The atomic nucleus: a finite open quantum many-body system

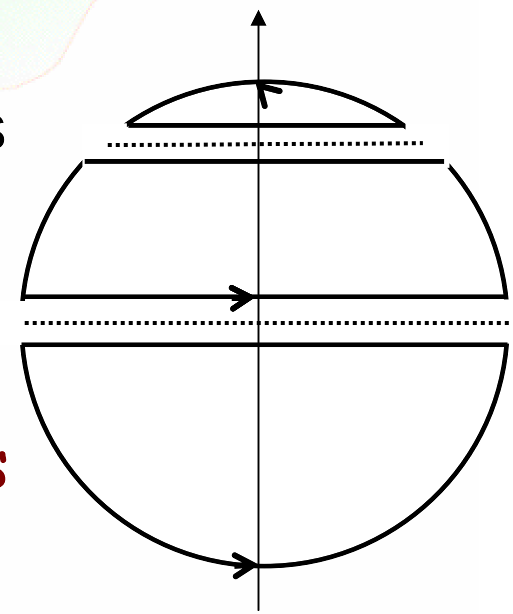
Witold Nazarewicz (Tennessee)

Cross talks in the physics of many body systems

Paris, December 2006

- Introduction: strategy
- Nuclear many-body problem'06
  - Ab initio techniques
  - Configuration interaction (shell model)
  - **Nuclear density functional theory**
- Large-amplitude collective motion
  - Fission and fusion
- Unifying structure and reaction aspects
  - **Rigged Hilbert space formulation**
- Super-heavy elements (?)

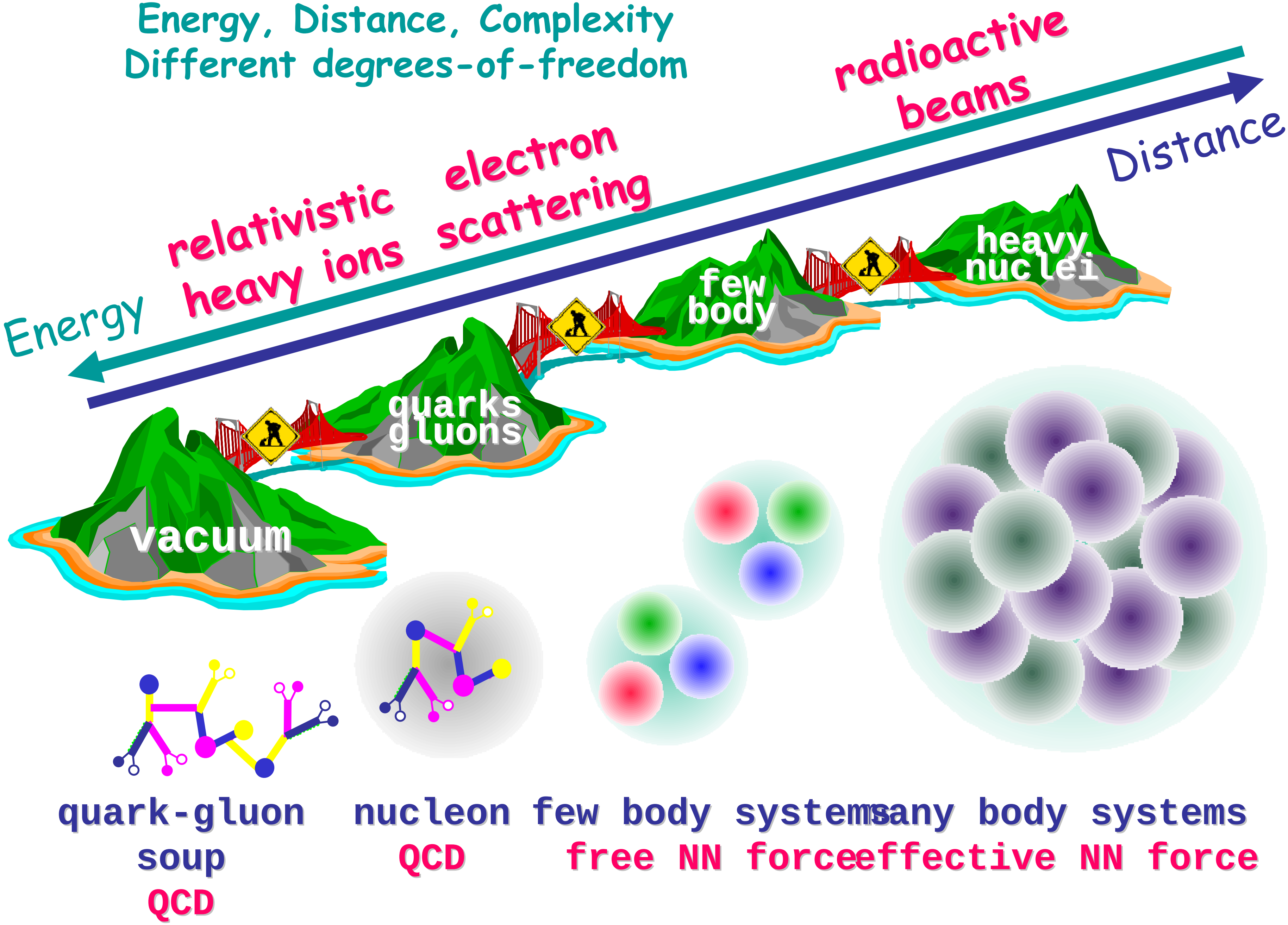
Summary



Emphasis on: novel aspects
differences
problems

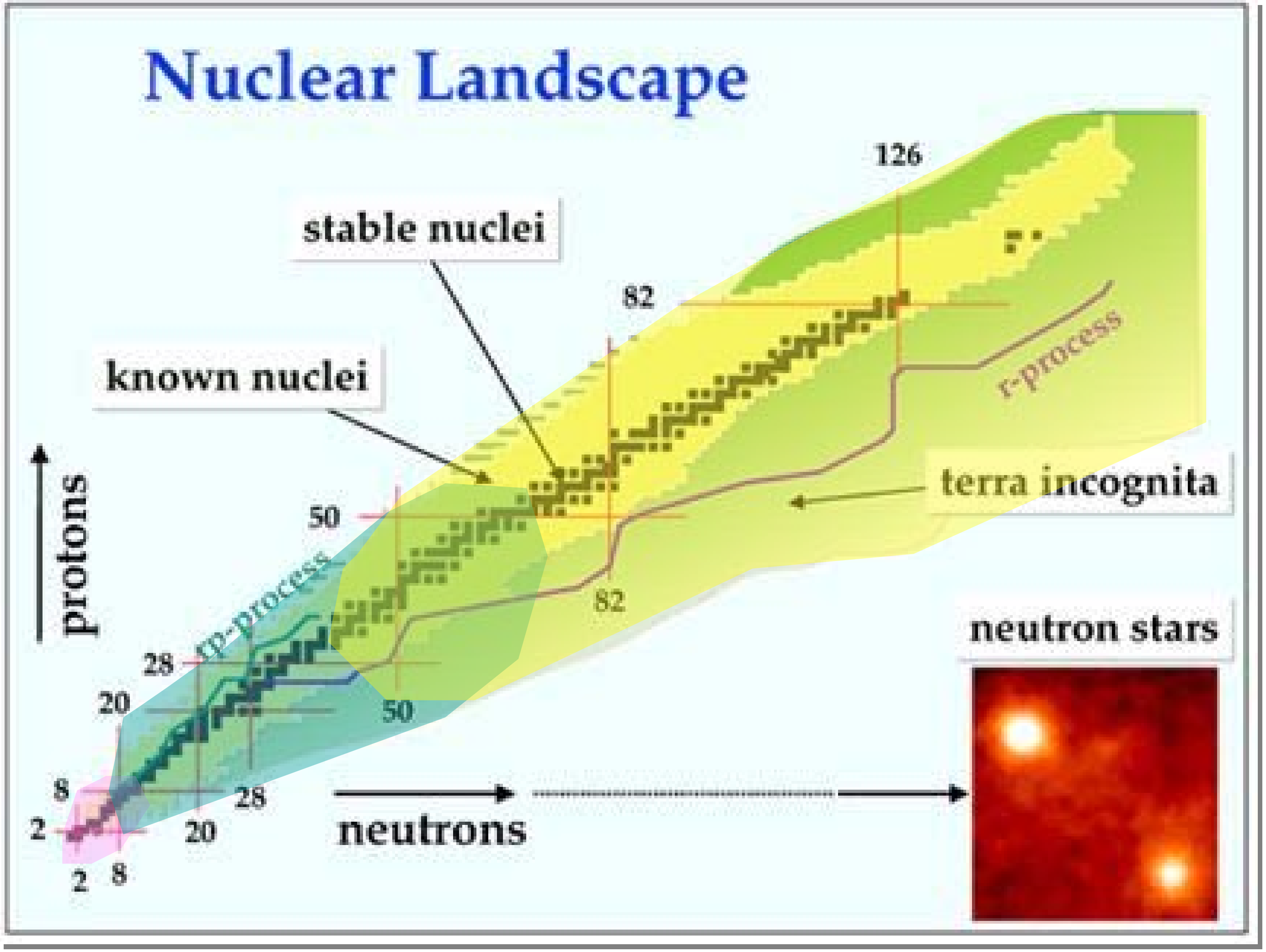
The Nuclear Many-Body Problem

Energy, Distance, Complexity
Different degrees-of-freedom



Bottom-up approaches to nuclear structure

Roadmap



Ab initio

Configuration interaction

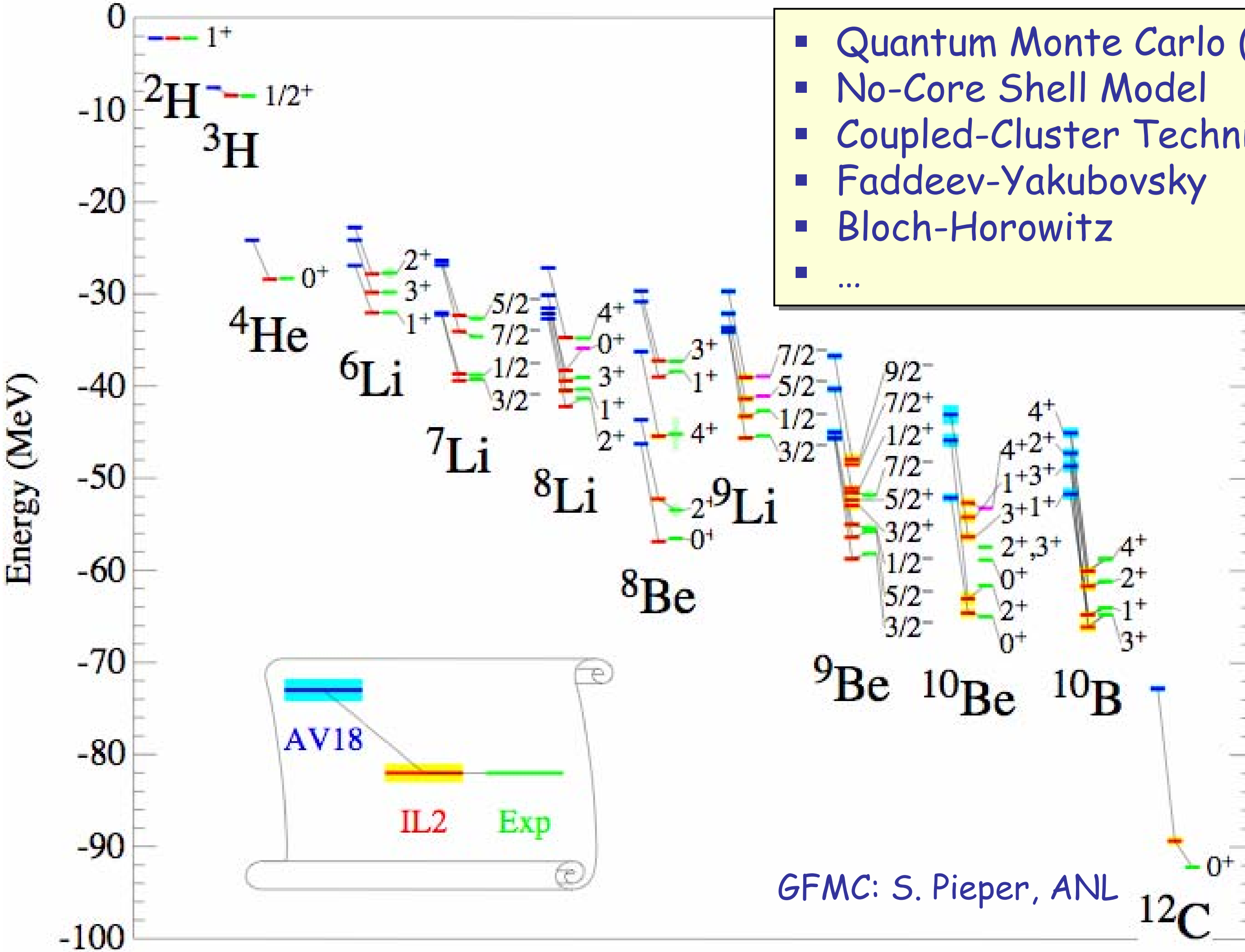
Density Functional Theory

Theoretical approaches overlap and need to be bridged

Ab initio: GFMC, NCSM, CCM

(nuclei, neutron droplets, nuclear matter)

- Quantum Monte Carlo (GFMC) ^{12}C
- No-Core Shell Model ^{13}C
- Coupled-Cluster Techniques ^{16}O
- Faddeev-Yakubovsky
- Bloch-Horowitz
- …

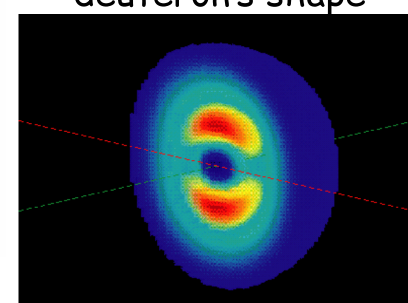


1-2% calculations of A = 6 – 12 nuclear energies are possible
excited states with the same quantum numbers computed

Input:

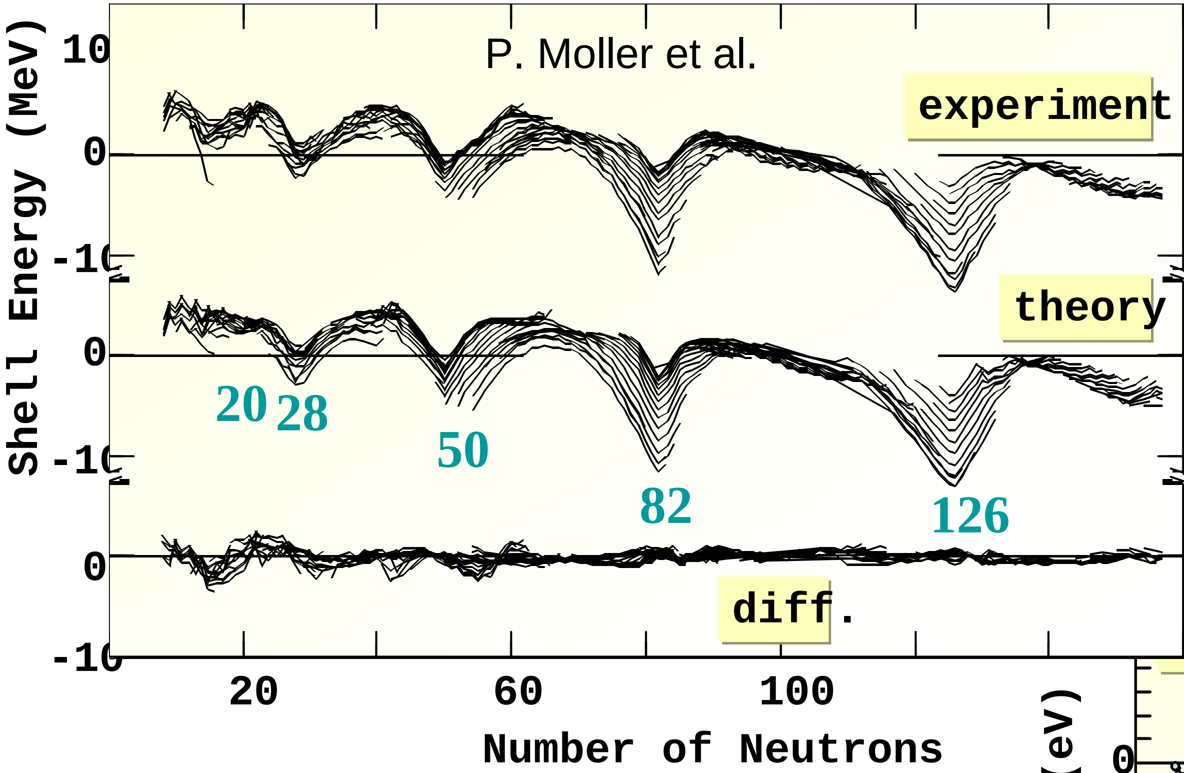
- Excellent forces based on the phase shift analysis
- EFT based nonlocal chiral NN and NNN potentials

deuteron's shape

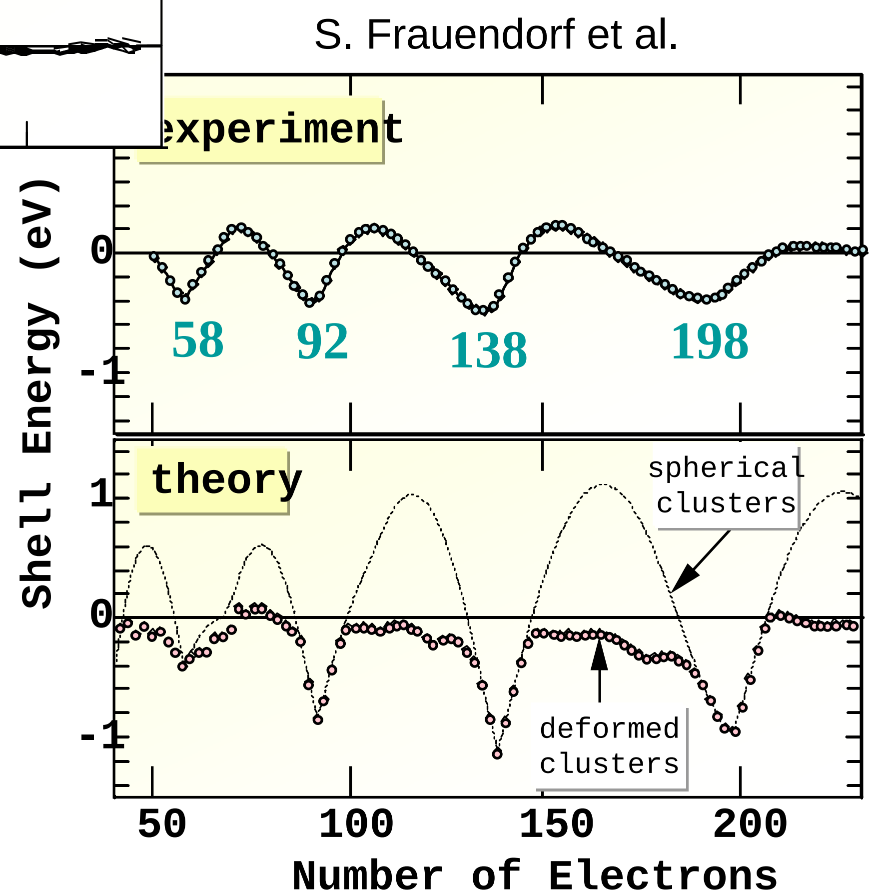


The nucleon-based description works to <0.5 fm

Shells



Nuclei



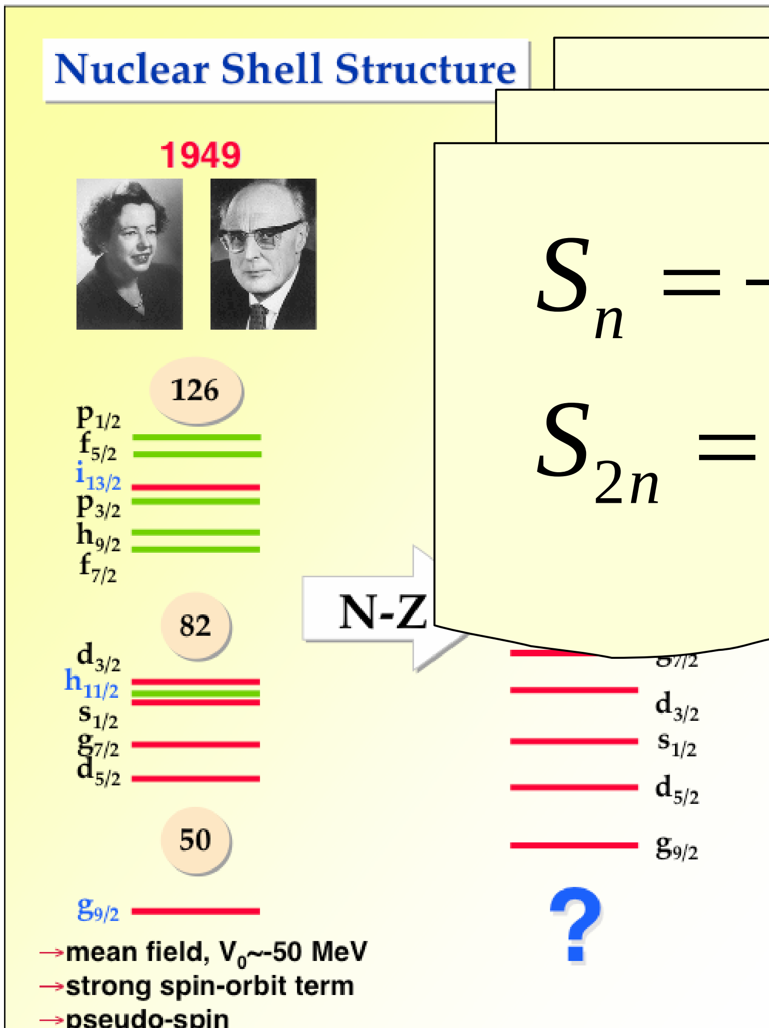
Sodium Clusters

- Mean-field an excellent starting point
- Single-particle motion a useful concept

…or is it???

Old paradigms, universal ideas, are not correct

Near the drip lines nuclear structure may be dramatically different.

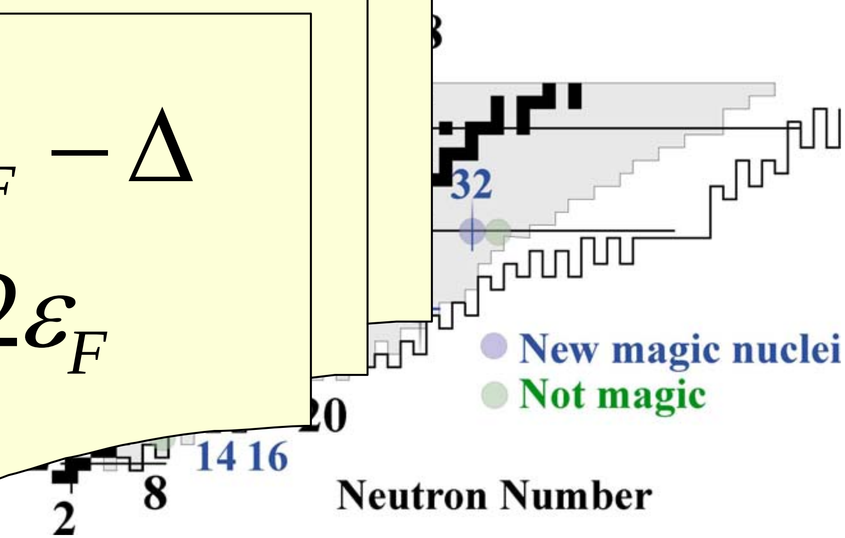


First experimental indications

ficant changes

$$S_n = -\varepsilon_F - \Delta$$

$$S_{2n} = -2\varepsilon_F$$



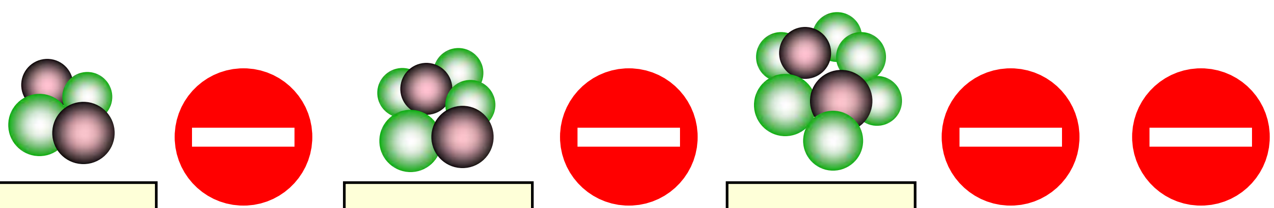
No shell closure for N=8 and 20 for drip-line nuclei; new shells at 14, 16, 32…

Neutron Drip line nuclei

HUGE

D i f f u s e d

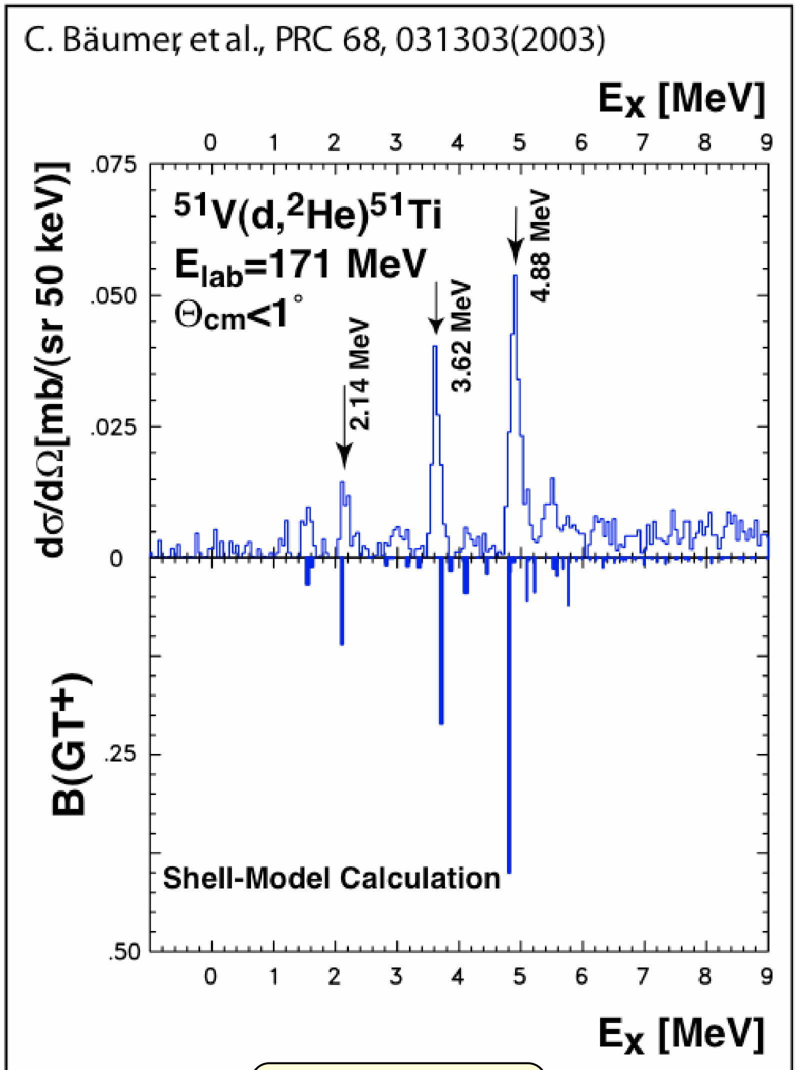
PA IR ED



^{4}He ^{5}He ^{6}He ^{7}He ^{8}He ^{9}He ^{10}He

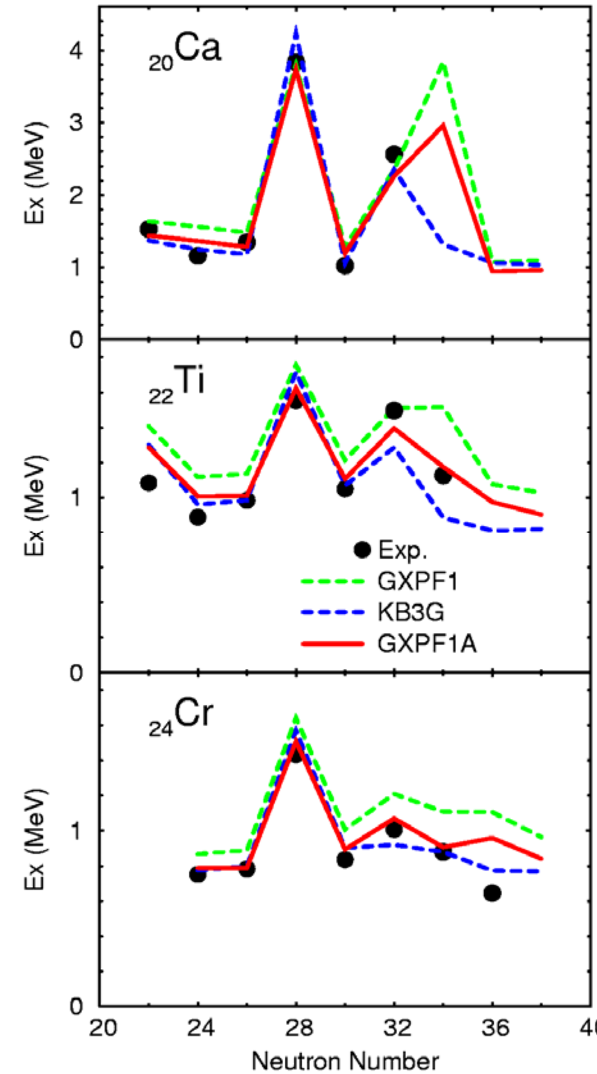
Diagonalization Shell Model (CI)

(medium-mass nuclei reached;dimensions 10^9!)



Martinez-Pinedo ENAM'04

Honma, Otsuka et al., PRC69, 034335 (2004) and ENAM'04



Configuration Interaction

One valence shell CI works great,
but… 10^{24} is not an option!!!

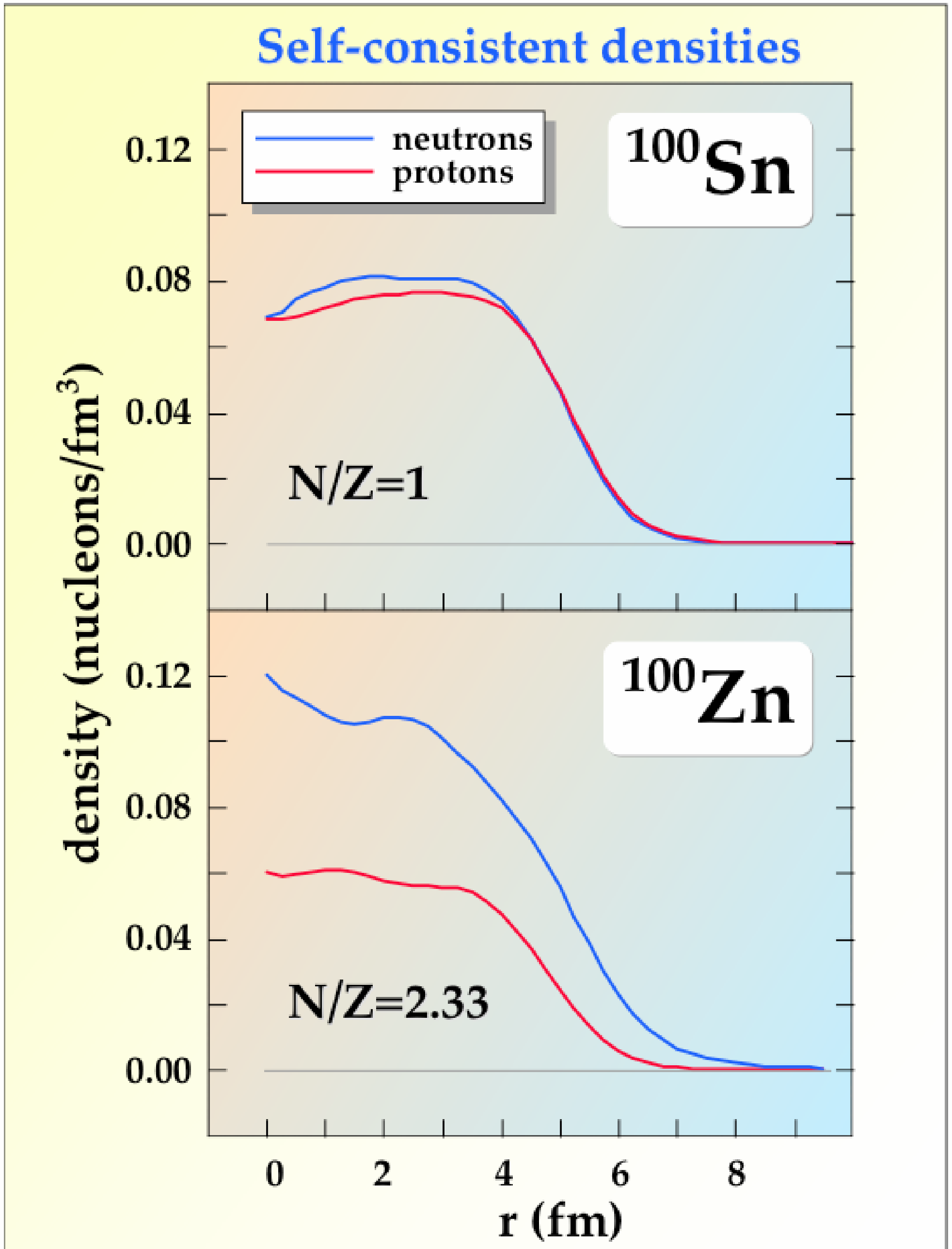
Smarter solutions are needed

- Monte Carlo Shell Model
- Density Matrix Renormalization Group
- Factorization schemes

Challenges:

Configuration space
Effective Interactions and operators
Open channels

Modern Mean-Field Theory = Energy Density Functional



mean-field ⇒ one-body densities

zero-range ⇒ local densities

finite-range ⇒ gradient terms

particle-hole and pairing channels

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

Towards the Universal Nuclear Energy Density Functional

- Two kinds of fermions
- Self-bound system
- Strong symmetry-breaking effects
- Short-ranged effective forces + Coulomb
- Major challenge: correlation energy (beyond mean field)

$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)$ 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 $(\rho_1 = \rho_n - \rho_p)$

$\vec{s}_0(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau)\vec{\sigma}_{\sigma'\sigma}$ 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

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

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

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

Local densities and currents + pairing…

Construction of the functional:
E. Perlinska et al.
Phys. Rev. C 69, 014316 (2004)

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

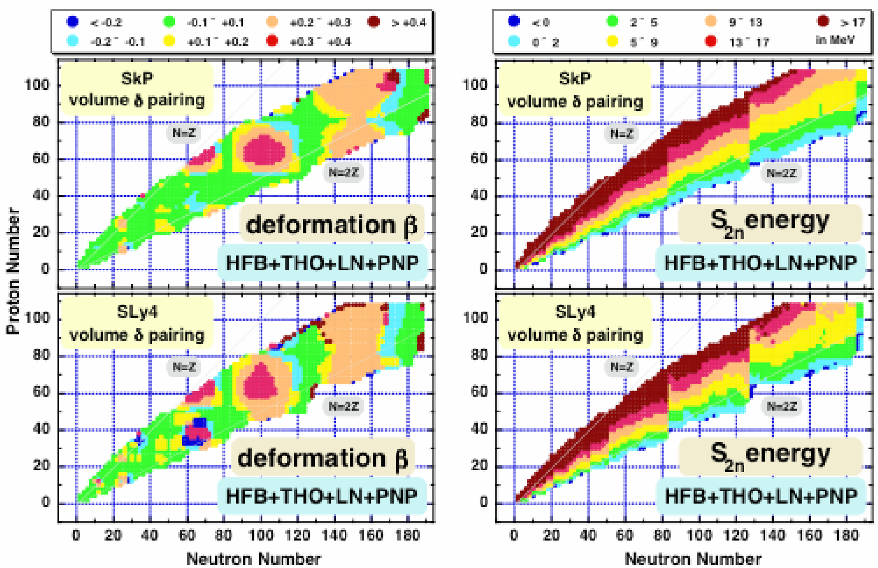
Total ground-state energy

Nuclear DFT

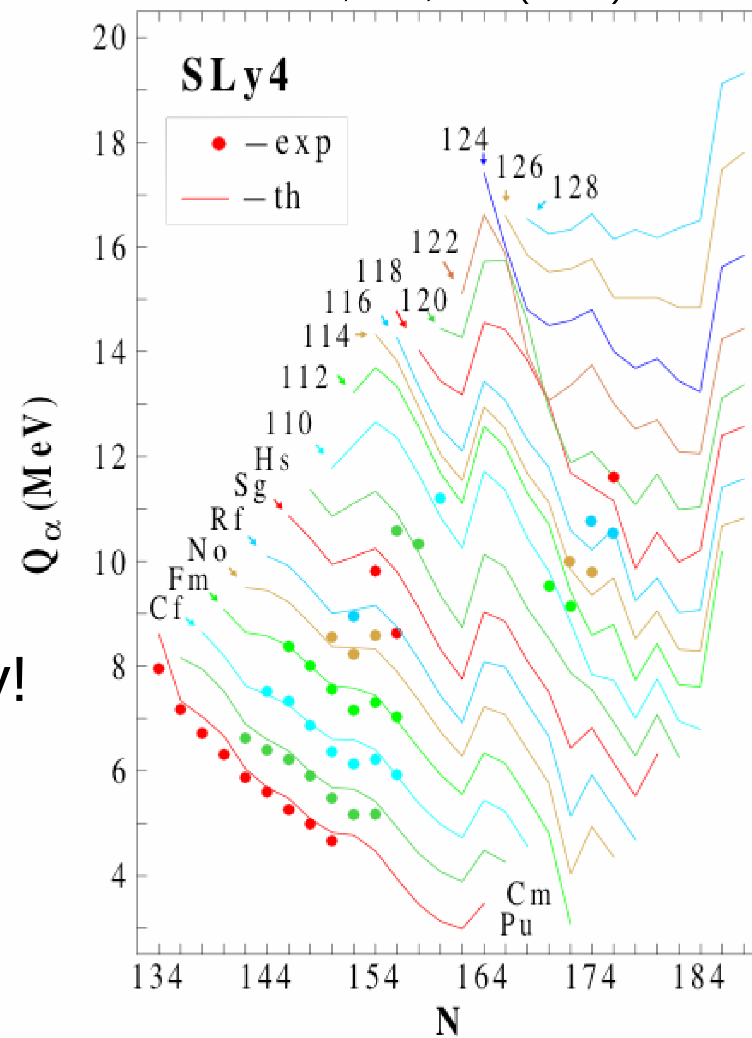
From Qualitative to Quantitative!

Microscopic Mass Table

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



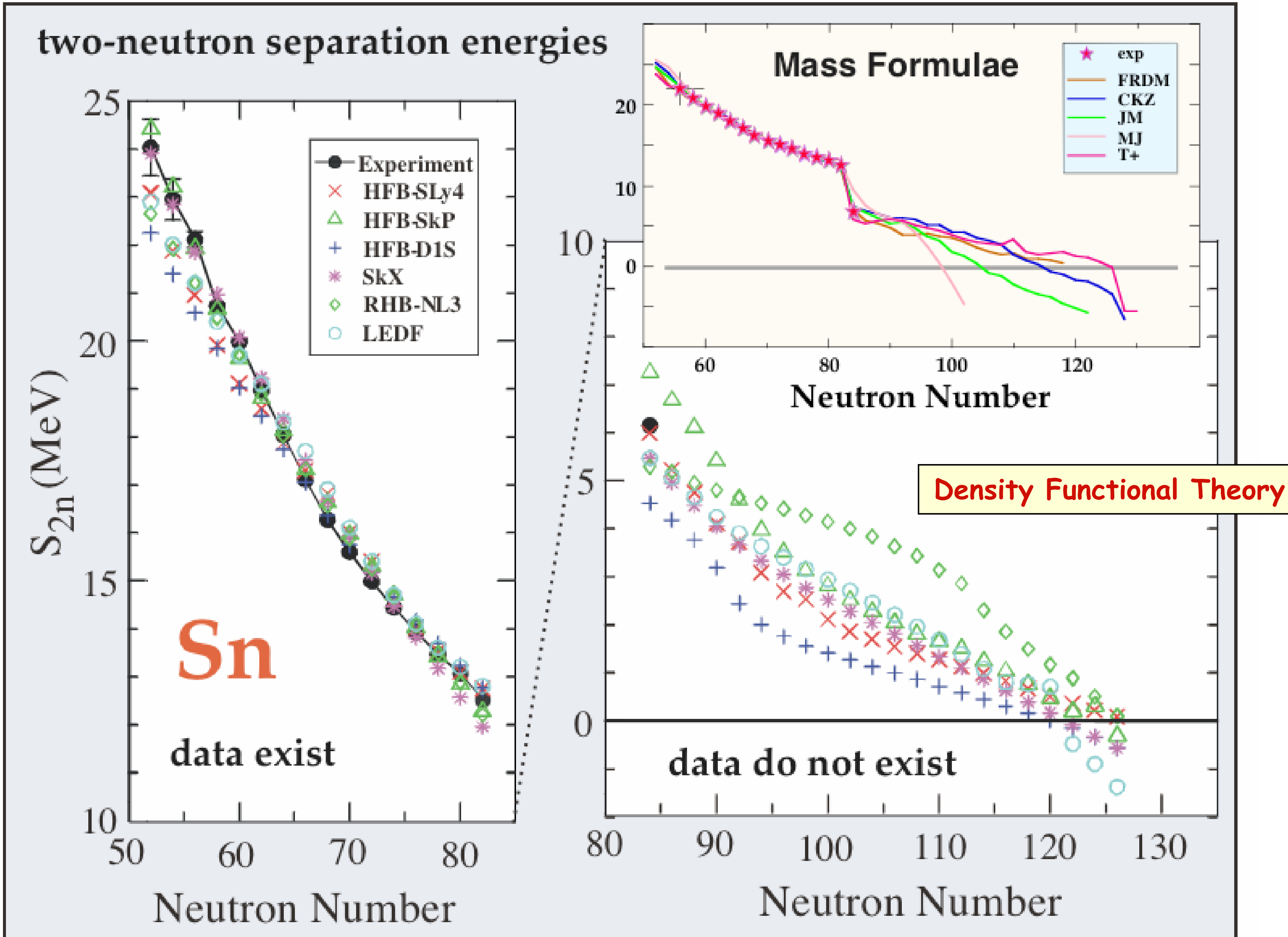
S. Cwiok, P.H. Heenen, W. Nazarewicz
Nature, 433, 705 (2005)



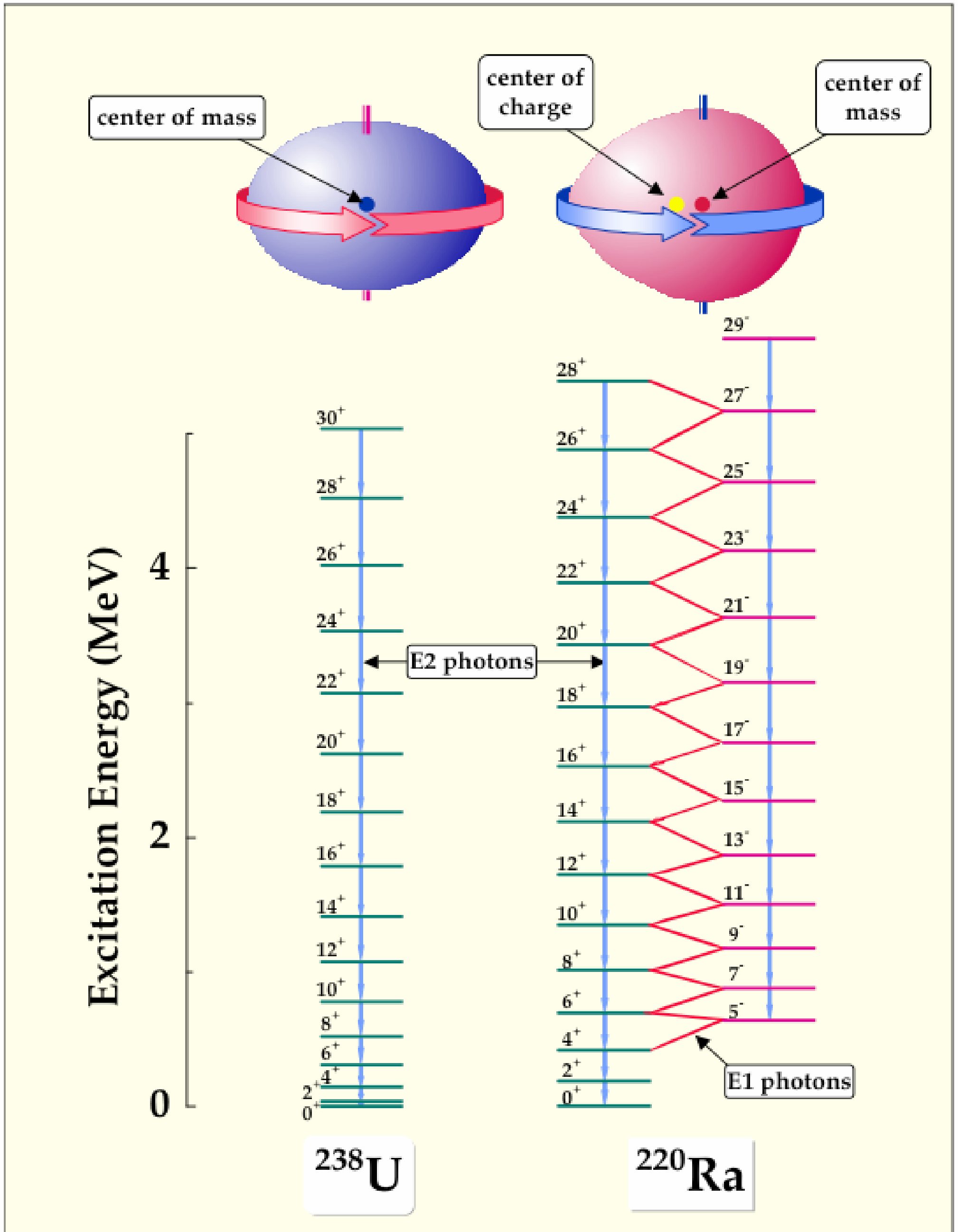
Deformed Mass Table in one day!

- HFB mass formula: Δm~700keV
- Good agreement for mass differences

What are the missing pieces?



Nuclear collective motion



molecules

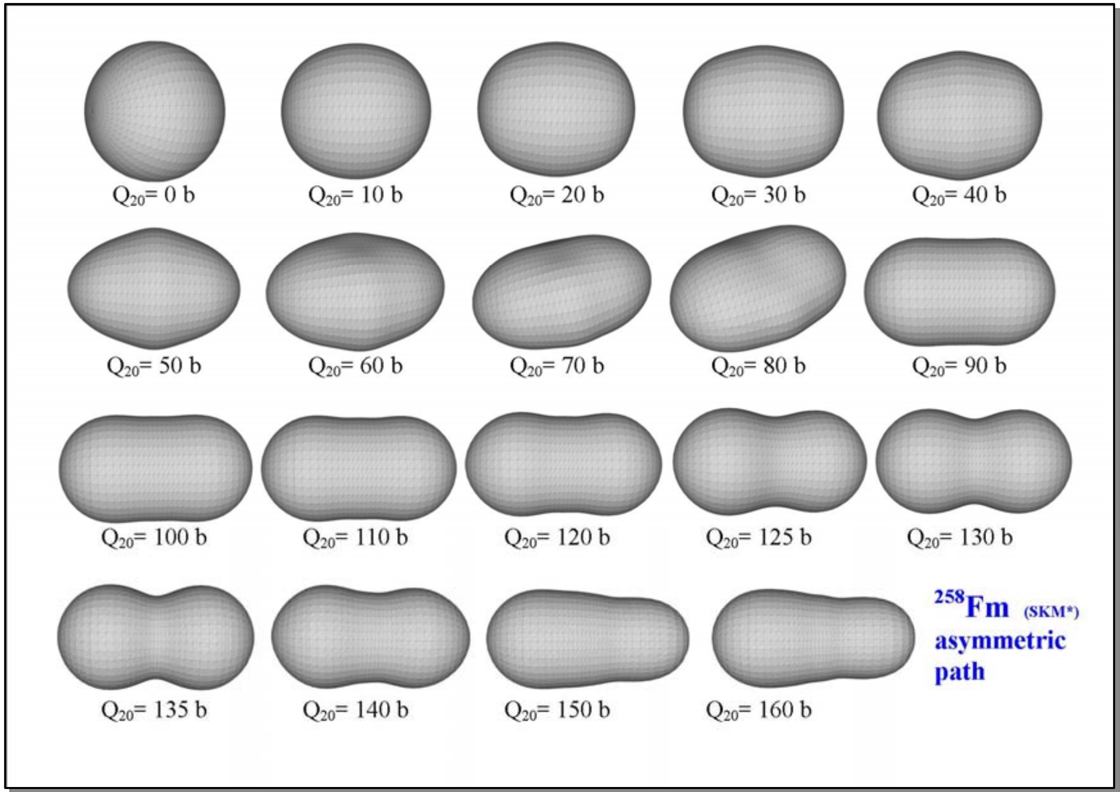
Rotational Transitions ~ 10 meV
Vibrational Transitions ~ 100 meV
Electronic Transitions ~ 1 eV

nuclei

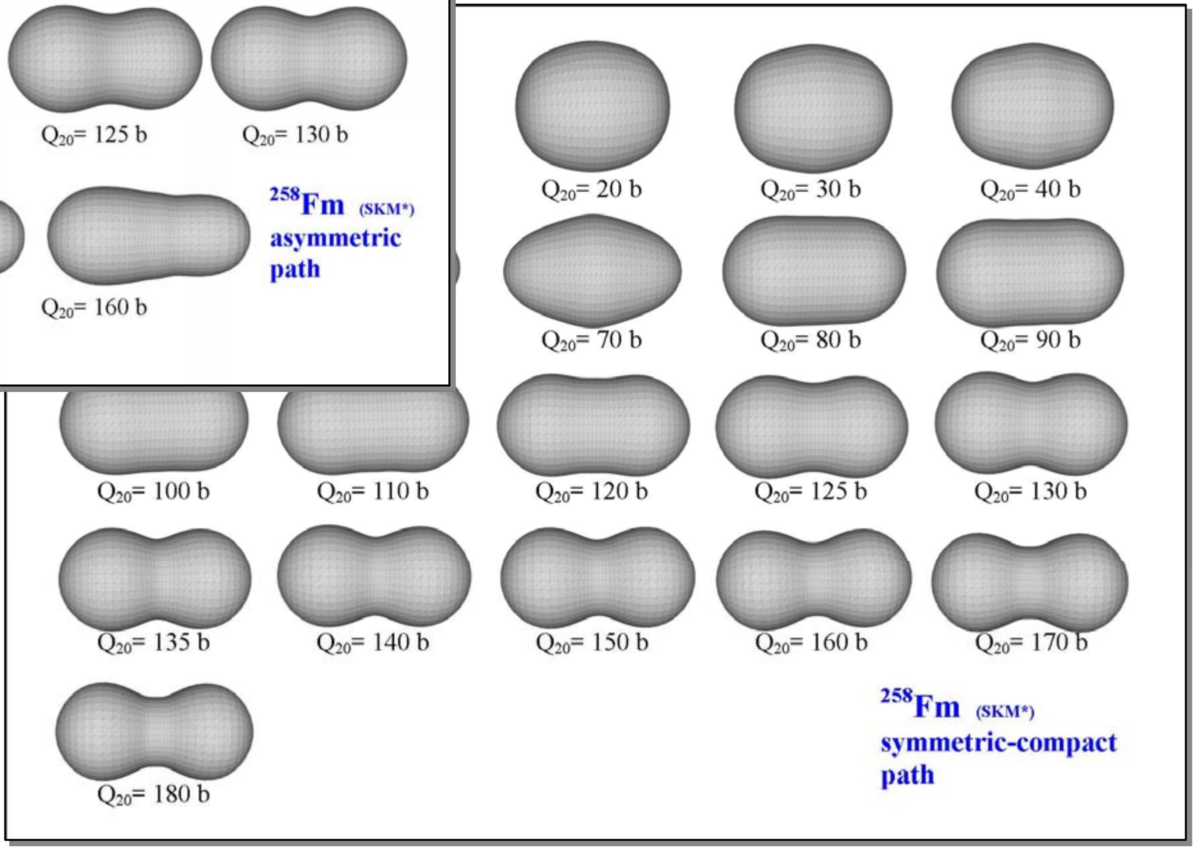
Rotational Transitions ~ 0.2-2 MeV
Vibrational Transitions ~ 0.5-12 MeV
Nucleonic Transitions ~ 7 MeV

Nuclear collective motion **is hardly** adiabatic

Fission: ultimate challenge (tunneling of a complex system)

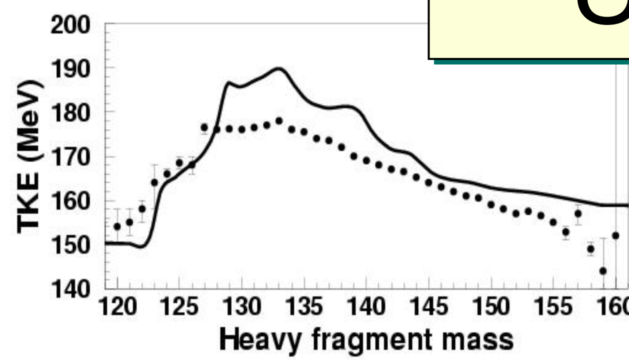


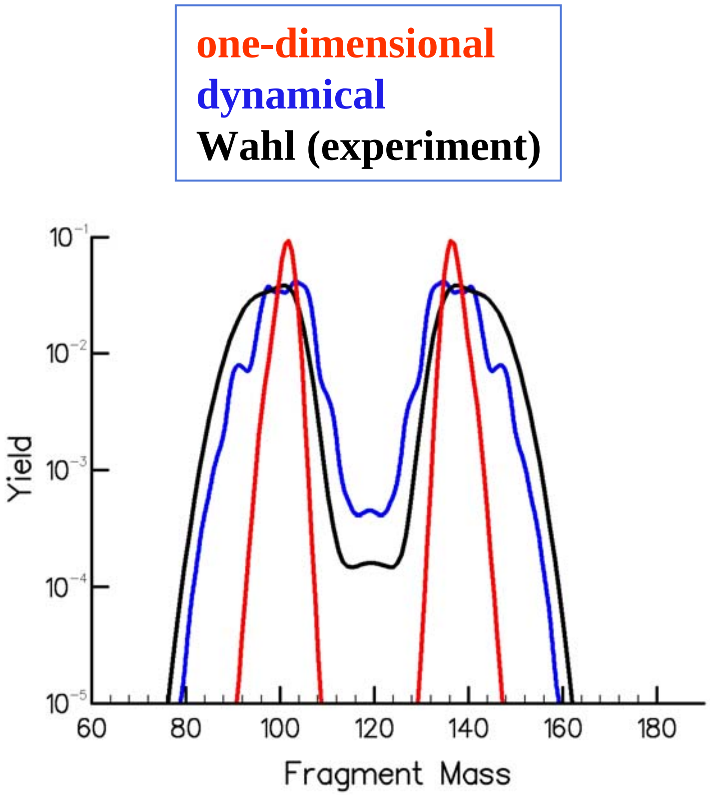
A. Staszczak, J. Dobaczewski
W. Nazarewicz, in preparation



Kinetic Energy and Mass Distributions
in HFB+TDGCM(GOA)

^{238}U





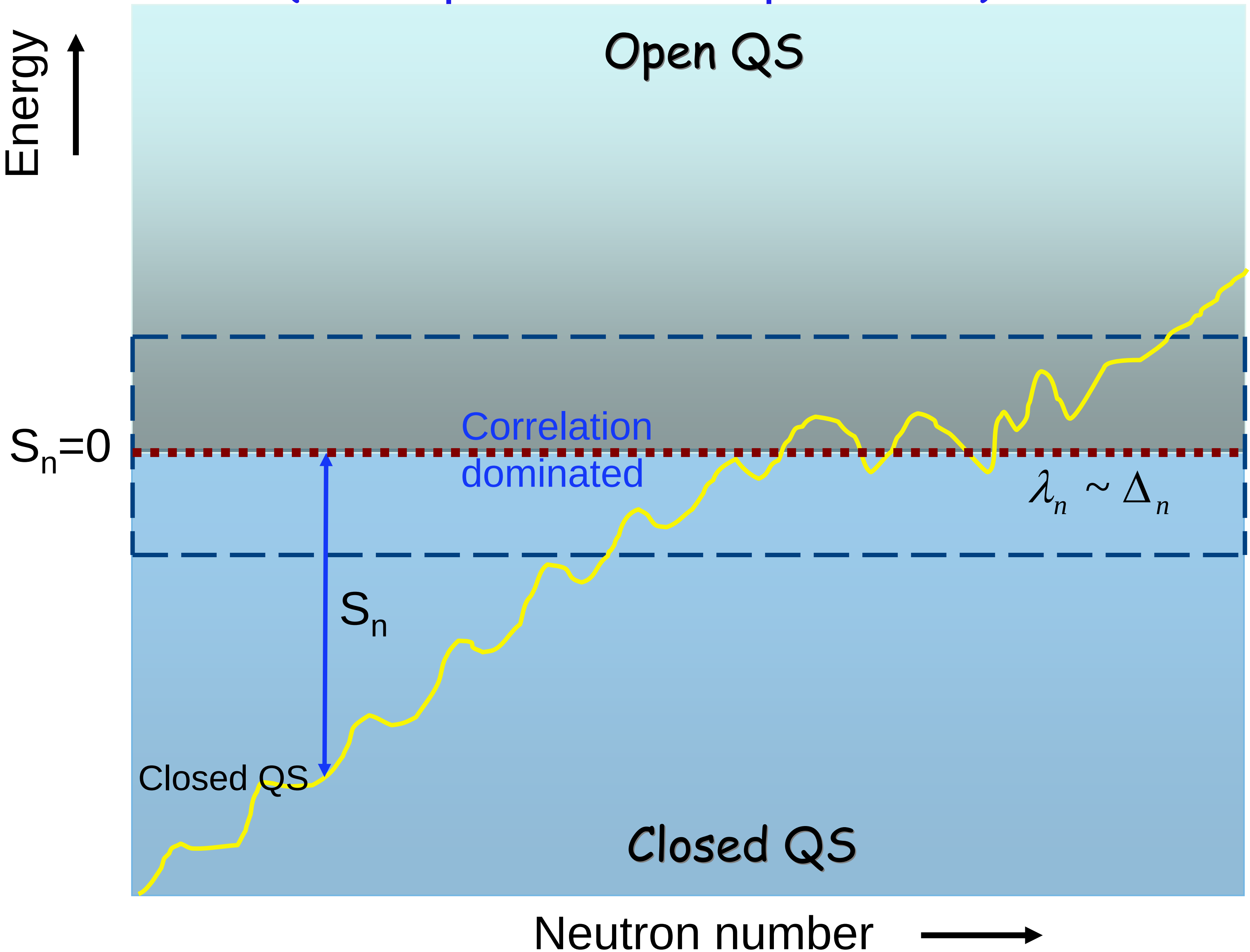
- Time-dependent microscopic collective Schroedinger equation
- Two collective degrees of freedom
- TKE and mass distributions reproduced
- Dynamical effects are responsible for the large widths of the mass distributions
- No free parameters

HFB + Gogny D1S + Time-Dependent GOA

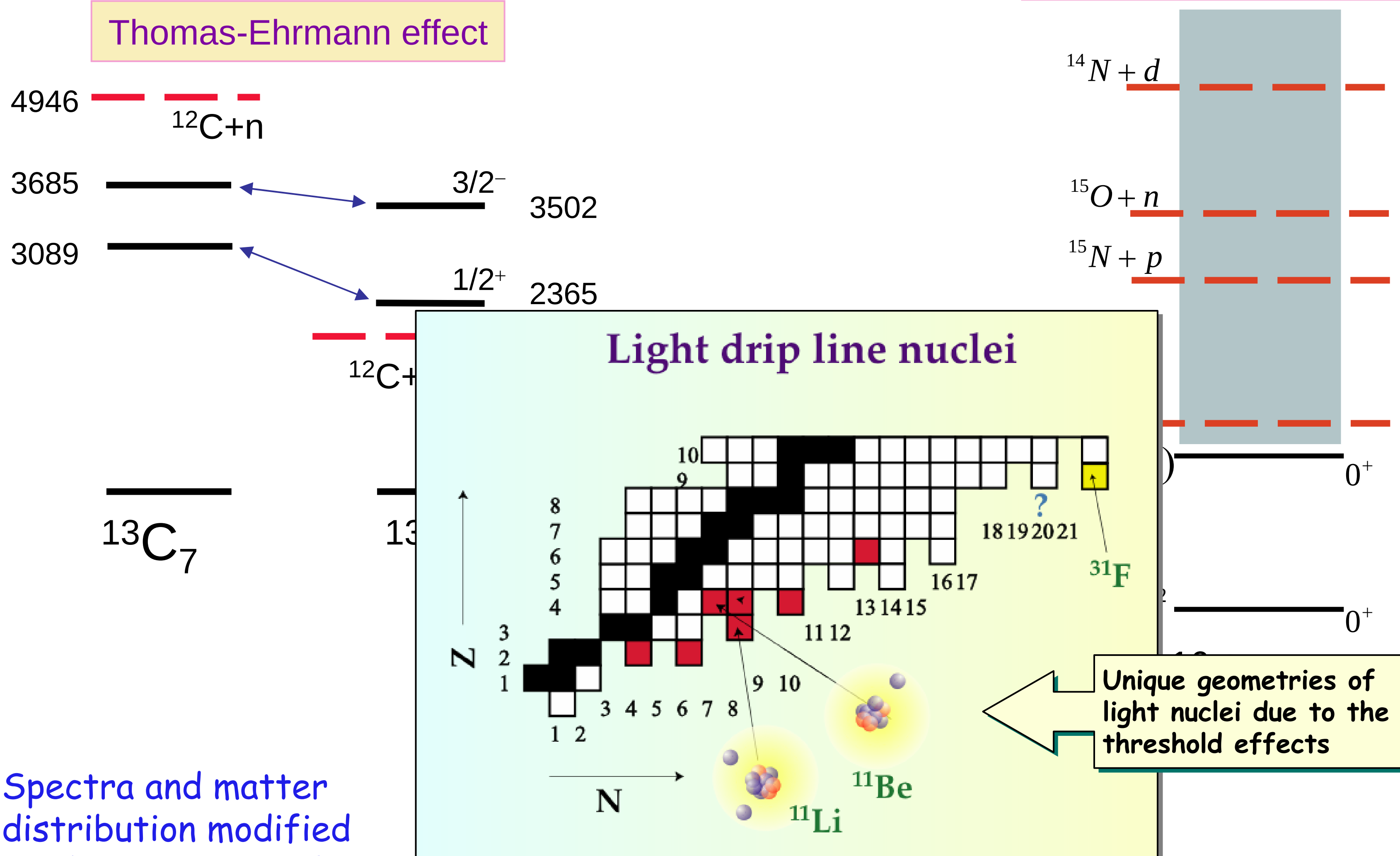
H. Goutte, P. Casoli, J.-F. Berger, D. Gogny, Phys. Rev. C71, 024316 (2005)

Coupling of nuclear structure and reaction theory

(microscopic treatment of open channels)



The nucleus is a correlated open quantum many-body system
Environment: continuum of decay channels



Spectra and matter distribution modified by the proximity of scattering continuum

The importance of the particle continuum was discussed in the early days of the multiconfigurational Shell Model and the mathematical formulation within the Hilbert space of nuclear states embedded in the continuum of decay channels goes back to H. Feshbach (1958-1962), U. Fano (1961), and C. Mahaux and H. Weidenmüller (1969)

- unification of structure and reactions
- resonance phenomena generic to many small quantum systems coupled to an environment of scattering wave functions: hadrons, nuclei, atoms, molecules, quantum dots, microwave cavities, …
- consistent treatment of multiparticle correlations

↓

Open quantum system many-body framework

Continuum (real-energy) Shell Model
(1977 - 1999 - 2005)
H.W.Bartz et al, NP A275 (1977) 111
R.J. Philpott, NP A289 (1977) 109
K. Bennaceur et al, NP A651 (1999) 289
J. Rotureau et al, PRL 95 (2005) 042503

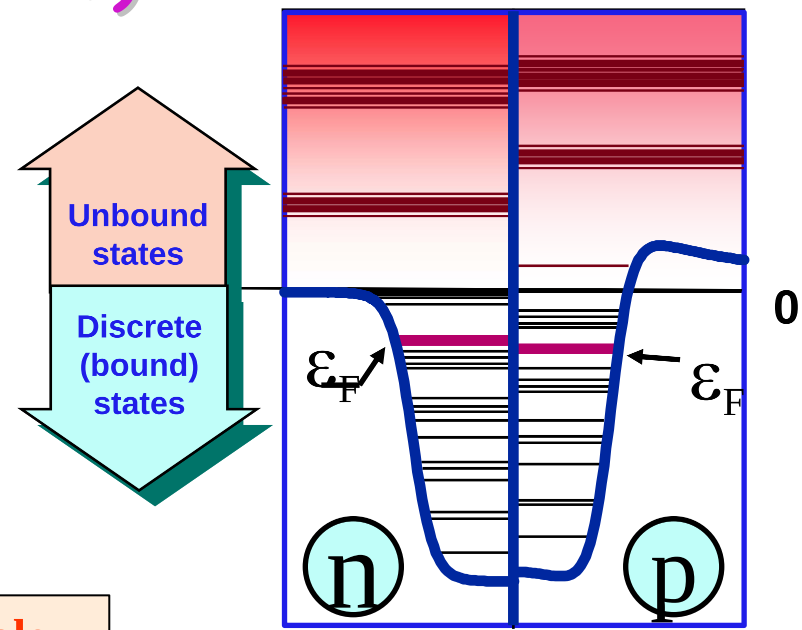
Gamow (complex-energy) Shell Model
(2002 -)
N. Michel et al, PRL 89 (2002) 042502
R. Id Betan et al, PRL 89 (2002) 042501
N. Michel et al, PRC 70 (2004) 064311
G. Hagen et al, PRC 71 (2005) 044314

Resonant (Gamow) states

$$\hat{H}\Psi = \left(e - i\frac{\Gamma}{2}\right)\Psi$$

outgoing solution

$$\Psi(0,k) = 0, \quad \Psi(\vec{r},k) \xrightarrow[r\to\infty]{} O_l(kr)$$



$$k_n = \sqrt{\frac{2m}{\hbar^2}\left(e_n - i\frac{\Gamma_n}{2}\right)}$$

complex pole of the S-matrix

- **Gamow, Z. Phys. 51, 204 (1928)**
- Siegert, Phys. Rev. **36**, 750 (1939)
- Humblet and Rosenfeld, Nucl. Phys. **26**, 529 (1961)

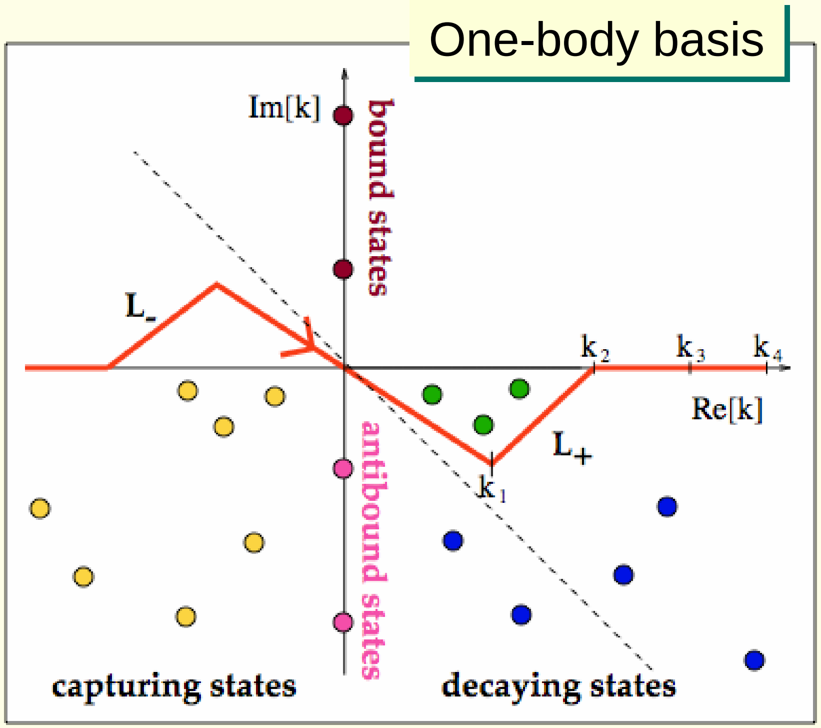
Rigged Hilbert space formulation of SM : Gamow Shell Model (2002)

(Gelfand triple, nested Hilbert space, equipped Hilbert space)

links the distribution and square-integrable aspects of functional analysis.

Gamow states and completeness relations

T. Berggren, Nucl. Phys. A109, 265 (1968); Nucl. Phys. A389, 261 (1982)
T. Lind, Phys. Rev. C47, 1903 (1993)



bound, anti-bound, and resonance states

non-resonant continuum

$$\sum_{n=b,r} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{L_+} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

particular case: Newton completeness relation

$$\sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{R} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

$$\sum\!\!\!\!\!\!\int_{\mathcal{B}} |u_{\mathcal{B}}\rangle\langle\widetilde{u_{\mathcal{B}}}| = 1$$

Contour is discretized

$$|SD_i\rangle = |u_{i_1}\cdots u_{i_A}\rangle$$

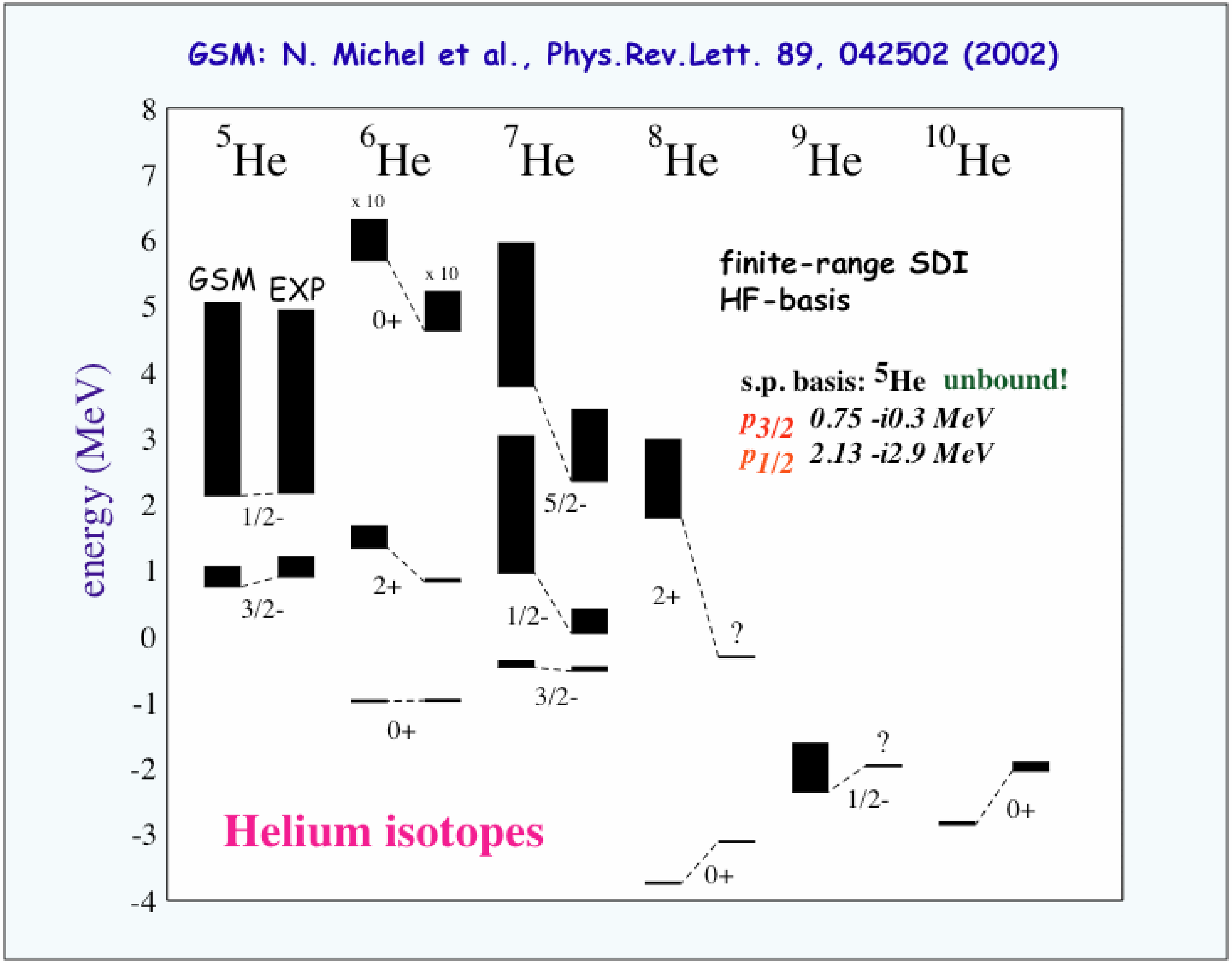
$$\sum_i |SD_i\rangle\langle\widetilde{SD_i}| \simeq 1$$

GSM Hamiltonian matrix is complex symmetric

DMRG-optimization of contour part
J. Rotureau et al., Phys. Rev. Lett. 97, 110603 (2006)

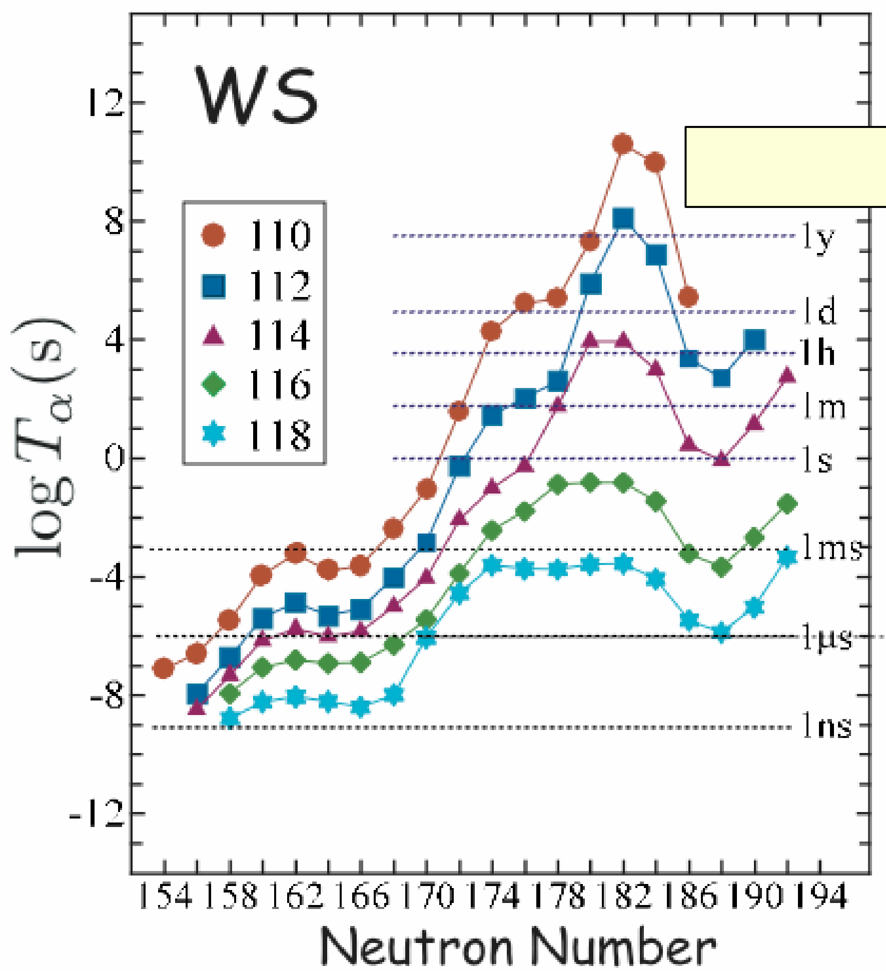
Virtual states not included explicitly in the GSM basis
Michel et al., Phys. Rev. C 74, 054305 (2006)

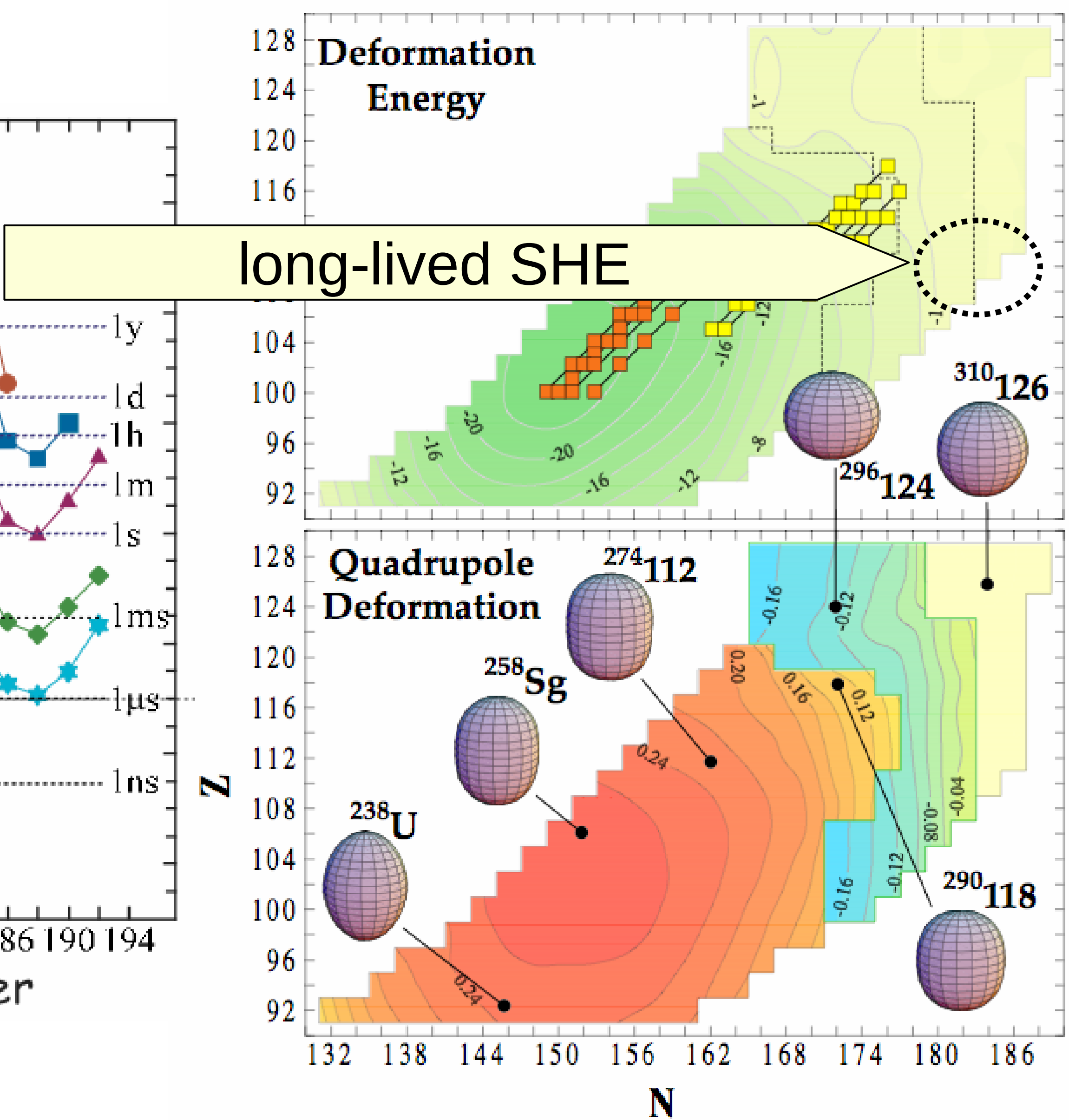
Tennessee - Caen collaboration



Bringing configuration mixing and continuum aspects together

Superheavy Elements in Nuclear DFT

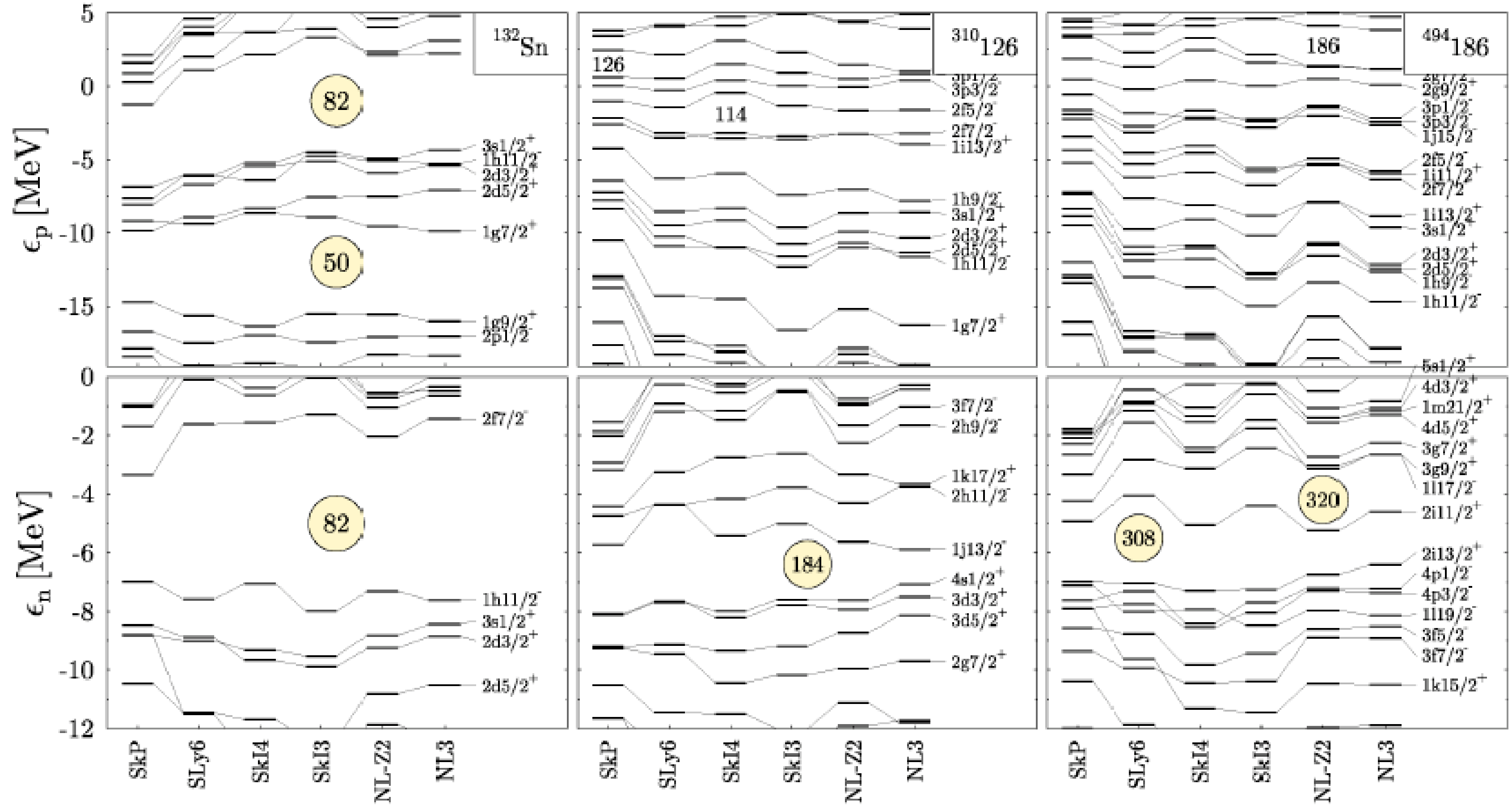




Shell structure in normal, superheavy, and hyperheavy nuclei

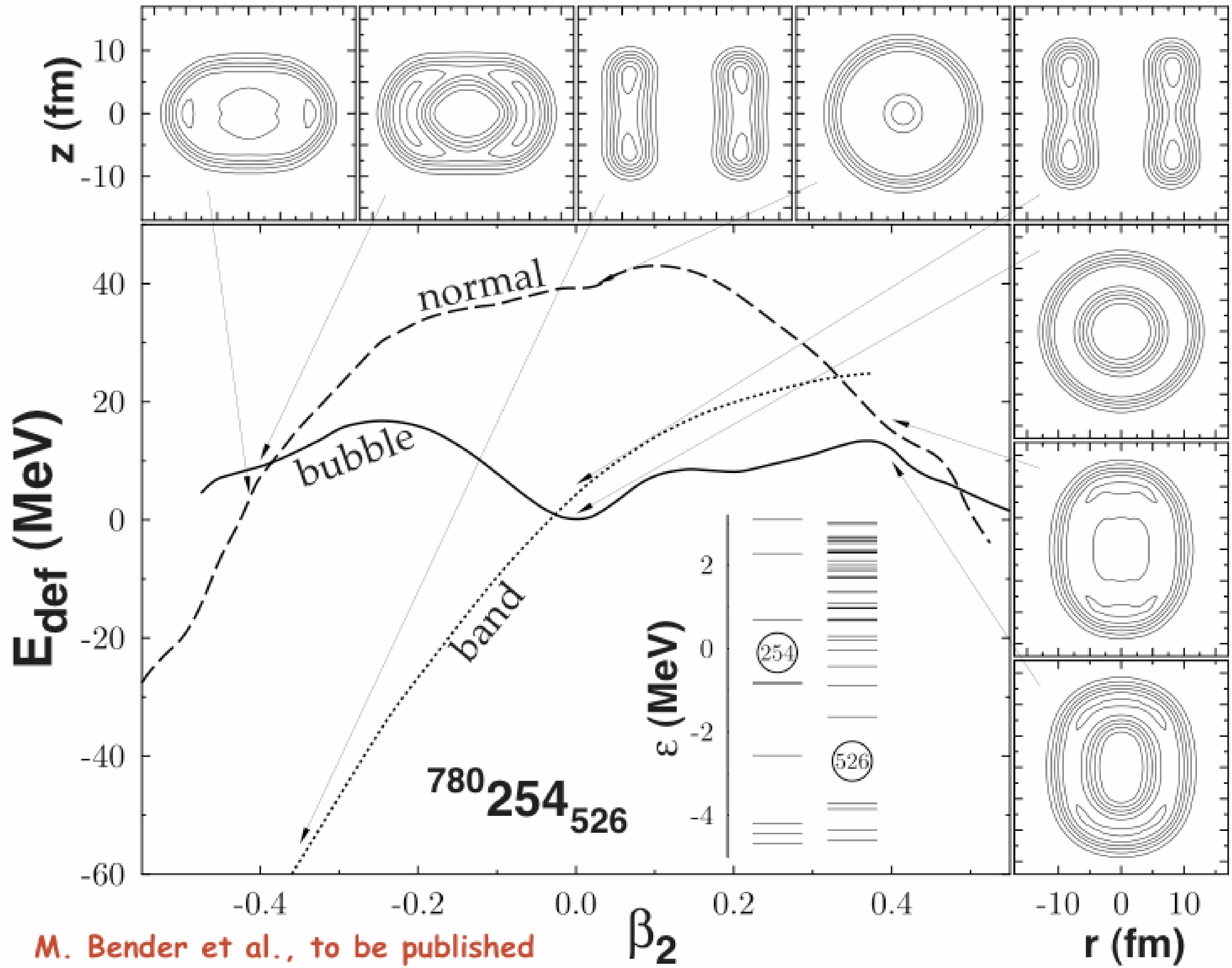
What is the next magic nucleus beyond ^{208}Pb?

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

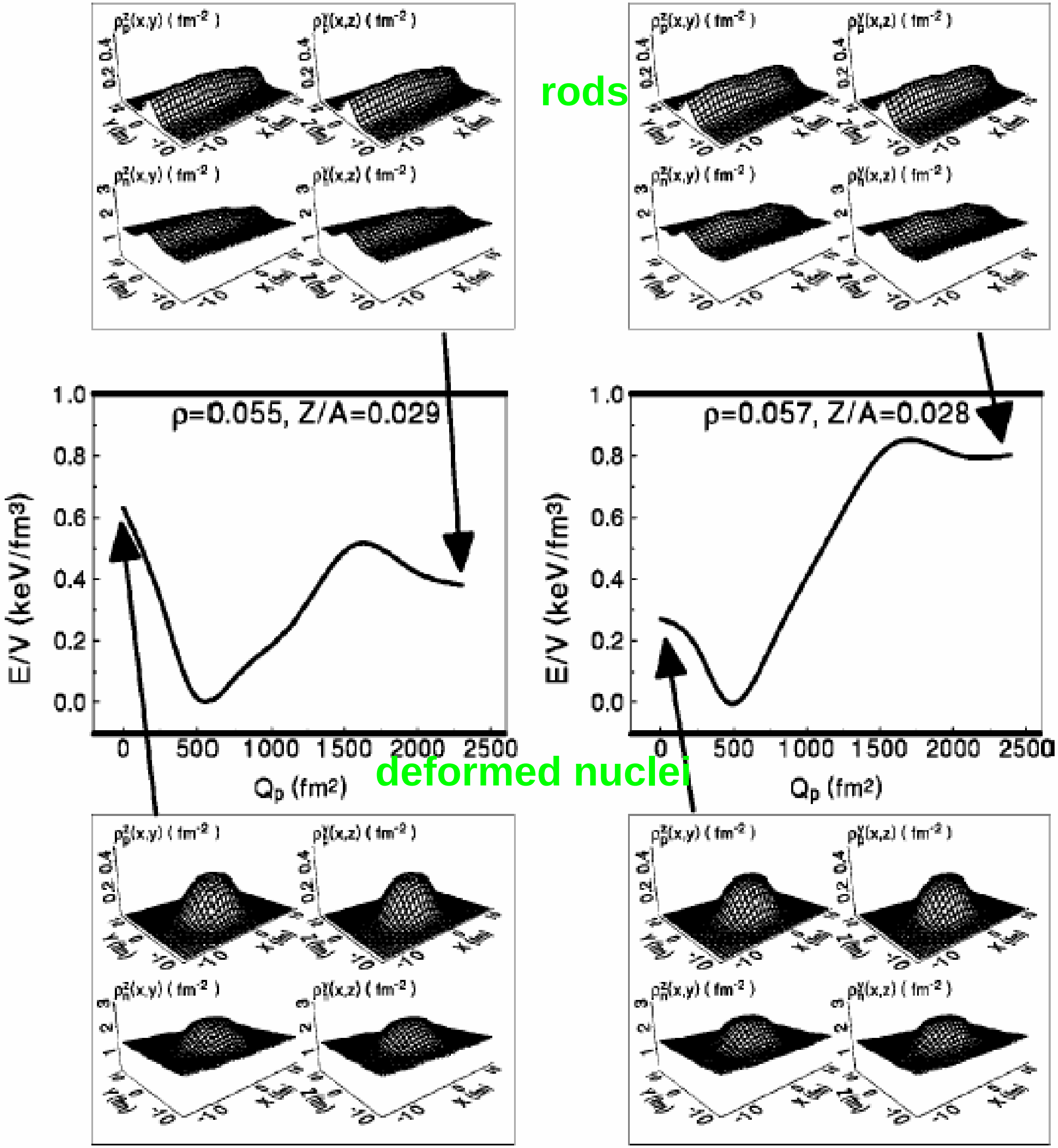


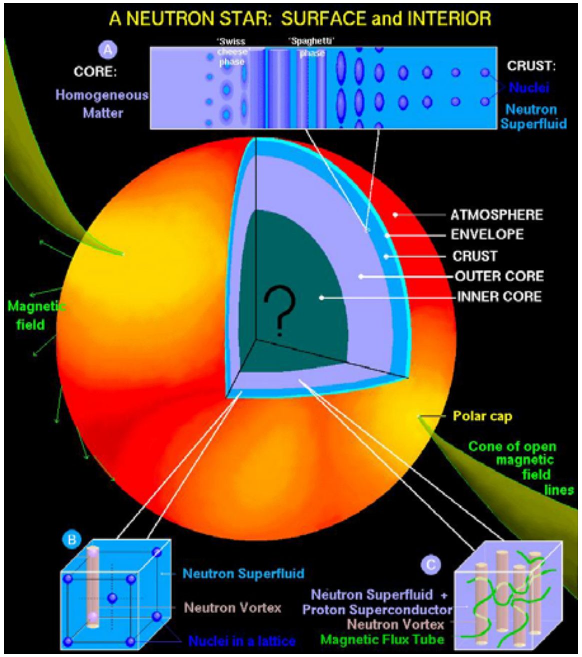
M.Bender, W.Nazarewicz, and P.-G.Reinhard, Phys. Lett. B515, 42 (2001)

Crazy topologies of superheavy nuclei due to the Coulomb frustration



M. Bender et al., to be published





Self-consistent calculations confirm the fact that the "pasta phase" might have a rather complex structure, various shapes can coexist, at the same time significant lattice distortions are likely and the neutron star crust could be on the verge of a disordered phase.

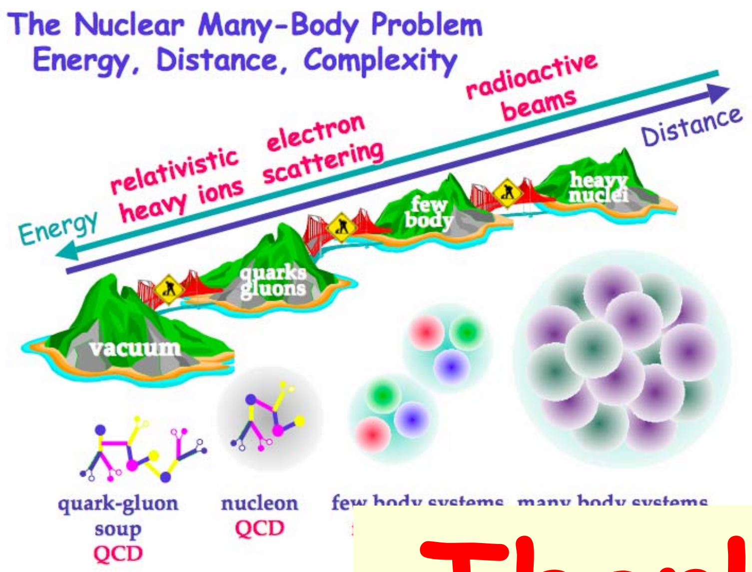
Liquid crystal structure?

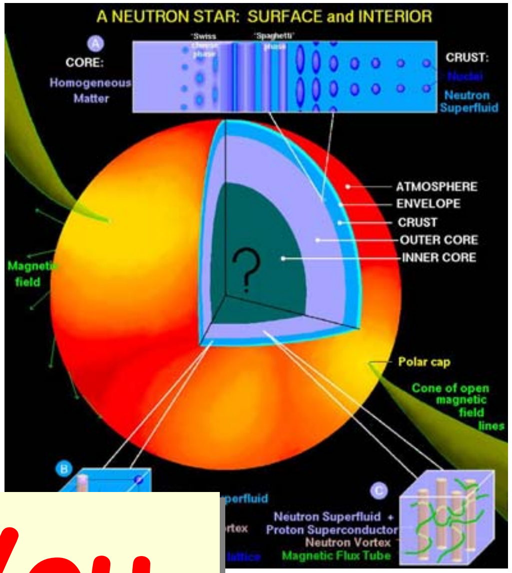
Skyrme HF with SLy4, Magierski and Heenen, Phys. Rev. C 65, 045804 (2002)

Conclusions

A comprehensive description of nuclei and their reactions is coming
Exotic nuclei are essential in this quest: they provide missing links

- Bridging theoretical approaches
  - Bridging ab-initio and SM (effective interactions)
  - Ab initio and DFT (nuclear matter, density dependence)
  - EFT, RGT and DFT (effective operators)
  - Fermionic and Bosonic (algebraic)
- Bridging structure with reactions (in both directions) CSM
- Bridging finite with bulk NDFT





Thank You

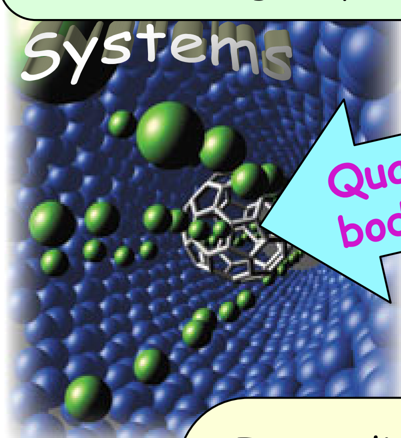
subfemto... QCD

- Origin of NN interaction
- Many-nucleon forces
- Effective fields

- How does complexity emerge from simple constituents?
- How can complex systems display astonishing simplicities?

femto...

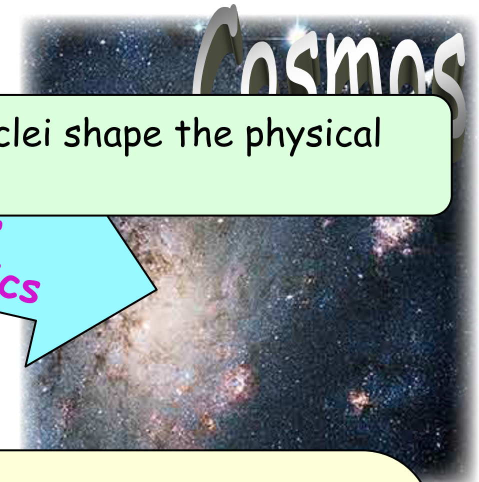
Giga...



Physics of Nuclei

Quantum many-body physics

Astrophysics



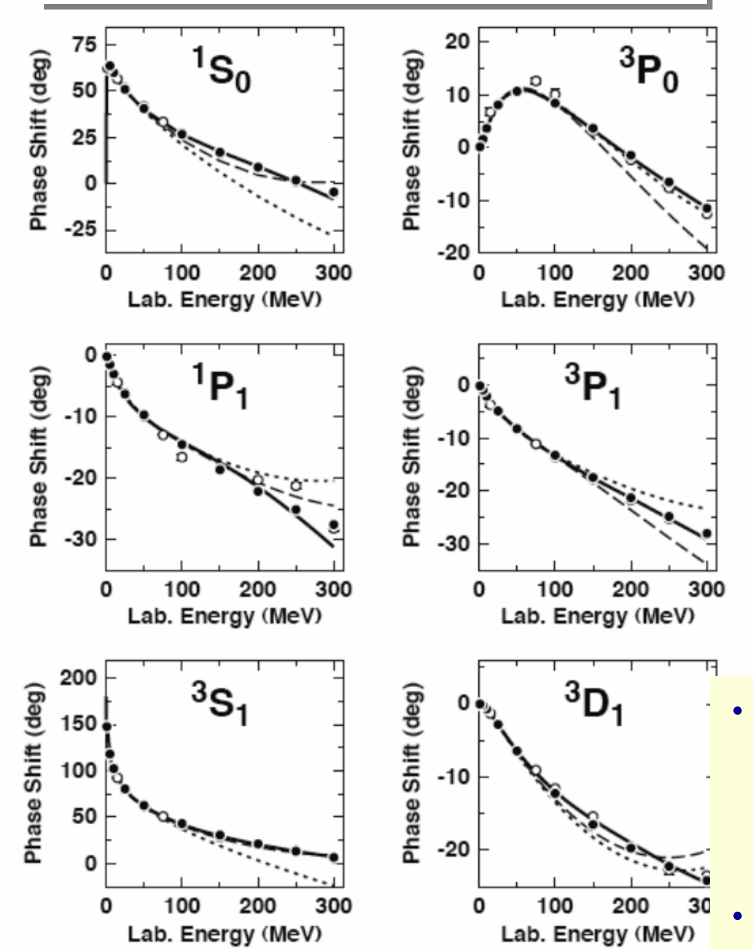
How do nuclei shape the physical universe?

- In-medium interactions
- Symmetry breaking
- Collective dynamics
- Phases and phase transitions
- Chaos and order
- Dynamical symmetries
- Structural evolution

- Origin of the elements
- Energy generation in stars
- Stellar evolution
- Cataclysmic stellar events
- Neutron-rich nucleonic matter
- Electroweak processes
- Nuclear matter equation of state

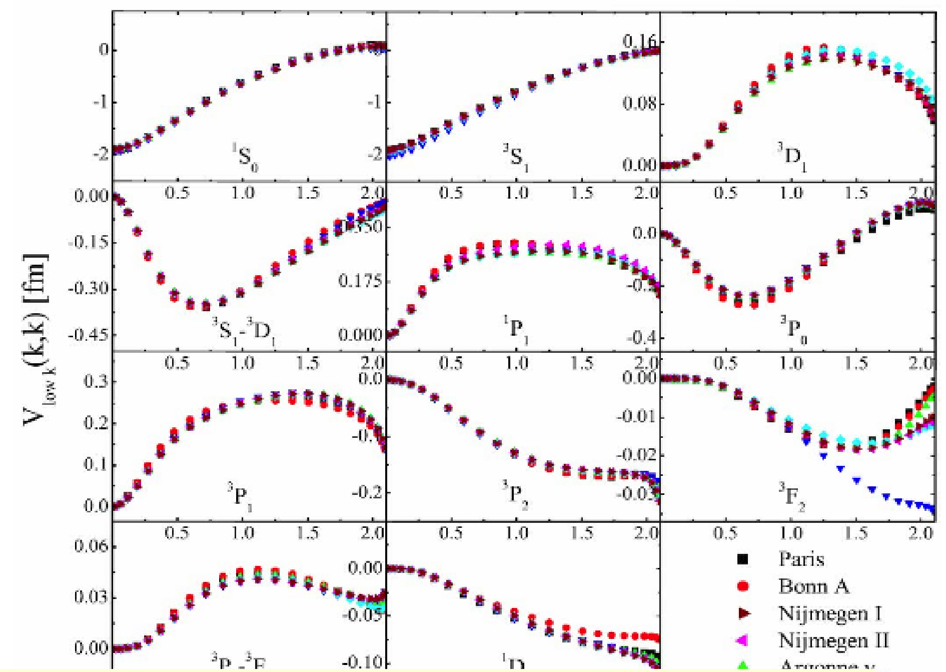
Nuclear Structure: the interaction

Effective-field theory (χ PT) potentials



N[3]LO: Entem et al., PRC68, 041001 (2003)
Epelbaum, Meissner, et al.

$V_{low\text{-}k}$: can it describe low-energy observables?



- Quality two- and three-nucleon interactions exist
    - Not uniquely defined (local, nonlocal)
    - Soft and hard-core
- The challenge is:
    - to understand their origin
    - to understand how to use them in nuclei

Effective Field Theory tells us that:

- Short-range (high-k) physics can be integrated out (no need to worry about explicit inclusion of hard core when dealing with low-k phenomena)
- Successive two-body scatterings with short-lived high-energy intermediate states unresolved $\rightarrow$ must be absorbed into three-body force
- Power counting can be controlled
- … but the operators have to be renormalized (i.e., consistent with the power counting)

Weinberg's Third Law of Progress in Theoretical Physics:
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

D. Furnstahl, INT Fall'05

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.

p-h density p-p density

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

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{j}}^2 + C_1^{\nabla j}\vec{\boldsymbol{s}}\cdot\circ(\boldsymbol{\nabla}\times\vec{\boldsymbol{j}}) + 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}$$

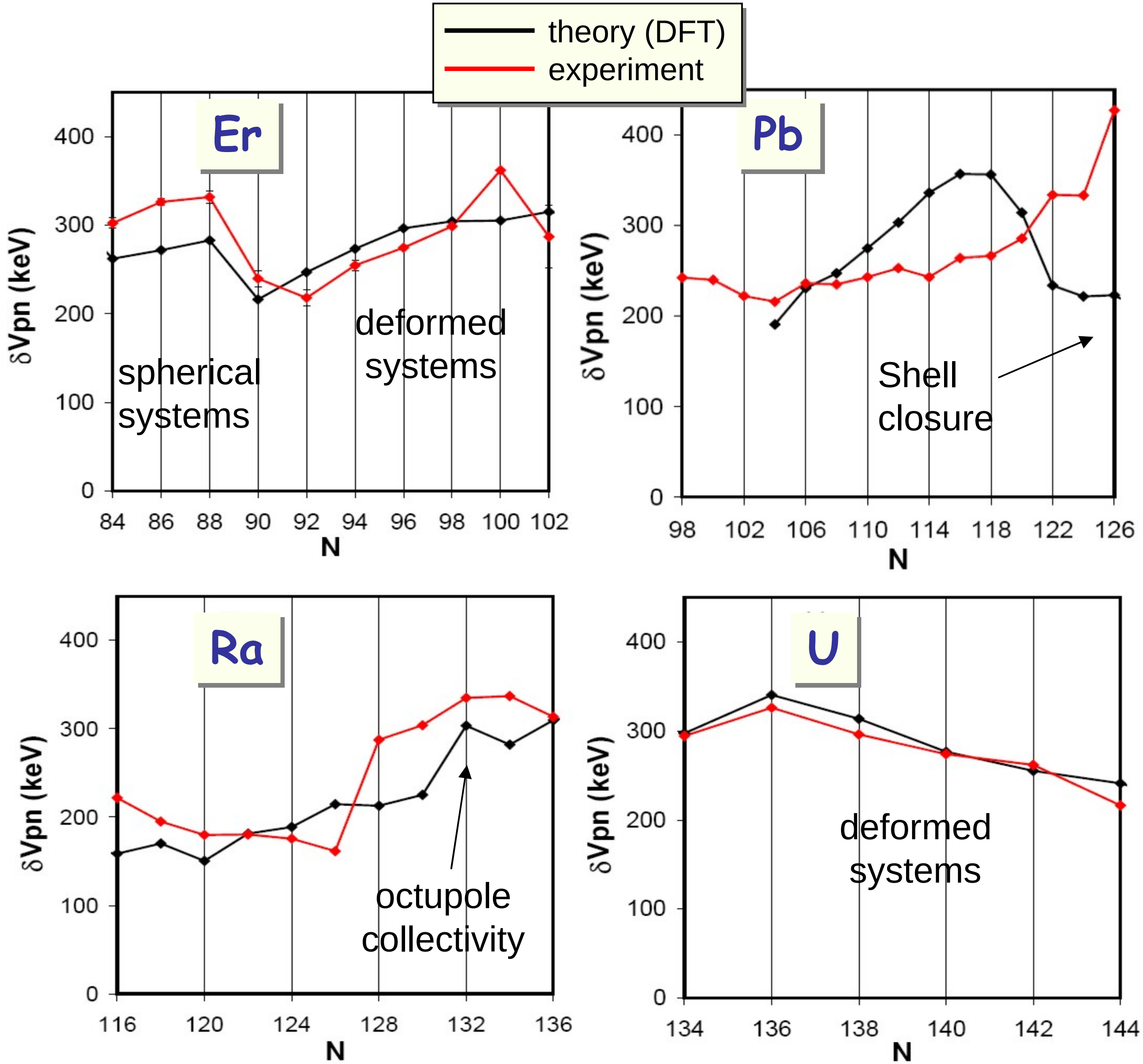
Not all terms are equally important! Some probe specific observables!

Example: pairing mean field

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

$$4\delta V_{pn} = +B(Z,N) - B(Z,N-2) - B(Z-2,N) + B(Z-2,N-2)$$

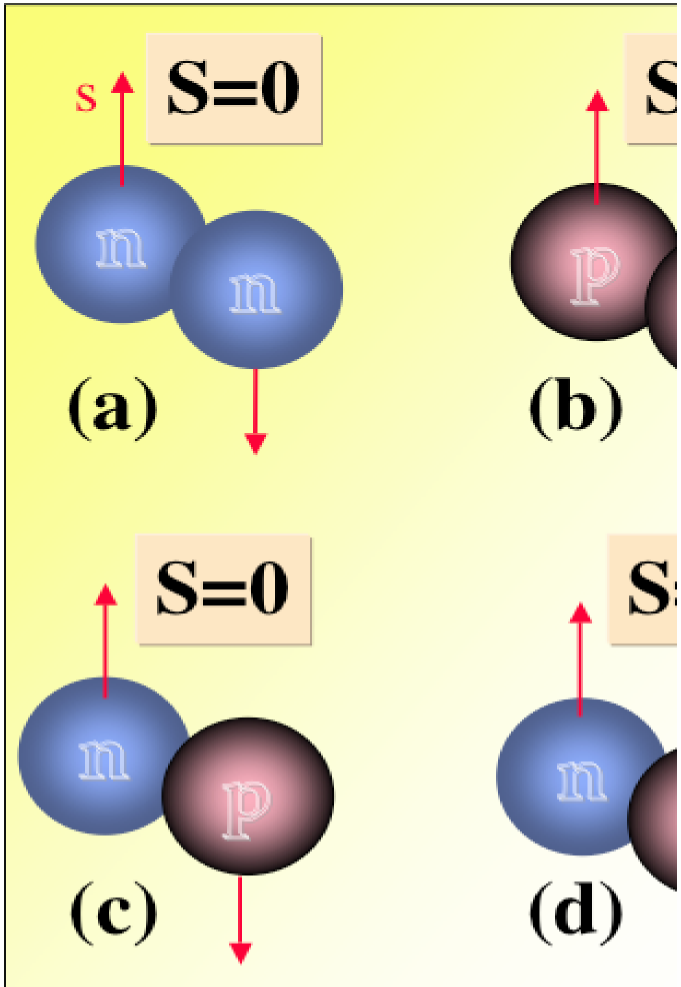
$$\delta V_{pn} \approx \frac{\partial^2 B}{\partial Z \partial N}$$



Average value: symmetry energy

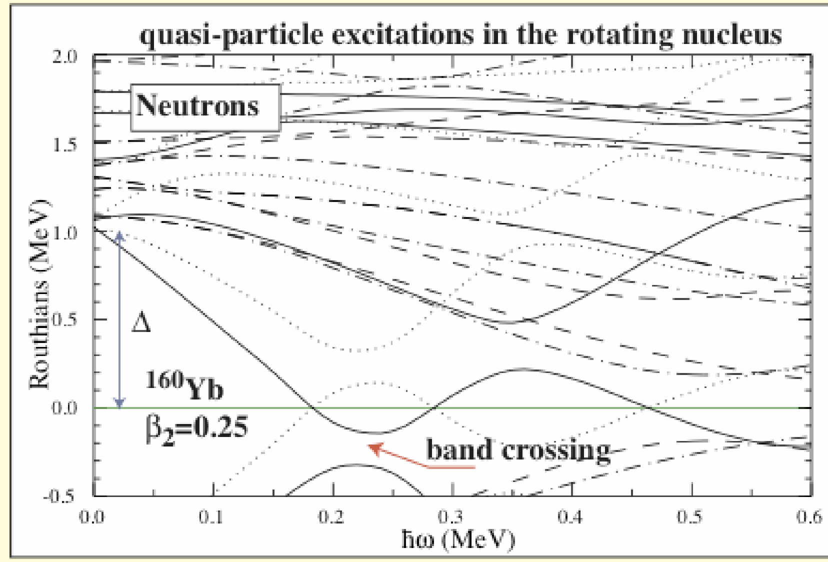
Stoitsov, Nazarewicz, Satula + Cakirli, Casten

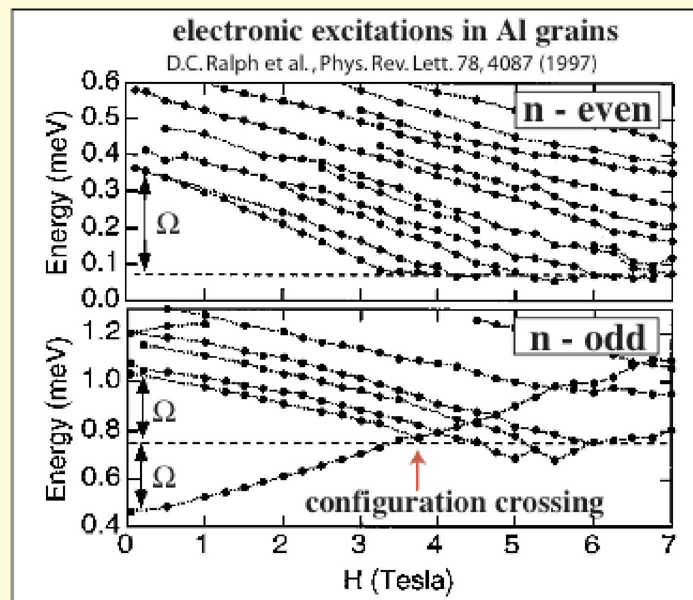
nucleonic superconduct



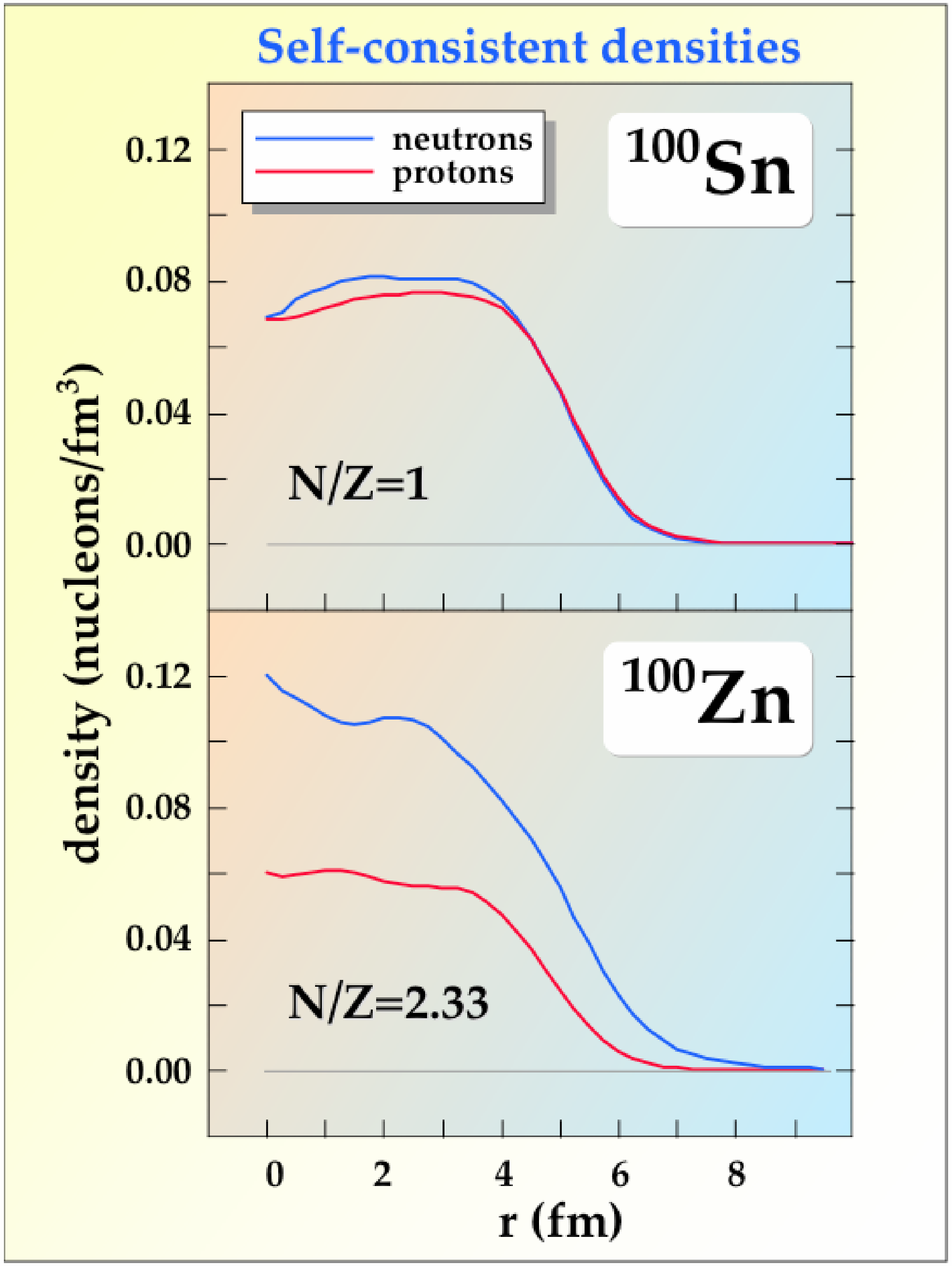
deuteron is bound but nn

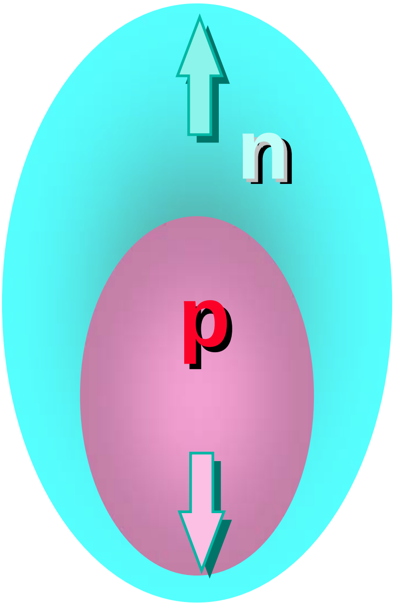
Quasi-particle excitations in finite fermion systems

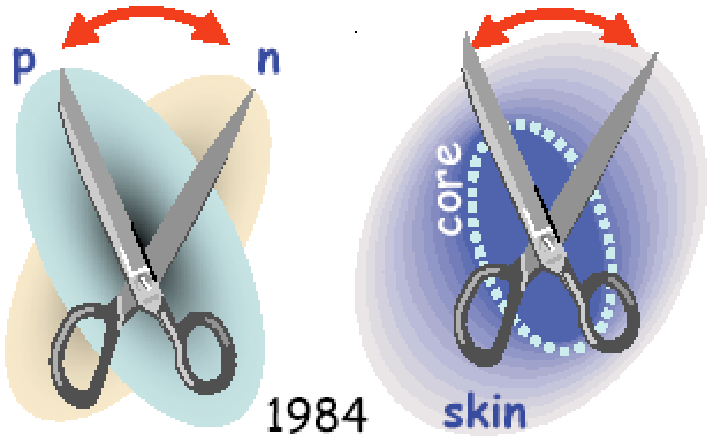


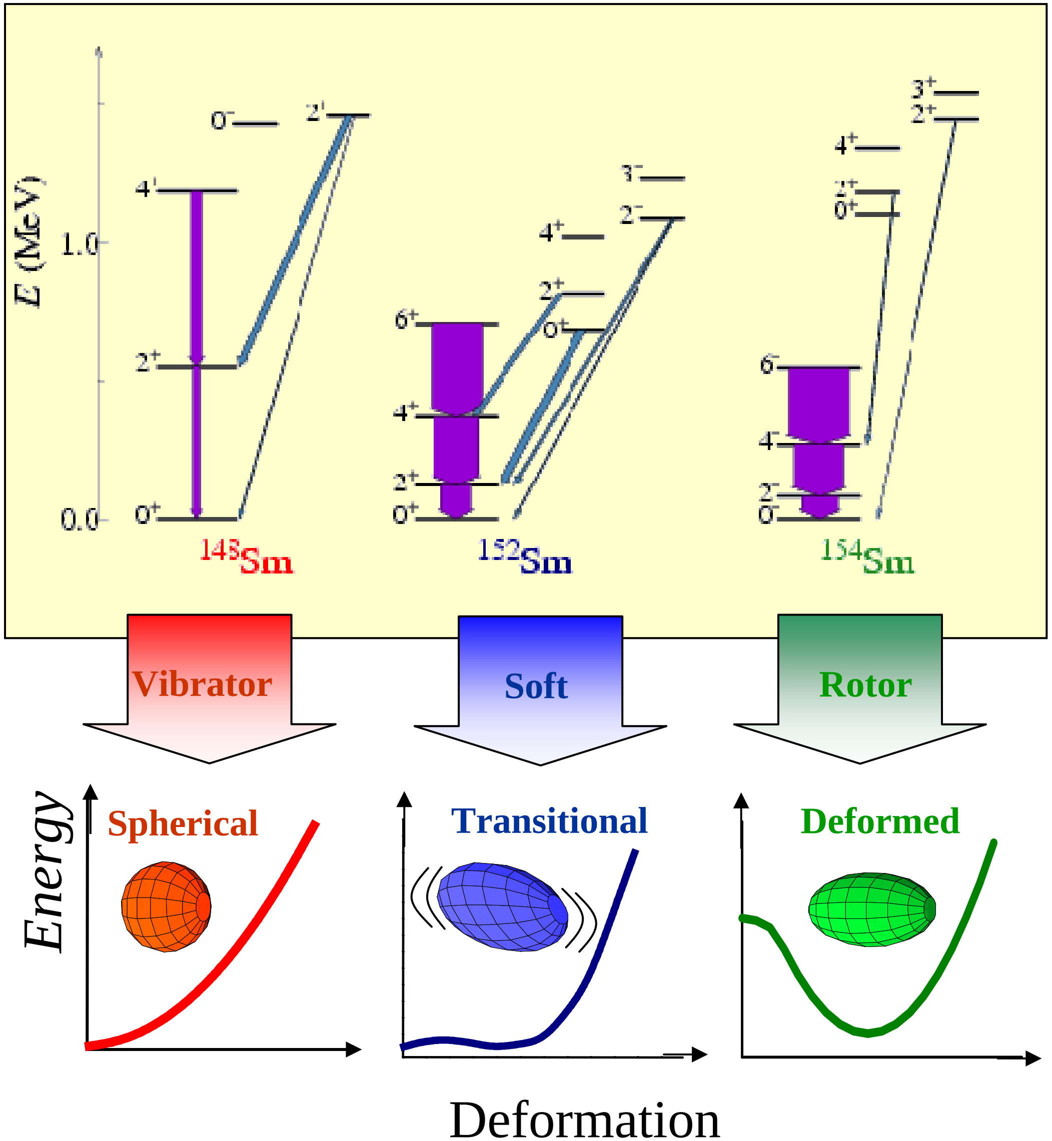


Skins and Skin Modes

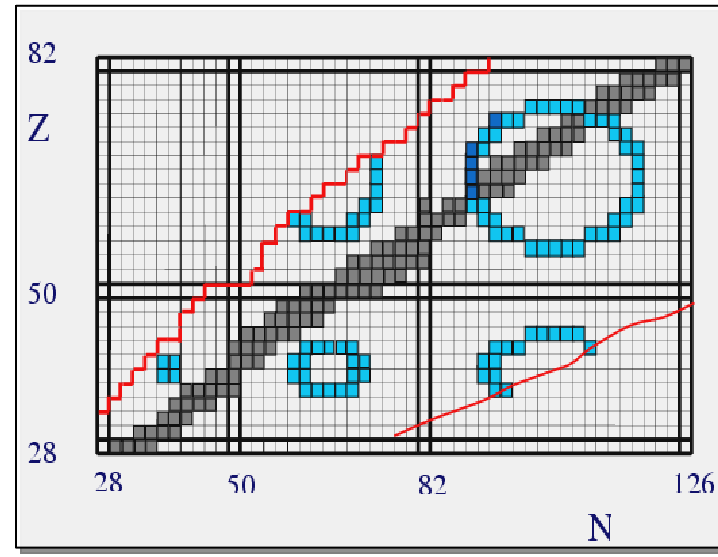








E (MeV)
1.0
0.0
^{148}Sm
^{152}Sm
^{154}Sm
Vibrator
Soft
Rotor
Energy
Spherical
Transitional
Deformed
Deformation



82
Z
50
28
28
50
82
126
N

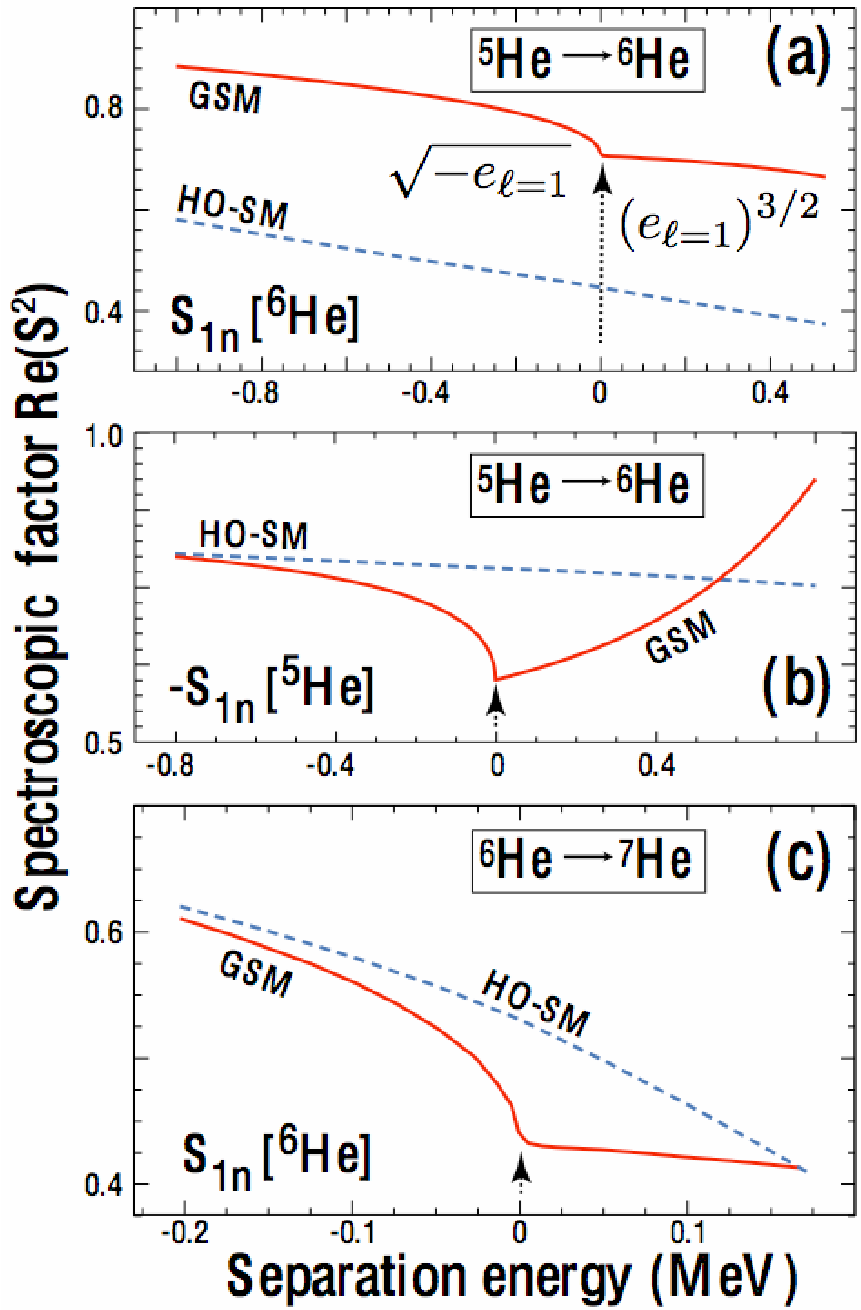
Example: Threshold anomaly

E.P. Wigner, Phys. Rev. 73, 1002 (1948), the Wigner cusp
G. Breit, Phys. Rev. 107, 923 (1957)
A.I. Baz', JETP 33, 923 (1957)
R.G. Newton, Phys. Rev. 114, 1611 (1959).
A.I. Baz', Ya.B. Zel'dovich, and A.M. Perelomov, Scattering Reactions and Decay in Nonrelativistic Quantum Mechanics, Nauka 1966
A.M. Lane, Phys. Lett. 32B, 159 (1970)
S.N. Abramovich, B.Ya. Guzhovskii, and L.M. Lazarev, Part. and Nucl. 23, 305 (1992).

- The threshold is a branching point.
- The threshold effects originate in conservation of the flux.
- If a new channel opens, a redistribution of the flux in other open channels appears, i.e. a modification of their reaction cross-sections.
- The shape of the cusp depends strongly on the orbital angular momentum.

Y(b,a)X	$\sigma_\ell \sim k^{2\ell-1}$
X(a,b)Y	$\sigma_\ell \sim k^{2\ell+1}$

$$a+X \longrightarrow \begin{cases} a+X \\ a_1+X_1 \text{ at } Q_1 \\ a_2+X_2 \text{ at } Q_2 \\ \\ a_n+X_n \text{ at } Q_n \end{cases}$$



WS potential depth decreased to bind ^{7}He. Monopole SGI strength varied

^{5}He+n ⟶ ^{6}He

WS potential depth varied

^{6}He+n ⟶ ^{7}He

Anomalies appear at calculated thresholds (many-body S-matrix unitary)

Scattering continuum essential