Nuclear structure II (global properties, shells)

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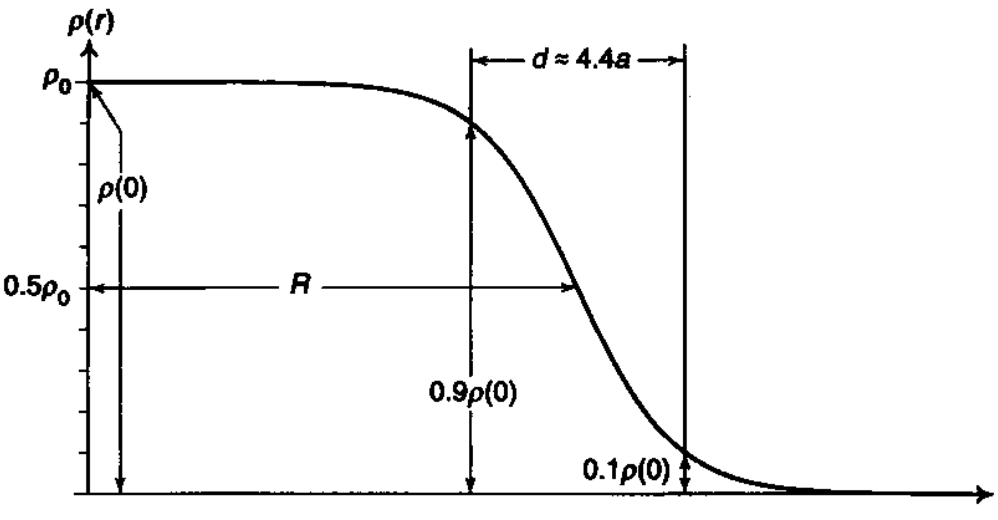
National Nuclear Physics Summer School 2014
William & Mary, VA

- Global properties of atomic nuclei
- Shell structure
- Nucleon-nucleon interaction
- Deuteron, Light nuclei

Global properties of atomic nuclei

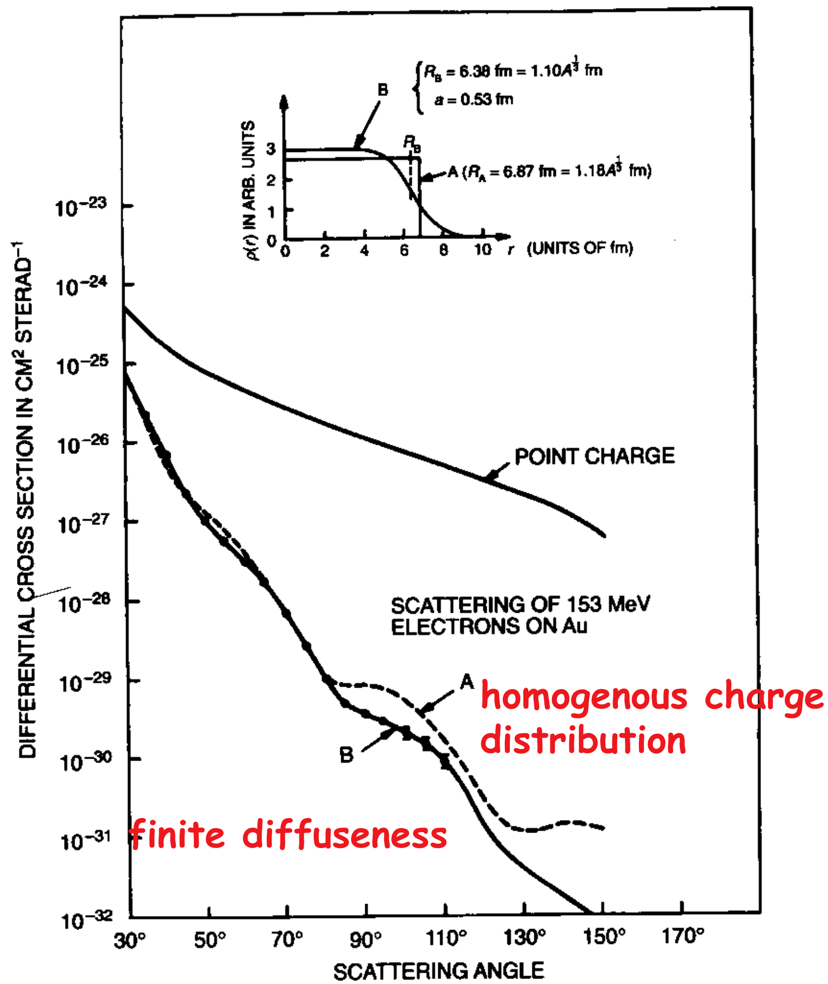
Sizes



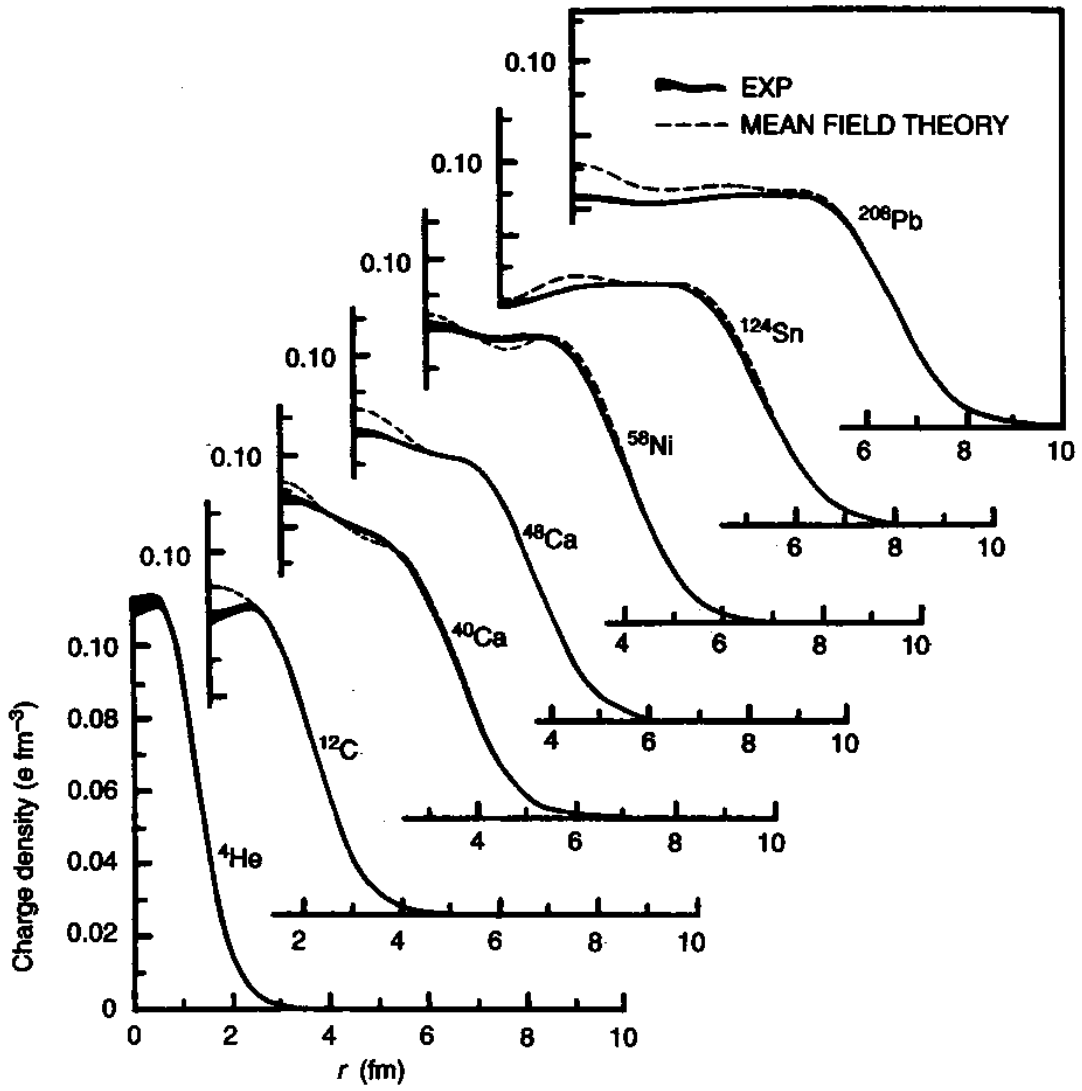
$$\rho(0) = 0.17 \text{nucleons/fm}^3$$

$$\rho(r) = \rho_0 \left[1 + \exp\left(\frac{r-R}{a} \right) \right]^{-1}$$

$$R \approx 1.2 A^{1/3} \text{fm}, \quad a \approx 0.6 \text{fm}$$



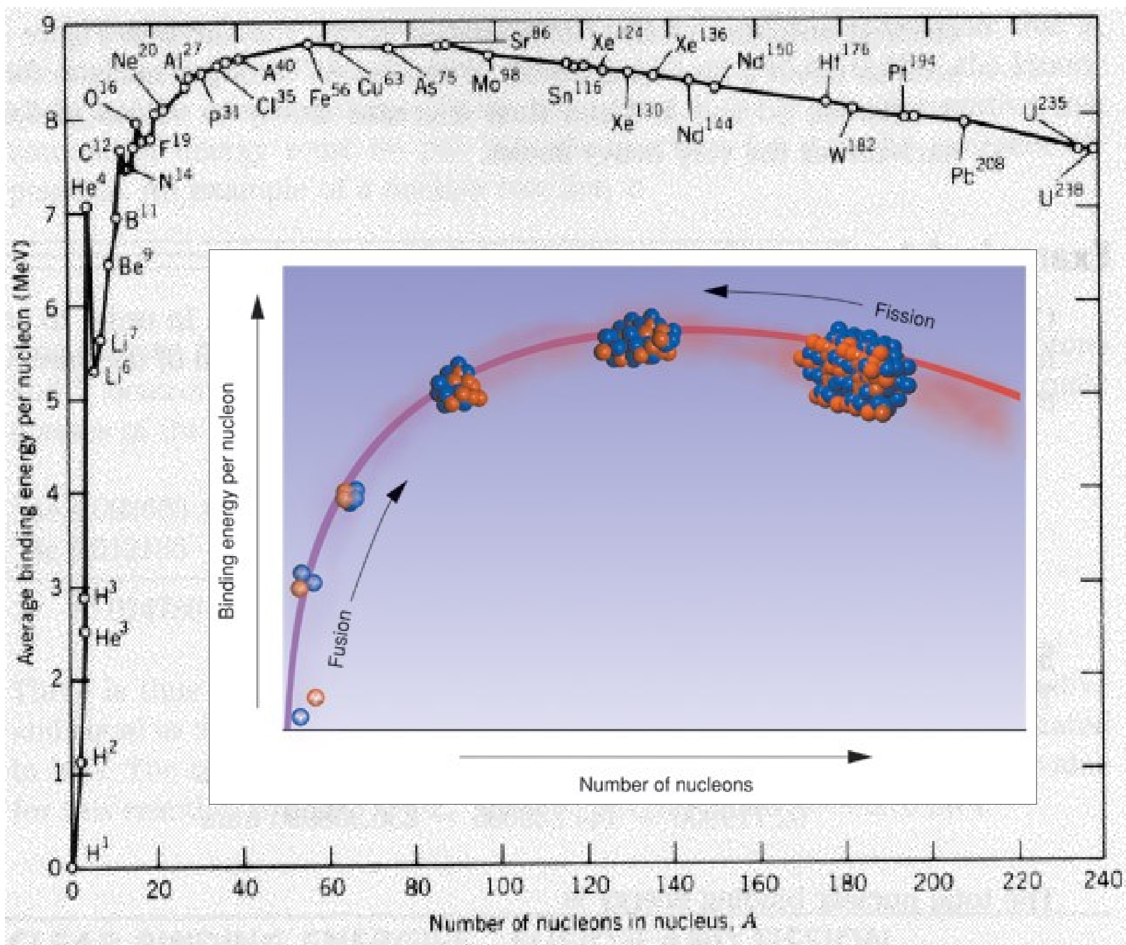
Calculated and measured densities



Binding

$$m(N,Z) = \frac{1}{c^2} E(N,Z) = NM_n + ZM_H - \frac{1}{c^2} B(N,Z)$$

The binding energy contributes significantly (~1%) to the mass of a nucleus. This implies that the constituents of two (or more) nuclei can be rearranged to yield a different and perhaps greater binding energy and thus points towards the existence of nuclear reactions in close analogy with chemical reactions amongst atoms.



The sharp rise of B/A for light nuclei comes from increasing the number of nucleonic pairs. Note that the values are larger for the 4n nuclei (α-particle clusters!). For those nuclei, the difference

4He

$$\Delta E \equiv B(N,Z) - nB(2,2)$$

divided by the number of alpha-particle pairs, n(n-1)/2, is roughly constant (around 2 (MeV). This is nice example of the saturation of nuclear force. The associated symmetry is known as SU(4), or Wigner supermultiplet symmetry.

Table 1-3: Binding energies (MeV) for some stable light nuclei.

Symbol	E_B	E_B/A	ΔE	Symbol	E_B	E_B/A	Symbol	E_B	E_B/A
^{2}H	2.22	1.11	—	^{3}H	8.48	2.83	^{3}He	7.72	2.57
^{4}He	28.30	7.07	—	^{5}He	27.41	5.48	^{5}Li	26.33	5.27
^{6}Li	32.00	5.33	—	^{7}Li	39.25	5.61	^{7}Be	37.60	5.37
^{8}Be	56.50	7.06	−0.09	^{9}Be	58.17	6.46	^{9}B	56.31	6.26
^{10}B	64.75	6.48	—	^{11}B	76.21	6.93	^{11}C	73.44	6.68
^{12}C	92.16	7.68	7.27	^{13}C	97.11	7.47	^{13}N	94.11	7.24
^{14}N	104.66	7.48	—	^{15}N	115.49	7.70	^{15}O	111.96	7.46
^{16}O	127.62	7.98	14.44	^{17}O	131.76	7.75	^{17}F	128.22	7.54
^{18}F	137.37	7.63	—	^{19}F	147.80	7.78	^{19}Ne	143.78	7.57
^{20}Ne	160.65	8.03	19.17	^{21}Ne	167.41	7.97	^{21}Na	163.08	7.77
^{22}Na	174.15	7.92	—	^{23}Na	186.57	8.11	^{23}Mg	181.73	7.90
^{24}Mg	198.26	8.26	28.48	^{25}Mg	205.59	8.22	^{25}Al	200.53	8.02

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The most tightly bound nucleus

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In many textbooks,[1–3] we are told that ^{56}Fe is the nuclide with the greatest binding energy per nucleon, and therefore is the most stable nucleus, the heaviest that can be formed by fusion in normal stars.

But we calculate the binding energy per nucleon BE/A, for a nucleus of mass number A, by the usual formula,

$$BE/A = (1/A)(Zm_H + Nm_n - M_{\text{atom}})c^2, \quad (1)$$

where m_H is the hydrogen atomic mass and m_n is the neutron mass, for the nuclides ^{56}Fe and ^{62}Ni (both are stable) using data from Wapstra and Audi.[4] The results are 8.790 MeV/nucleon for ^{56}Fe and 8.795 MeV/nucleon for ^{62}Ni. The difference,

$$(0.005\ \text{MeV/nucleon})(\approx 60\ \text{nucleons}) = 300\ \text{keV}, \quad (2)$$

is much too large to be accounted for as the binding energy of the two extra electrons in ^{62}Ni over the 26 electrons in ^{56}Fe.

^{56}Fe is readily produced in old stars as the end product of the silicon-burning series of reactions.[5] How, then, do we explain the relative cosmic deficiency of ^{62}Ni compared with ^{56}Fe? In order to be abundant, it is not enough that ^{62}Ni be the most stable nucleus. To be formed by charged-particle fusion (the energy source in normal stars), a reaction must be available to bridge the gap from ^{56}Fe to ^{62}Ni. To accomplish this with a single fusion requires a nuclide with $Z = 2$, $A = 6$. But no such stable nuclide exists. The other possibility is two sequential fusions with ^{3}H, producing first ^{59}Co then ^{62}Ni. However, the ^{3}H nucleus is unstable and is not expected to be present in old stars synthesizing heavy elements. We are aware that there are element-generating processes other than charged-particle fusion, such as processes involving neutron capture, which could generate nickel. However, these processes apparently do not occur in normal stars, but rather in supernovas and post-supernova phases, which we do not address.

We conclude that ^{56}Fe is the end product of normal stellar fusion not because it is the most tightly bound nucleus, which it is not, but that it is in close, but unbridgeable, proximity to ^{62}Ni, which is the most tightly bound nucleus.

[1] Arthur Beiser, *Concepts of Modern Physics* (McGraw-Hill, New York, 1987), 4th ed., p. 421.
[2] Frank Shu, *The Physical Universe* (University Science Books, Mill Valley, CA, 1982), 1st ed., pp. 116–117.
[3] Donald D. Clayton, *Principles of Stellar Evolution and Nucleosynthesis* (McGraw-Hill, New York, 1968), p. 518.
[4] A. H. Wapstra and G. Audi, Nucl. Phys. A **432**, 1 (1985).
[5] William K. Rose, *Astrophysics* (Holt, Rinehart and Winston, New York, 1973), p. 186.

Binding (summary)

- For most nuclei, the binding energy per nucleon is about 8MeV.
- Binding is less for light nuclei (these are mostly surface) but there are peaks for *A* in multiples of 4. (But note that the peak for 8Be is slightly lower than that for 4He.
- The most stable nuclei are in the A~60 mass region
- Light nuclei can gain binding energy per nucleon by fusing; heavy nuclei by fissioning.
- The decrease in binding energy per nucleon for *A*>60 can be ascribed to the repulsion between the (charged) protons in the nucleus: the Coulomb energy grows in proportion to the number of possible pairs of protons in the nucleus Z(Z-1)/2
- The binding energy for massive nuclei (*A*>60) thus grows roughly as *A*; if the nuclear force were long range, one would expect a variation in proportion to the number of possible pairs of nucleons, i.e. as A(A-1)/2. The variation as *A* suggests that the force is *saturated*; the effect of the interaction is only felt in a neighborhood of the nucleon.

Nuclear liquid drop

The semi-empirical mass formula, based **on the liquid drop model**, considers five contributions to the binding energy (Bethe-Weizacker 1935/36)

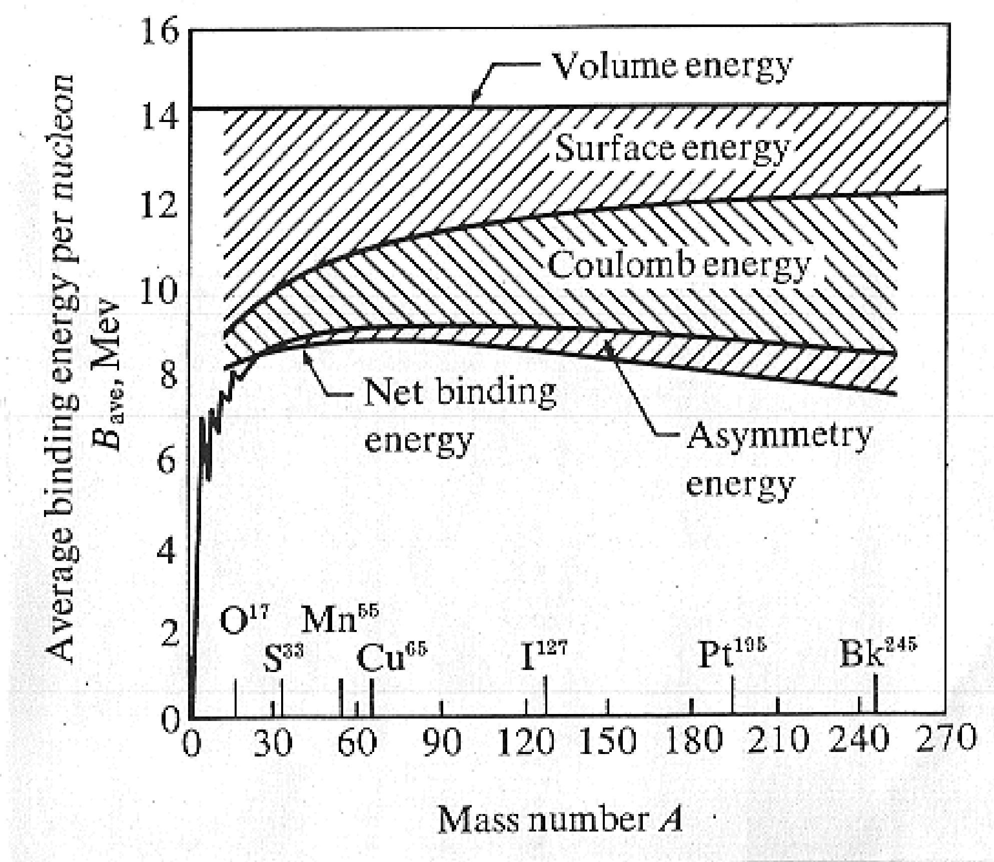
$$B = a_{vol}A - a_{surf}A^{2/3} - a_{sym}\frac{(N-Z)^2}{A} - a_C\frac{Z^2}{A^{1/3}} - \delta(A)$$

15.68   -18.56   -28.1   -0.717

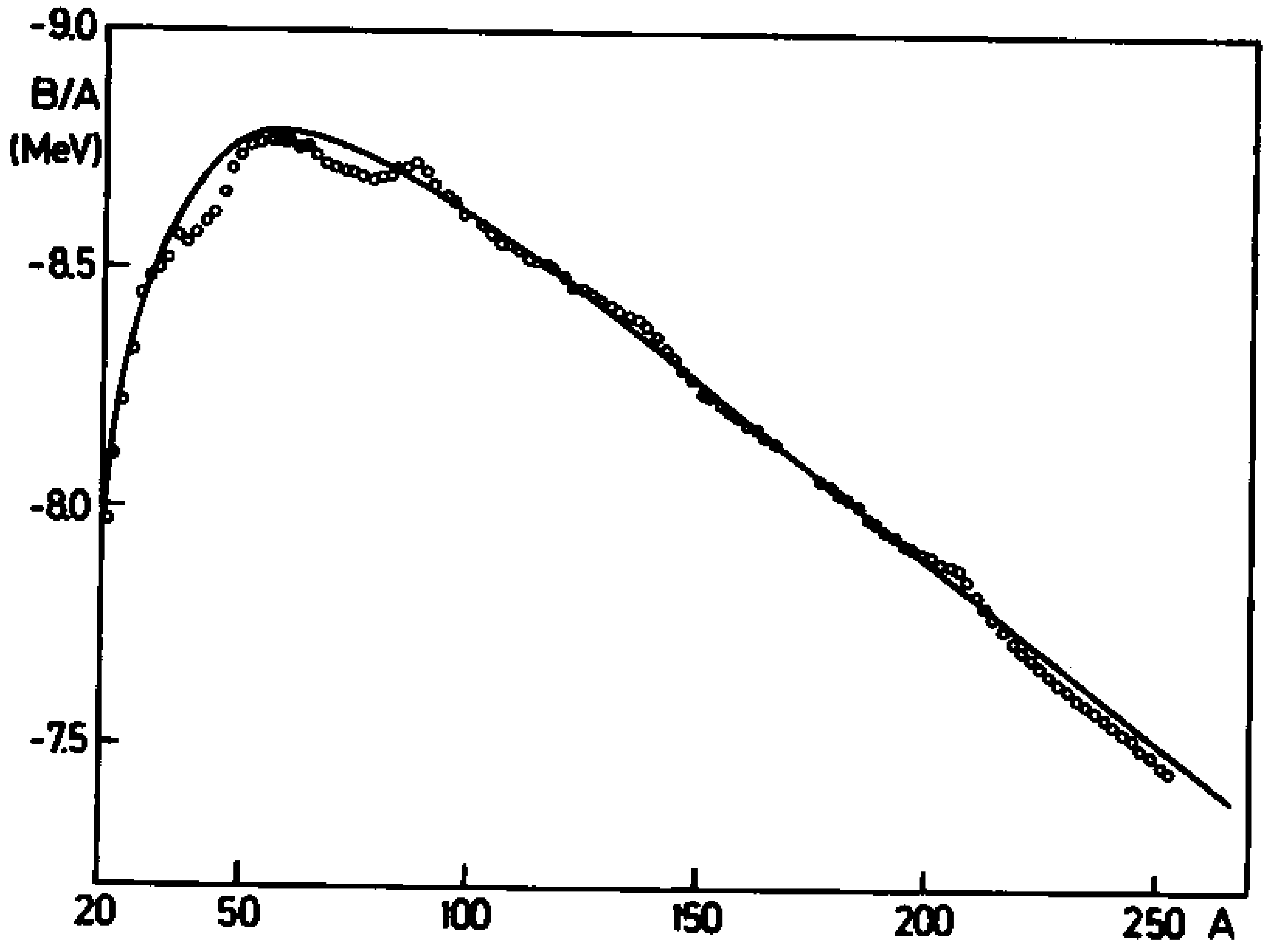
pairing term

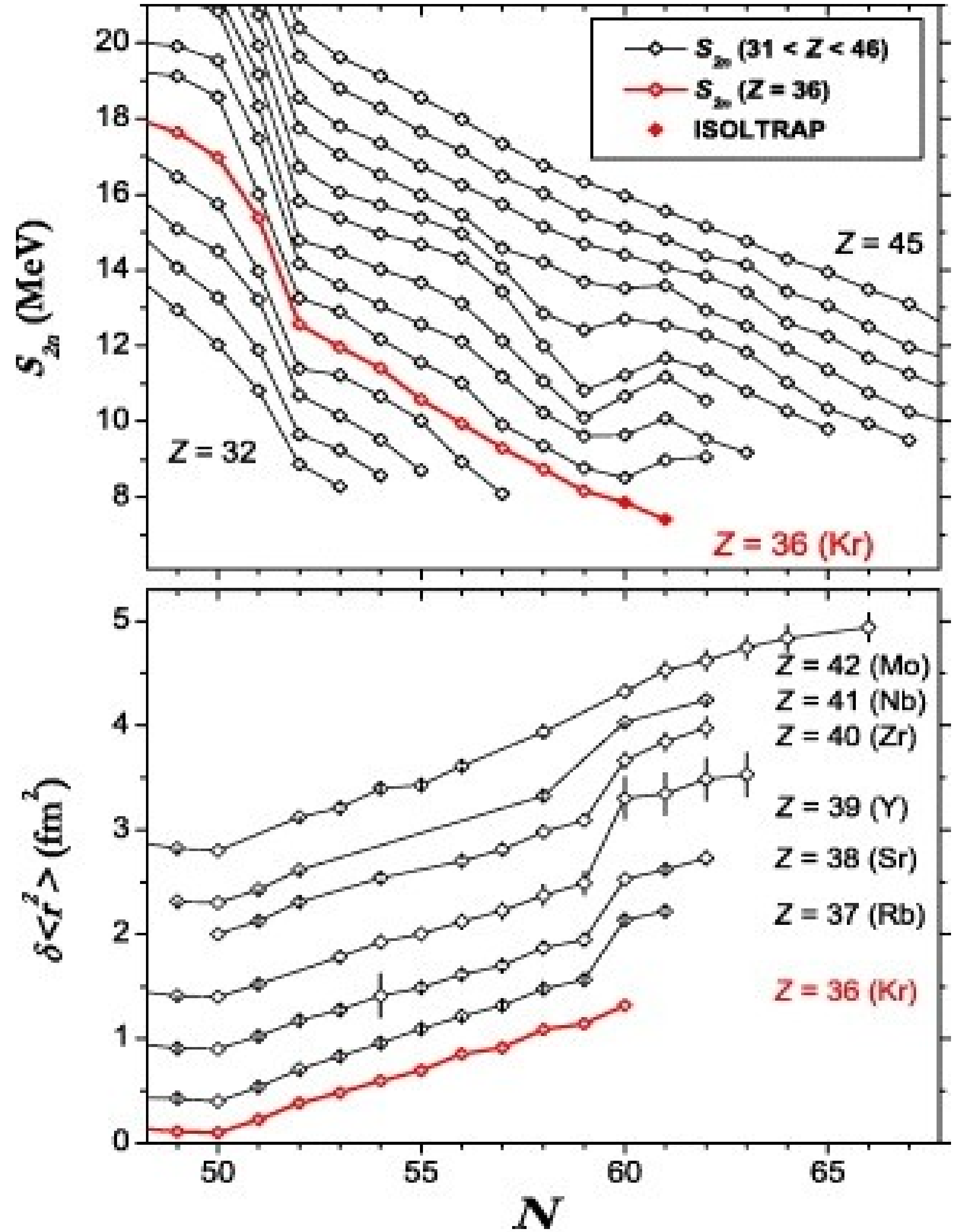
$$\delta(A) = \begin{cases} -34A^{-3/4} & \text{for even - even} \\ 0 & \text{for even - odd} \\ 34A^{-3/4} & \text{for odd - odd} \end{cases}$$

Leptodermous expansion



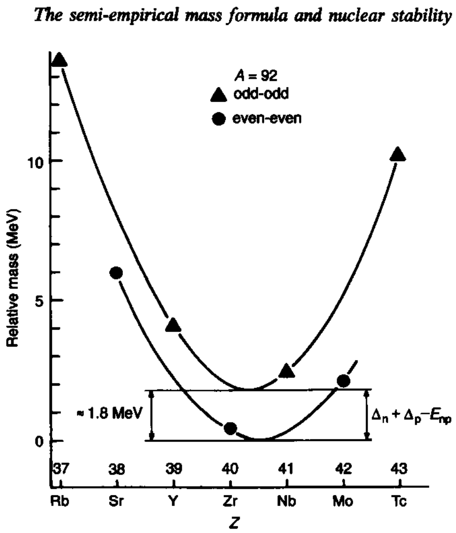
The semi-empirical mass formula, based **on the liquid drop model**, compared to the data

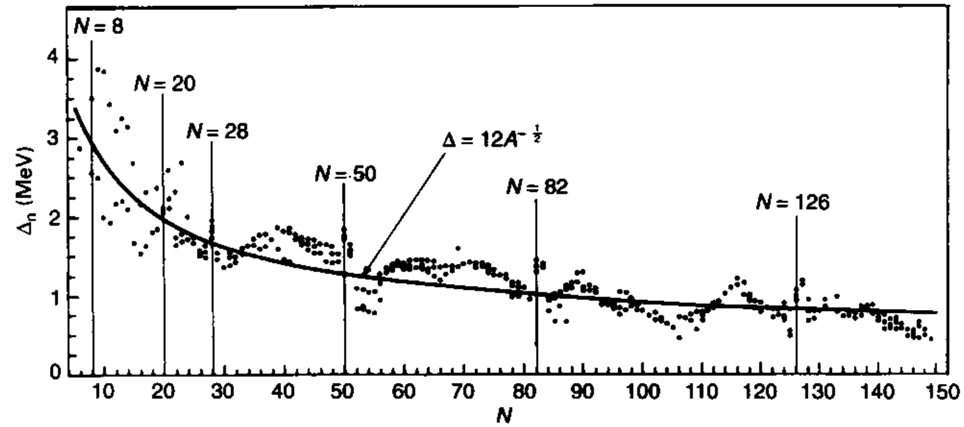


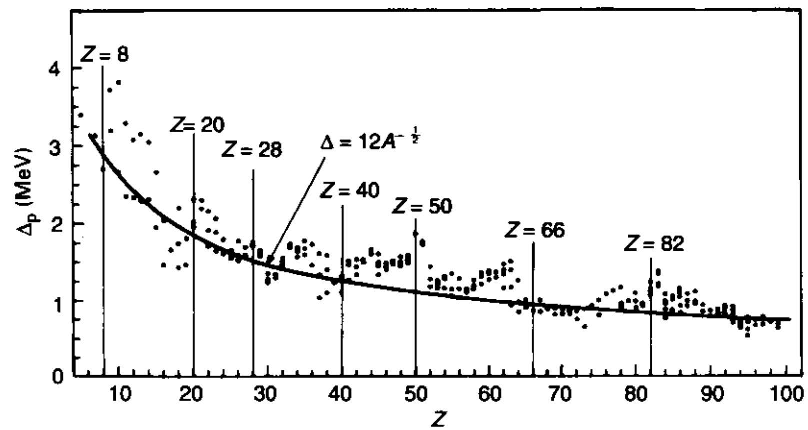


S_{2n} (31 < Z < 46)
S_{2n} (Z = 36)
ISOLTRAP
Z = 45
Z = 32
Z = 36 (Kr)
S_{2n} (MeV)
Z = 42 (Mo)
Z = 41 (Nb)
Z = 40 (Zr)
Z = 39 (Y)
Z = 38 (Sr)
Z = 37 (Rb)
Z = 36 (Kr)
$\delta<r^2>$ (fm^2)
N

Pairing energy





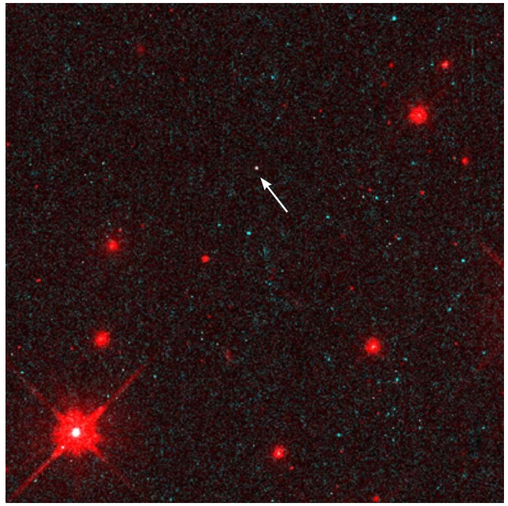


$$\Delta_n = B(N,Z) - \frac{B(N+1,Z) + B(N-1,Z)}{2}$$

$$\Delta_p = B(N,Z) - \frac{B(N,Z+1) + B(N,Z-1)}{2}$$

A common phenomenon in mesoscopic systems!

Neutron star, a bold explanation



A lone neutron star, as seen by NASA's Hubble Space Telescope

$$B = a_{vol}A - a_{surf}A^{2/3} - a_{sym}\frac{(N-Z)^2}{A} - a_C\frac{Z^2}{A^{1/3}} - \delta(A) + \frac{3}{5}\frac{G}{r_0 A^{1/3}}M^2$$

Let us consider a giant neutron-rich nucleus. We neglect Coulomb, surface, and pairing energies. Can such an object exist?

$$B = a_{vol}A - a_{sym}A + \frac{3}{5}\frac{G}{r_0 A^{1/3}}(m_n A)^2 = 0$$

limiting condition

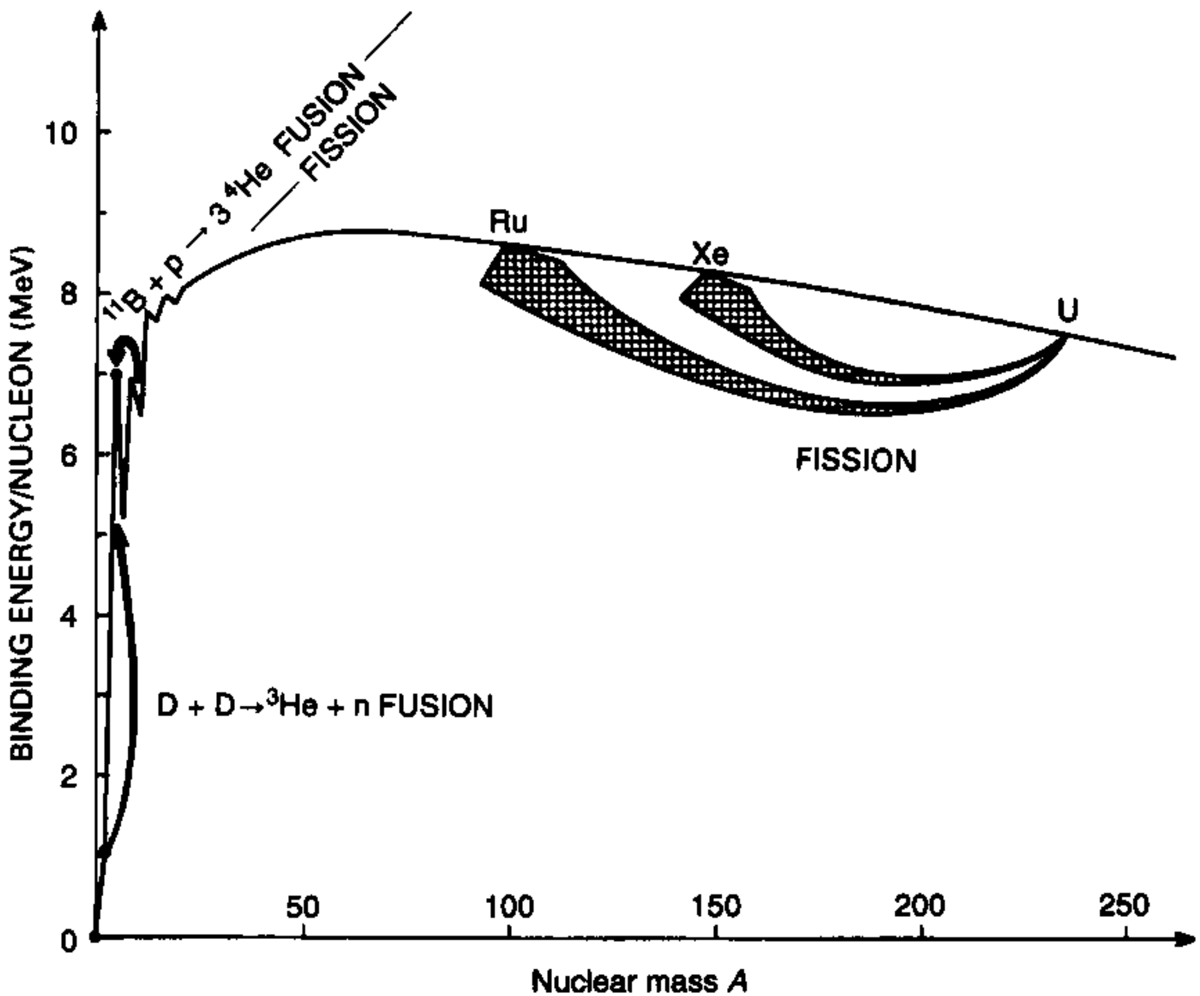
$$\frac{3}{5}\frac{G}{r_0}m_n^2 A^{2/3} = 7.5\,\mathrm{MeV} \Rightarrow A \cong 5\times10^{55},\ R \cong 4.3\,\mathrm{km},\ M \cong 0.045 M_\odot$$

More precise calculations give M(min) of about 0.1 solar mass ($M_\odot$). Must neutron stars have

$$R \cong 10\,\mathrm{km},\ M \cong 1.4\,M_\odot$$

Fission

- All elements heavier than A=110-120 are fission unstable!
- But… the fission process is fairly unimportant for nuclei with A<230. Why?



Deformed liquid drop (Bohr & Wheeler, 1939)

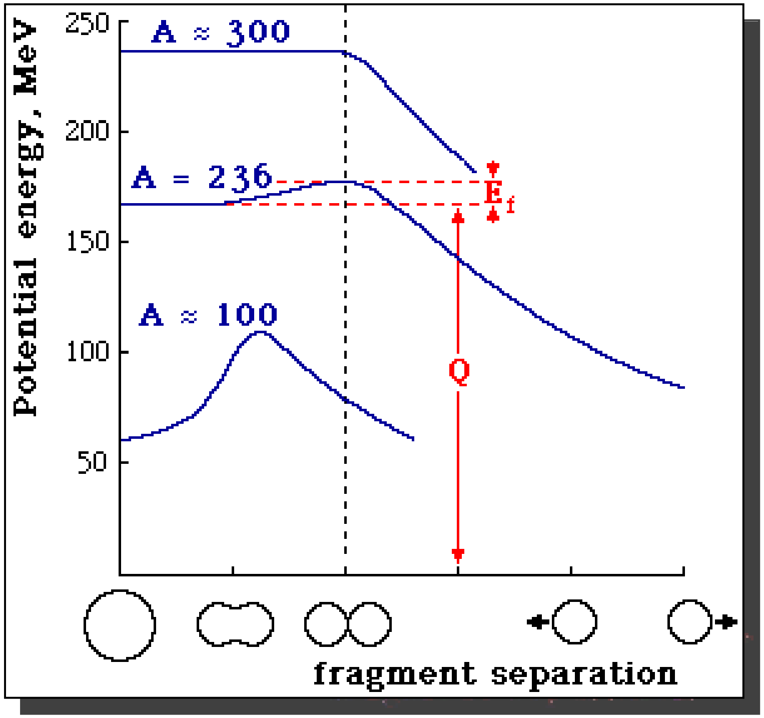
$$E_{LDM}(def) = E_S(0)\left[B_S(def) - 1 + 2x\left(B_C(def) - 1\right)\right]$$

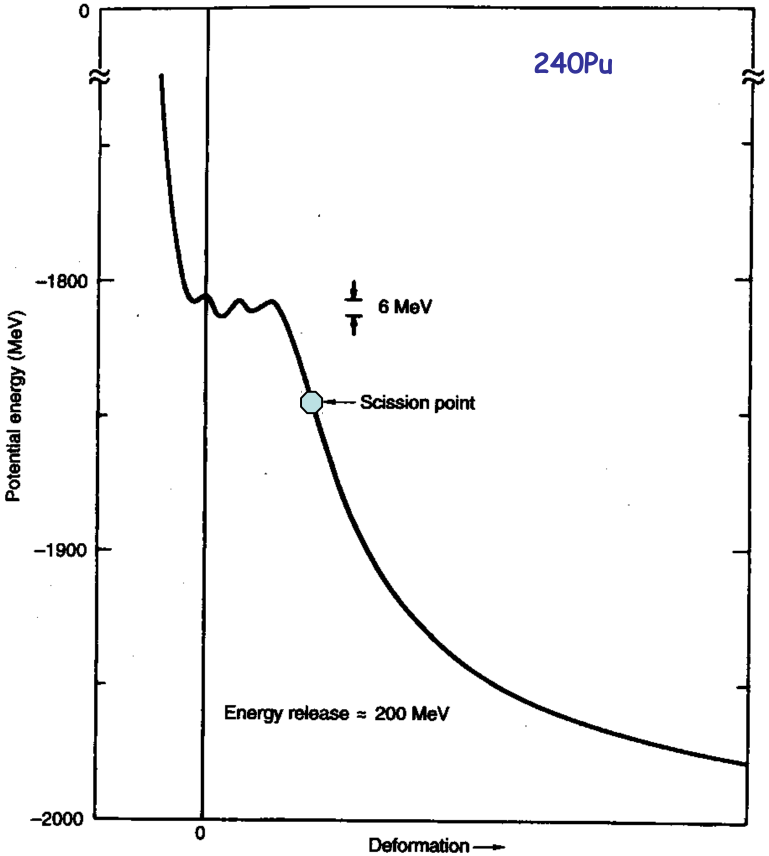
$$B_S(def) = \frac{E_S(def)}{E_S(0)}, \quad B_C(def) = \frac{E_C(def)}{E_C(0)}$$

$$x = \frac{E_C(0)}{2E_S(0)} = \frac{Z^2/A}{\left(Z^2/A\right)_{crit}} \approx \frac{Z^2}{50A}$$

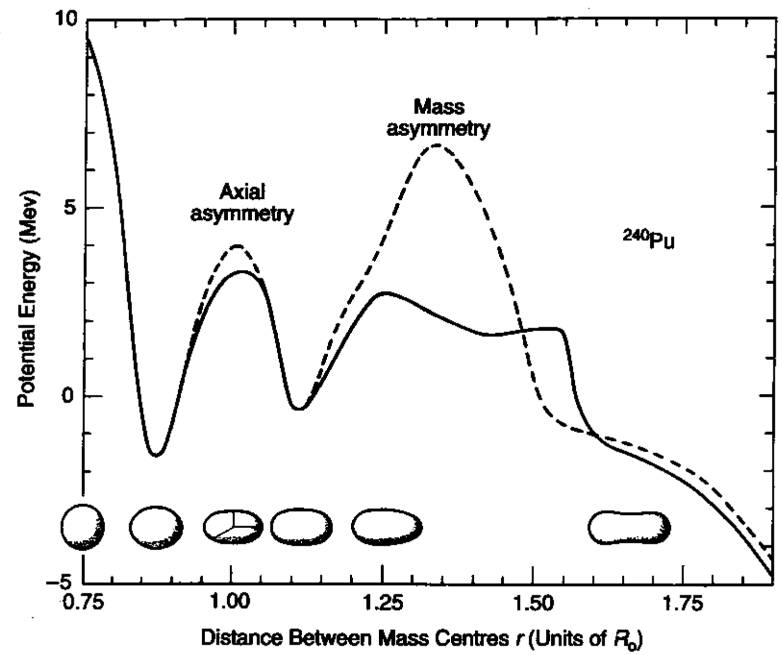
fissibility parameter

The classical droplet stays stable and spherical for x<1.
For x>1, it fissions immediately.
For 238U, x=0.8.





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



Realistic calculations

Nuclear shapes

The first evidence for a non-spherical nuclear shape came from the observation of a quadrupole component in the hyperfine structure of optical spectra. The analysis showed that the electric quadrupole moments of the nuclei concerned were more than an order of magnitude greater than the maximum value that could be attributed to a single proton and suggested a deformation of the nucleus as a whole.

- Schüler, H., and Schmidt, Th., Z. Physik 94, 457 (1935)
- Casimir, H. B. G., On the Interaction Between Atomic Nuclei and Electrons, Prize Essay, Taylor's Tweede Genootschap, Haarlem (1936)

The question of whether nuclei can rotate became an issue already in the very early days of nuclear spectroscopy

- Thibaud, J., Comptes rendus 191, 656 (1930)
- Teller, E., and Wheeler, J. A., Phys. Rev. 53, 778 (1938)
- Bohr, N., Nature 137, 344 (1936)
- Bohr, N., and Kalckar, F., Mat. Fys. Medd. Dan. Vid. Selsk. 14, no, 10 (1937)

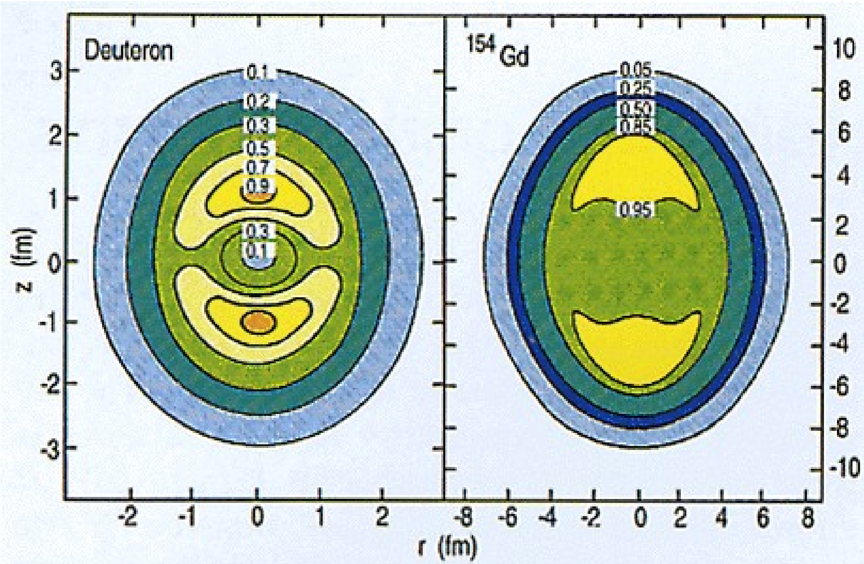
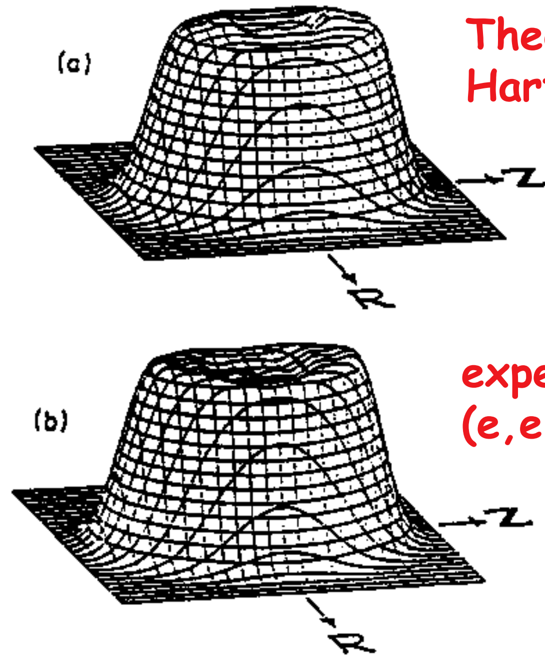


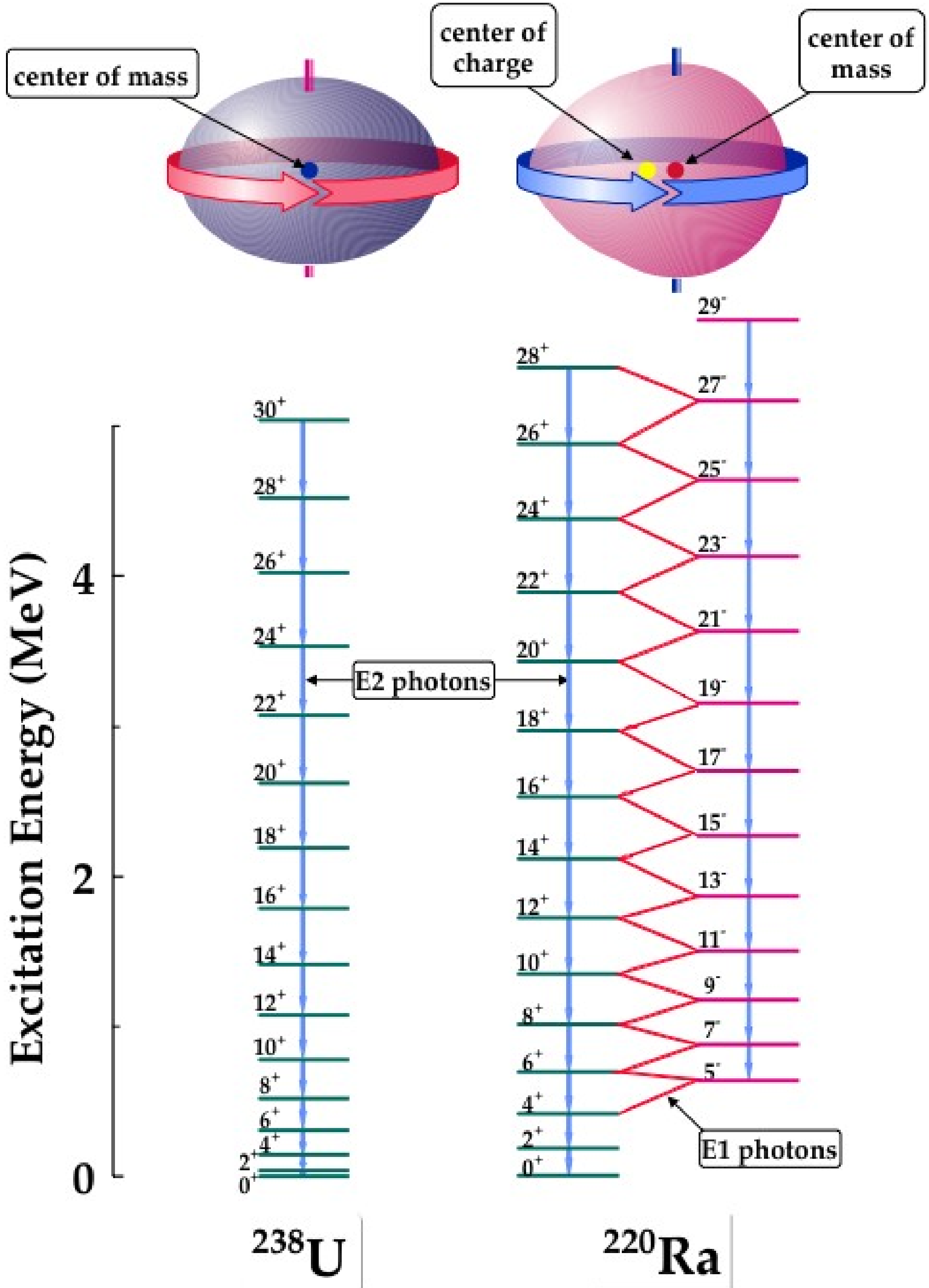
Figure I.1: Matter density contours for the deuteron (left) and the ^{154}Gd nucleus (right) deduced from experiment.



Theory: Hartree-Fock

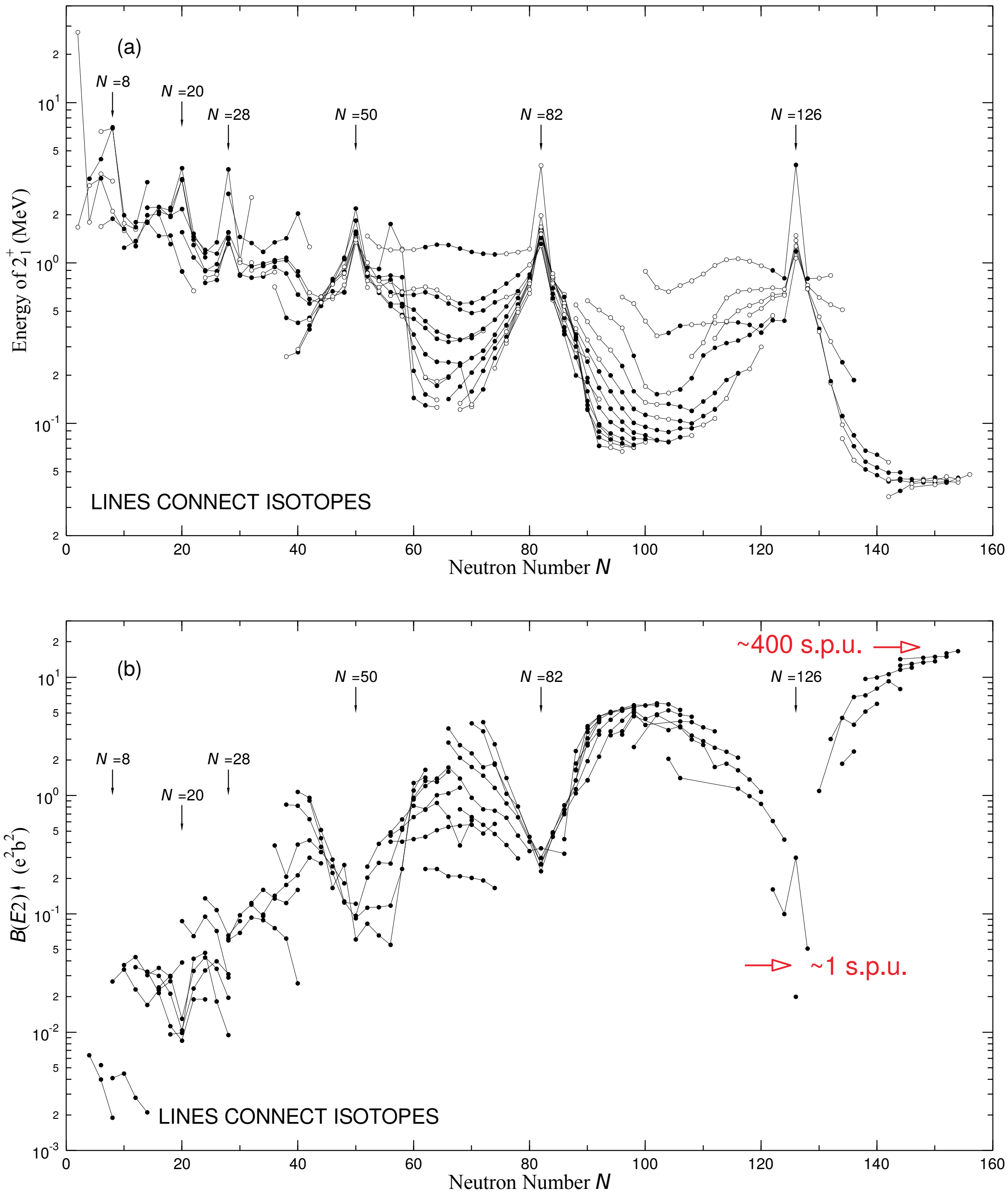
experiment: (e,e') Bates

Shape of a charge distribution in ^{154}Gd

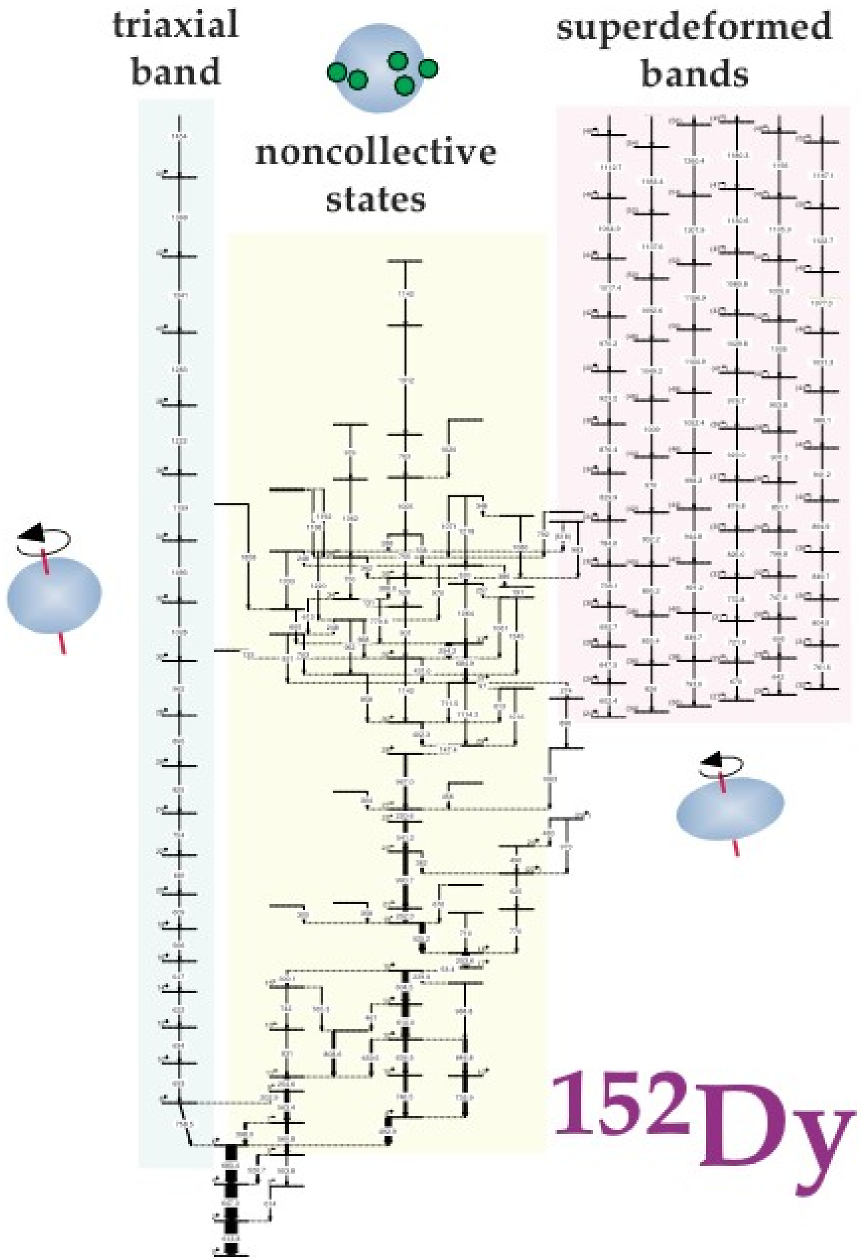


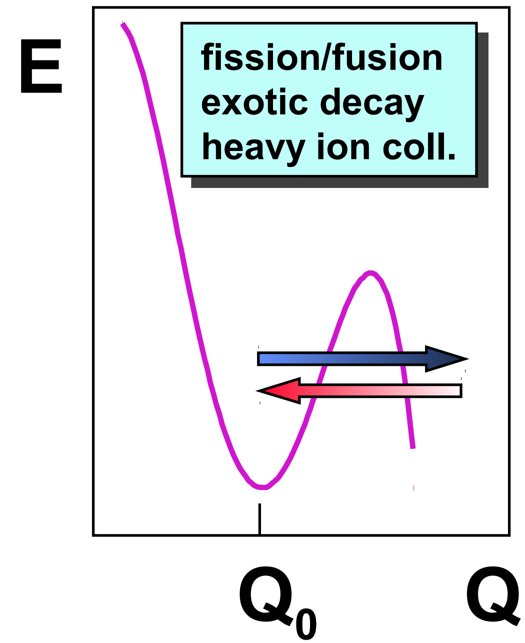
center of mass
center of charge
center of mass
Excitation Energy (MeV)
0
2
4
E2 photons
E1 photons
30+
28+
26+
24+
22+
20+
18+
16+
14+
12+
10+
8+
6+
4+
2+
0+
29-
27-
25-
23-
21-
19-
17-
15-
13-
11-
9-
7-
5-
238U
220Ra

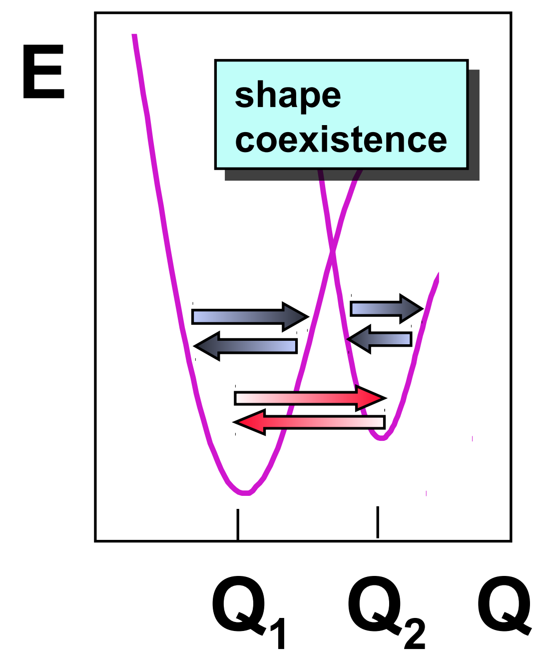
S. Raman et al., Atomic Data & Nuclear Data Tables 78, 1



Coexistence of collective and noncollective motion







Nucleonic Shells

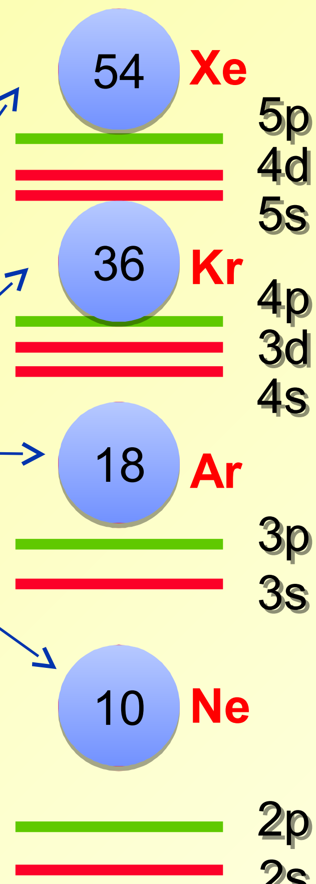
1912

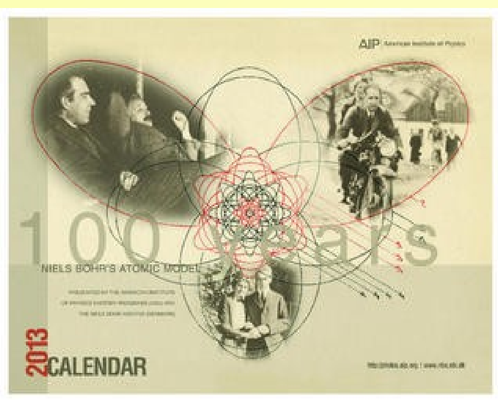
Nobel Prize 1922

Bohr's picture still serves as an elucidation of the physical and chemical properties of the elements.

electronic shells of the atom

noble gases (closed shells)



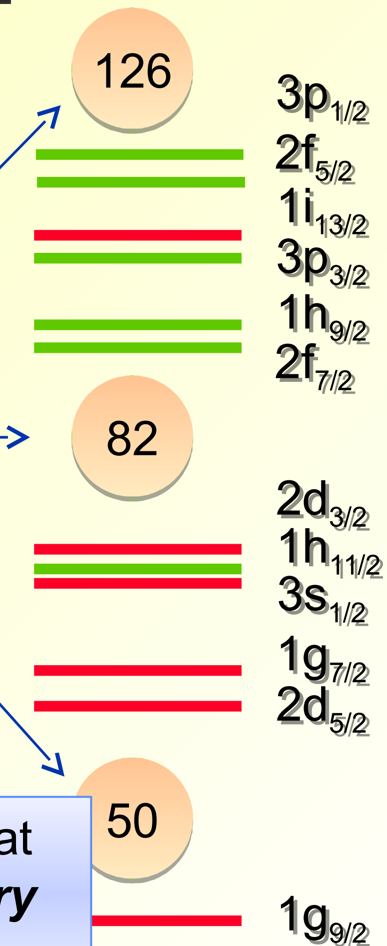


1949

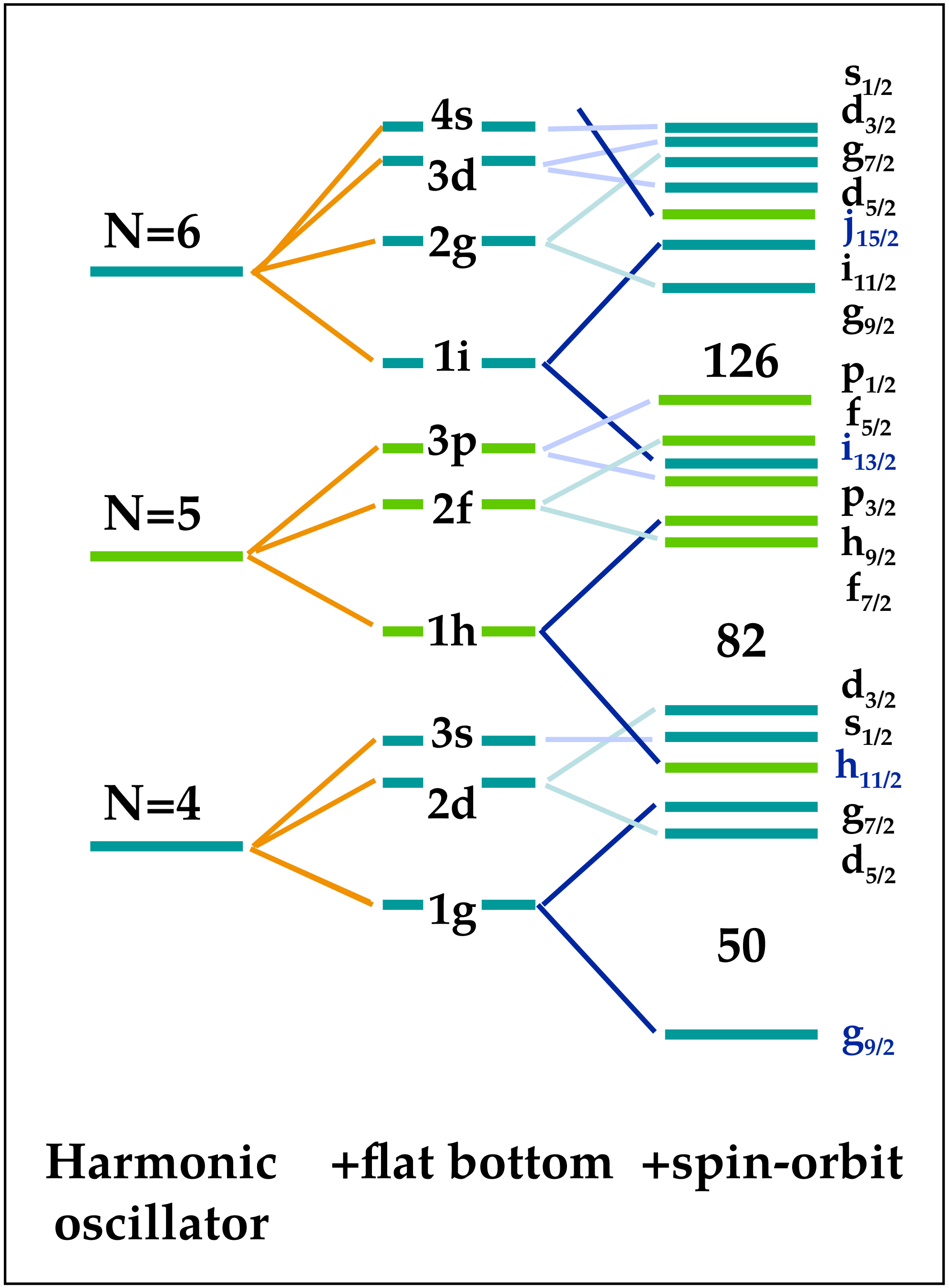
Nobel Prize 1963

nucleonic shells of the nucleus

magic nuclei (closed shells)

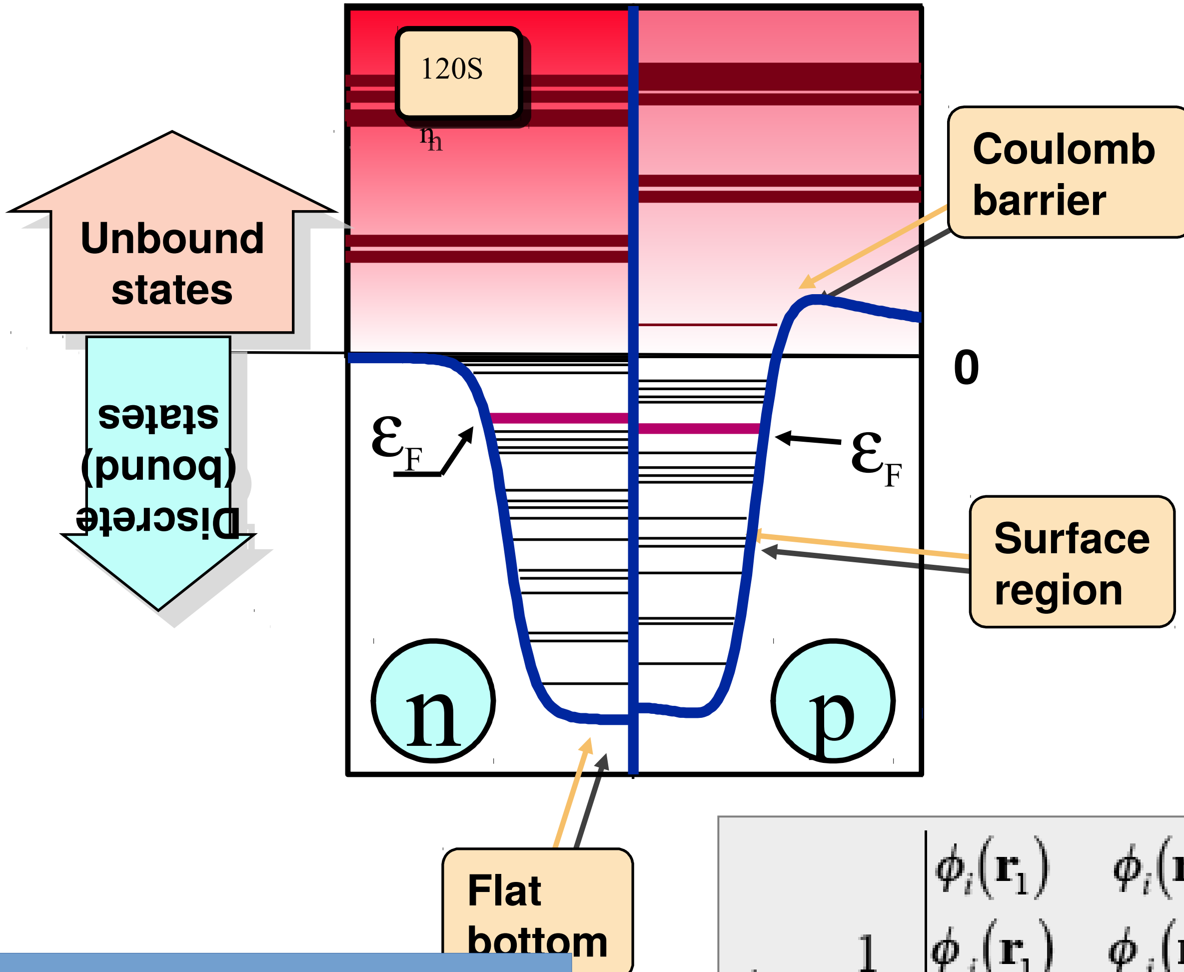


We know now that this picture is ***very*** incomplete…



N=6
N=5
N=4
4s
3d
2g
1i
3p
2f
1h
3s
2d
1g
126
82
50
s1/2
d3/2
g7/2
d5/2
j15/2
i11/2
g9/2
p1/2
f5/2
i13/2
p3/2
h9/2
f7/2
d3/2
s1/2
h11/2
g7/2
d5/2
g9/2
Harmonic oscillator
+flat bottom
+spin-orbit

Average one-body Hamiltonian



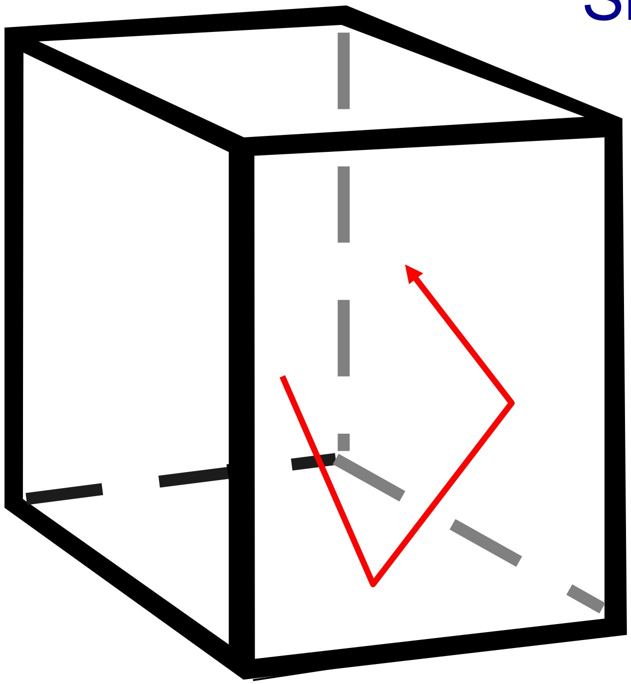
$$\hat{H}_0 = \sum_{i=1}^{A} h_i, \quad h_i = -\frac{\hbar^2}{2M}\nabla_i^2 + V_i$$

$$h_i \phi_k(i) = \varepsilon_k \phi_k(i)$$

$$\phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \cdots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \cdots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^+ \ldots a_j^+ a_i^+ |0\rangle$$

Shell effects and classical periodic orbits



$$\hat{H} = \hat{H}_1 + \hat{V}_2 \cdots$$

$$\hat{H}_1 = \sum_{i=1}^{A} \hat{h}_i = \sum_{i=1}^{A} \left(\frac{\hat{p}_i^2}{2m_i} + \hat{V}_i \right)$$

$$\hat{h}\varphi_\alpha = \epsilon_\alpha \varphi_\alpha$$

Shells

One-body field
- Not external (self-bound)
- Hartree-Fock

- Product (independent-particle) state is often an excellent starting point
- Localized densities, currents, fields
- Typical time scale: babyseconds (10^{-22}s)
- Closed orbits and s.p. quantum numbers

But…

- Nuclear box is not rigid: motion is seldom adiabatic
- The walls can be transparent
- In weakly-bound nuclei, residual interaction may dominate the picture: shell-model basis does not govern the physics!
- Shell-model basis not unique (many equivalent Hartree-Fock fields)

Shell effects and classical periodic orbits

Balian & Bloch, Ann. Phys. **69** (1971) 76
Bohr & Mottelson, Nuclear Structure vol 2 (1975)
Strutinski & Magner, Sov. J. Part. Nucl. **7** (1976) 138

Trace formula, Gutzwiller, J. Math. Phys. 8 (1967) 1979

$$g(\varepsilon) = \tilde{g}(\varepsilon) + \sum_{\gamma} A_{\gamma}(\varepsilon) \cos\left[S_{\gamma}(\varepsilon) / \hbar - \alpha_{\gamma} \right]$$

$$S_{\gamma}(\varepsilon) = \oint_{\gamma} p\,dq$$

The action integral for the periodic orbit γ

$$\varepsilon(n_1, n_2, n_3) = \varepsilon(n_{10}, n_{20}, n_{30}) + (n_1 - n_{10}) \left(\frac{\partial \varepsilon}{\partial n_1} \right)_0 + (n_2 - n_{20}) \left(\frac{\partial \varepsilon}{\partial n_2} \right)_0 + (n_3 - n_{30}) \left(\frac{\partial \varepsilon}{\partial n_3} \right)_0 + \ldots$$

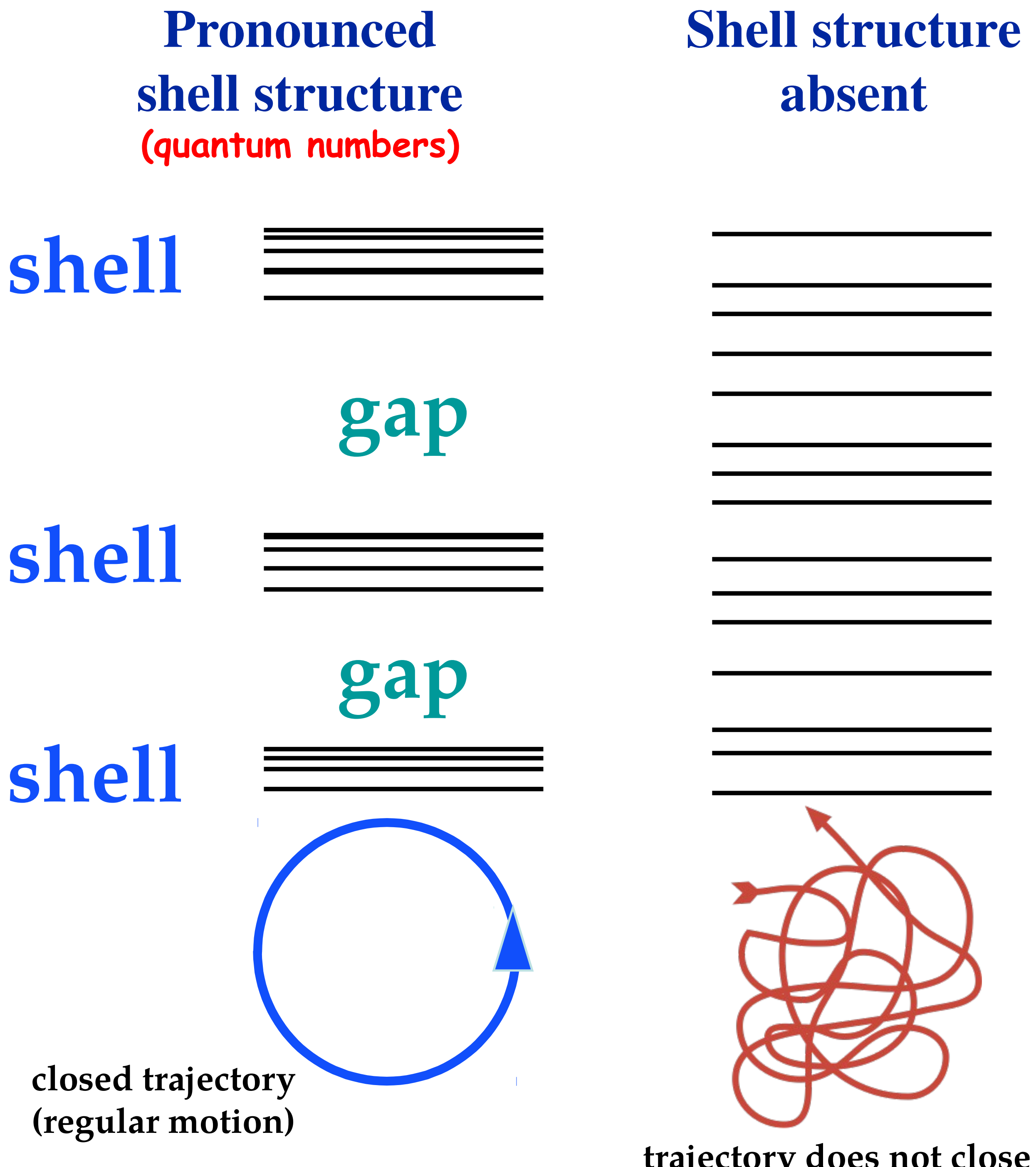
$$\left(\frac{\partial \varepsilon}{\partial n_1} \right)_0 : \left(\frac{\partial \varepsilon}{\partial n_2} \right)_0 : \left(\frac{\partial \varepsilon}{\partial n_3} \right)_0 = k_1 : k_2 : k_3$$

on for
ructure

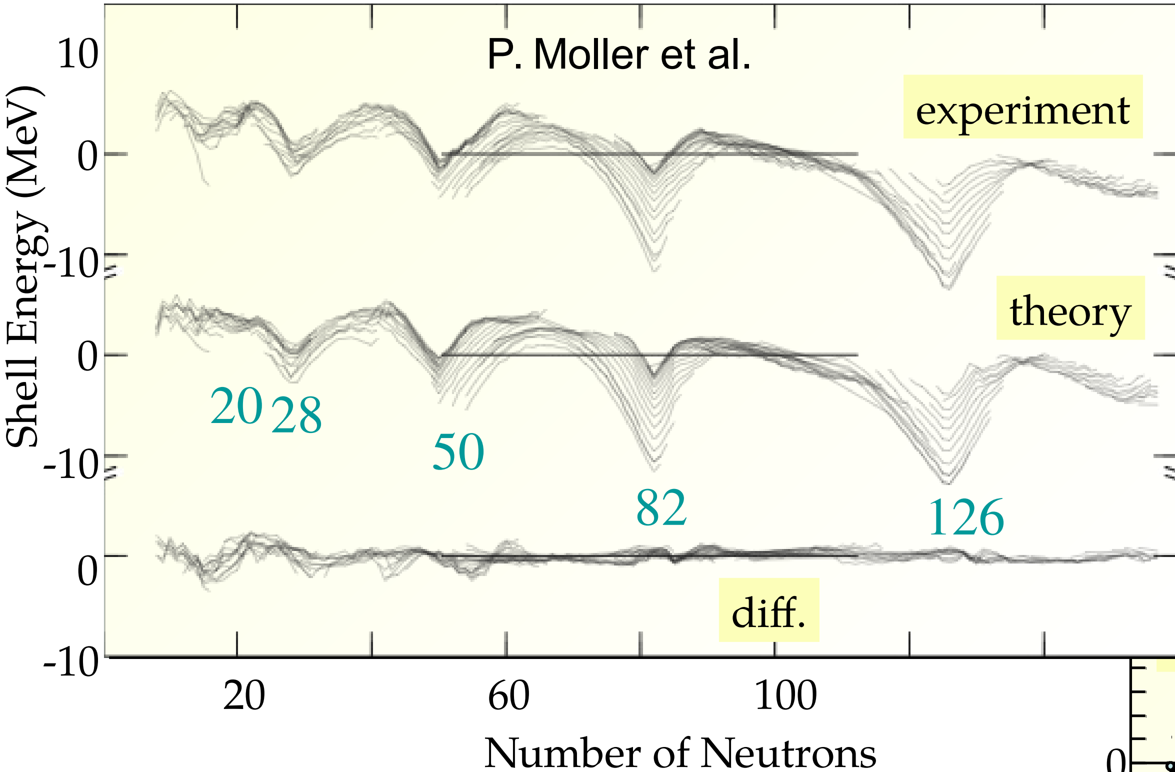
$$N_{shell} = k_1 n_1 + k_2 n_2 + k_3 n_3, \qquad \hbar\omega_{shell} = \frac{1}{k_i} \left(\frac{\partial \varepsilon}{\partial n_i} \right)_0$$

Principal shell
quantum number

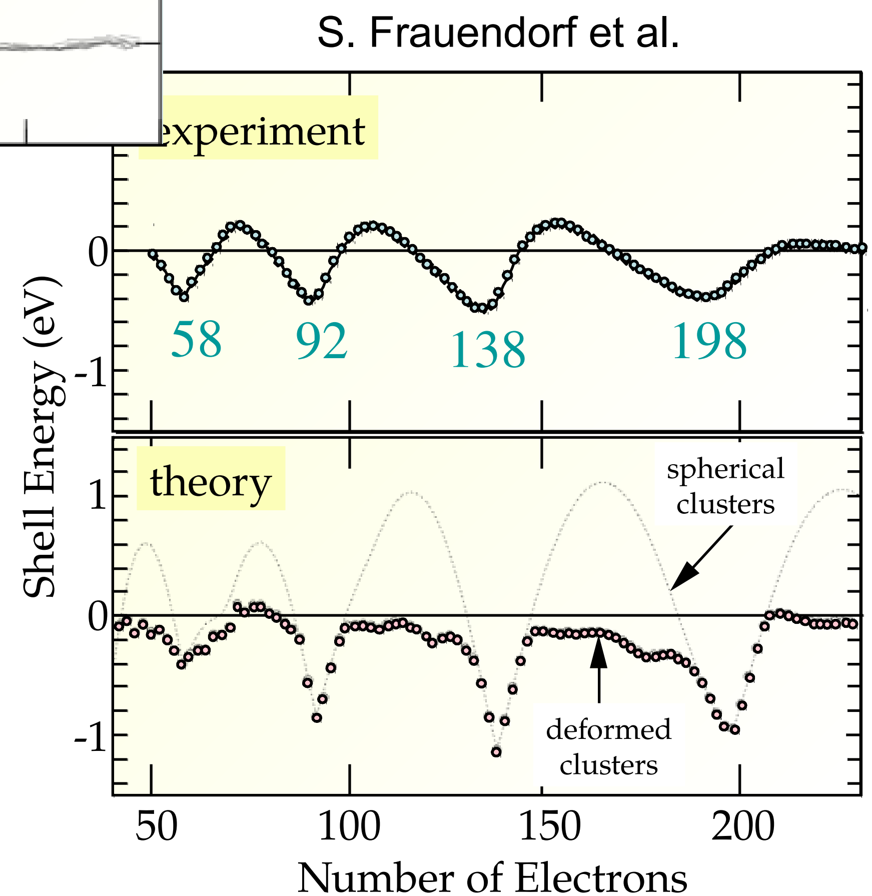
Distance between shells
(frequency of classical orbit)


Pronounced shell structure
(quantum numbers)
Shell structure absent
shell
gap
shell
gap
shell
closed trajectory
(regular motion)
trajectory does not close

Shells in mesoscopic systems



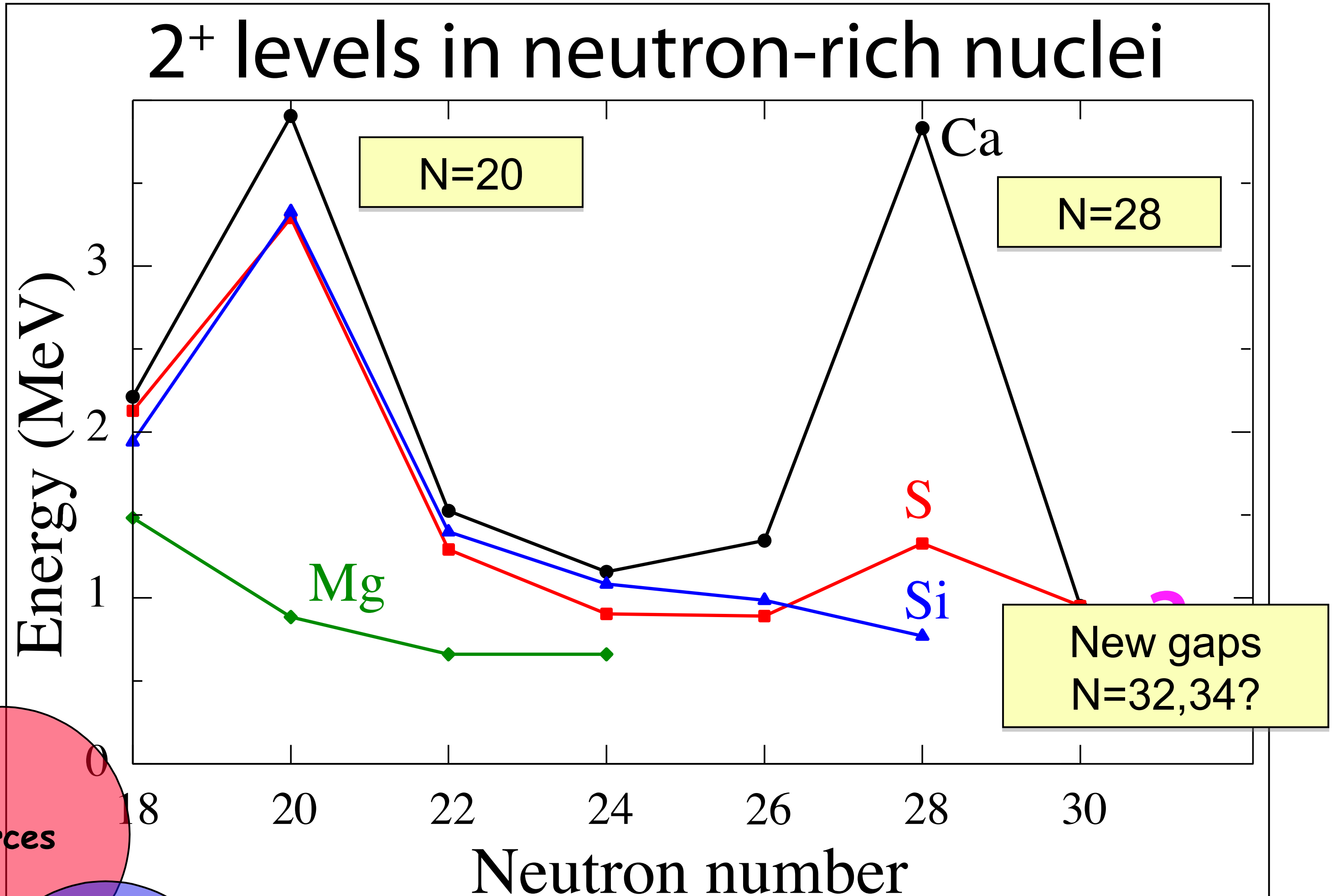
Nuclei

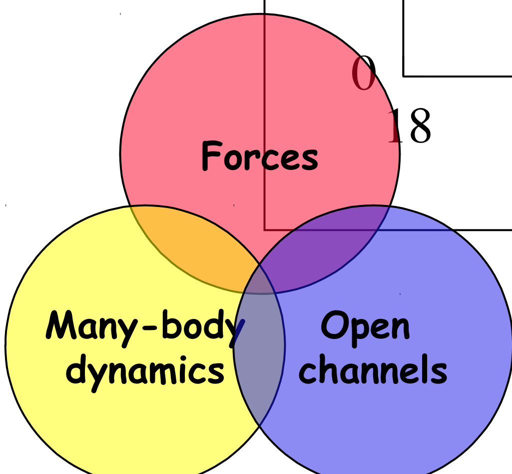


Sodium Clusters

- Jahn-Teller Effect (1936)
- Symmetry breaking and deformed (HF) mean-field

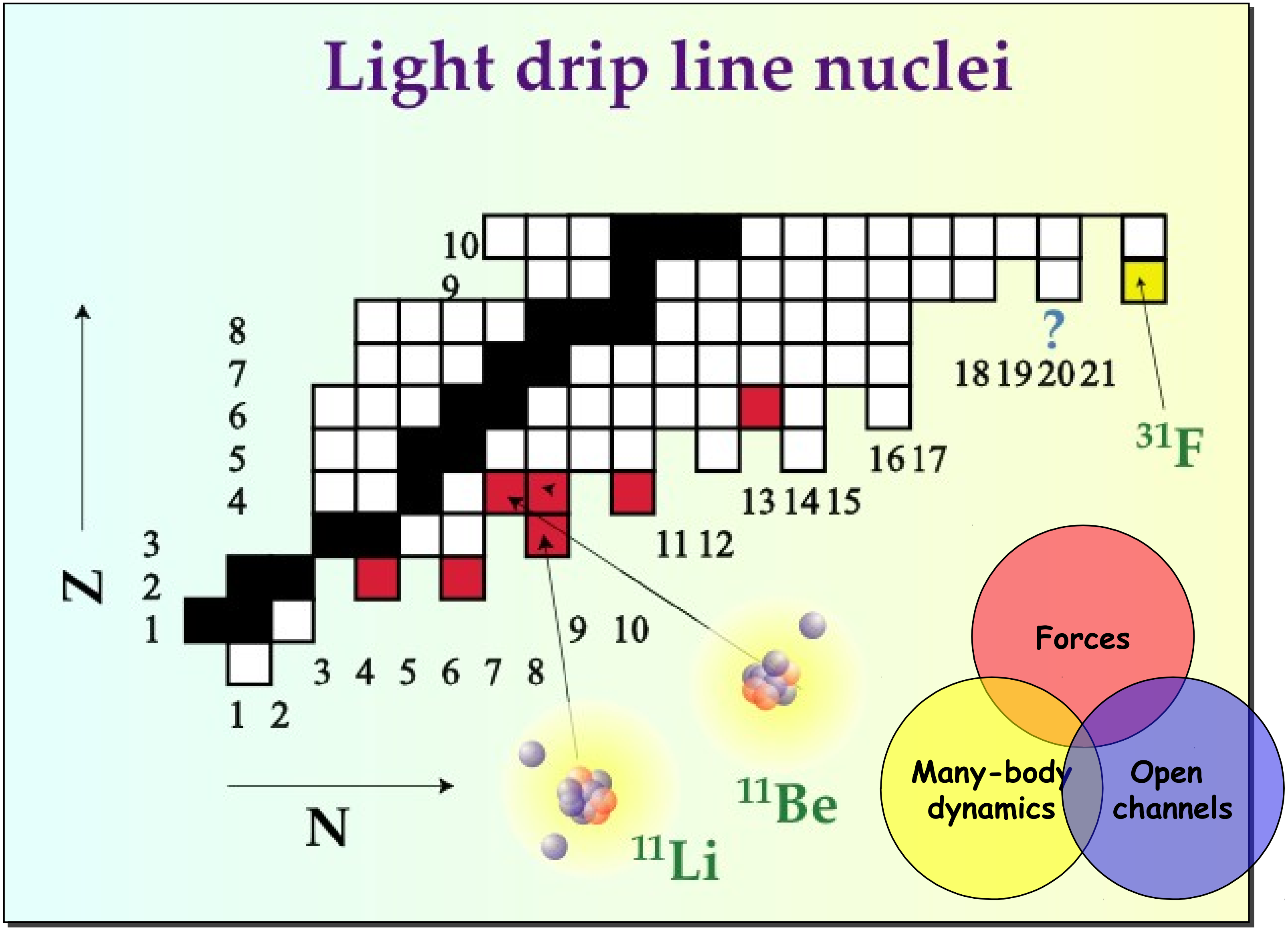
Revising textbooks on nuclear shell model…





from A. Gade

Living on the edge… Correlations and openness

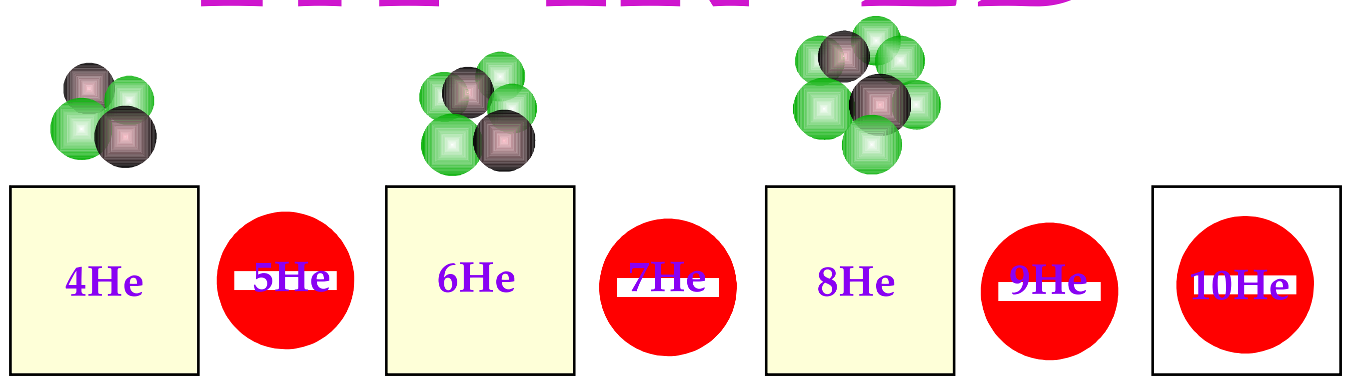


Neutron Drip line nuclei

HUGE

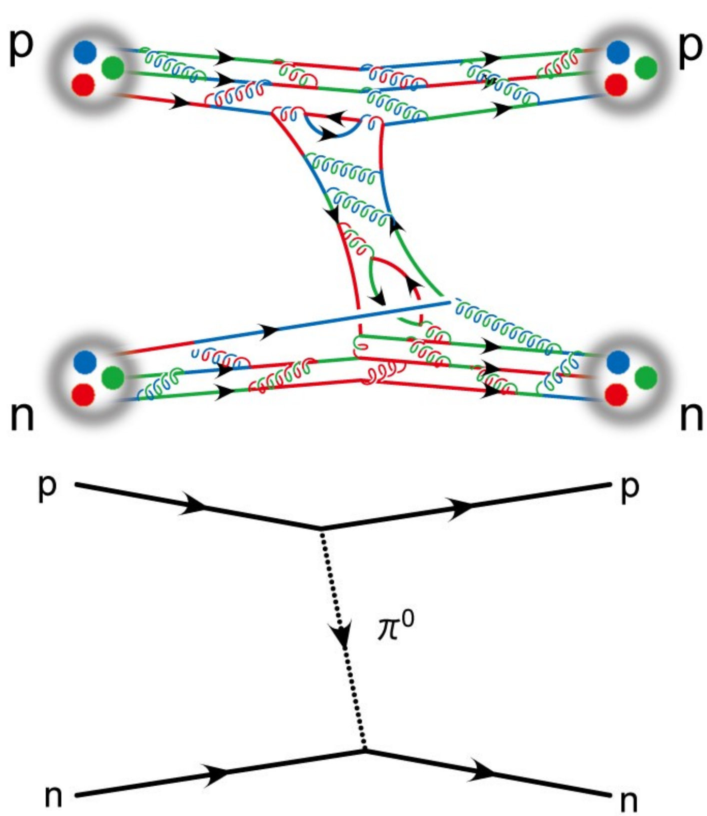
D i f f u s e d

PA IR ED



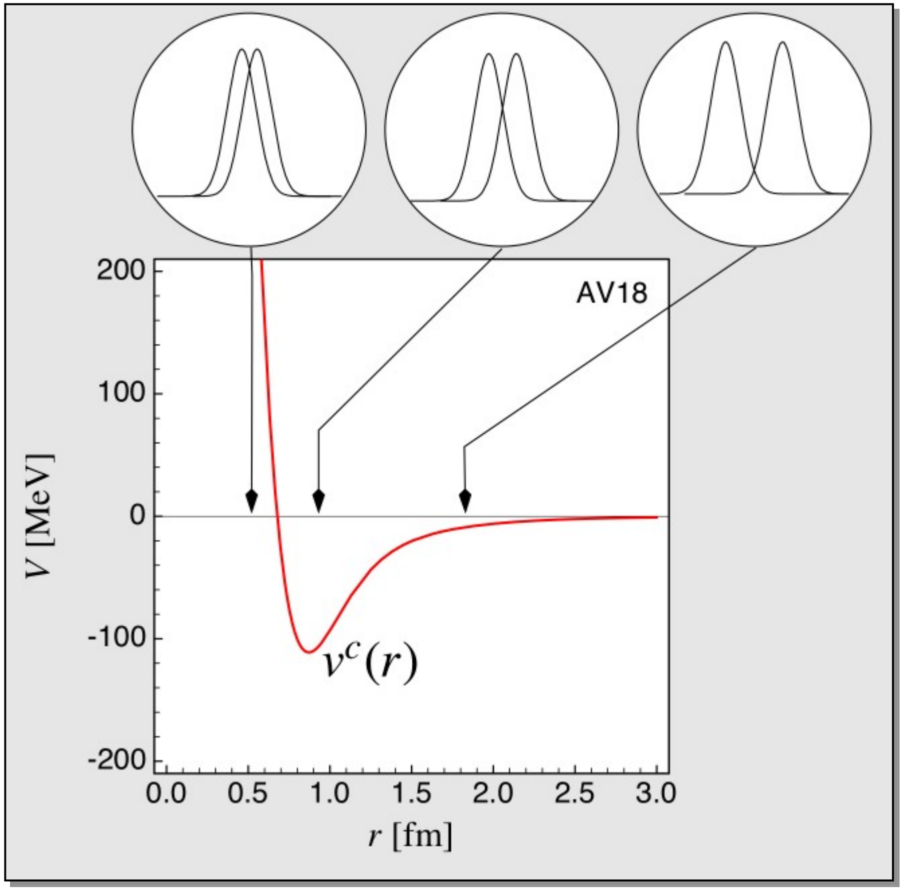
The Force

Nuclear force

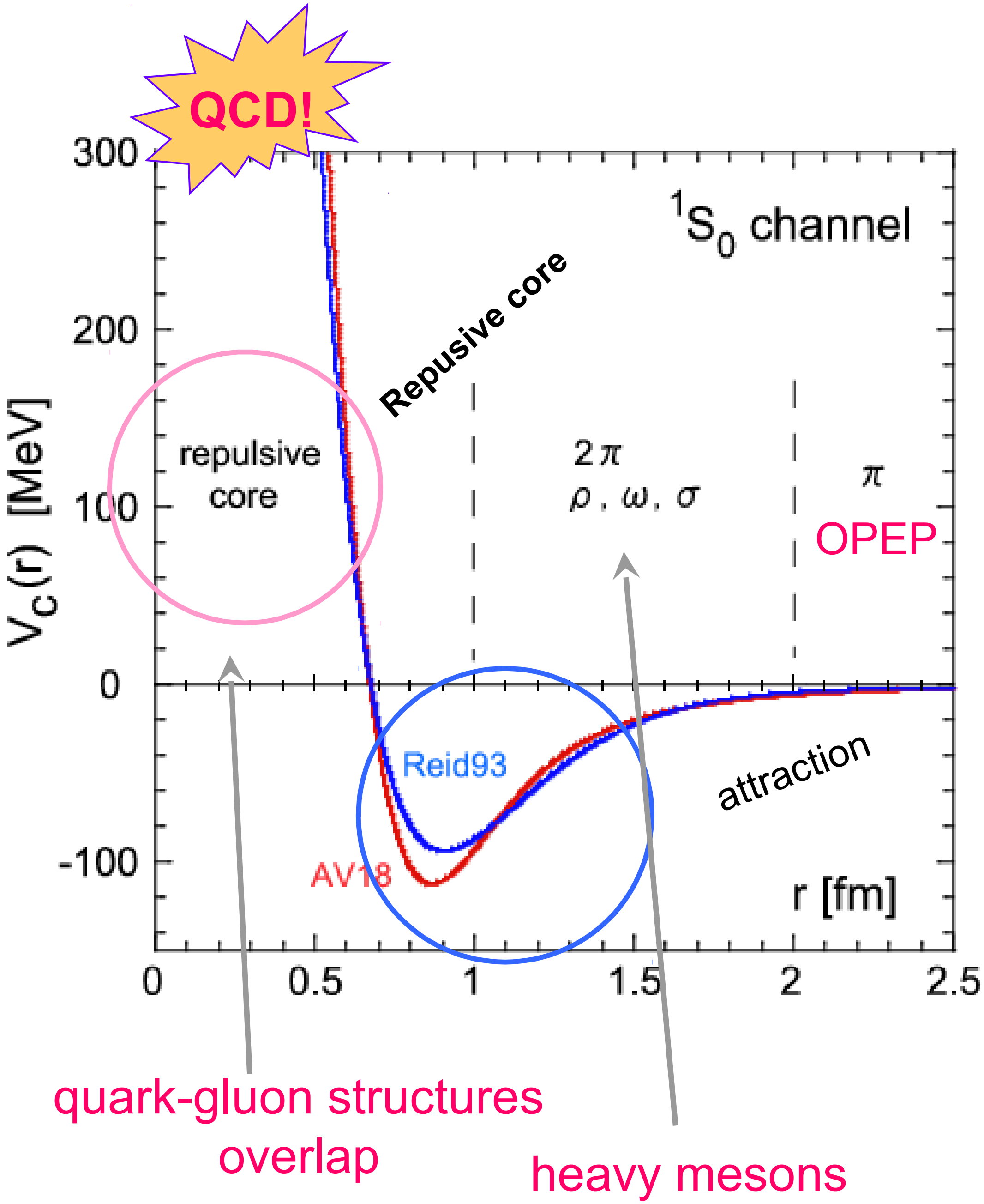


- Nucleon r.m.s. radius ~0.86 fm
- Comparable with interaction range
- Half-density overlap at max. attarction
- V_{NN} not fundamental (more like inter-molecular van der Waals interaction)
- Since nucleons are composite objects, three-and higher-body forces are expected.

A realistic nuclear force force: schematic view



Nucleon-Nucleon interaction (qualitative analysis)



There are infinitely many equivalent nuclear potentials!

$$\hat{H}\Psi = E\Psi$$

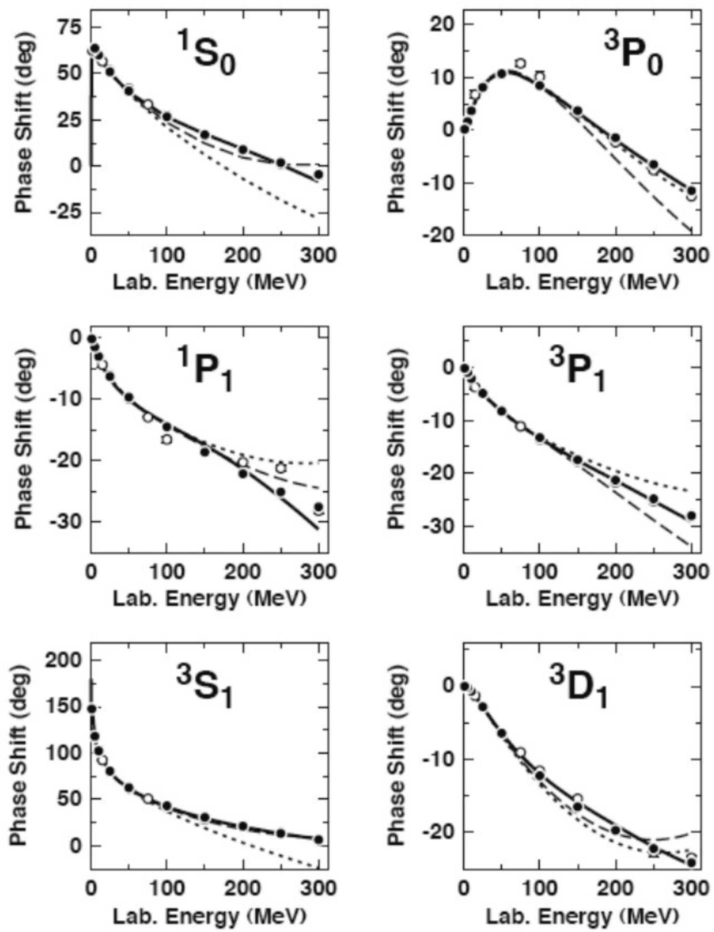
$$(\hat{U}\hat{H}\hat{U}^{-1})\hat{U}\Psi = E\hat{U}\Psi$$

Reid93 is from
V.G.J.Stoks et al., PRC**49**, 2950 (1994).

AV16 is from
R.B.Wiringa et al., PRC**51**, 38 (1995).

nucleon-nucleon interactions

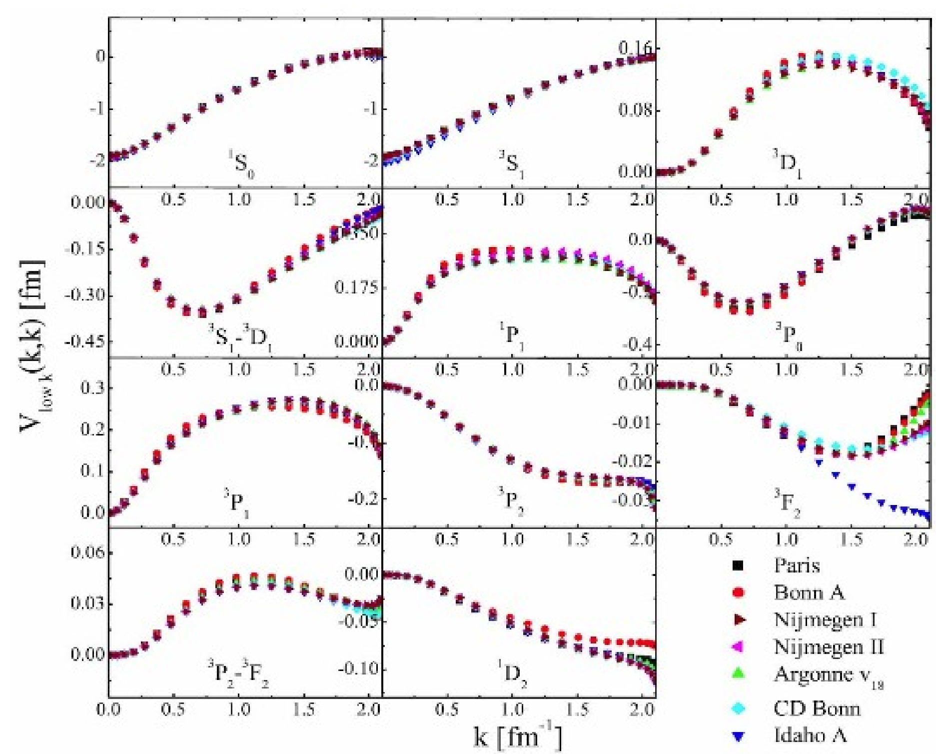
Effective-field theory potentials



N3LO: Entem et al., PRC68, 041001 (2003)
Epelbaum, Meissner, et al.

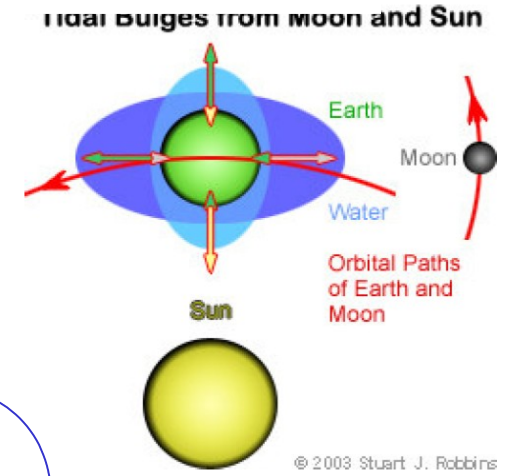
Renormalization group (RG) evolved nuclear potentials

$V_{\text{low-k}}$ unifies NN interactions at low energy



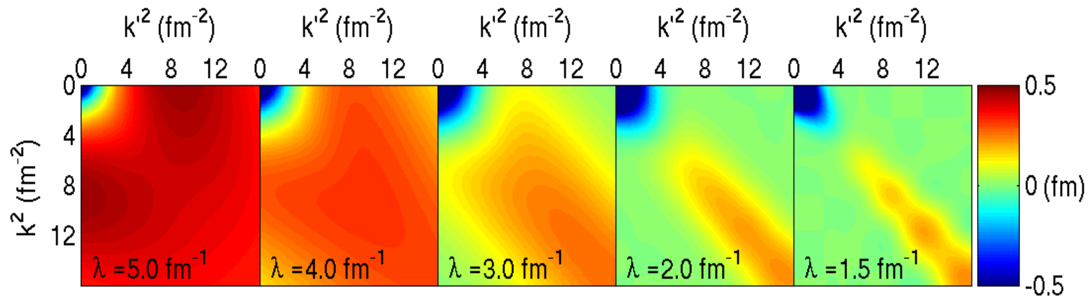
Bogner, Kuo, Schwenk, Phys. Rep. 386, 1 (2003)

three-nucleon interactions



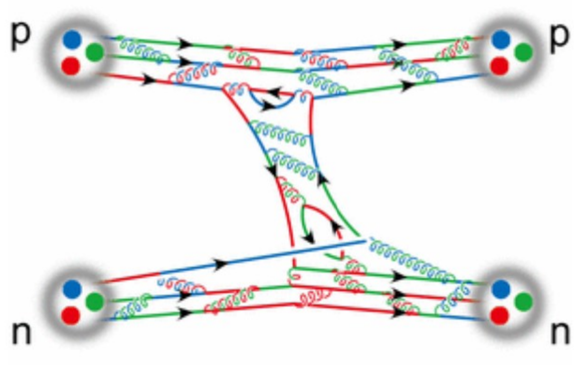
Three-body forces between protons and neutrons are analogous to tidal forces: the gravitational force on the Earth is *not* just the sum of Earth-Moon and Earth-Sun forces (if one employs point masses for Earth, Moon, Sun)

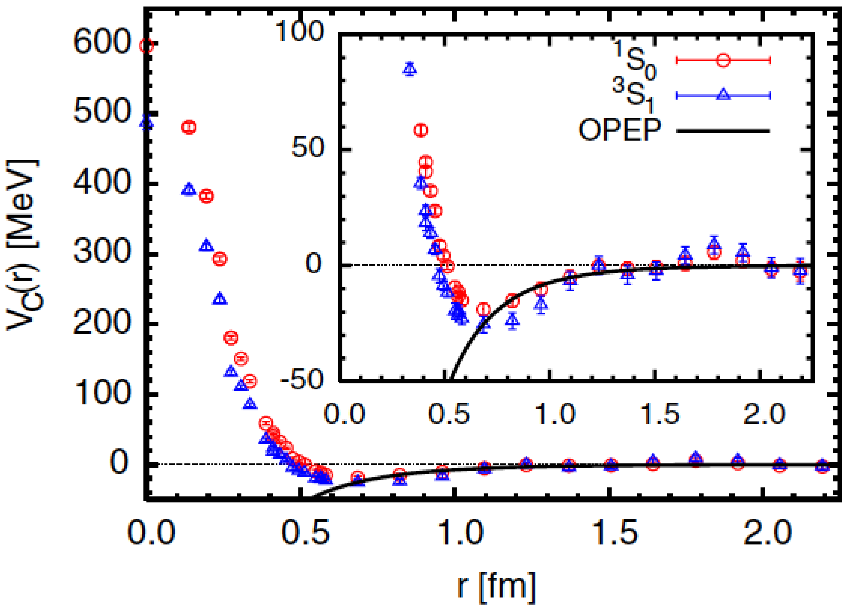
The computational cost of nuclear 3-body forces can be greatly reduced by decoupling low-energy parts from high-energy parts, which can then be discarded.



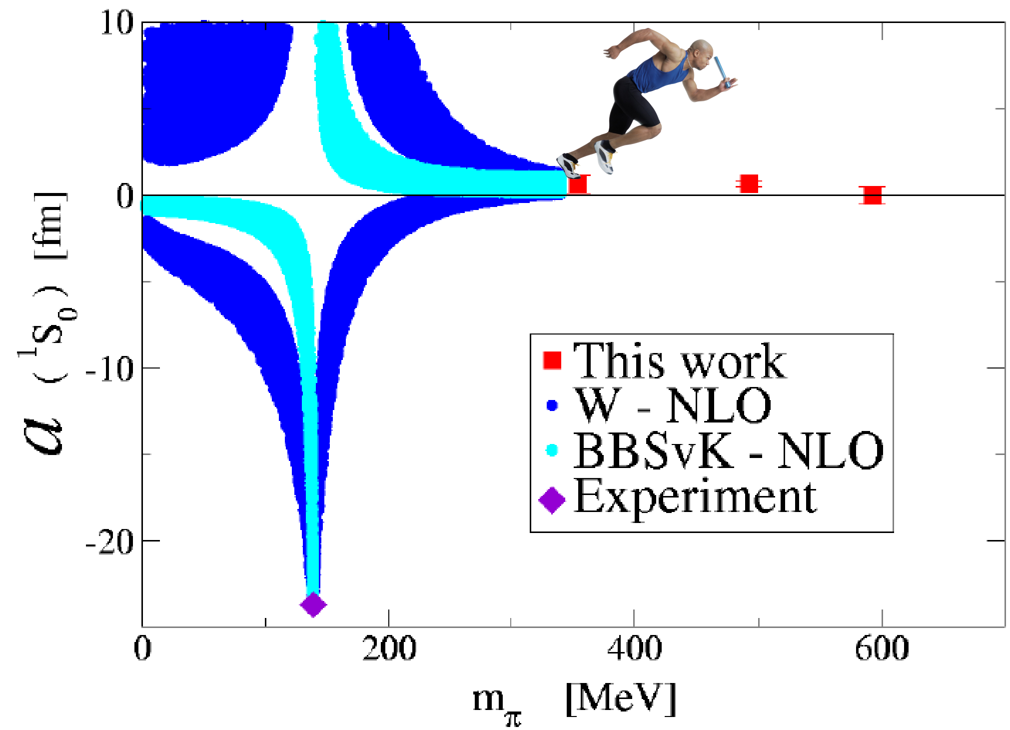
Recently the first consistent Similarity Renormalization Group softening of three-body forces was achieved, with rapid convergence in helium. With this faster convergence, calculations of larger nuclei are possible!

The challenge and the prospect: NN force





Ishii et al. PRL 99, 022001 (2007)



Beane et al. PRL 97, 012001 (2006)
and Phys. Rev. C 88, 024003 (2013)

Optimizing the nuclear force

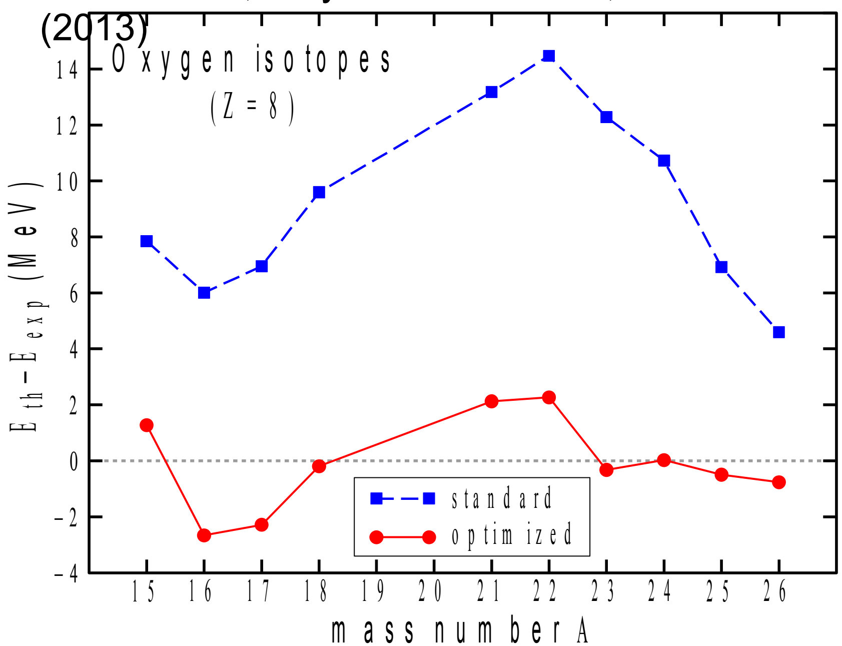
input matters: garbage in, garbage out

- The derivative-free minimizer POUNDERS was used to systematically optimize NNLO chiral potentials
- The optimization of the new interaction $NNLO_{opt}$ yields a χ^2/datum ≈ 1 for laboratory NN scattering energies below 125 MeV. The new interaction yields very good agreement with binding energies and radii for A=3,4 nuclei and oxygen isotopes
- Ongoing: Optimization of NN + 3NF

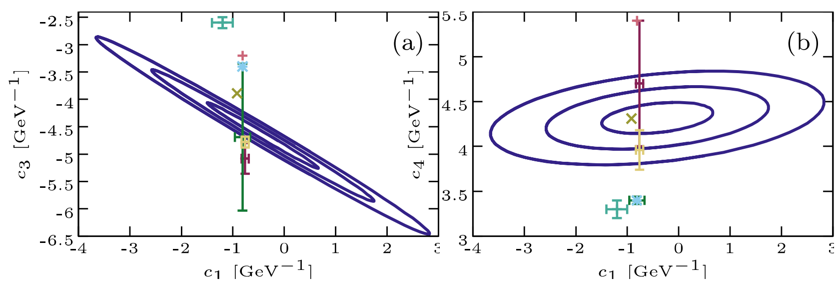
- Used a coarse-grained representation of the short-distance interactions with 30 parameters
- The optimization of a chiral interaction in NNLO yields a χ^2/datum ≈ 1 for a mutually consistent set of 6713 NN scattering data
- Covariance matrix yields correlation between LECCs and predictions with error bars.

Navarro Perez, Amaro, Arriola, Phys. Rev. C 89, 024004 (2014) and arXiv:1406.0625

A. Ekström et al., Phys. Rev. Lett. 110, 192502 (2013)



http://science.energy.gov/np/highlights/2014/np-2014-05-e/



	This work	Emp./Rec. [36–41]	δ she
E_d (MeV)	Input	2.224575(9)	In
η	0.02473(4)	0.0256(5)	0.02
A_S (fm$^{1/2}$)	0.8854(2)	0.8845(8)	0.88
r_m (fm)	1.9689(4)	1.971(6)	1.96
Q_D (fm^2)	0.2658(5)	0.2859(3)	0.26
P_D	5.30(3)	5.67(4)	5.62
$\langle r^{-1} \rangle$ (fm^{-1})	0.4542(2)		0.45

Deuteron, Light Nuclei

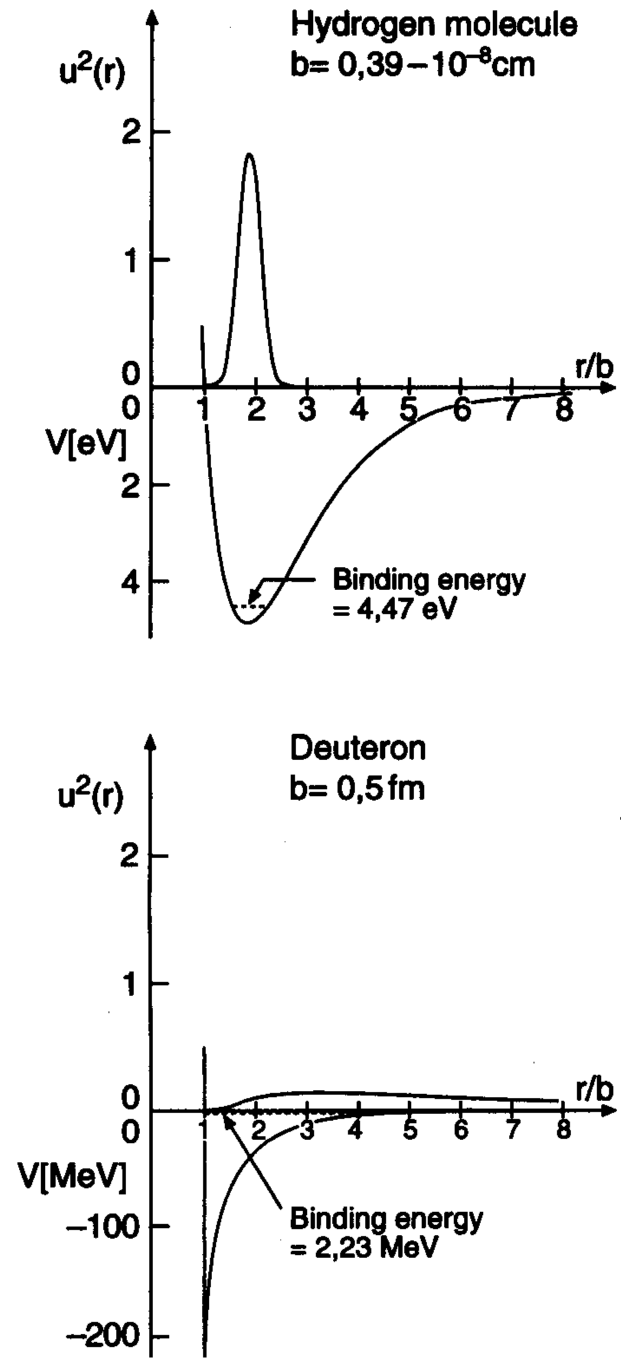
Deuteron

Binding energy	2.225 MeV
Spin, parity	1^+
Isospin	0
Magnetic moment	μ=0.857 μ_N
Electric quadrupole moment	Q=0.282 e fm^2

$$\mu_p + \mu_n = 2.792\mu_N - 1.913\mu_N = 0.879\mu_N$$

$$|\psi_d\rangle = 0.98\,|{}^3S_1\rangle + 0.20\,|{}^3D_1\rangle$$

produced by tensor force!



Nucleon-Nucleon Interaction

NN, NNN, NNNN,…, forces

GFMC calculations tell us that:

$$\langle V_\pi \rangle / \langle V \rangle \sim 70-80\%$$

$$\langle V_\pi \rangle \sim -15\,\text{MeV/pair}$$

$$\langle V^R \rangle \sim -5\,\text{MeV/pair}$$

ge

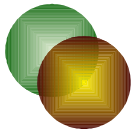
$$\langle V^3 \rangle \sim -1\,\text{MeV/three}$$

dy

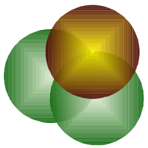
$$\langle T \rangle \sim 15\,\text{MeV/nucleon}$$

$$\langle V_C \rangle \sim 0.66\,\text{MeV/pair of protons}$$

Few-nucleon systems
(theoretical struggle)

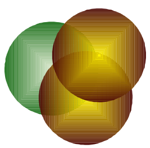


A=2: many years ago…

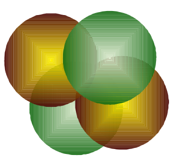


3H: 1984 (1% accuracy)

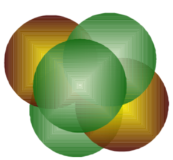
- **Faddeev**
- **Schroedinger**



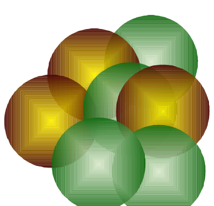
3He: 1987



4He: 1987



5He: 1994 (n-α resonance)



A=6,7,..12: 1995-2014