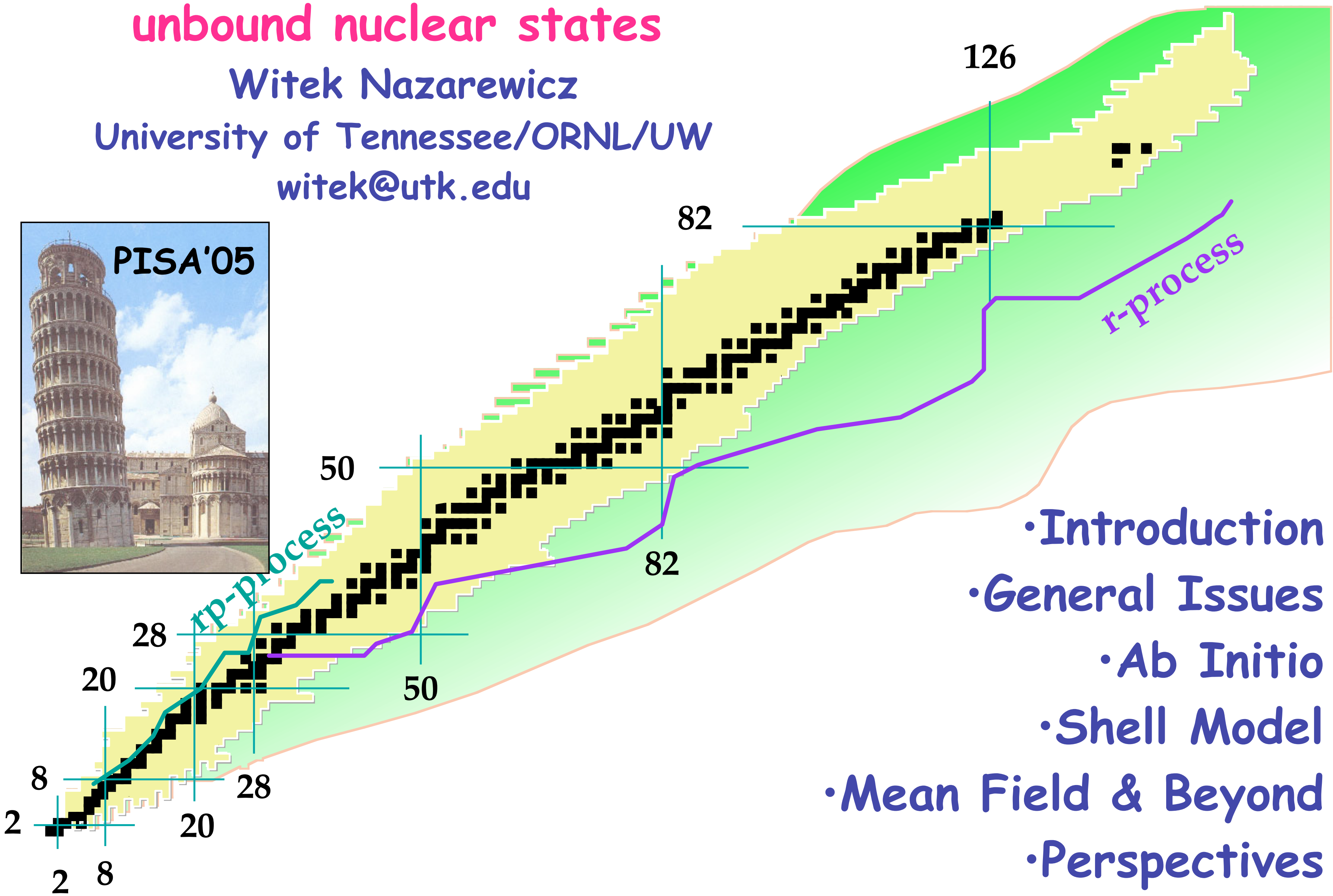
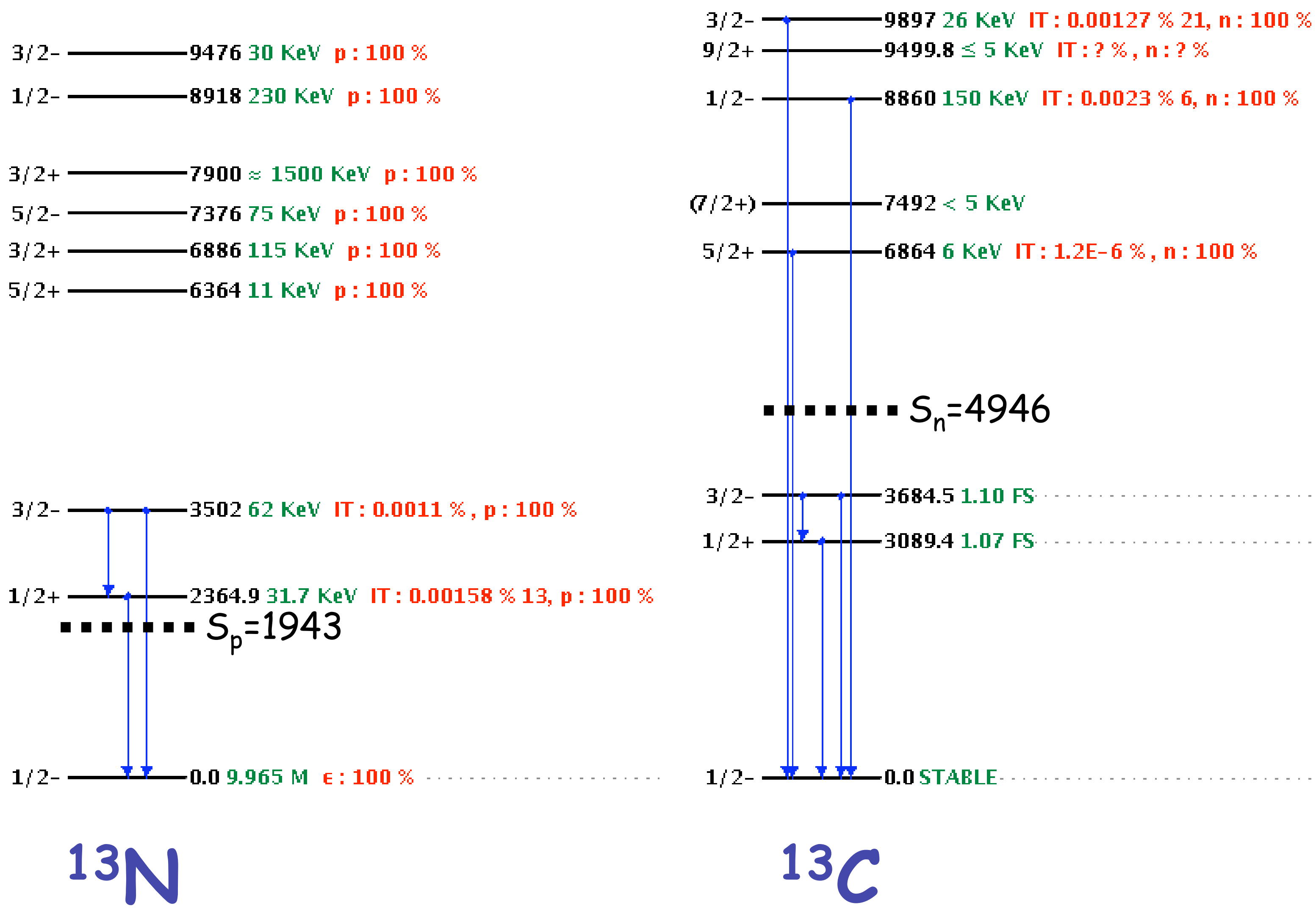
Unified description of bound and unbound nuclear states

Witek Nazarewicz
University of Tennessee/ORNL/UW
witek@utk.edu

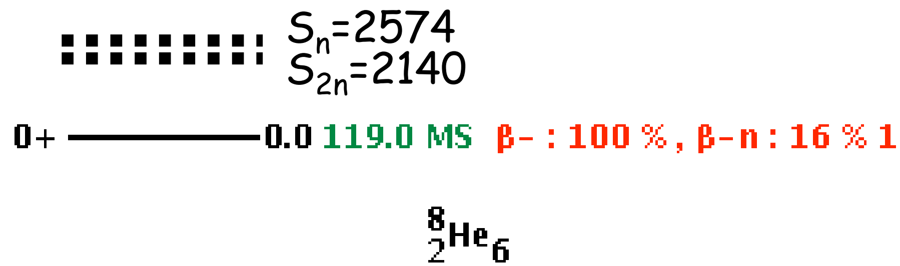


- Introduction
- General Issues
- Ab Initio
- Shell Model
- Mean Field & Beyond
- Perspectives

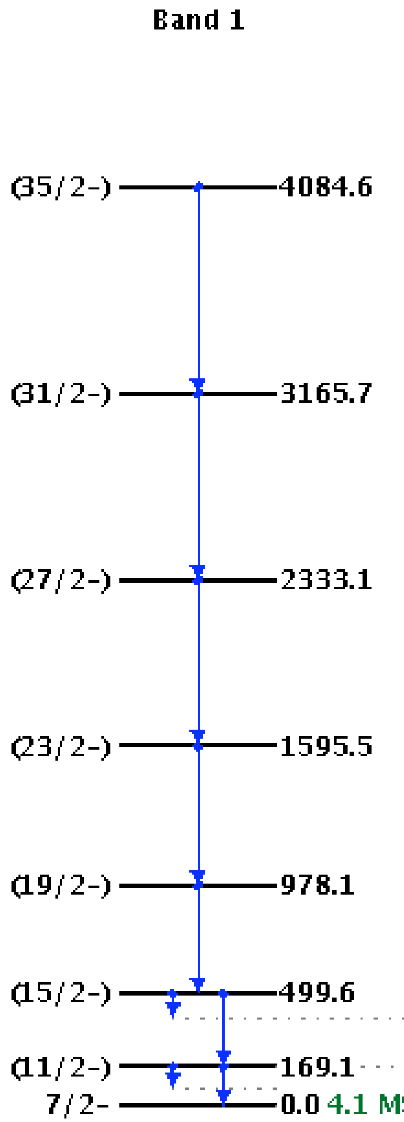
Thomas-Ehrman Shift (1951/52)

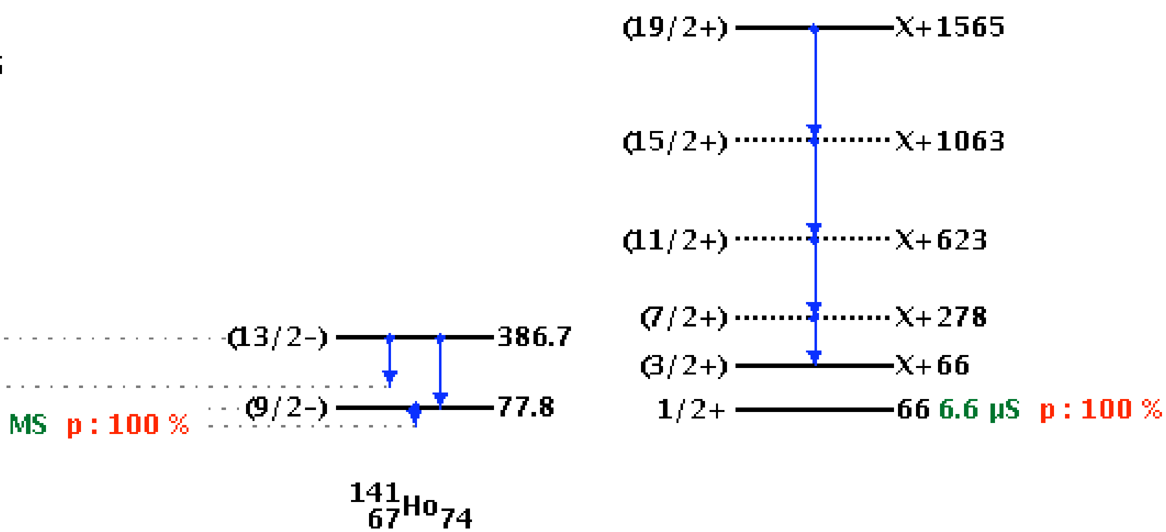


^{8}He: neutron halo

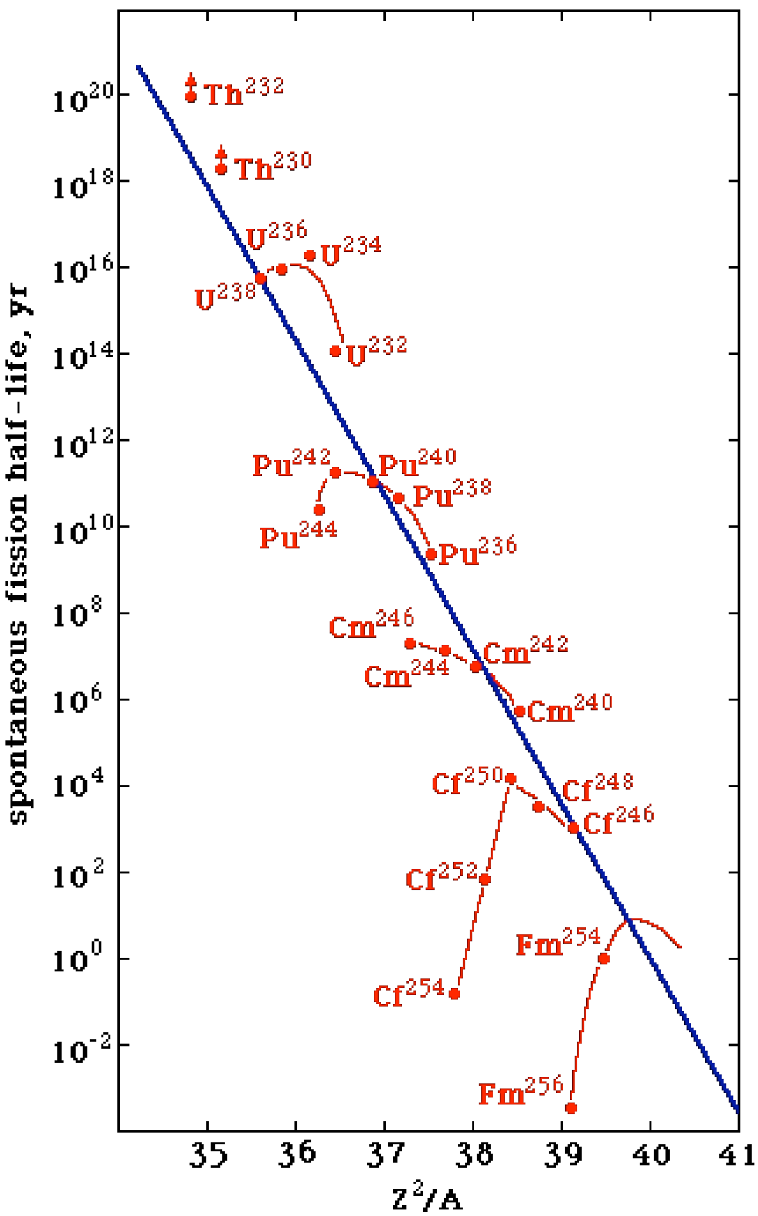


^{141}Ho: proton emitter





Spontaneous fission



NSAC Theory Report: opportunities

Microscopic Nuclear Structure Theory
•novel quantum many-body techniques (ab initio)
•handling enormous configuration spaces
•microscopic effective forces and effective operators

Nucleon-Nucleon Effective Field Theory
•nuclear NN and NNN interactions constrained by EFT
•applications to few-body systems
•DFT applications

Towards the universal microscopic energy density functional
•description of nuclei and asymmetric nucleonic matter
•better understanding of isovector and density dependence
•improved treatment of many-body correlations
•nuclear matter equation of state; low density limit and clustering

Coupling of nuclear structure and reaction theory
•*ab-initio* description of reactions with light nuclei
•consistent treatment of open channels: continuum shell model

Complex nuclei: nuclear dynamics and symmetries
•long term goal: microscopic understanding of nuclear collective dynamics
•important challenge: large amplitude collective motion

Coupling of nuclear structure and reaction theory

(microscopic treatment of open channels)

The major theoretical challenge in the microscopic description of nuclei, especially weakly bound ones, is the rigorous treatment of both the many-body correlations and the continuum of positive-energy states and decay channels. The importance of continuum for the description of resonances is obvious. Weakly bound states cannot be described within the closed quantum system formalism since there always appears a virtual scattering into the continuum phase space involving intermediate scattering states. A unified description of excited states in weakly bound nuclei and reactions on weakly bound nuclei is one of the main goals of modern nuclear structure physics.

Ab-initio, EFT,…

ab-initio description (GFMC, NCSM, Faddeyev, …)

realistic wave functions and electroweak currents

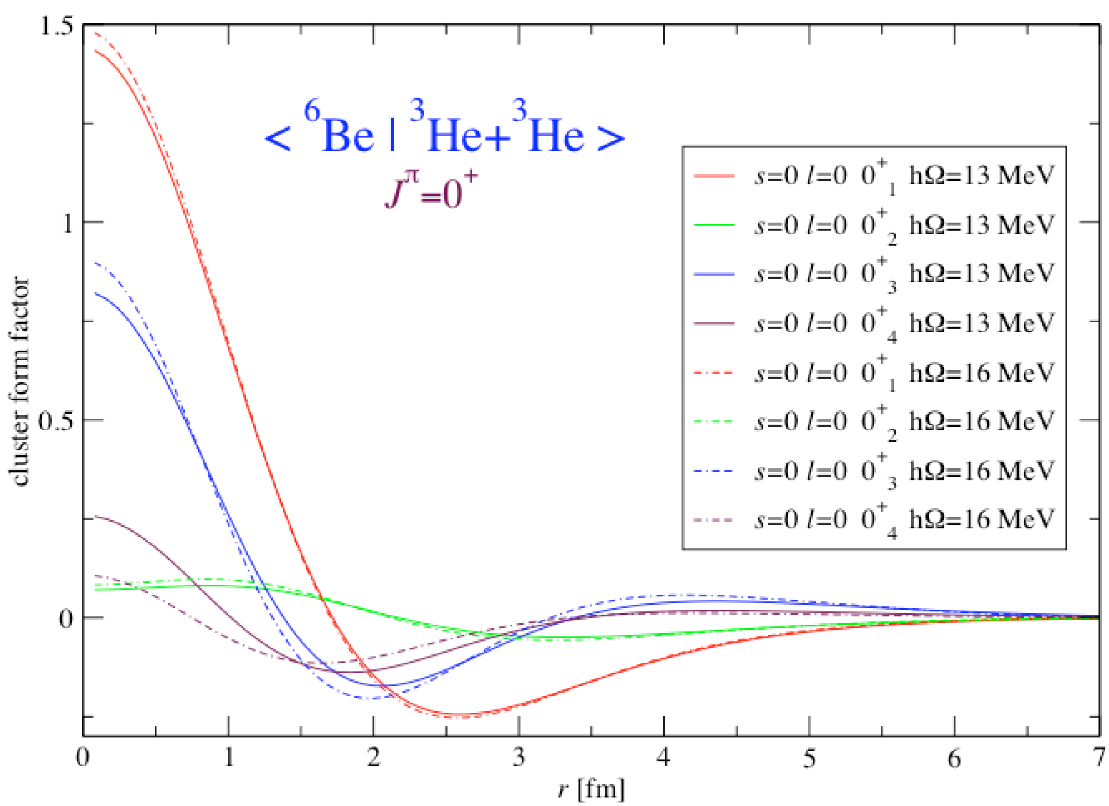
applications to radiative capture reactions

cluster form factors, spectroscopic factors

EFT description

reactions on deuterium, halo nuclei

P. Navratil, nucl-th/0410052



Challenges:

- Treatment of continuum in VMC and GFMC
- NCSM calculations with A=4 projectiles
- Low-energy reactions in NCSM

K. Nollett, Phys.Rev. C63, 05400 (2001)

L.E. Marcucci et al., nucl-th/0402078

P. Navratil, nucl-th/0410052

Resonance states, properties

$$\Psi(t) = \exp\left(-\frac{i}{\hbar}t\left(e - i\frac{\Gamma}{2}\right)\right)\Psi(\vec{r},k)$$

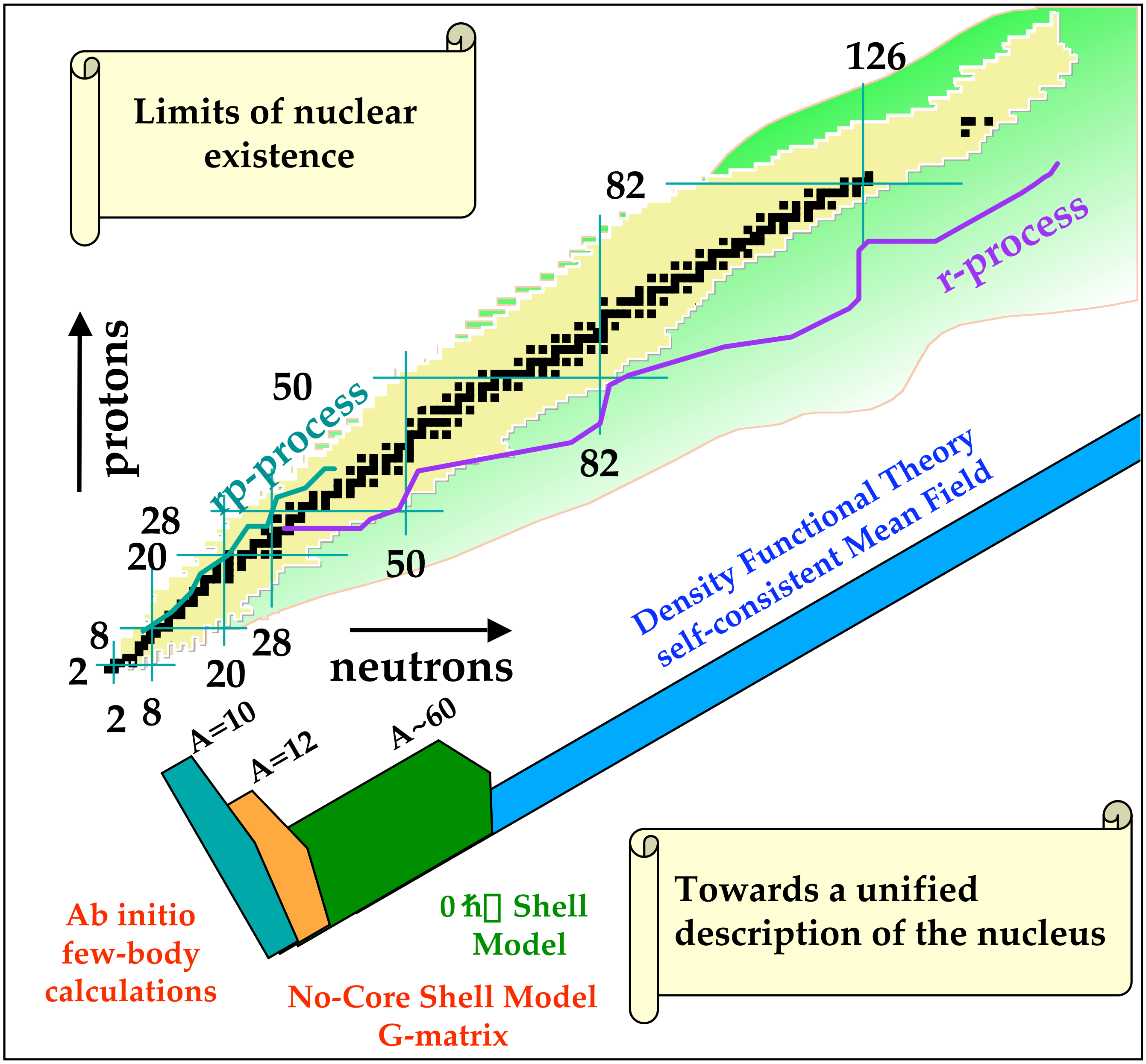
$$\langle\Psi(t)|\Psi(0)\rangle = \exp\left(-\frac{\Gamma}{2\hbar}t\right)\langle\Psi(\vec{r},k)|\Psi(\vec{r},k)\rangle$$

$$T_{1/2} = \ln 2\,\frac{\hbar}{\Gamma}, \qquad \hbar = 6.58\cdot 10^{-22}\ \mathrm{MeV}\cdot\mathrm{sec}$$

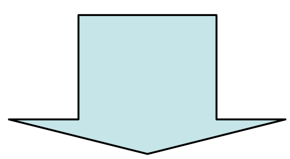
Can one calculate Γ with sufficient accuracy?

$$T_{s.p.} \approx 3\cdot 10^{-22}\,\mathrm{sec} = 3\,\mathrm{baby\,sec}.$$

For narrow resonances, explicit time propagation impossible!



Weakly bound nuclei are open systems



Structure and Reactions intertwined

Average one-body Hamiltonian

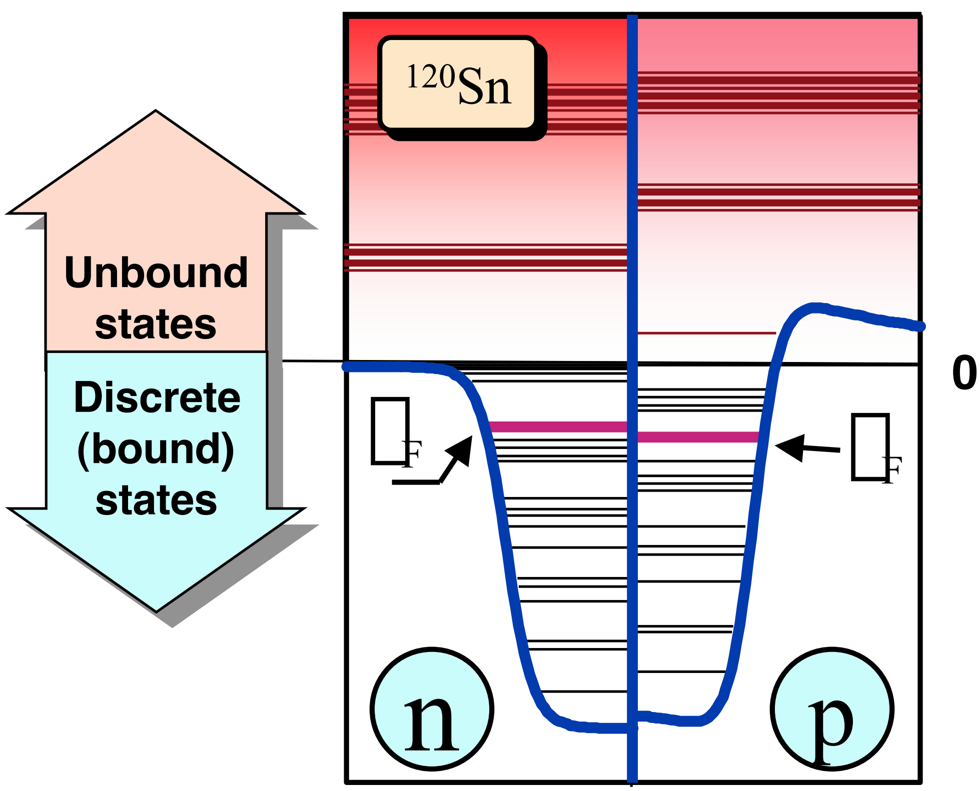
Single-particle orbitals

$$\hat{H}_0 = \sum_{i=1}^{A} h_i, \quad h_i = -\frac{\hbar^2}{2M}\nabla_i^2 + V_i, \quad h_i\phi_k(i) = \varepsilon_k\phi_k(i)$$

$$\left|\Phi_{k_1 k_2 \ldots k_A}\right\rangle = c_{k_1}^{+} c_{k_2}^{+} \ldots c_{k_A}^{+} |0\rangle,$$

$$E_{k_1 k_2 \ldots k_A} = \varepsilon_{k_1} + \varepsilon_{k_2} + \ldots + \varepsilon_{k_A}$$

$$V = V_n + V_{LS} + V_{Coul}$$



Continuum Shell Model -an old tool!

- U. Fano, Phys. Rev. 124, 1866 (1961)
- C. Mahaux and H. Weidenmüller: "Shell Model Approach to Nuclear Reactions" 1969
- H. W. Bartz et al., Nucl. Phys. A275, 111 (1977)
- D. Halderson and R.J. Philpott, Nucl. Phys. A345, 141
- …
- J. Okolowicz, M. Ploszajczak, I. Rotter, Phys. Rep. 374, 271 (2003)

Recent Developments:

SMEC

- K. Bennaceur et al., Nucl. Phys. A651, 289 (1999)
- K. Bennaceur et al., Nucl. Phys. A671, 203 (2000)
- N. Michel et al., Nucl. Phys. A703, 202 (2002)
- Y. Luo et al., nucl-th/0201073

Gamow Shell Model

- N. Michel et al., Phys. Rev. Lett. 89, 042502 (2002)
- N. Michel et al., Phys. Rev. C67, 054311 (2003)
- N. Michel et al., Phys. Rev. C70, 064313 (2004)
- R. Id Betan et al., Phys. Rev. Lett. 89, 042501 (2002)
- R. Id Betan et al., Phys. Rev. C67, 014322 (2003)
- R. Id Betan et al., Phys. Lett. B584, 48 (2004)
- G. Hagen et al., nucl-th/0410114

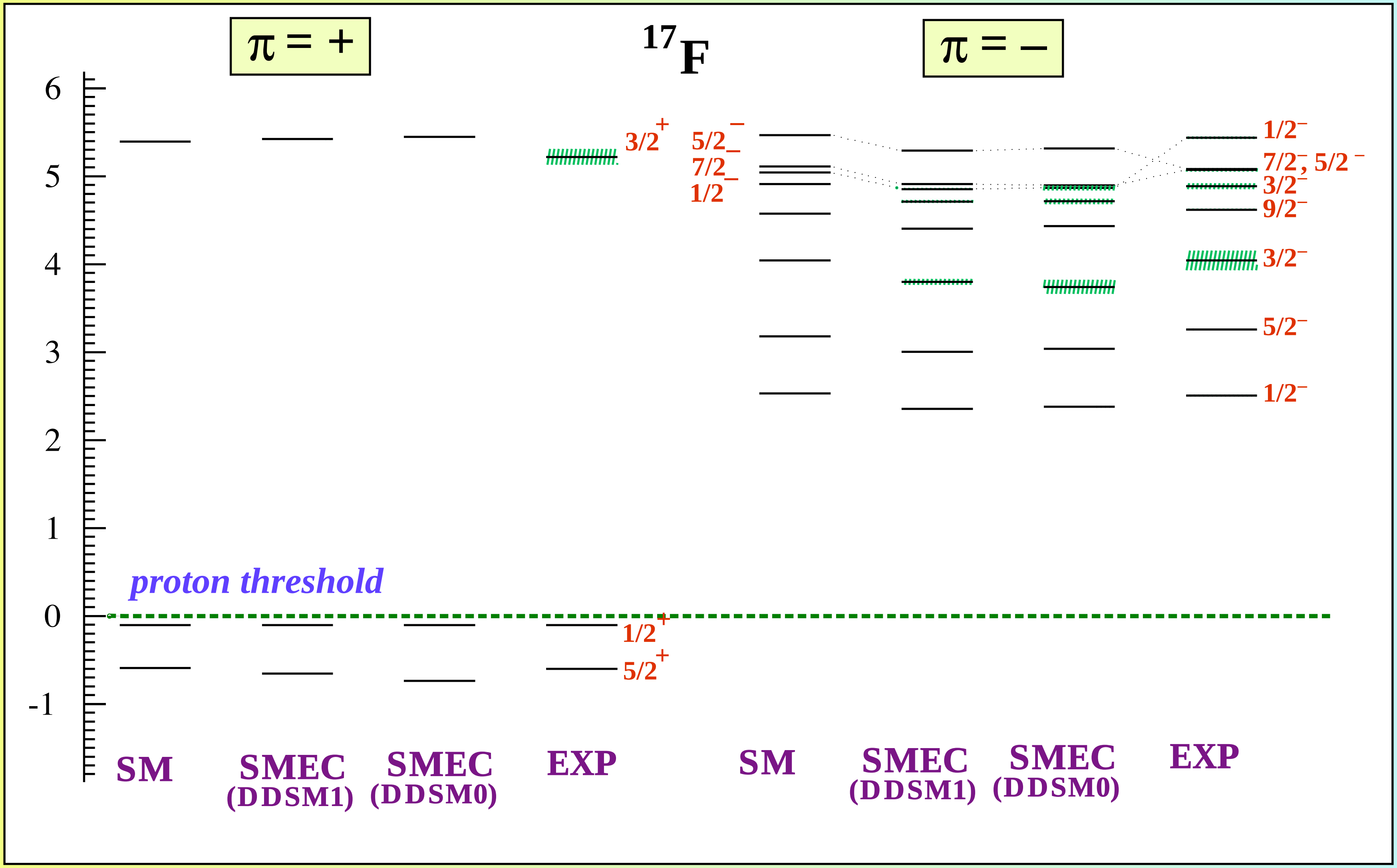
Other

- A. Volya and V. Zelevinsky, nucl-th/0406019

Continuum Shell Model

Q - quasi-bound states P - scattering states

H_{QQ} - shell model Hamiltonian; H_{PQ} - density-dependent

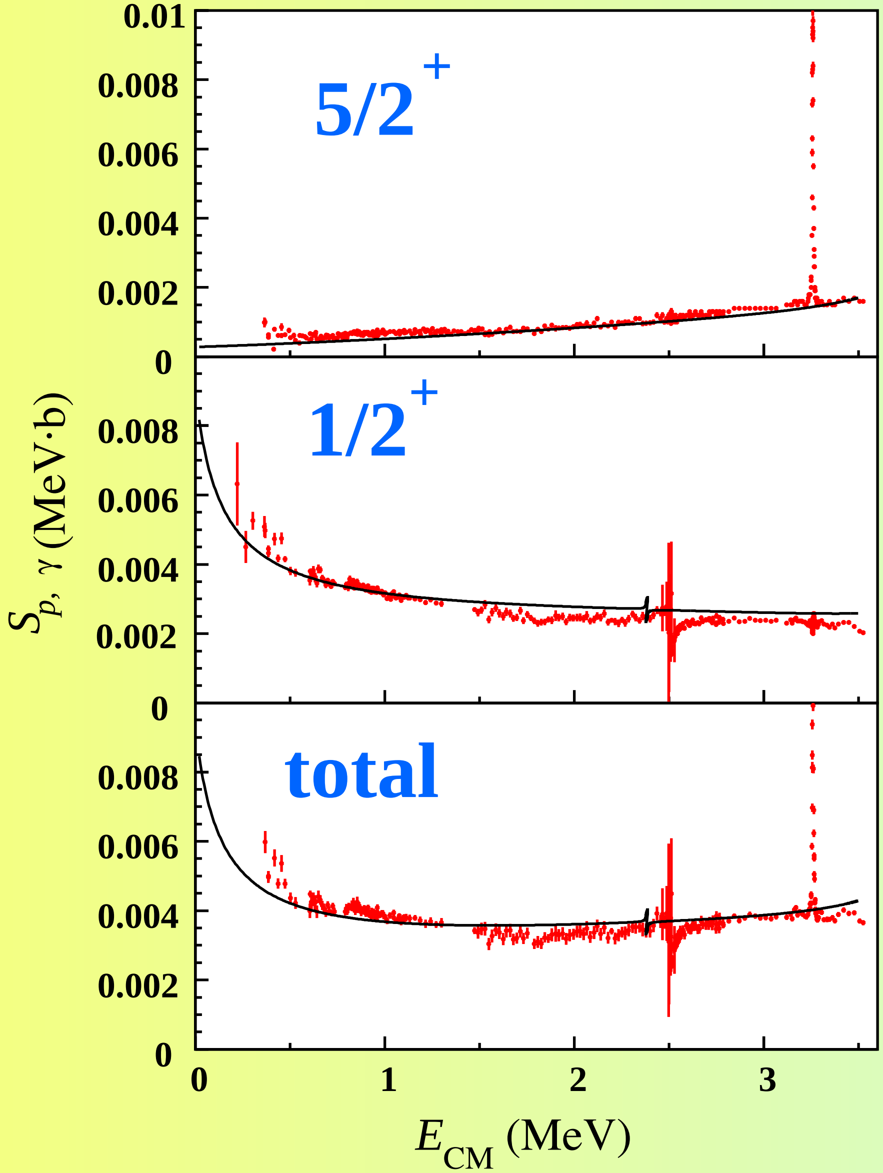


Theory: K. Bennaceur et al., Nucl. Phys. A651, 289 (1999); Phys. Lett. B488, 75 (2000)

Continuum Shell Model

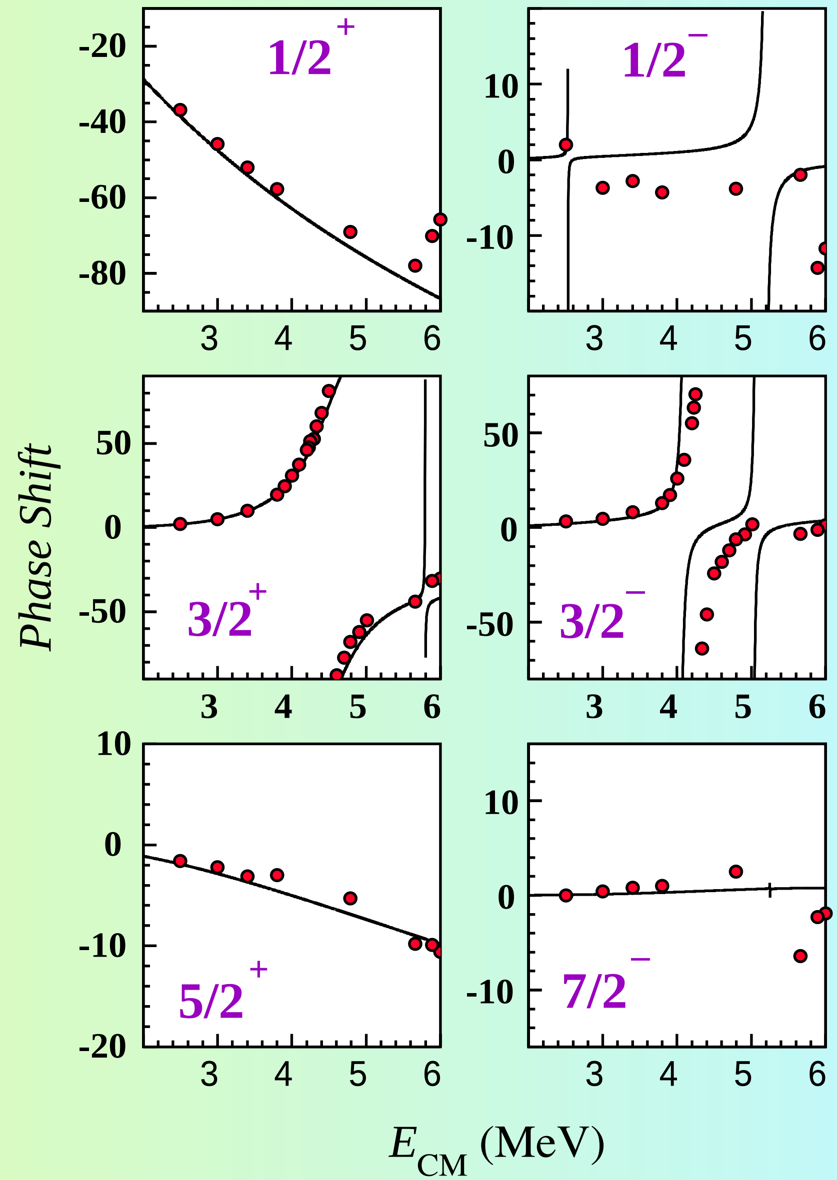
$^{16}O(p,\gamma)^{17}F$

Exp: Morlock et al., Phys. Rev. Lett. 79, 3837 (1997)



p+^{16}O elastic scattering

Exp: Blee and Haeberli , Phys. Rev. 137, B284 (1965)



Theory: K. Bennaceur et al., Nucl. Phys. A651, 289 (1999); Phys. Lett. B488, 75 (2000)

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

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

S-matrix has poles at k_n:

- Bound states ($k_n = i\kappa_n$)
- Antibound states ($k_n = -i\kappa_n$)
- Resonances: ($k_n = \pm\kappa_n - i\gamma_n$)

Only bound states are square integrable!

Resonance states, properties

Humblet and Rosenfeld: Nucl. Phys. **26,** 529 (1961)

$$\left[\hat{T}+\hat{V}\right]\psi = \left(e - i\frac{\Gamma}{2}\right)\psi$$

$$\left[\hat{T}+\hat{V}\right]\psi^{*} = \left(e + i\frac{\Gamma}{2}\right)\psi^{*}$$

$$\hbar \oint_S \vec{j}\, d\vec{S} = -\Gamma \int_V \rho\, d^3 r$$

$$\vec{j} = \frac{\hbar}{2mi}\left(\psi^{*}\vec{\nabla}\psi - \psi\vec{\nabla}\psi^{*}\right), \quad \rho = \psi^{*}\psi$$

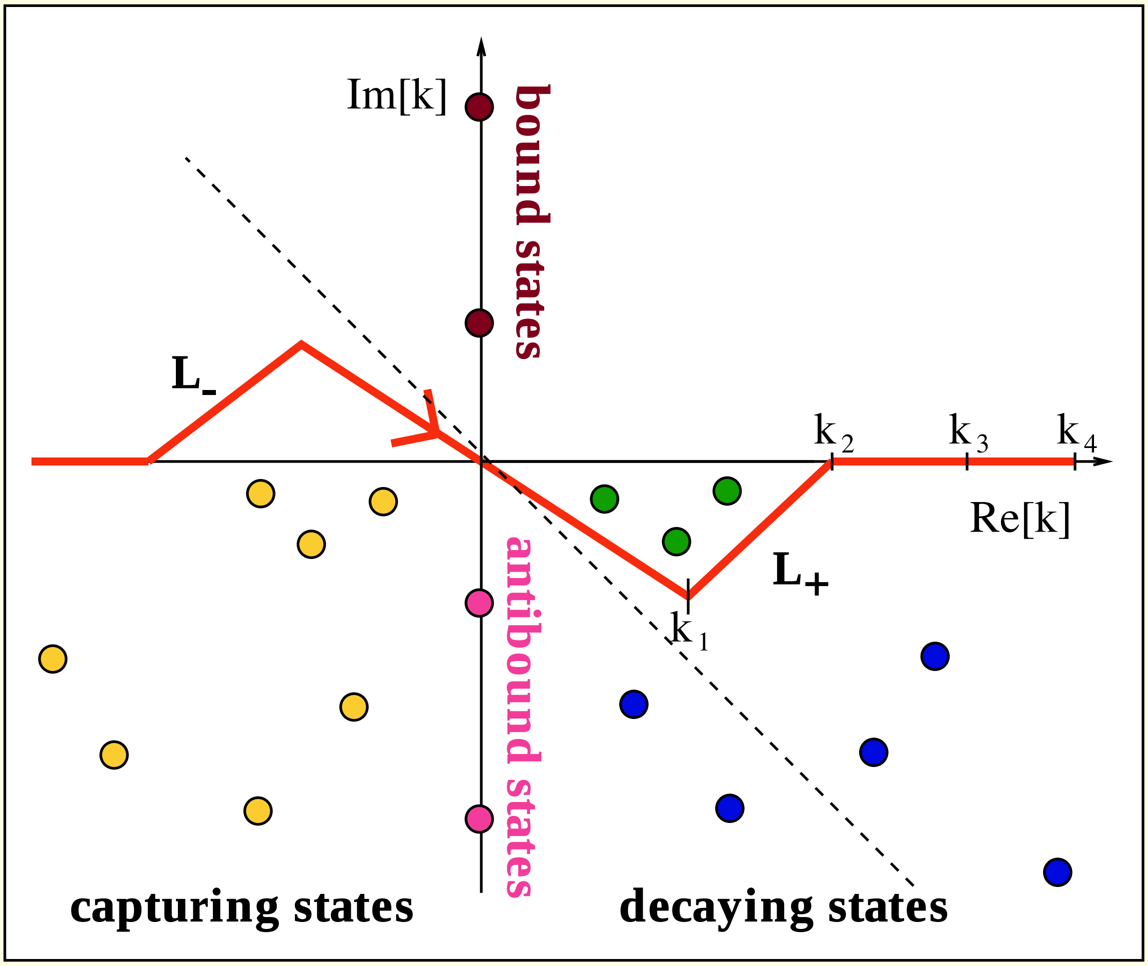
S can be taken as a sphere of radius R:

$$\Gamma = \frac{\hbar R^2 \oint j_r\, d\Omega}{\int_{V_R} \rho\, d^3 r}$$

$$\vec{\nabla}\vec{j} + \frac{\Gamma}{\hbar}\rho = 0 \quad \left(\vec{\nabla}\vec{j} + \frac{\partial\rho}{\partial t} = 0\right)$$

Gamow states and completeness relations

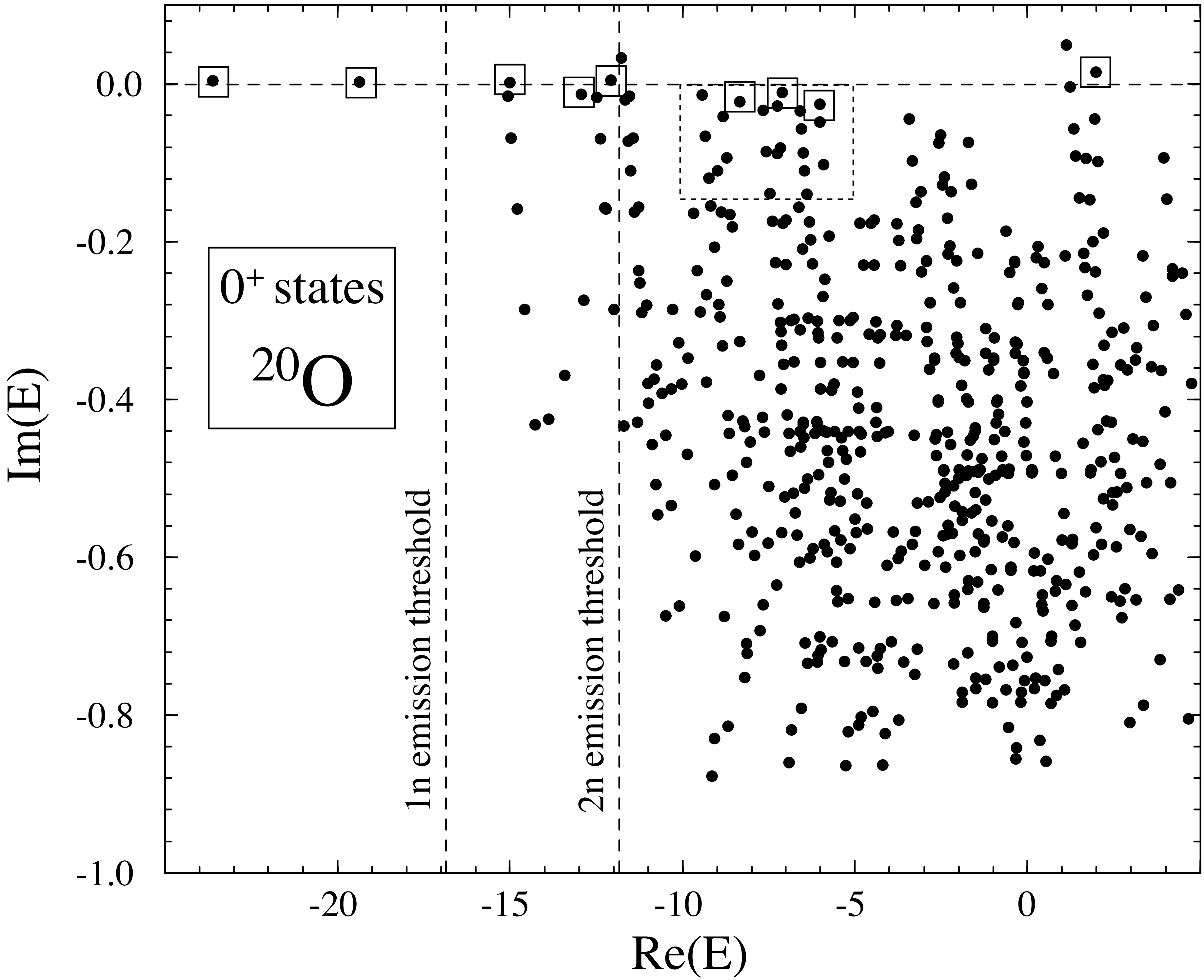
T. Berggren, Nucl. Phys. A109, 265 (1968); Nucl. Phys. A389, 261 (1982)
T. Lind, Phys. Rev. C47, 1903 (1993)



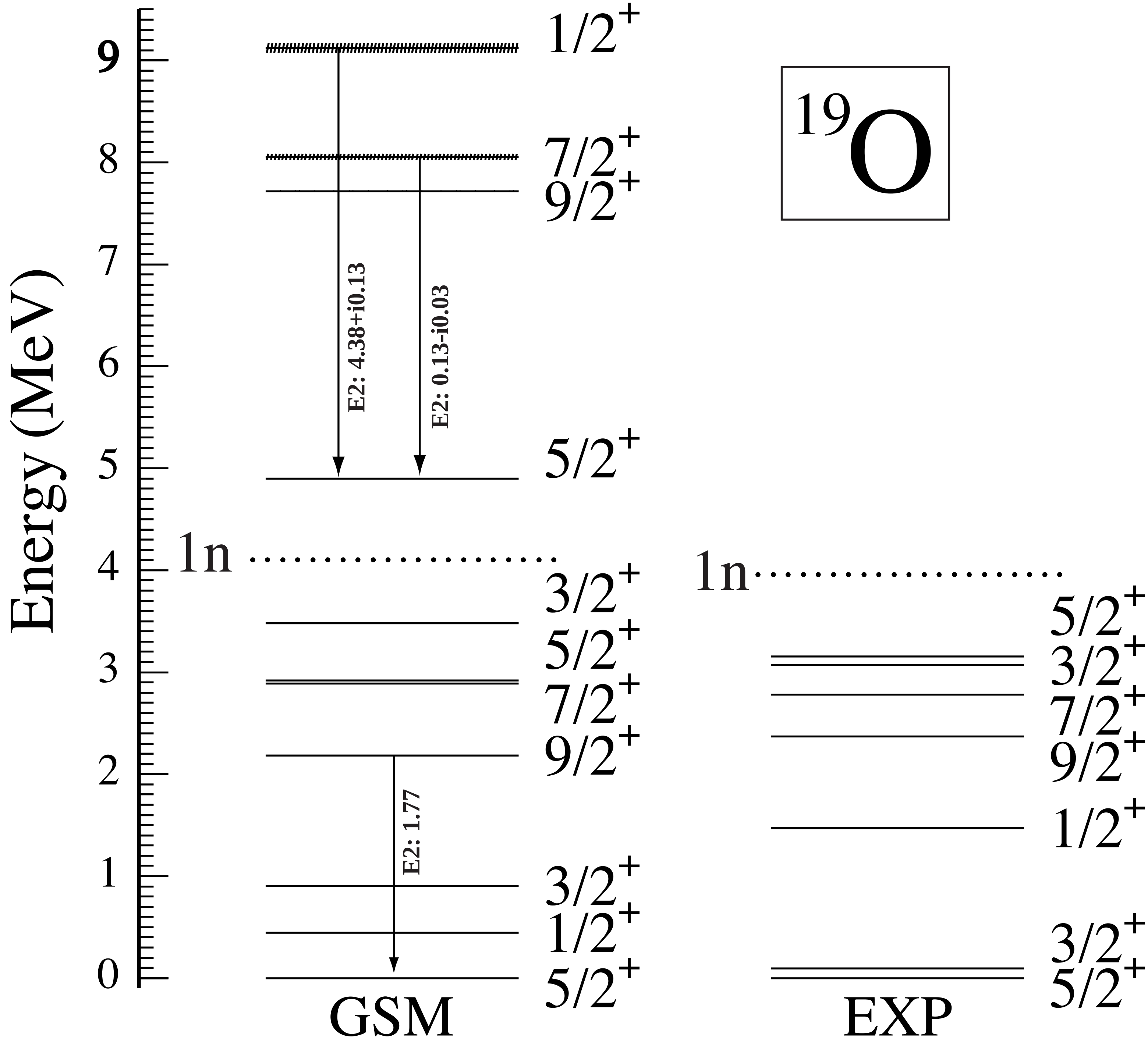
$$\sum_{n=b,r} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{L_+} |u(k)\rangle\langle u(k^*)|\, dk = 1$$

particular case: Newton completeness relation

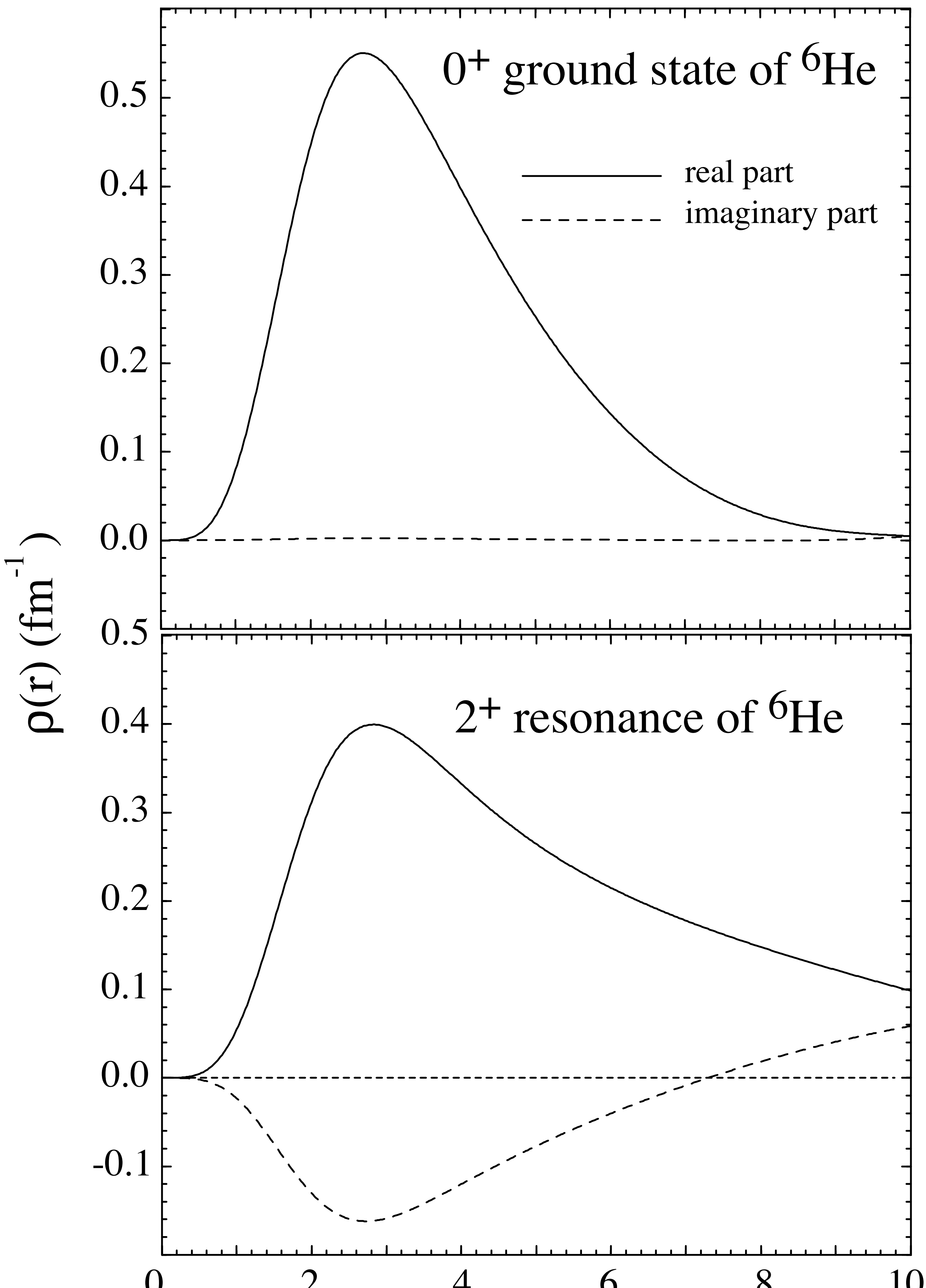
$$\sum_{n=b} |u_n\rangle\langle\tilde{u}_n| + \frac{1}{\pi}\int_{R} |u(k)\rangle\langle u(k^*)|\, dk = 1$$



0.0
-0.2
-0.4
-0.6
-0.8
-1.0
Im(E)
-20
-15
-10
-5
0
Re(E)
0+ states
20O
1n emission threshold
2n emission threshold

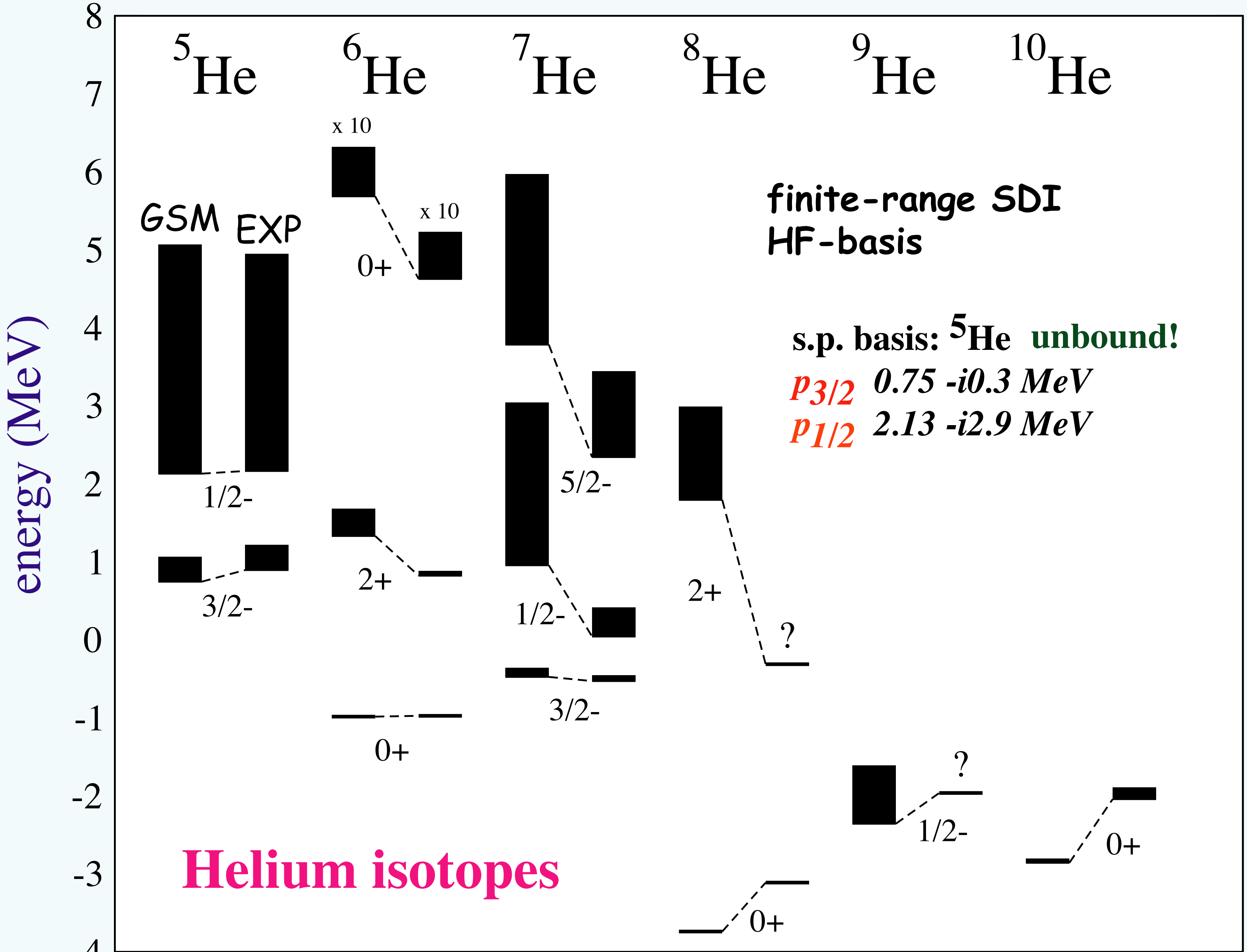


Energy (MeV)
0
1
2
3
4
5
6
7
8
9
1n
1/2+
7/2+
9/2+
5/2+
3/2+
5/2+
7/2+
9/2+
3/2+
1/2+
5/2+
E2: 4.38+i0.13
E2: 0.13-i0.03
E2: 1.77
GSM
19O
1n
5/2+
3/2+
7/2+
9/2+
1/2+
3/2+
5/2+
EXP

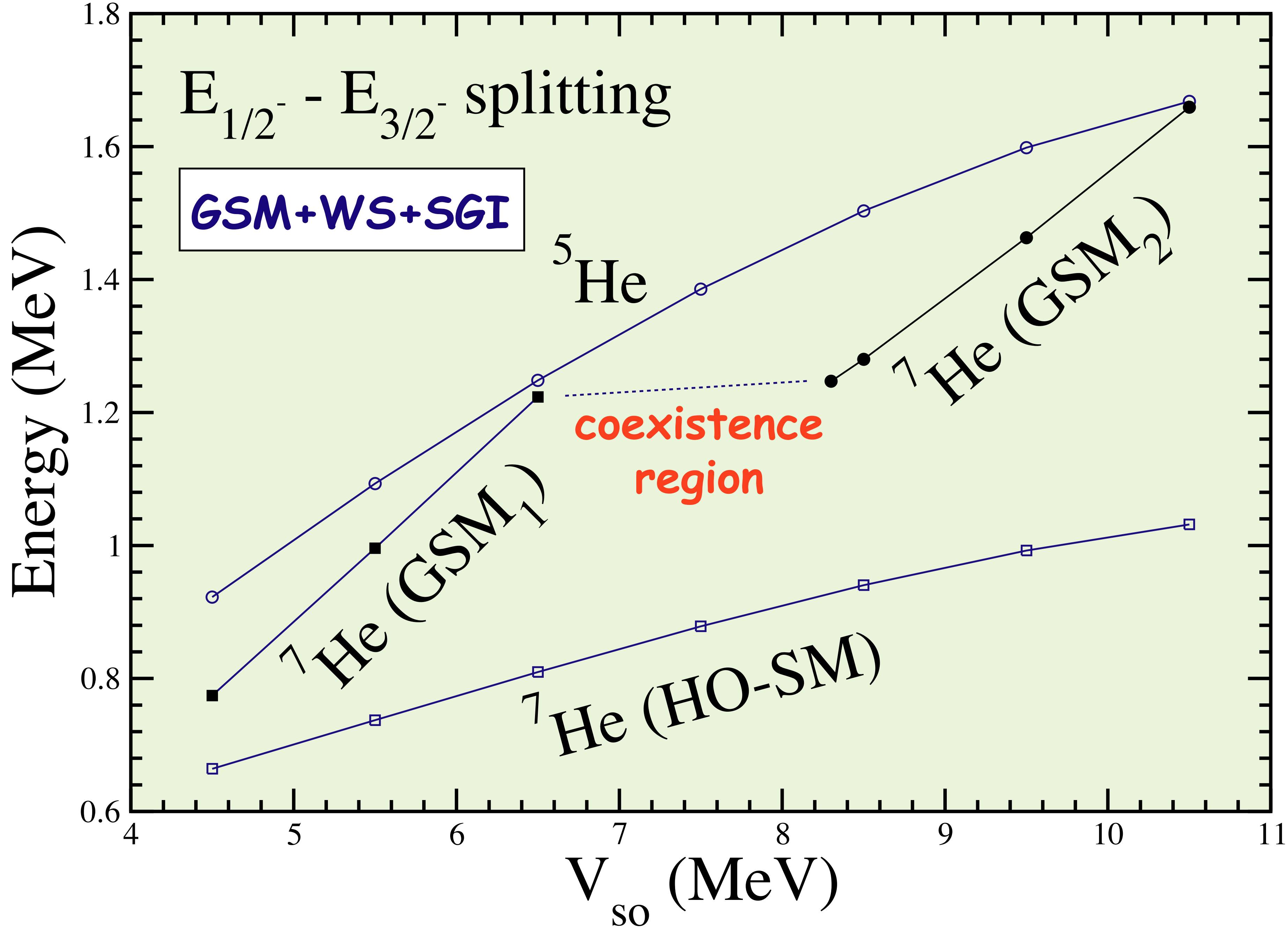


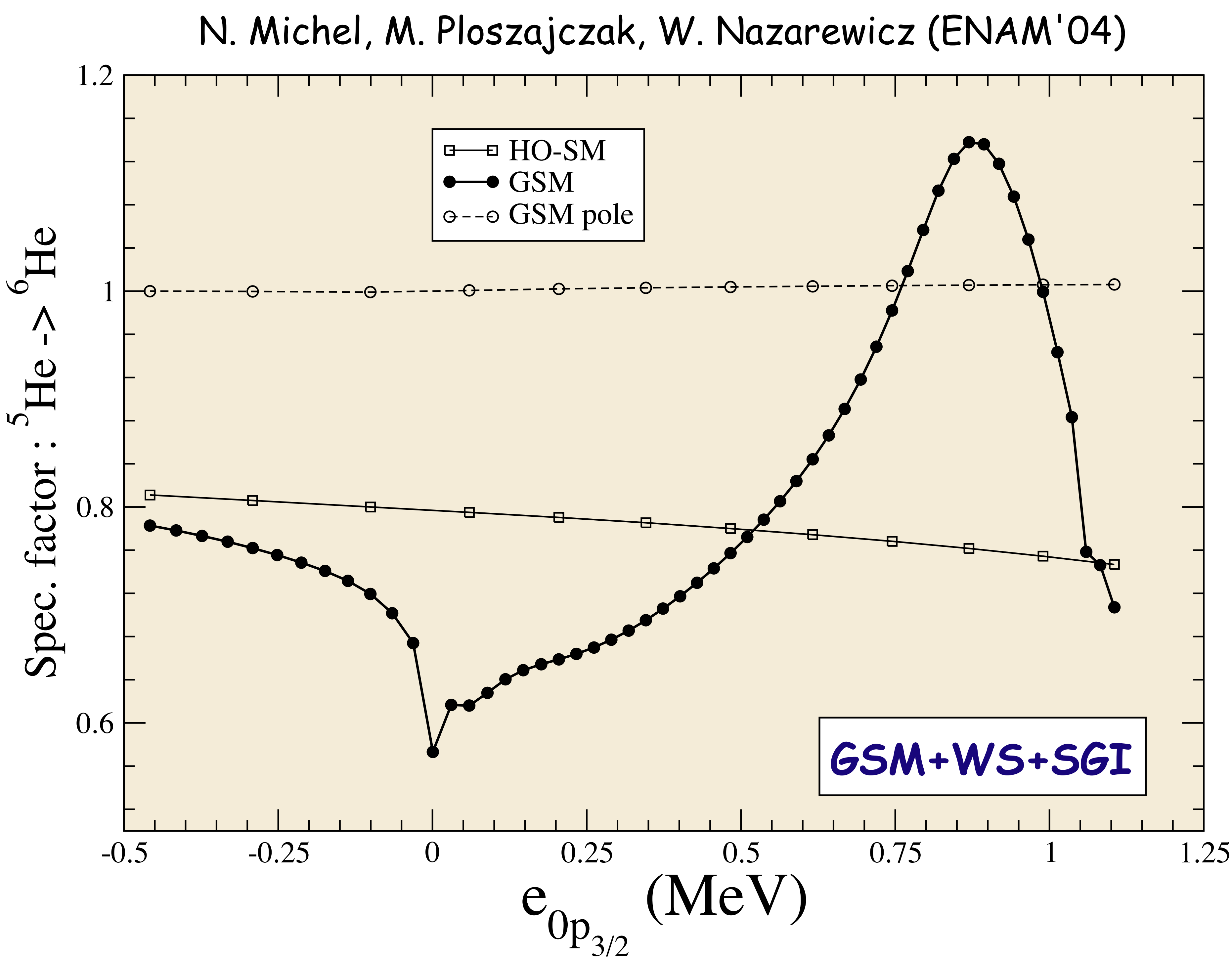
0+ ground state of 6He
real part
imaginary part
2+ resonance of 6He
ρ(r) (fm-1)
r (fm)
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
0
2
4
6
8
10

GSM: N. Michel et al., Phys.Rev.Lett. 89, 042502 (2002)

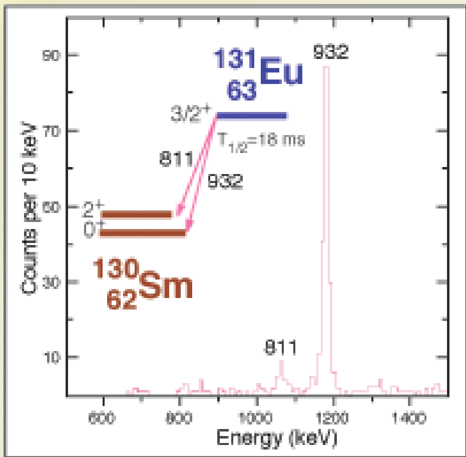


N. Michel, M. Ploszajczak, W. Nazarewicz (ENAM'04)



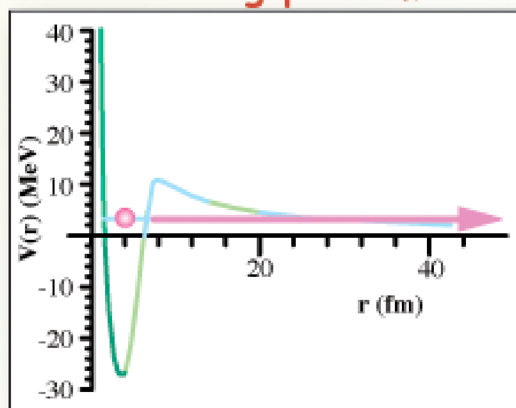

N. Michel, M. Ploszajczak, W. Nazarewicz (ENAM'04)
HO-SM
GSM
GSM pole
GSM+WS+SGI
Spec. factor : ^{5}He -> ^{6}He
$e_{0p_{3/2}}$ (MeV)
1.2
1
0.8
0.6
-0.5
-0.25
0
0.25
0.5
0.75
1
1.25

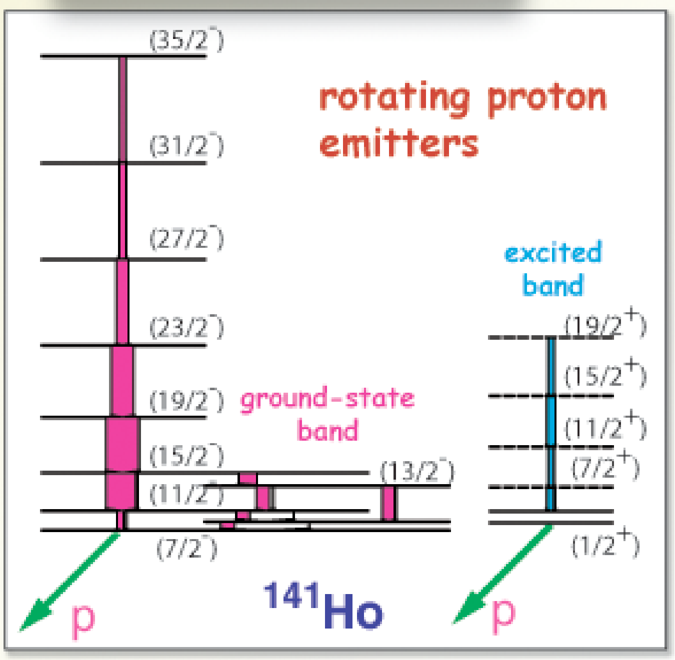
fine structure in proton decay

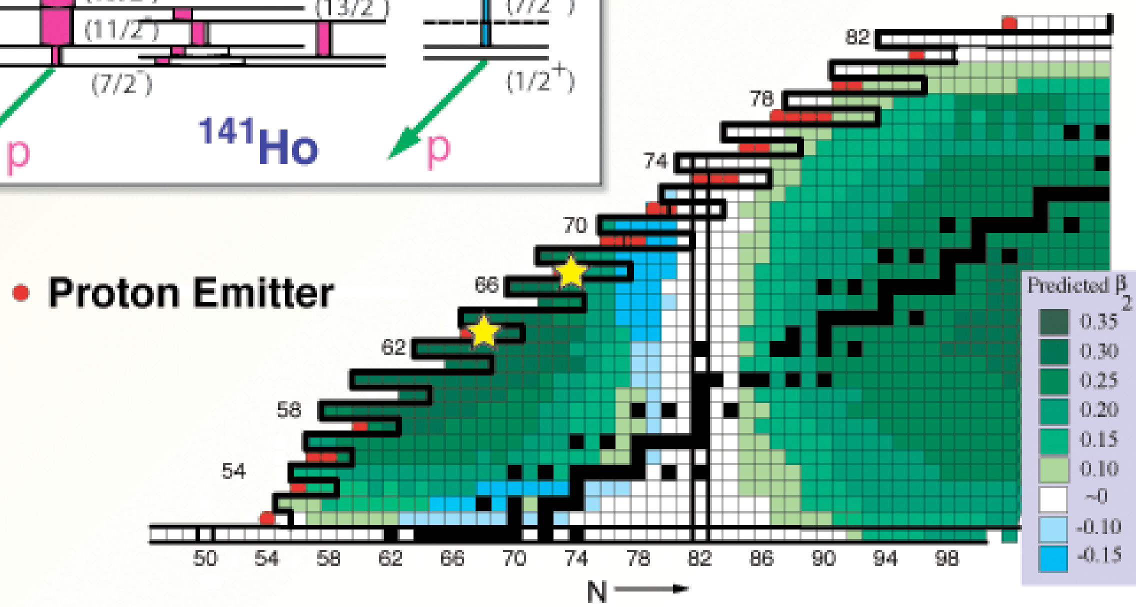


Life beyond the proton drip line

proton emission - tunnelling phenomenon







Proton Emitters, narrow resonances
(Some Recent References)

Particle-core vibration coupling

C.N.Davids, H.Esbensen, Phys.Rev. C69, 034314 (2004)
M.Karny et al., Phys.Rev.Lett. 90, 012502 (2003)
K.Hagino, Phys.Rev. C64, 041304 (2001)
C.N.Davids, H.Esbensen, Phys.Rev. C64, 034317 (2001)
H. Esbensen and C.N. Davids, Phys. Rev. C64, 034317 (2001)

Deformed proton emitters, coupled-channels

B.Barmore et al., Phys.Rev. C62, 054315 (2000)
H.Esbensen, C.N.Davids, Phys.Rev. C63, 014315 (2001)
W.Krolas et al., Phys.Rev. C65, 031303 (2002)
A.T. Kruppa and W. Nazarewicz, Phys. Rev. C69, 054311 (2004)

BCS treatment of pairing

G.Fiorin, E.Maglione, L.S.Ferreira, Phys.Rev. C67, 054302 (2003)
A. Volya and C. Davids, nucl-th/0410053

Odd-odd proton emitters

L.S. Ferreira, E. Maglione, Phys.Rev. Lett. 86, 1721 (2001)

Two-potential approach

S.A. Gurvitz, P.B. Semmes, W. Nazarewicz, T. Vertse,
Phys. Rev. A69, 042705 (2004)

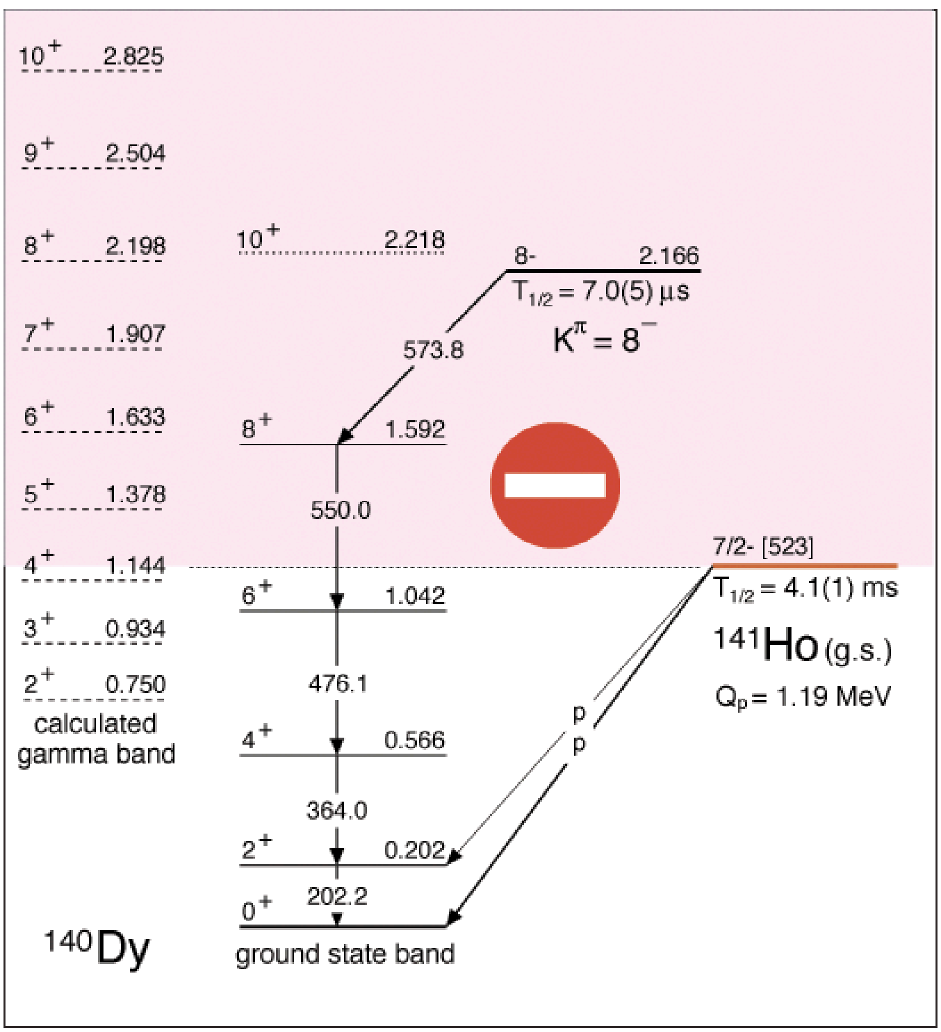
Weak Coupling Description

$$H_{\mathrm{tot}} = H_{\mathrm{d}} - \frac{\hbar^2}{2m} \Delta_{\mathbf{r}} + V_{\mathrm{def}}(\mathbf{r}, \omega)$$

collective Hamiltonian

nucleon-daughter relative energy

nucleon-core interaction



HFB theory in coordinate space

J. Dobaczewski, H. Flocard, and J. Treiner,
Nucl. Phys. A422 (1984) 103

$$x = (\vec{r}, \sigma), \quad \sum_{\sigma} \int d^3\vec{r} \equiv \int dx$$

$$\int dx' \begin{pmatrix} h(x,x') & \Delta(x,x') \\ \Delta(x,x') & -h(x,x') \end{pmatrix} \begin{pmatrix} u(x') \\ v(x') \end{pmatrix} = \begin{pmatrix} E+\lambda & 0 \\ 0 & E-\lambda \end{pmatrix} \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}$$

$h(\vec{r},\vec{r}\,') \to 0$ and $\Delta(\vec{r},\vec{r}\,') \to 0$ for large $\vec{r},\vec{r}\,'$

$$\Rightarrow \begin{cases} \left(-\frac{\hbar^2}{2M}\nabla^2\right) u(x) = (\lambda + E) u(x) \\ \left(-\frac{\hbar^2}{2M}\nabla^2\right) v(x) = (\lambda - E) v(x) \end{cases}$$

- For λ>0 the entire spectrum is continuous.
- For $|E|>-\lambda$ both components are localized

$$u(x) \sim \begin{cases} r^{-1}\cos(k_1 r + \delta_1) & \text{for } \lambda + E > 0 \\ r^{-1}\exp(-\kappa_1 r) & \text{for } \lambda + E < 0 \end{cases}$$

$$v(x) \sim \begin{cases} r^{-1}\cos(k_2 r + \delta_2) & \text{for } \lambda - E > 0 \\ r^{-1}\exp(-\kappa_2 r) & \text{for } \lambda - E < 0 \end{cases}$$

Localized!

$$\kappa(x,x') = \sum_{0<E_n<E_{\max}} v_n(x) v_n^*(x')$$

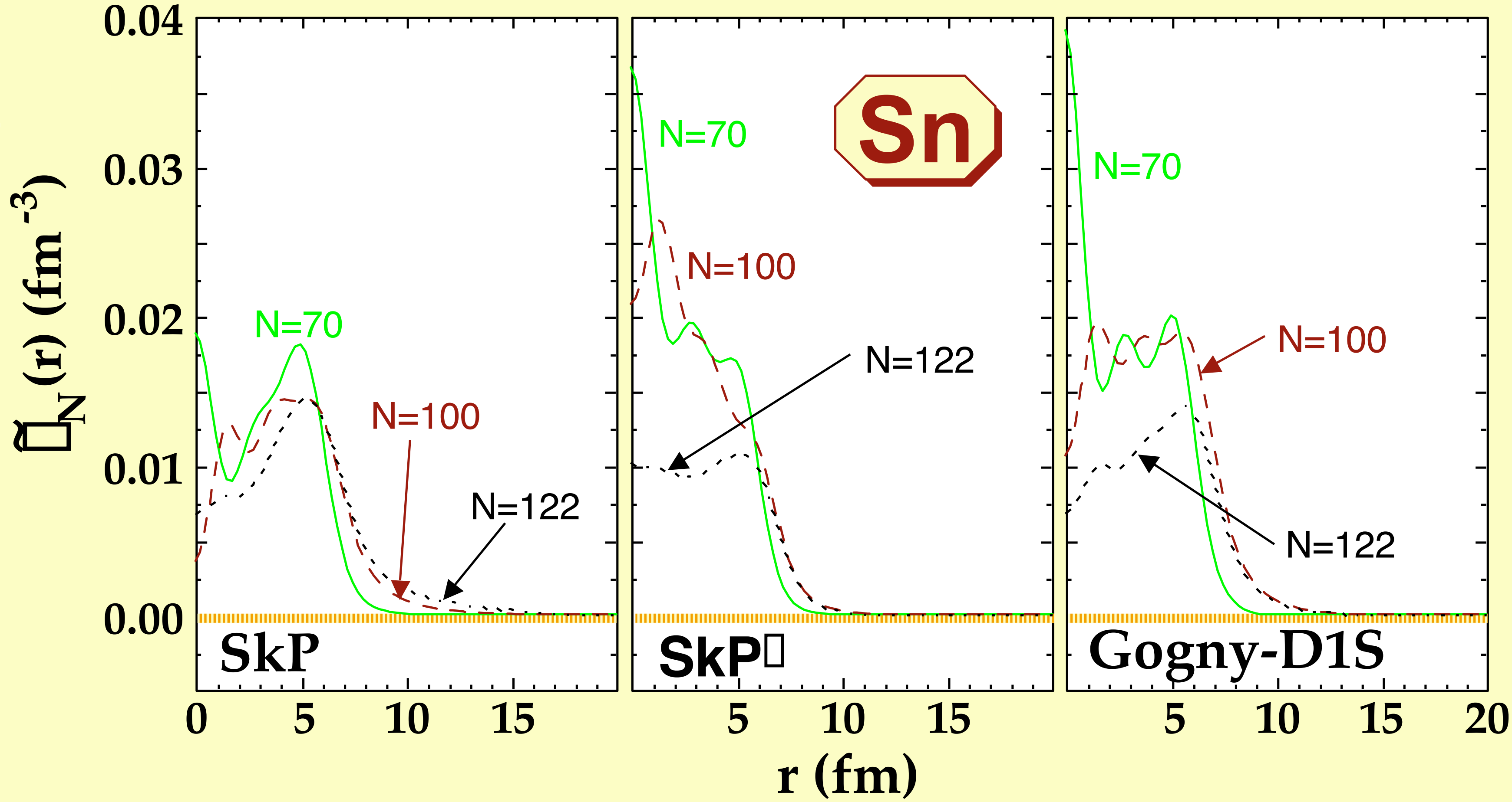
Localized!

HF+BCS

$$\Delta_{BCS}(\vec{r},\vec{r}\,') = \Delta\,\delta(\vec{r} - \vec{r}\,')$$

Pairing is not localized inside the nucleus. Completely different asymptotic properties!

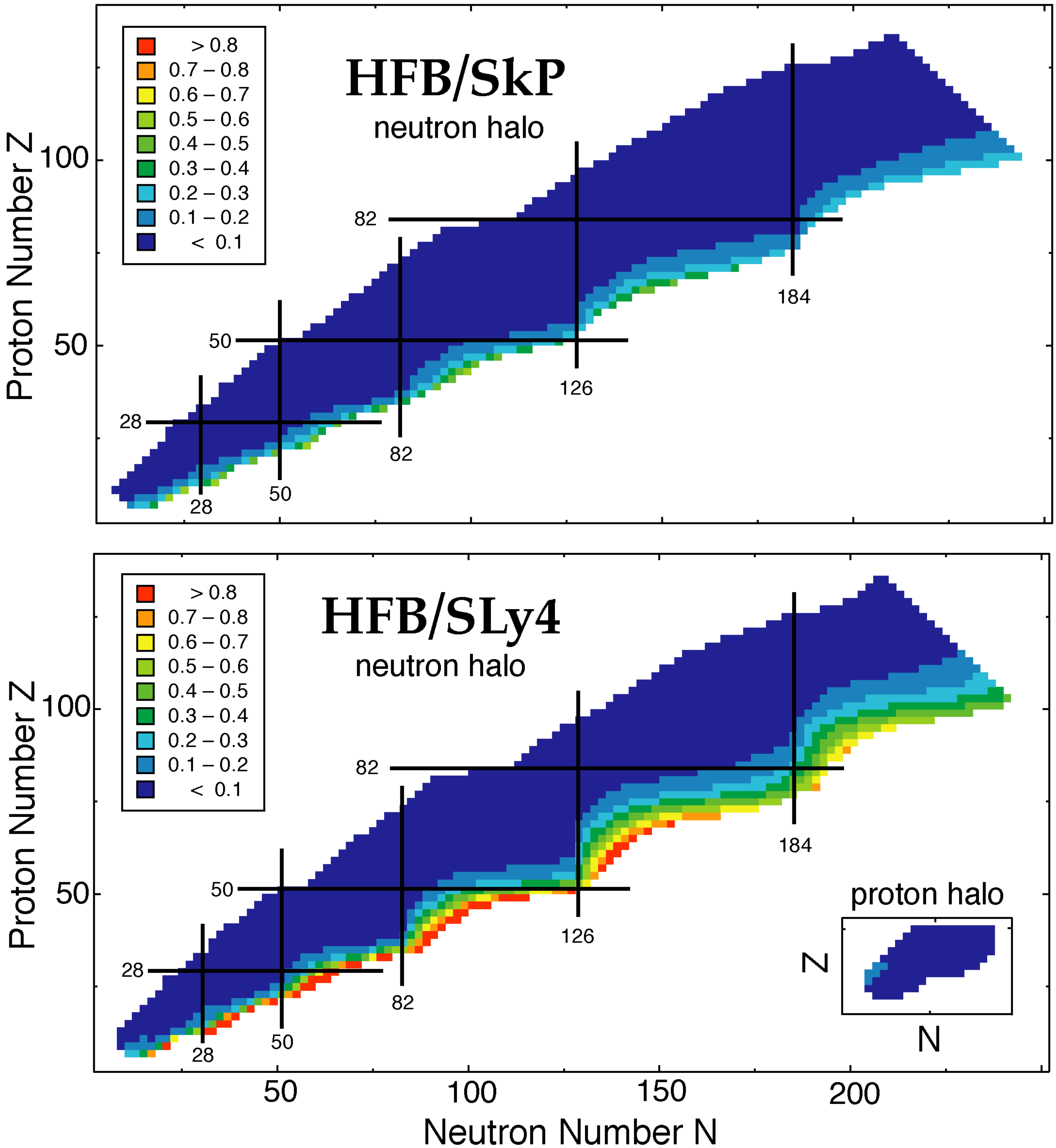
HFB: Pairing density



Phys. Rev. C53, 2809 (1996)

Neutron Halo

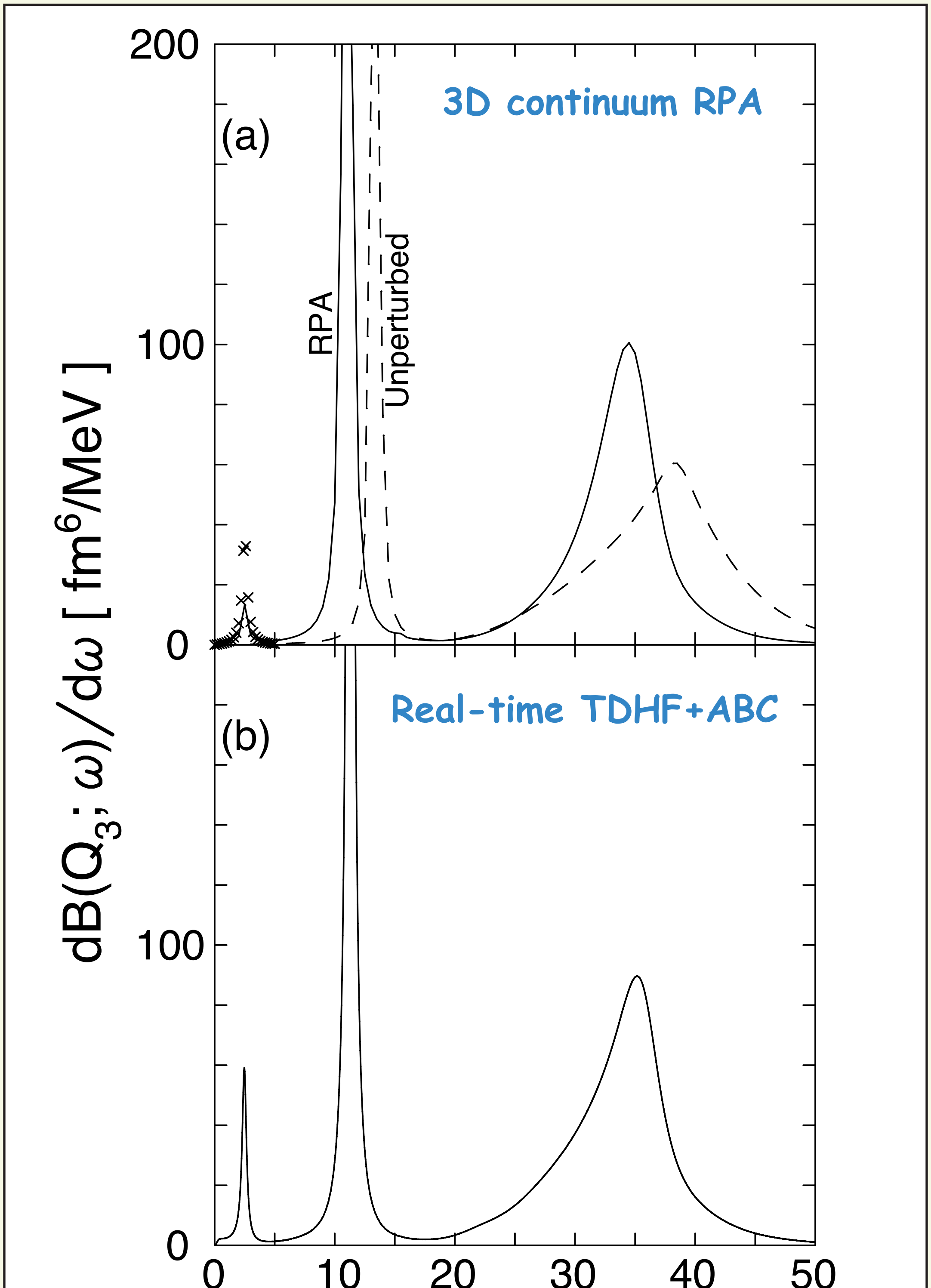
S. Mizutori et al., Phys. Rev. C61, 044326 (2000)



Halo is strongly influenced by pairing!

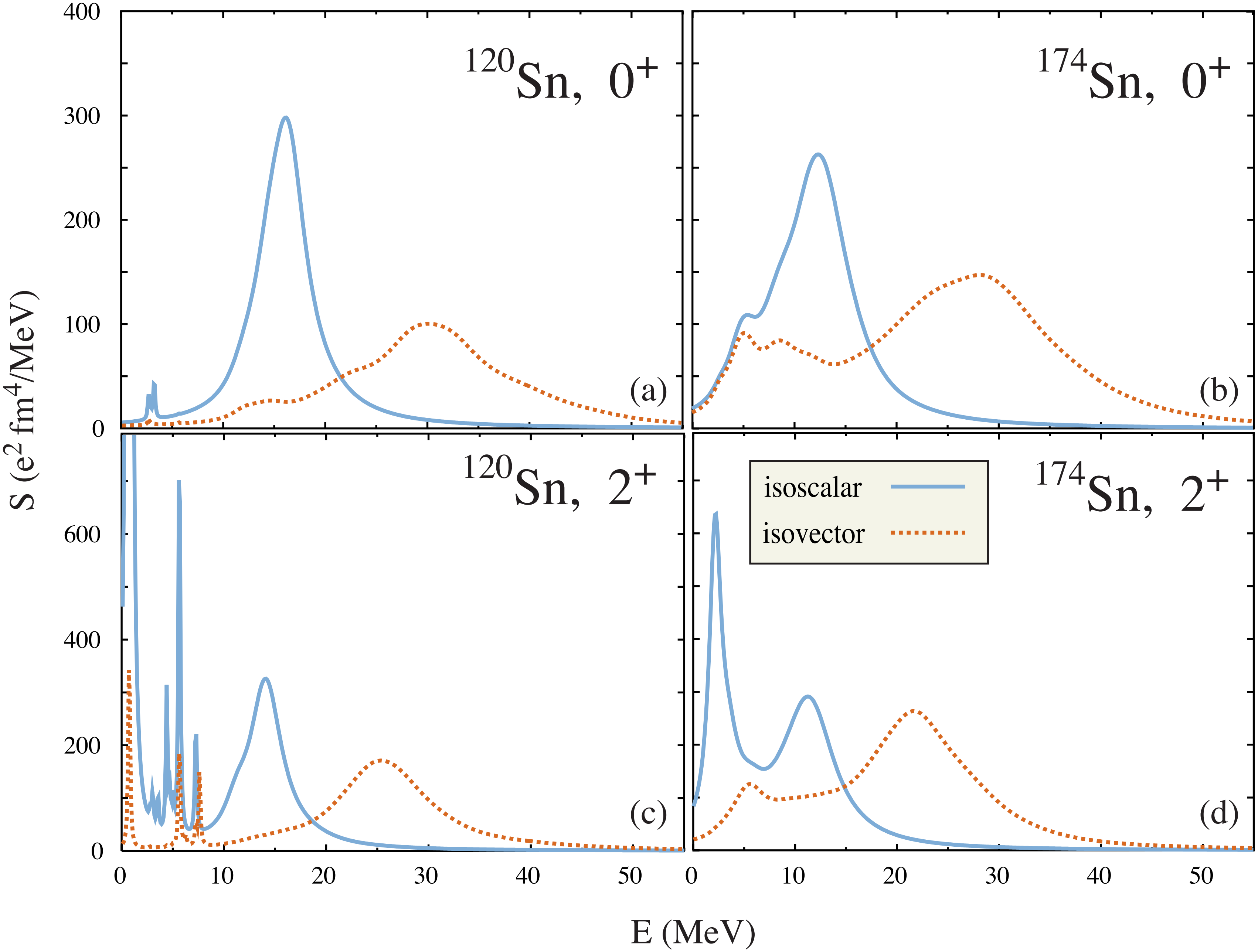
Linear response theory in the continuum for deformed nuclei: Green's function vs. time-dependent Hartree-Fock with the absorbing-boundary condition

Nakatsukasa and Yabana, nucl-th/0409013



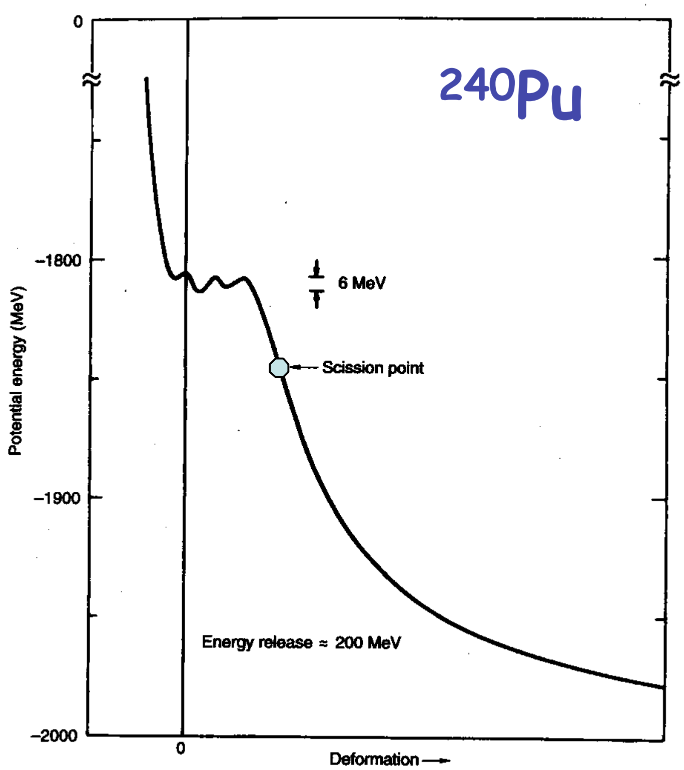
Skyrme-QRPA (self-consistent, coordinate space, canonical basis)

Jun Terasaki et al., nucl-th/0407111 (Phys. Rev. C, in press)

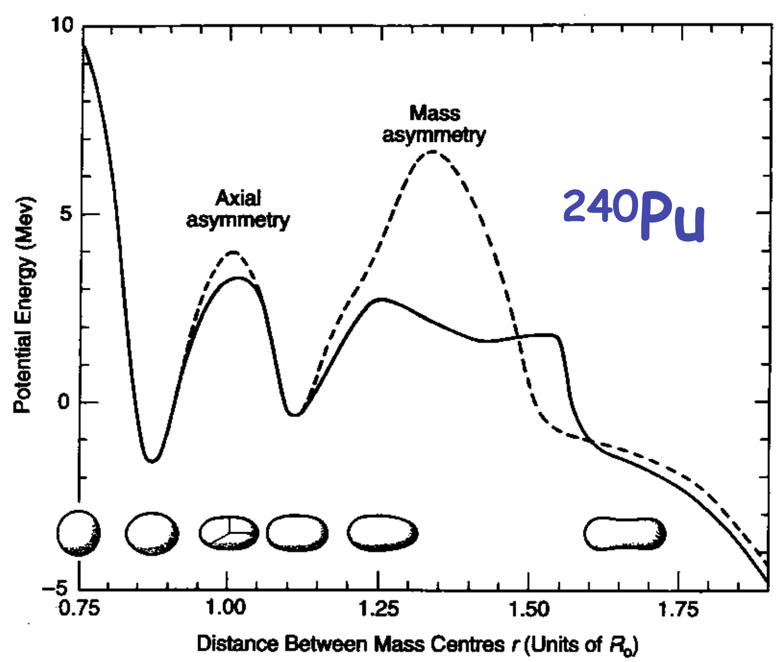


Spontaneous fission

1938 - Hahn & Strassmann
1939 Mwitner & Frisch
1939 Bohr & Wheeler
1940 Petrzhak & Flerov



Realistic calculations



Coupling of nuclear structure and reaction theory

(NSAC Nuclear Theory Report)

Tying nuclear structure directly to nuclear reactions within a coherent framework applicable throughout the nuclear landscape is an important goal. For light nuclei, ab-initio methods hold the promise of direct calculation of low-energy scattering processes, including those important in nuclear astrophysics, and tests of fundamental symmetries. In nuclear structure for heavier nuclei, the continuum shell model and modern mean-field theories allow for the consistent treatment of open channels, thus linking the description of bound and unbound nuclear states and direct reactions. On the reaction side, better treatment of nuclear structure aspects is equally crucial. The battleground in this task is the newly opening territory of weakly bound nuclei where the structure and reaction aspects are interwoven and where interpretation of future data will require advances in understanding of the reaction mechanism.