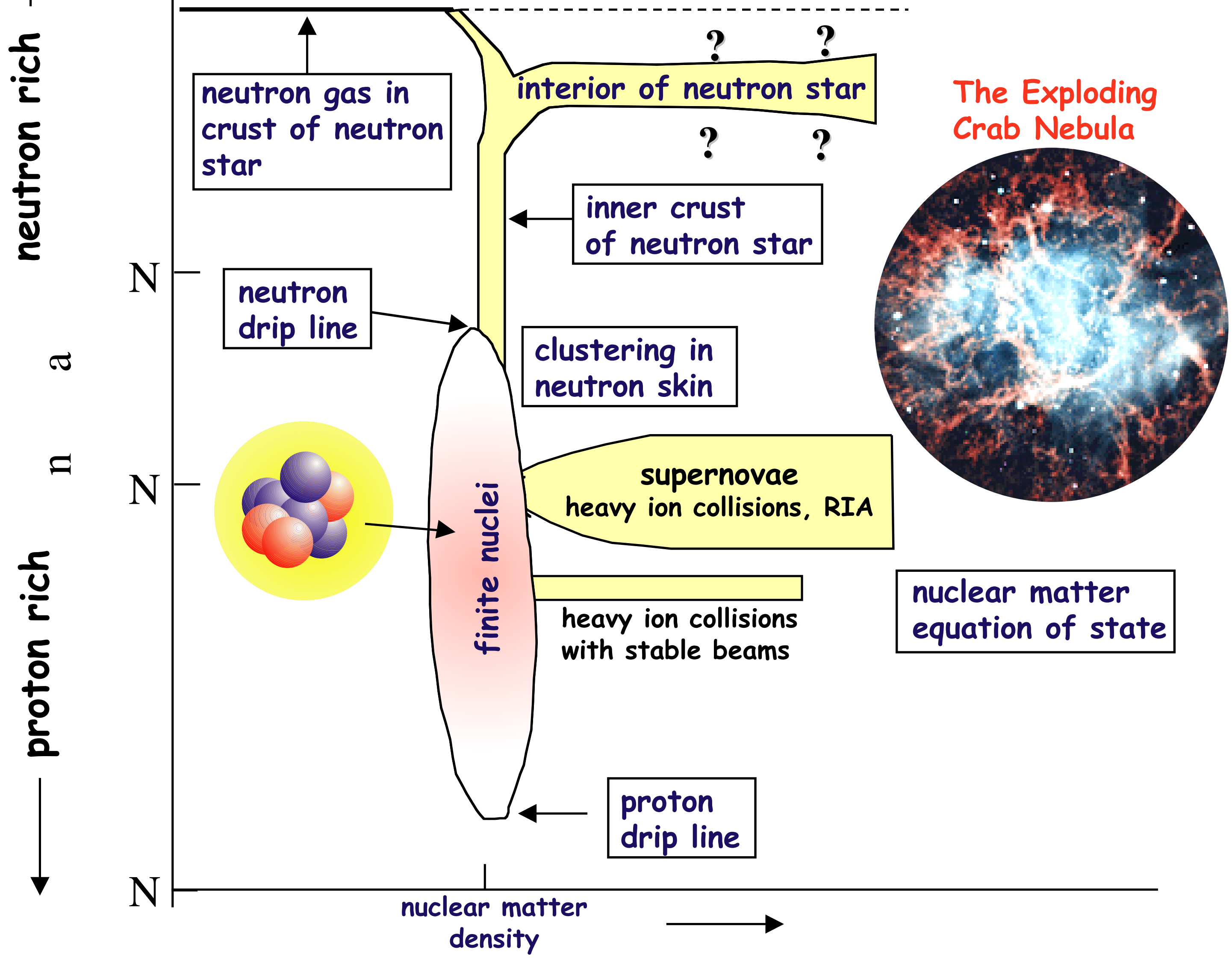
Engel et al. Phys.Rev. C60, 014302 (1999)

HFB+QRPA: J. Terasaki et al. nucl-th/0407111



From finite nuclei to extended nuclear matter


Vela Pulsar



The Exploding Crab Nebula

nuclear matter equation of state