

Atomic nuclei as building blocks of the interdisciplinary quantum many-body science

Gianluca Colò



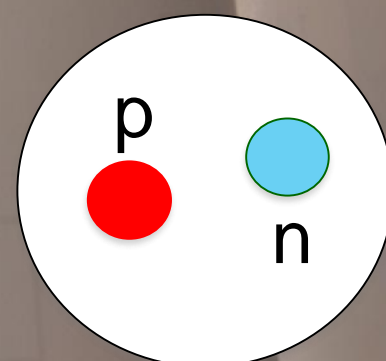
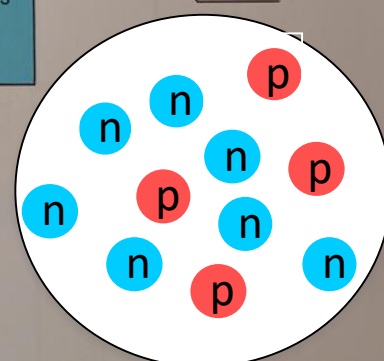
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ILL, July 2nd, 2018



- Which nuclei, i.e. which aggregates of neutrons and protons, exist?
- How do the complex phenomena of nuclear physics emerge? (Nuclei are made up by nucleons but often behave as a whole, they are stiff under compression but look different when they undergo fission...)
- Which is the role of the mutual interaction and which is the role of many-body correlations? (Common to other quantum many-body systems).
- How were atomic nuclei made? (The nucleosynthesis problem)

	5730 a	2.45 s	0.747 s	193 ms	92 ms	49 ms	14 ms	<30 ns	6.2 ms
	$\beta^- 0.2$ no γ	$\beta^- 4.5; 9.6...$ $\gamma 5298...$	$\beta^- 4.7; 7.9...$ $\beta n 0.79; 1.72$	β^- $\beta n 1.62...$ $\gamma 1375; 1849;$ 1906...	β^- $\gamma 2614; 880;$ 2499...	β^- $\beta n 1.01; 0.46...$ $\beta 2n$	β^- βn	n ?	β^- βn $\beta 2n ?$
B 12 20.20 ms	B 13 17.33 ms	B 14 13.8 ms	B 15 10.4 ms	B 16 <190·10 ⁻¹² s	B 17 5.1 ms	B 18 <26 ns	B 19 2.92 ms		
$\beta^- 13.4...$ $\gamma 4439...$ $\beta \alpha 0.2$	$\beta^- 13.4...$ $\gamma 3684$ $\beta n 3.0; 2.4$	$\beta^- 14.0...$ $\gamma 6090; 6730$ βn	β^- $\beta n 1.77; 3.20...$	n ?	β^- $\beta n; \beta 2n;$ $\beta 3n; \beta 4n$	n ?	β^- βn $\beta 2n$		
Be 11 13.8 s	Be 12 23.6 ms	Be 13 0.5 ns	Be 14 4.35 ms						
				12	14				
		0.13E-4	1.58E-4						
		0.47E-4	3.01E-4	10					
Li 10 30 keV · 10 ⁻²¹ s	Li 11 8.5 ms								
$\beta^- 18.5; 20.4$ $\gamma 3368^*;$ 320...									
$\beta n; \beta 2n; \beta 3n;$ $\beta \alpha; \beta \gamma; \beta \delta$									

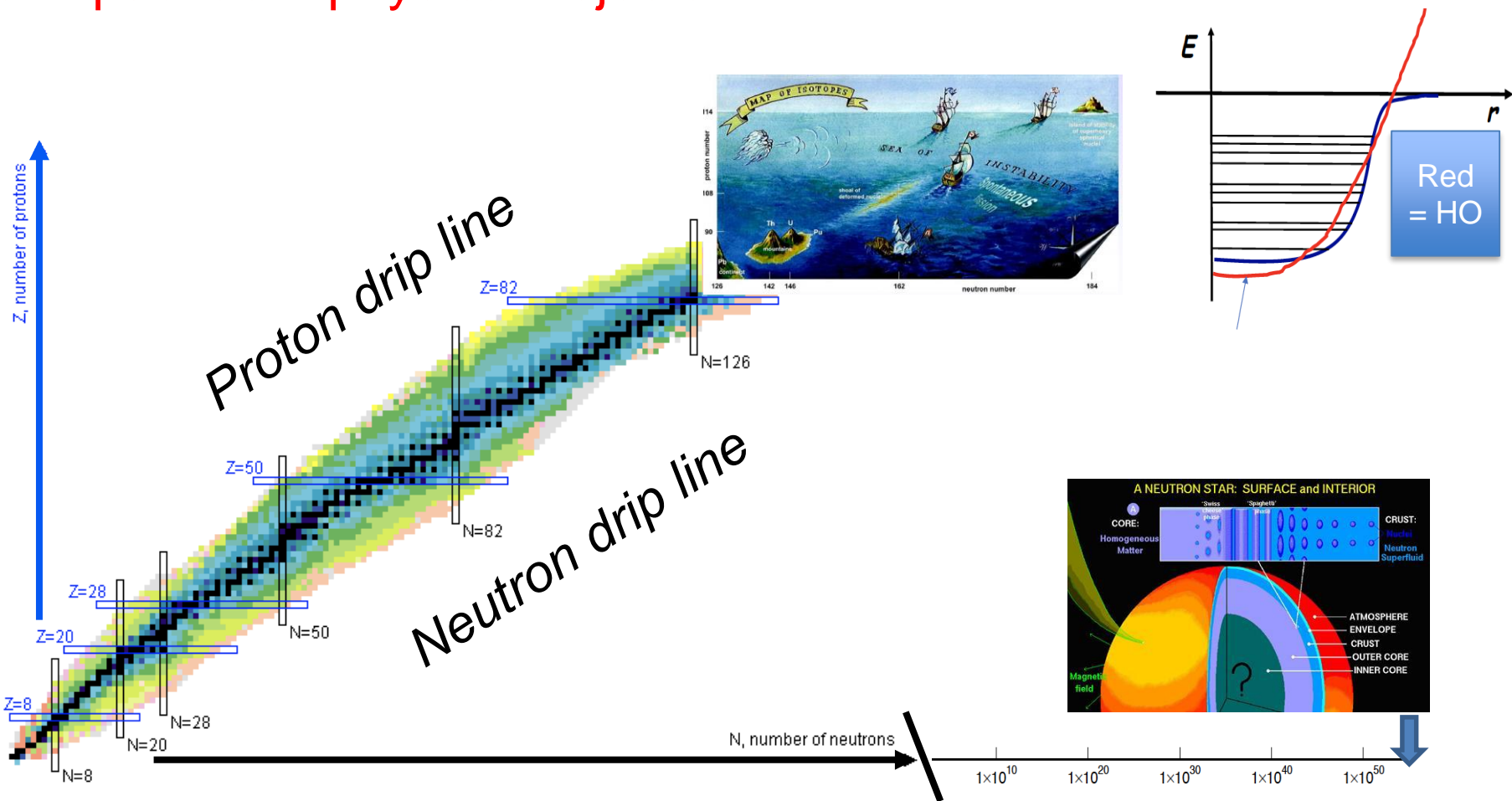


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Discovering the limits of the nuclear existence is still underway

Three **new territories**: nuclei at the drip lines, super-heavies, compact astrophysical objects



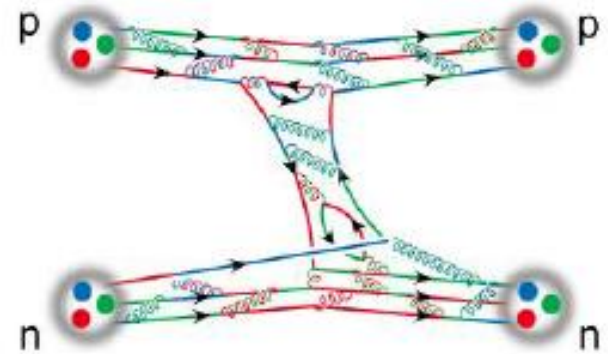
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Theory: *ab initio* ?

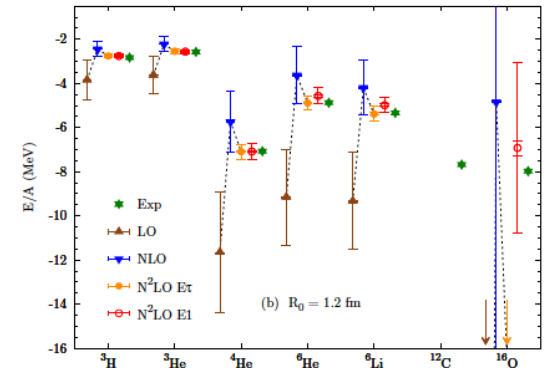
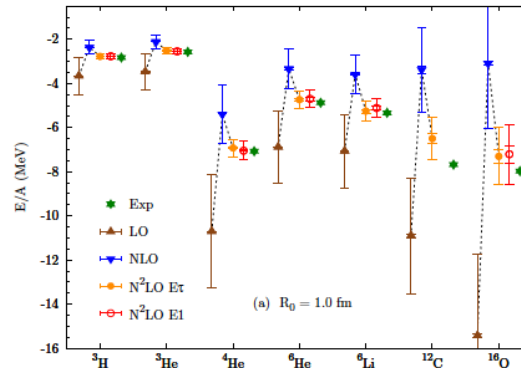
- There are attempts to derive the interaction between nucleons from the dynamics of quarks inside nucleons (**Quantum Chromo Dynamics, QCD**).

No bound two- or three-nucleon system.
 BE (^4He) around 5 MeV.
 T. Inoue *et al.*, PRL 111, 112503 (2013)



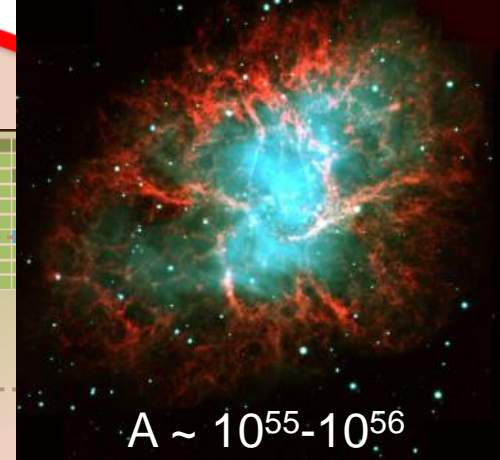
- Most often, **effective** theories are used. (Very) demanding from the computational viewpoint.

D. Lonardoni *et al.*, PRC 97, 044318 (2018)

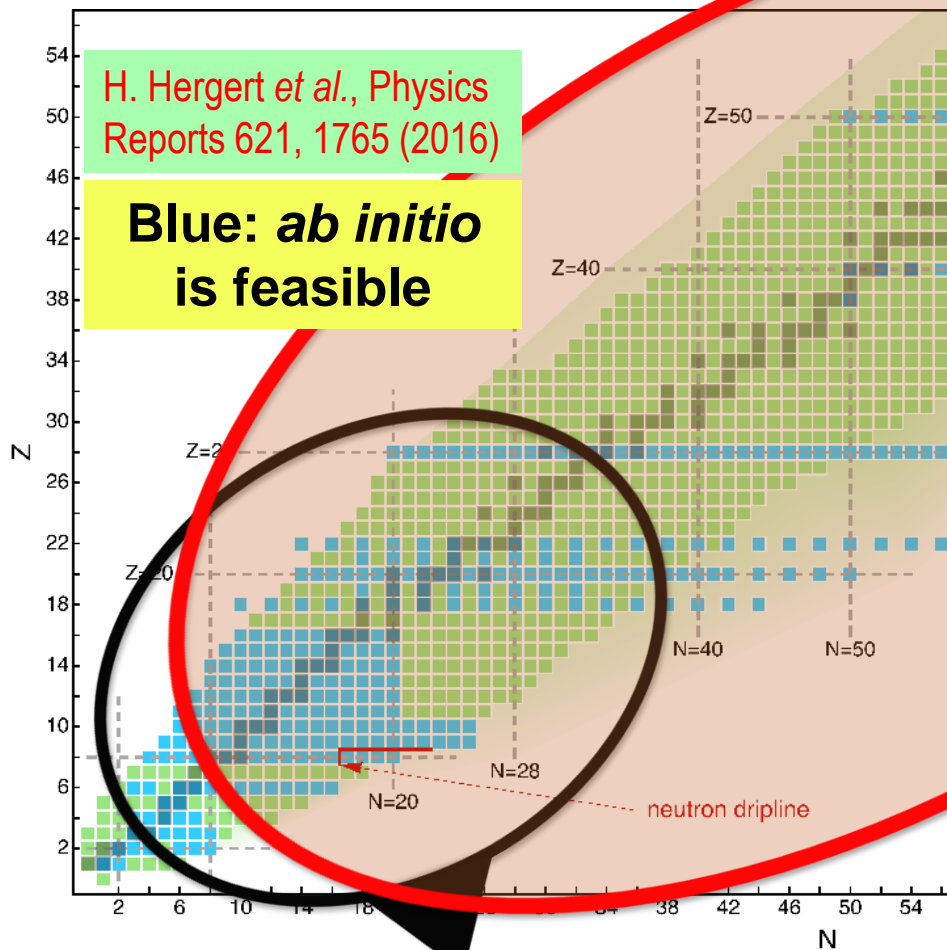


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$A \sim 10^{55}-10^{56}$



H. Hergert *et al.*, Physics Reports 621, 1765 (2016)

Blue: *ab initio* is feasible

Density Functional Theory, DFT

- Can access a very large part of the **nuclear chart**, if not all
- Can explore **large E_x**
- Link with nuclear matter and compact objects like **neutron stars**

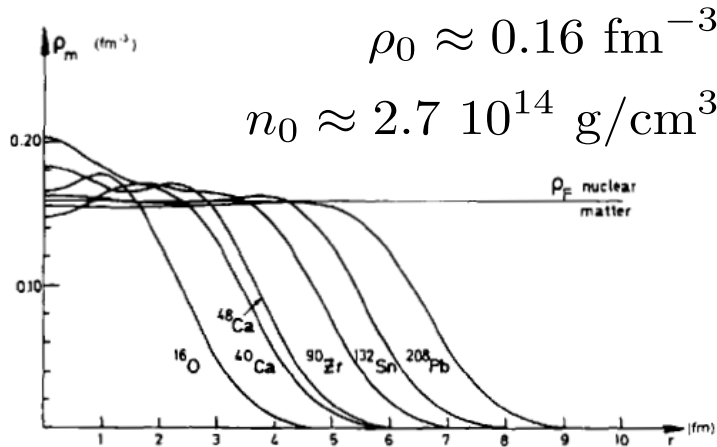
**Shell model
(Configuration interaction, CI)**



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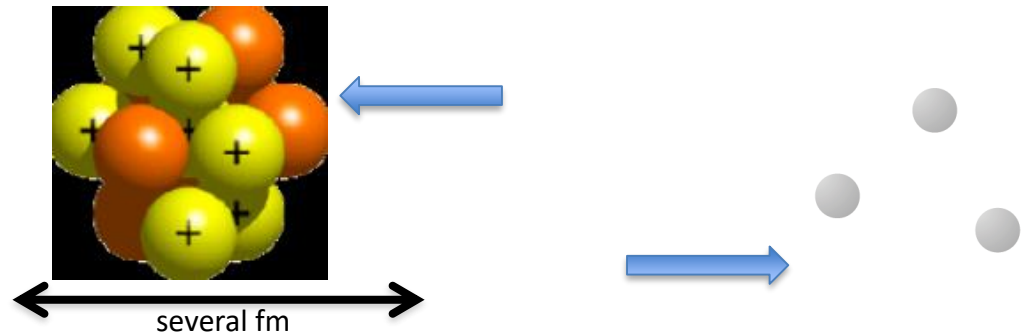
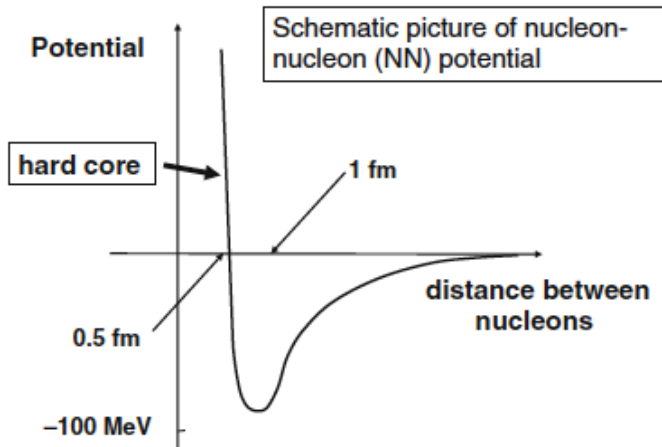
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Why does DFT work if the force is strong?



$$\frac{1}{\rho} = \frac{4}{3} \pi r_0^3$$

- The nuclear system is rather **dilute**: distance r_0 between particles $>$ interaction range.
- Nucleons do not feel so often the strongest part of V_{NN} .



Nuclear Density Functional Theory

$$E = \int \mathcal{E}[\rho] d^3r$$

Energy density = \mathcal{E}
E is a functional

“DFT is an exactification of Hartree-Fock”
(W. Kohn).



Courtesy: M. Pössel

- Mechanism for saturation
- Flexibility (i.e., enough terms) to account for the many features of finite nuclei
- Suitable for extensive computational efforts
- “Guaranteed” by the Hohenberg-Kohn theorem (1964)

$$E_{\text{ground state}} = \min_{\rho} E[\rho]$$

The **exact** functional has a minimum at the exact ground-state density, where it assumes the exact energy as a value.



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The principle is relatively **simple**: write the energy of a system as a functional of the density and minimize !

- Masses $M(N, Z) = Zm_p c^2 + Nm_n c^2 - BE(N, Z)$

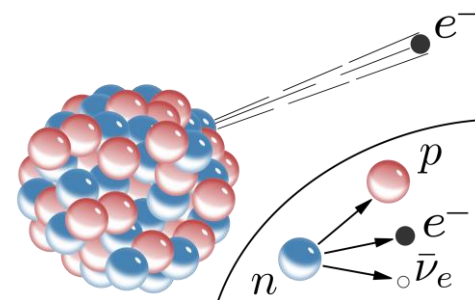
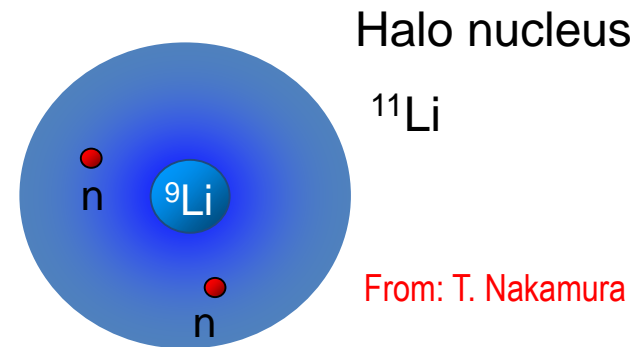
- Radii

- Deformations

- Excited states: vibrations, rotations

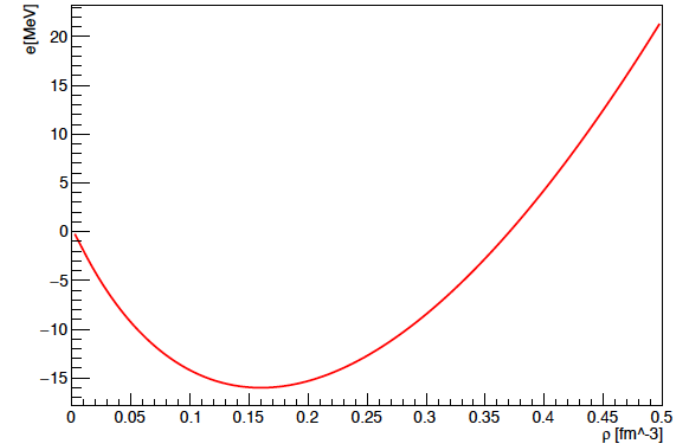
- Decays (for instance, β and $\beta\beta$ transitions)

...



Simplistic / realistic functional(s)

$$\begin{aligned}
 \mathcal{H} = & \frac{\hbar^2}{2m}\tau \\
 & + \frac{1}{4}t_0[(2+x_0)\rho^2 - (2x_0+1)(\rho_p^2 + \rho_n^2)] \\
 & + \frac{1}{24}t_3\rho^\sigma[(2+x_3)\rho^2 - (2x_3+1)(\rho_p^2 + \rho_n^2)] \\
 & + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau\rho \\
 & + \frac{1}{8}[t_2(2x_2+1) - t_1(2x_1+1)](\tau_p\rho_p + \tau_n\rho_n) \\
 & + \frac{1}{32}[3t_1(2+x_1) - t_2(2+x_2)](\vec{\nabla}\rho)^2 \\
 & - \frac{1}{32}[3t_1(2x_1+1) + t_2(2x_2+1)][(\vec{\nabla}\rho_p)^2 + (\vec{\nabla}\rho_n)^2] \\
 & + \frac{1}{2}W_0[\vec{J} \cdot \vec{\nabla}\rho + \vec{J}_p \cdot \vec{\nabla}\rho_p + \vec{J}_n \cdot \vec{\nabla}\rho_n] \\
 & - \frac{1}{16}(t_1x_1 + t_2x_2)J^2 + \frac{1}{16}(t_1 - t_2)(J_p^2 + J_n^2).
 \end{aligned}$$



$$\tau = \sum_i |\vec{\nabla}\phi_i|^2 \quad \vec{J} = \sum_{i,\sigma,\sigma'} \phi_i^\dagger \vec{\nabla}\phi_i \times \langle \sigma' | \vec{\sigma} | \sigma \rangle$$

- Skyrme: local functionals
- Gogny: non local f.
- Relativistic EDFs: covariant formulation



Chemical Accuracy



exact exchange and exact partial correlation

exact exchange and compatible correlation

meta-generalized gradient approximation $E_{xc}^{mGGA} = \int d^3r f(\rho, \nabla\rho, \nabla^2\rho, \tau)$

generalized gradient approximation

$$E_{xc}^{GGA} = \int d^3r f(\rho, \nabla\rho)$$

local spin density approximation

$$E_{xc}^{LDA} \text{ or } LSDA = \int d^3r \rho(r) e_{xc}^{unif}[\rho]$$

World

FIGURE 1. Jacob's ladder of density functional approximations. Any resemblance to the Tower of Babel is purely coincidental. Also shown are angels in the spherical approximation, ascending and descending. Users are free to choose the rungs appropriate to their accuracy requirements and computational resources. However, at present their safety can be guaranteed only on the two lowest rungs.

J. Perdew, K. Schmidt, AIP
Conf. Proc. 577, 1 (2001).

**Error (th. vs. exp.) in the
atomization energies of 20
molecules [eV]**

**(average of these energies
≈ 8.21 eV)**

LSDA	GGA	mGGA
1.4	0.3	0.1

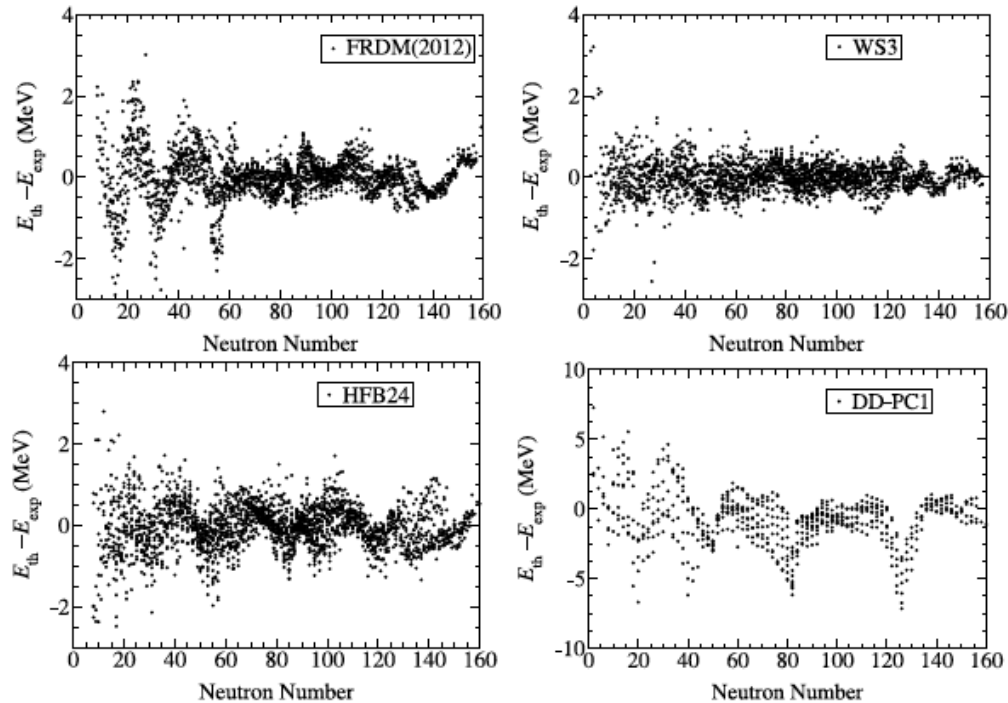


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Masses/binding energies of nuclei

X. Roca-Maza and N.Paar, PPNP 101, 96 (2018)



Model	Type	N ^a par.	σ_M [MeV]
FRDM(2012)	Mac-Mic	38 ^a	0.559 ^b
WS4 ^c	Mac-Mic	18	0.298 ^d
HFB24	EDF	30 ^e	0.549 ^f
UNEDF1	EDF	12	1.88 ^g
DD-PC1	EDF	9	2.01 ^h

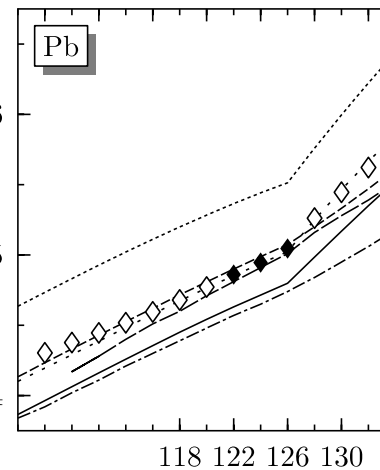
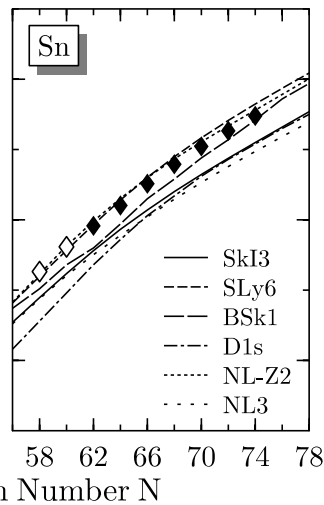
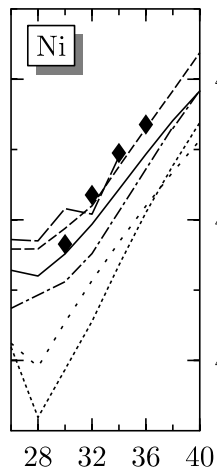
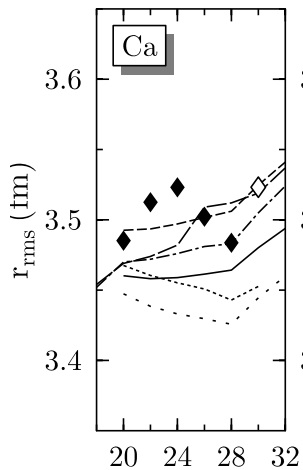
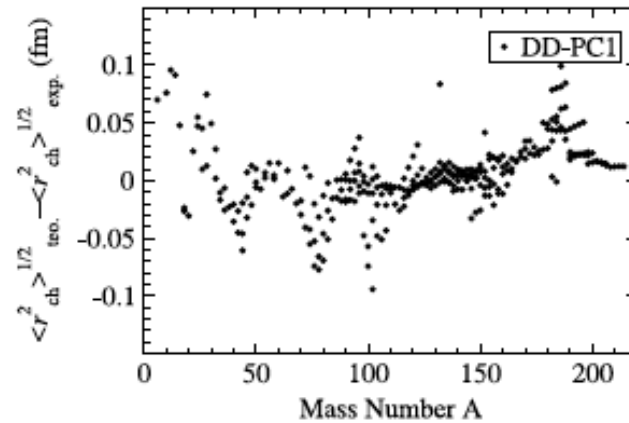
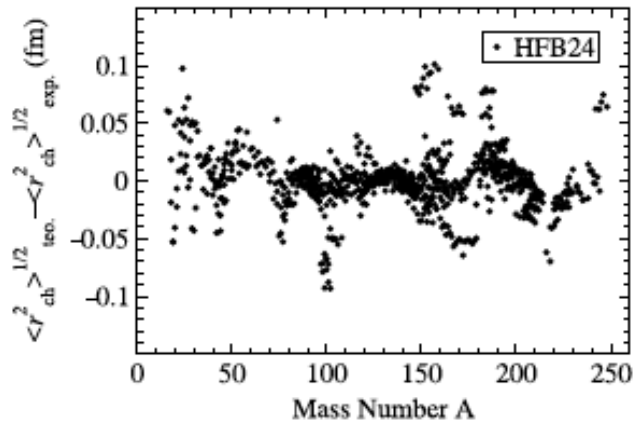
- Typical EDFs have errors \approx MeV for the masses. 0.1 % to 1 % (!).
- More *ad hoc* parameters may push errors down (not necessarily the predictive power).
- **Arches** unavoidable?



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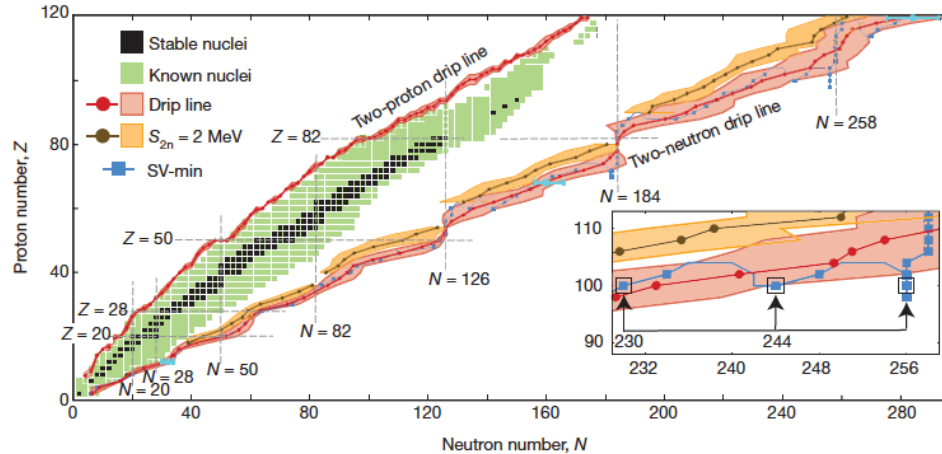
Charge radii



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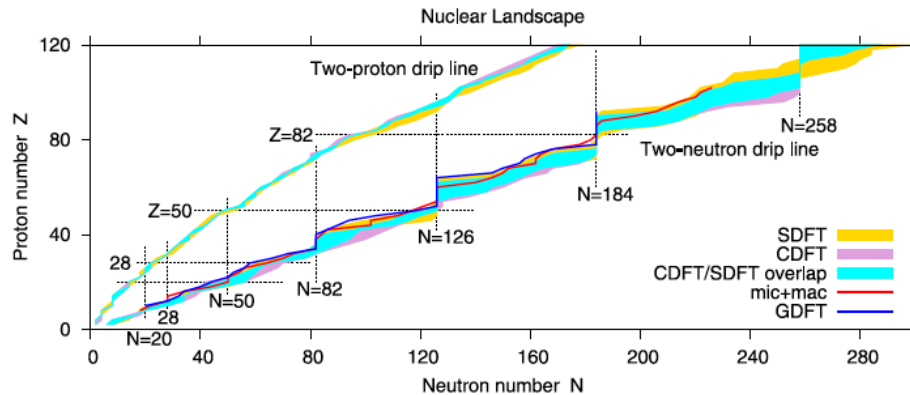
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Theoretical predictions of the drip lines



J. Erler *et al.*, Nature
486, 509 (2012) - SEDF

Evaluation of theoretical uncertainties.



A.V. Afanasjev *et al.*,
Phys. Lett. B726, 680
(2013) - CEDF

The uncertainty on the drip lines position can increase up to about 10 mass units for large A.

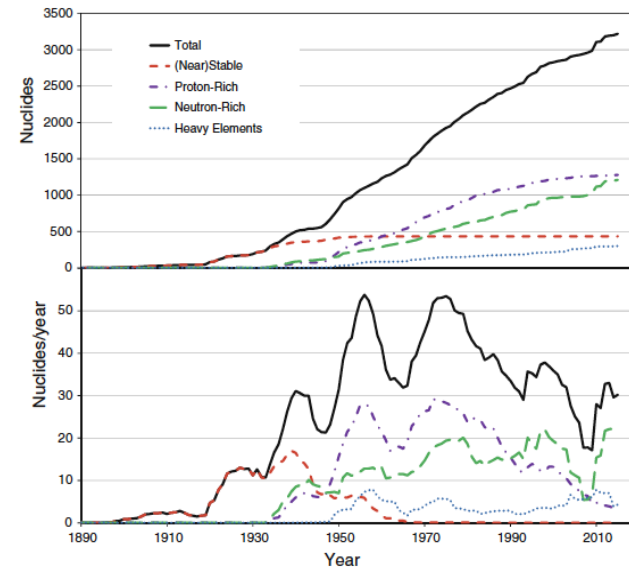
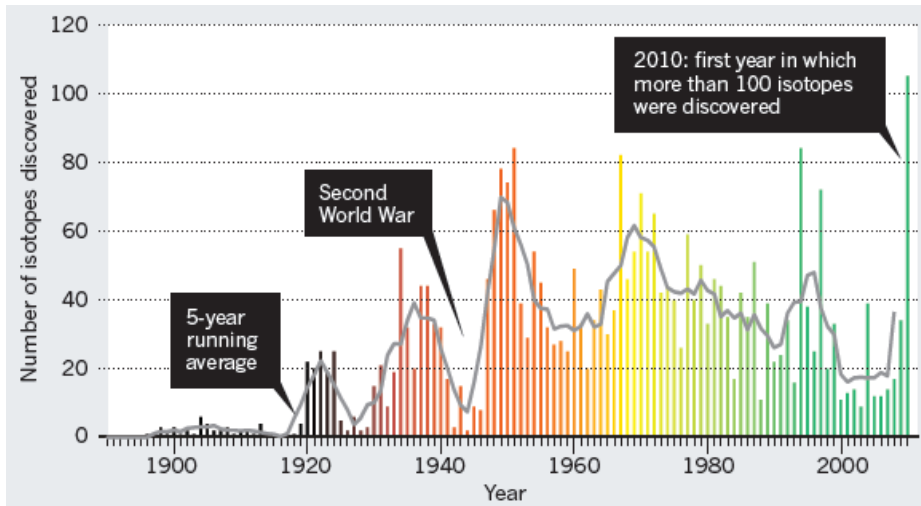
Fig. 4. The comparison of the uncertainties in the definition of two-proton and two-neutron drip lines obtained in CDFT and SDFT. The shaded areas are defined by the extremes of the predictions of the corresponding drip lines obtained with different parametrizations. The blue shaded area shows the area where the CDFT and SDFT results overlap. Non-overlapping regions are shown by dark yellow and plum colors for SDFT and CDFT, respectively. The results of the SDFT calculations are taken from the supplement to Ref. [2]. The two-neutron drip lines obtained by microscopic + macroscopic (FRDM [3]) and Gogny D1S DFT [5] calculations are shown by red and blue lines, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this Letter.)



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Discovering new “exotic” isotopes



M. Thoennessen, B. Sherrill, *Nature* 473, 25 (2011)

M. Thoennessen, *Int. J. Mod. Phys. E* 26, 1730003 (2017)

<http://www.nsl.msu.edu/~thoennessen/isotopes/>

Nuclear isotopes can be produced in the lab, but how does or did Nature produce them ?



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The nucleosynthesis problem

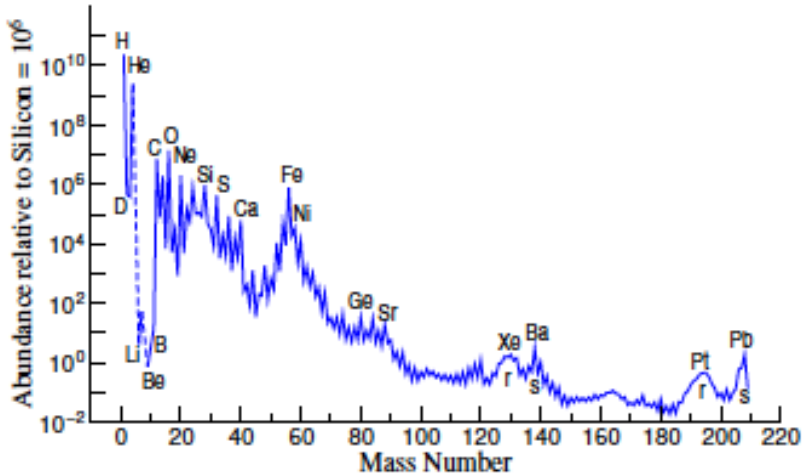
The 11 Greatest Unanswered Questions of Physics | DiscoverMagazine.com

FROM THE FEBRUARY 2002 ISSUE

The 11 Greatest Unanswered Questions of Physics

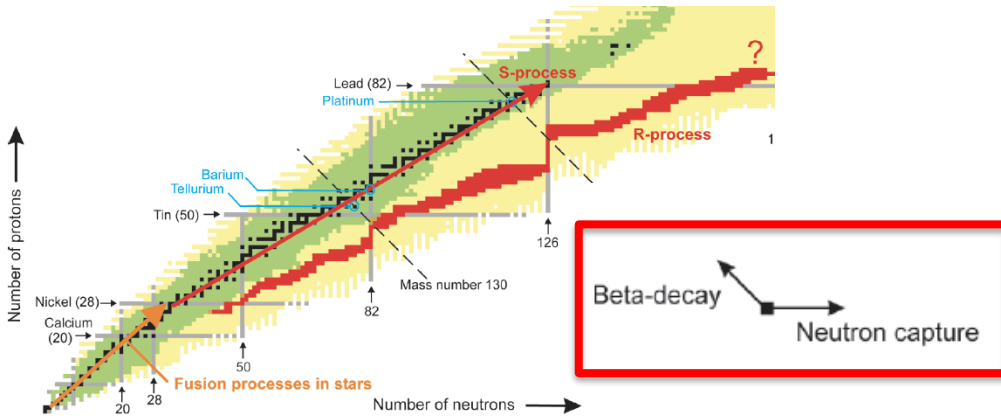
How were the heavy elements from iron to uranium made?

“How” means in which environment and by means of which nuclear processes

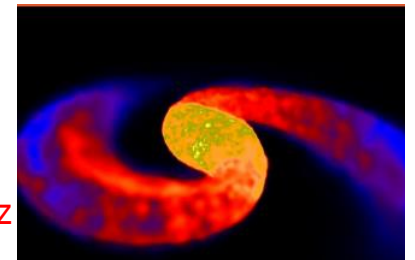


s-process and r-process.

Where does the r-process take place?



Figures: G. Martinez-Pinedo and H. Schatz

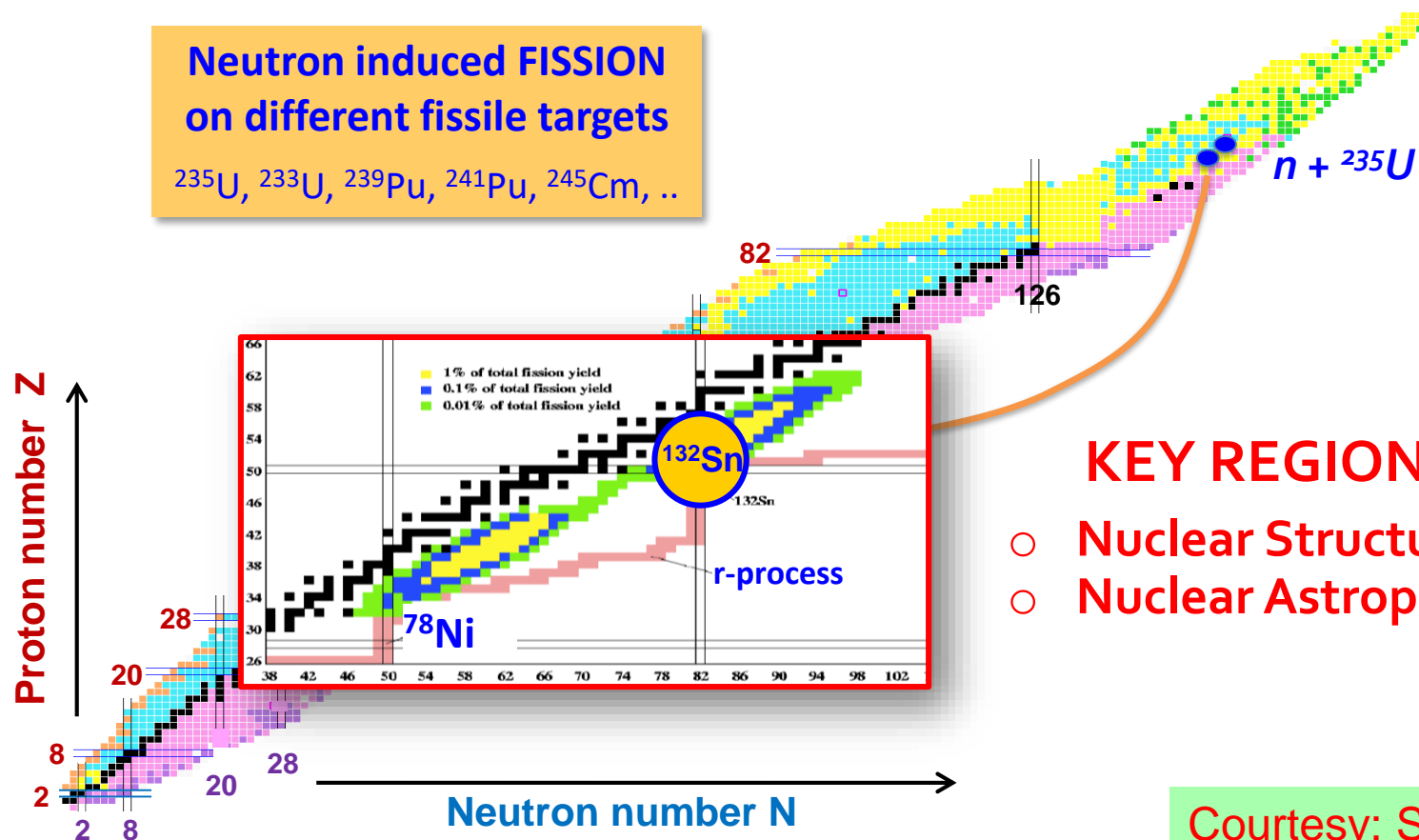


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UNIQUE OPPORTUNITIES OFFERED BY ILL INTENSE and very CLEAN thermal neutron beam

**Neutron induced FISSION
on different fissile targets**
 ^{235}U , ^{233}U , ^{239}Pu , ^{241}Pu , ^{245}Cm , ..



- KEY REGIONS for**
- Nuclear Structure
 - Nuclear Astrophysics

Courtesy: S. Leoni



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The nuclear Equation of State (EoS): neutron stars, nuclear excitations, nuclear reactions



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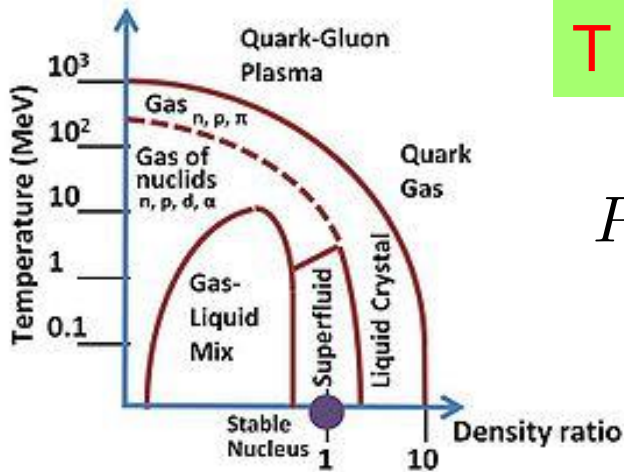
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Nuclear matter

- Nuclear matter is an idealized **UNIFORM** system of neutrons and protons having constant density. (The Coulomb interaction among protons must be taken out).
- It is analogous to the uniform electron gas for condensed matter physicists.

**WE STICK TO
T = 0 !**

$$\rho = \frac{A}{\Omega} \text{ with } A \text{ fixed !}$$



$$P = -\frac{\partial E}{\partial \Omega} = -\frac{d\rho}{d\Omega} \frac{\partial E}{\partial \rho} = \frac{A}{\Omega^2} \frac{\partial E}{\partial \rho} = \rho^2 \frac{\partial}{\partial \rho} \frac{E}{A}$$

- We call **E/A** the “**equation of state**” of nuclear matter.



The EoS and the symmetry energy

Nuclear matter EOS

$$\frac{E}{A}(\rho, \beta) = \frac{E}{A}(\rho, \beta \stackrel{\downarrow}{=} 0) + \underset{\downarrow}{S(\rho)}\beta^2$$

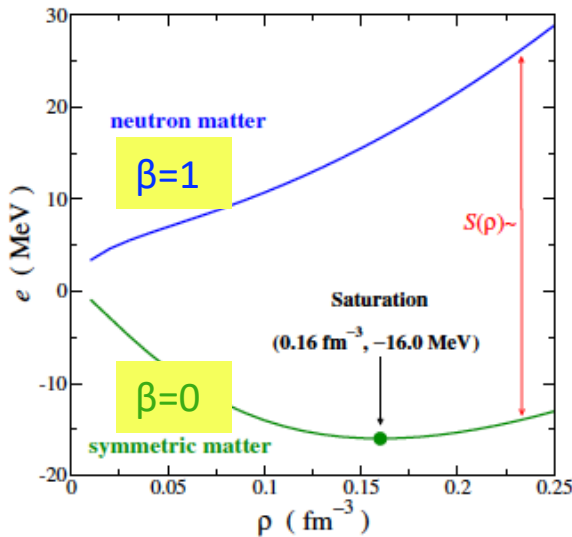
Symmetric matter EOS

Symmetry energy S

$$\beta \equiv \frac{\rho_n - \rho_p}{\rho}$$

$$S \equiv \frac{E}{A}(\text{neutron matter}) - \frac{E}{A}(\text{symmetric matter})$$

Expansion around
 $\rho_0 = 0.16 \text{ fm}^{-3}$
SATURATION
POINT of SNM



$$\frac{E}{A}(\rho, \beta = 0) = E_0 + \frac{1}{2}K_\infty \left(\frac{\rho - \rho_0}{3\rho_0}\right)^2 + \dots$$

$$S(\rho) = J + L \left(\frac{\rho - \rho_0}{3\rho_0}\right) + \frac{1}{2}K_{\text{sym}} \left(\frac{\rho - \rho_0}{3\rho_0}\right)^2 + \dots$$

J = 31.6 ± 2.7 MeV
L = 58.9 ± 31.6 MeV
 B.A. Li, 2016

$S(\rho_0) \equiv J$
 $S'(\rho_0) \equiv L/3\rho_0$
 $S''(\rho_0) \equiv K_{\text{sym}}/9\rho_0^2$

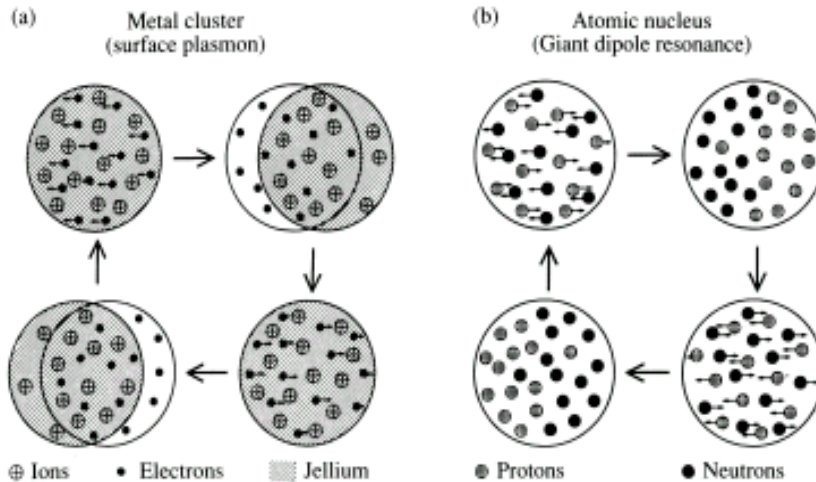


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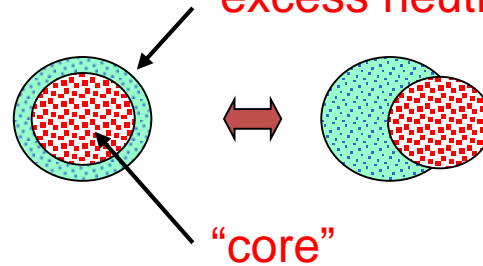
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Isvector dipole collective motion

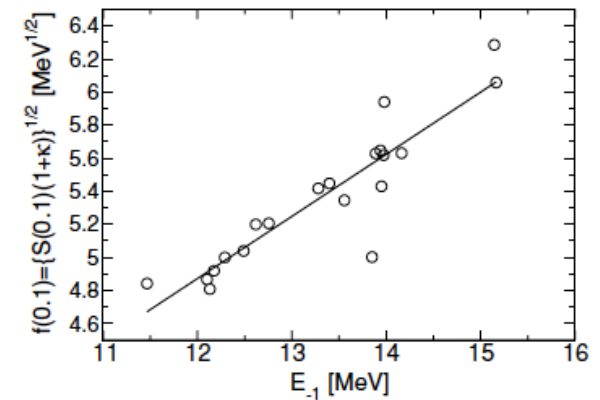
- **GDR (Giant Dipole Resonance)**: excited by e.g. a photon beam impinging on a nucleus.



- Neutron-rich nuclei can display other kinds of **excess neutrons** modes.



The larger the symmetry energy (energy per particle to change neutrons into protons), the higher the energy of this kind of oscillation modes



L. Trippa *et al.*, PRC 77, 061304(R) (2008)

$$E_{IVGR} \approx \sqrt{\frac{\partial^2 E}{\partial \beta^2}} \approx \sqrt{S(\rho)}$$



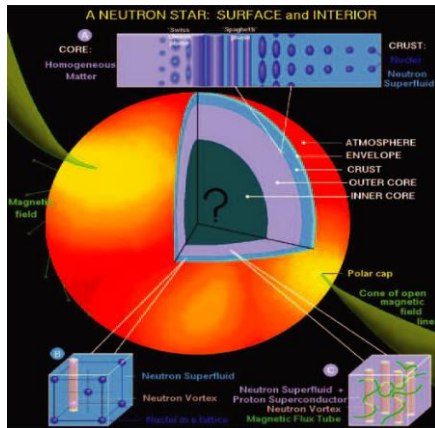
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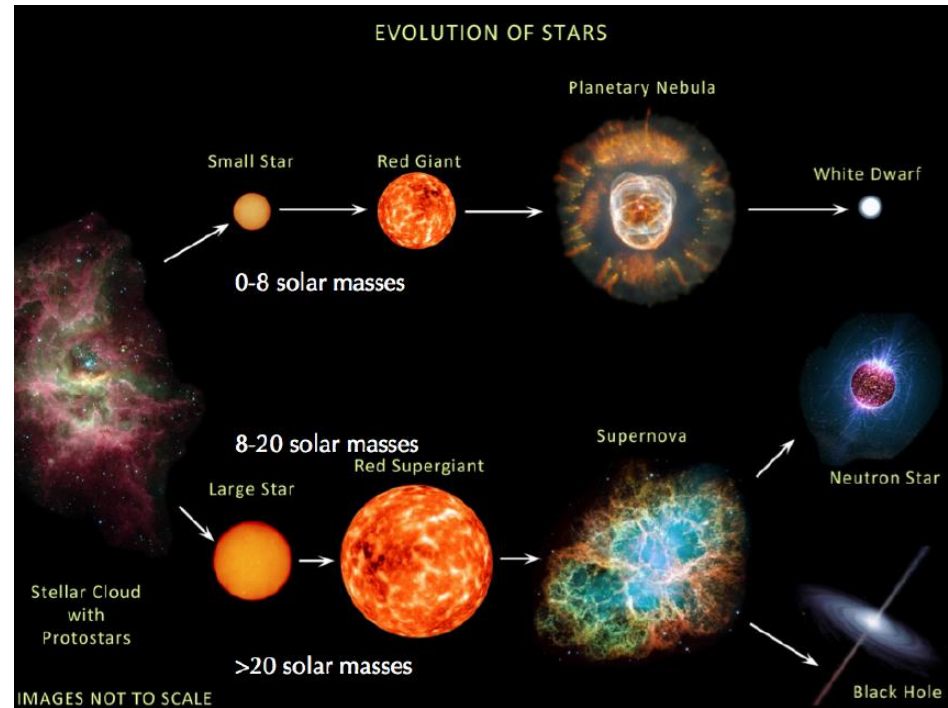
The existence of stars is determined by the balance between gravitational pressure and thermonuclear reactions.

If **exothermic nuclear reactions** are no longer possible, the star ends its life. The after-life destiny depends on the initial mass of the star.

Neutron stars: a possible outcome. Balance between gravitational pressure and energy of neutron matter.



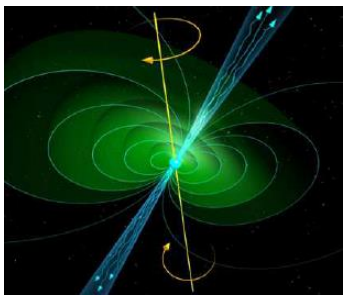
Courtesy: D. Page



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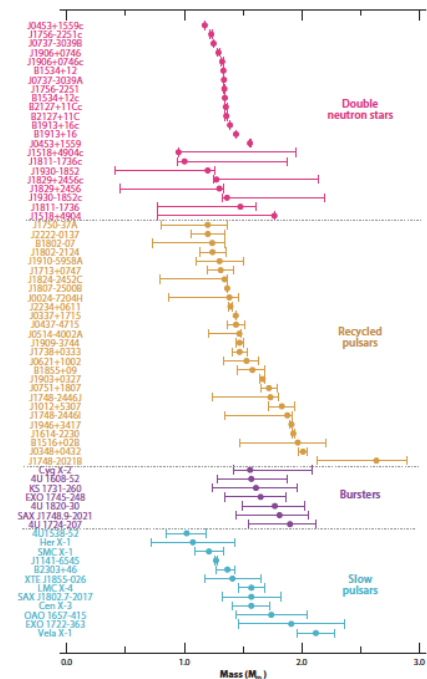
Neutron stars

- Postulated by **Landau** after the neutron was discovered
<http://www.ift.uni.wroc.pl/%7Ekarp44/talks/yakovlev.pdf>
- Discovered many years later by **J. Bell and A. Hewish** (Nobel prize 1974)
- Masses known much more precisely than radii
- Characterised by huge magnetic fields



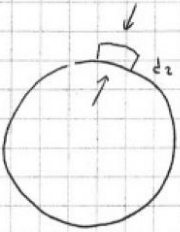
$$B \sim 10^{12} \text{ G}$$

F. Özel and P. Freire,
 ARAA 54, 401 (2016)



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Tolman-Oppenheimer-Volkov equation



$$\rho(r+dz) = F(r+dz) / A$$

$$\rho(r) = F(r) / A$$

$$\frac{d\rho}{dz} = \frac{1}{A} \frac{dF}{dz} = \frac{1}{4\pi r^2} (-G) \frac{M(r) \overbrace{4\pi r^2 \rho(r) dz}^{dm}}{r^2} \frac{1}{dz}$$

$$\frac{d\rho}{dz} = -G \frac{\rho(r) M(r)}{r^2} \quad (*)$$

$$\frac{dM}{dz} = 4\pi r^2 \rho(r), \quad M(r) = 4\pi \int_0^r dz' r'^2 \rho(r')$$

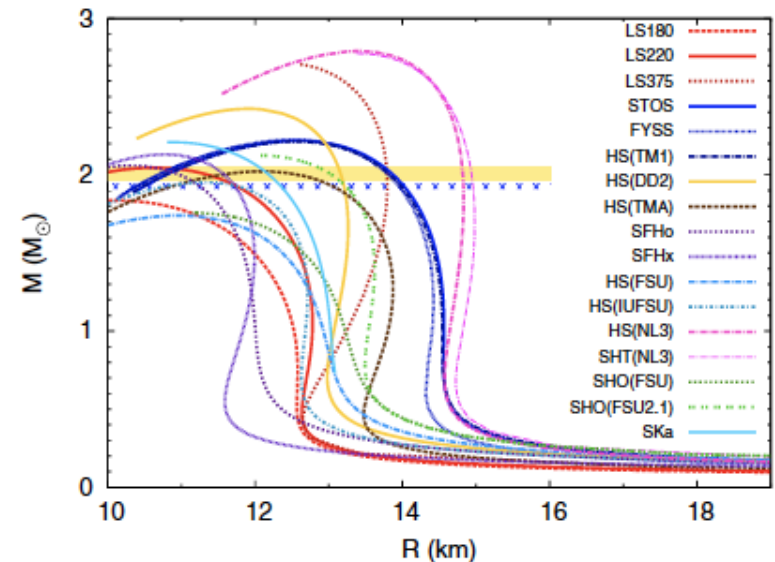
Classical gravity (Newton)

$$\frac{dP(r)}{dr} = -\frac{Gm(r)\varepsilon(r)}{r^2 c^2}$$

General relativity corrections (TOV)

$$\frac{dP(r)}{dr} = -\frac{Gm(r)\varepsilon(r)}{r^2 c^2} \left(1 + \frac{P(r)}{\varepsilon(r)}\right) \left(1 + \frac{4\pi r^3 P(r)}{\varepsilon(r)}\right) \frac{1}{1 - \frac{2Gm(r)}{rc^2}}$$

One has to input $P(\rho)$ from the nuclear EoS and solve a simple differential equation.



M. Oertel, M. Hempel, T. Klähn, S. Typel, Rev. Mod. Phys. 89, 015007 (2017)



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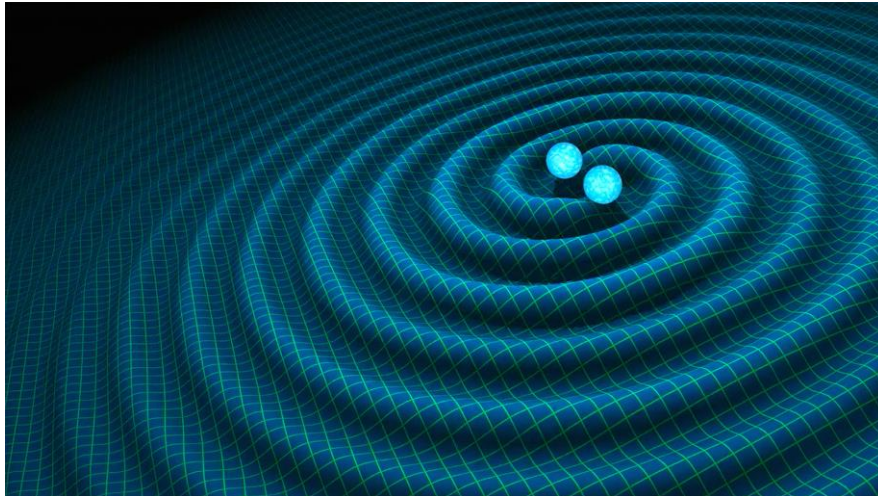
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The merging of neutron stars

- 2015: first observation of Gravitational Waves (GW), awarded Nobel 2017.
- 17/8/2017 "multi-messenger" observation of NS merging (GW, GRB, X-rays...).

GW170817 Press Release
LIGO and Virgo make first
detection of gravitational
waves produced by colliding
neutron stars

B.P. Abbott et al., *Astrophysical J. Lett.* 848:L12 (2017)



In the simulations tidal effects are quite relevant and they depend on the uncertainties on the nuclear EoS

$$\Lambda = \frac{2}{3} k_2 \left(\frac{c^2 R}{GM} \right)^2$$

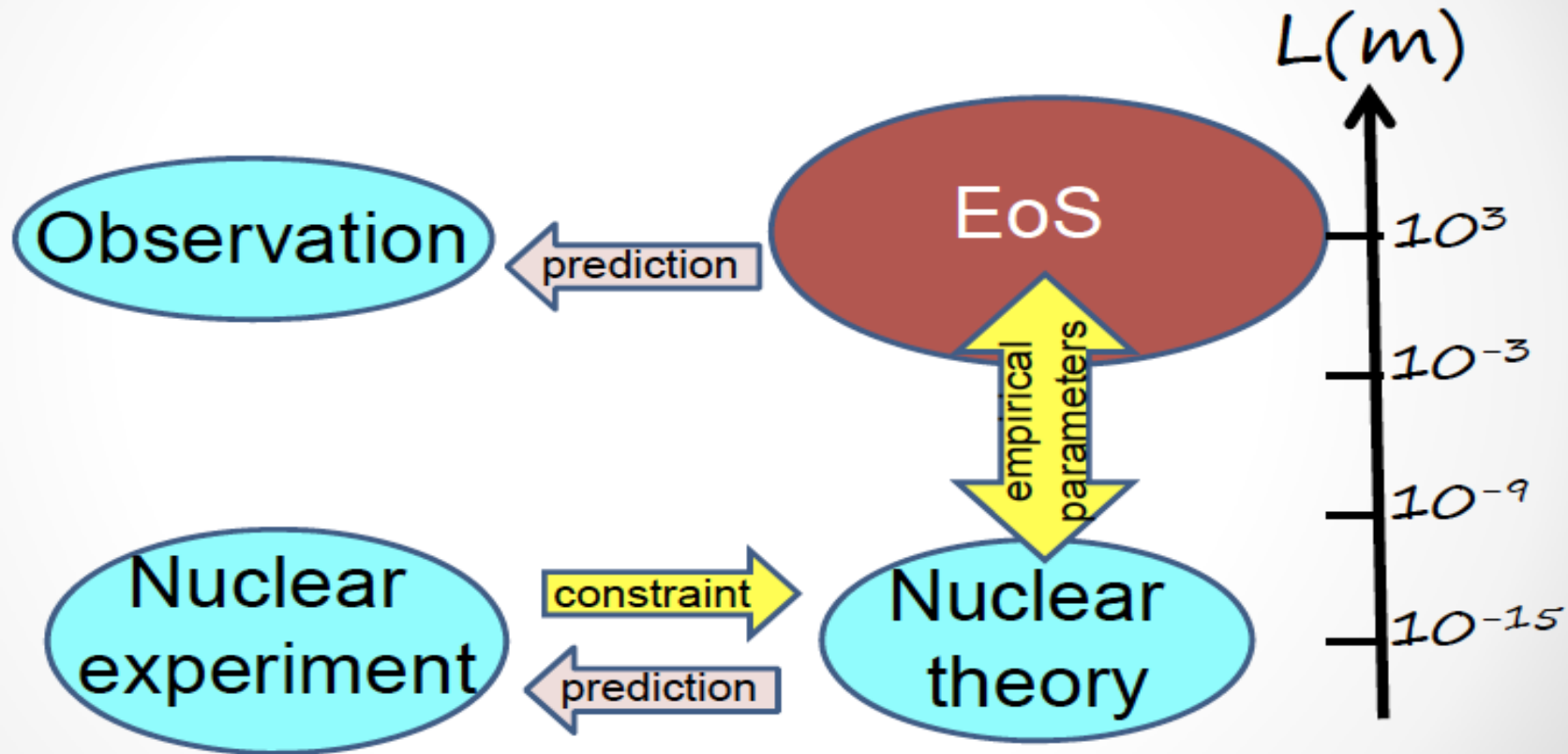
Nuclear experiments on isovector observables are relevant for the physics of GWs



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Constraining the empirical parameters: jumping across the scales!



Courtesy: F. Gulminelli

Milano, April 2018



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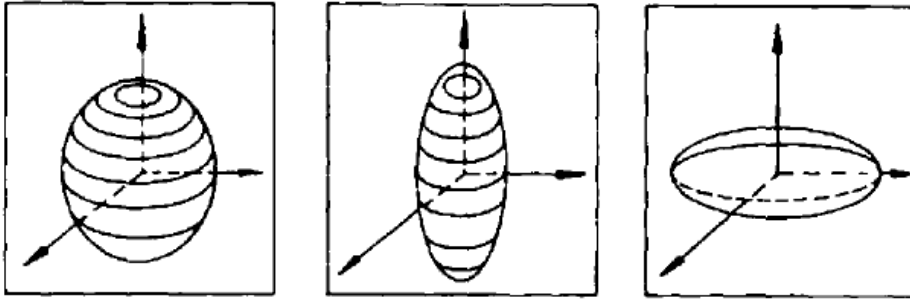
Nuclear correlations: coupling between single-particle and nuclear shapes



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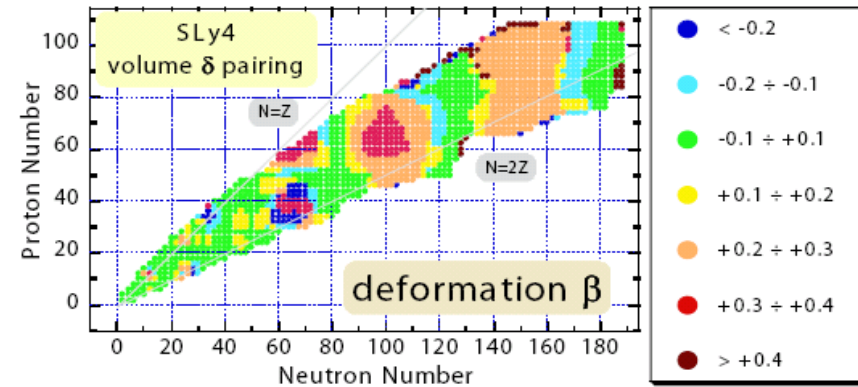
Nuclear deformation



In the case of axial quadrupole deformations:

$$\frac{\delta R}{R} \sim \beta$$

Intrinsic quadrupole moment $\langle Q \rangle \sim \beta$



The gain in energy due to deformation is correlated with the number of protons and neutrons outside closed shells.

There are non-axial deformations:

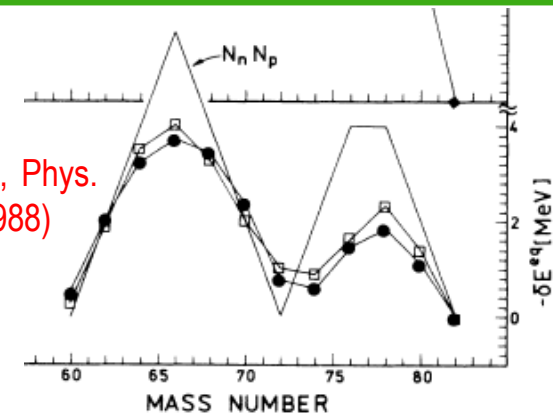
$$\delta R_x = R\left(\frac{\pi}{2}, 0\right) - R_0 = R_0 \sqrt{\frac{5}{4\pi}} \beta \cos\left(\gamma - \frac{2\pi}{3}\right)$$

$$\delta R_y = R\left(\frac{\pi}{2}, \frac{\pi}{2}\right) - R_0 = R_0 \sqrt{\frac{5}{4\pi}} \beta \cos\left(\gamma + \frac{2\pi}{3}\right)$$

$$\delta R_z = R(0, 0) - R_0 = R_0 \sqrt{\frac{5}{4\pi}} \beta \cos \gamma$$

^{A}Ge

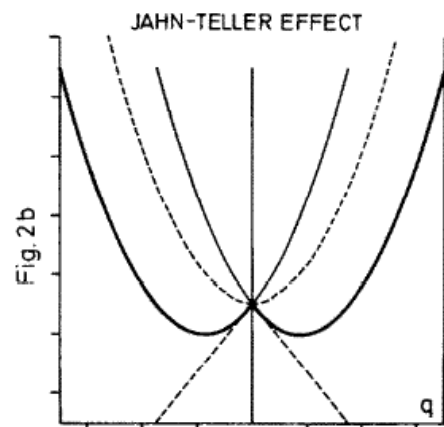
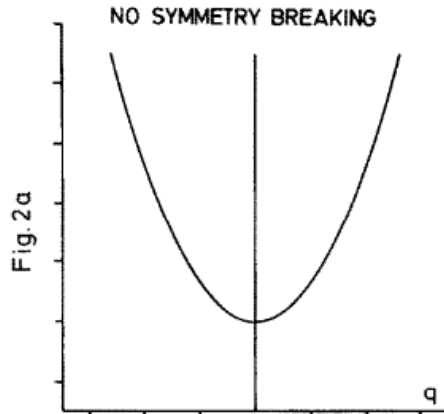
J. Dobaczewski et al., Phys. Rev. Lett. 60, 2254 (1988)



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The nuclear Jahn-Teller effect



In molecules, the coupling with vibrations breaks the degeneracy between electronic states.

In nuclei the **energy scale** is rather different: both **nucleons and shape vibrations are at the MeV scale.**

Nonetheless, in medium-heavy nuclei there are many, almost degenerate single-nucleon levels.

Coupling with shape vibrations can be strong.

In the case of quadrupole vibrations, this has been recognised long ago.

P.-G. Reinhard and E. W. Otten, Nucl. Phys. A 420, 173 (1984)



Octupole correlations/shapes

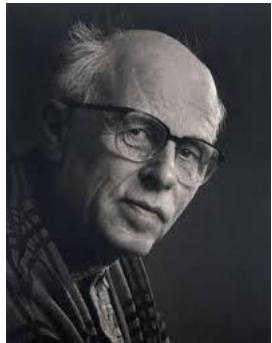
^{224}Ra



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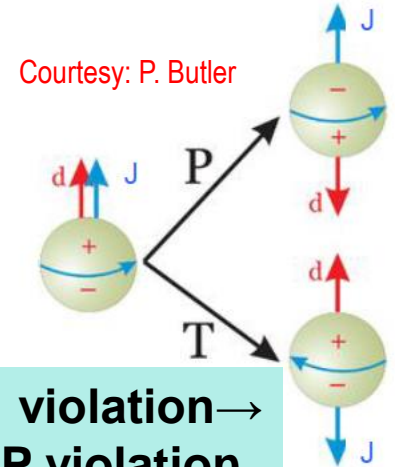
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Tests of the standard model in nuclei

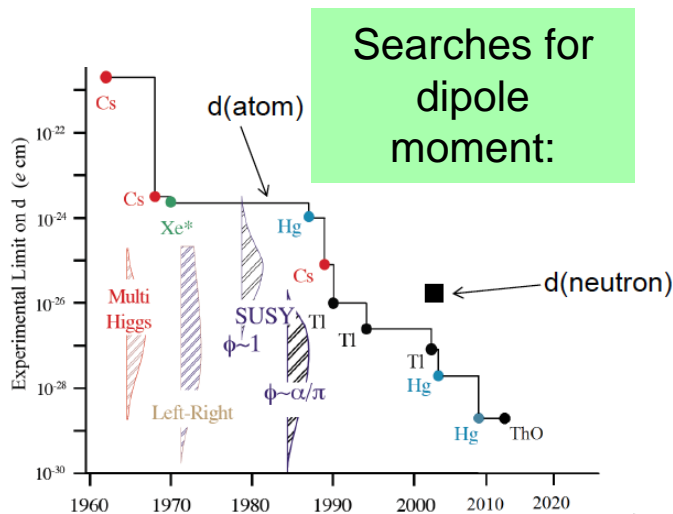


CP violation may be needed to explain matter-antimatter asymmetry. Cf. A. Sacharov.

A static dipole moment violates CP:



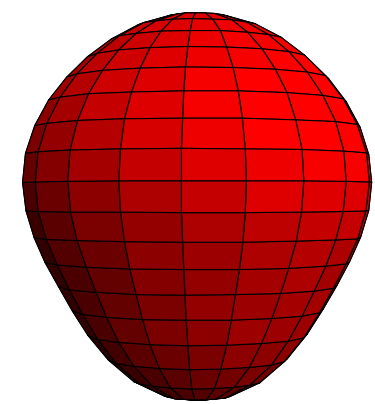
T violation → CP violation



Searches for dipole moment:

Schiff:
If a nucleus is pointlike its dipole moment cancels exactly the electronic dipole moment. ☹️

Pear-shape nucleus:
Something left (quenching may be around 10^{-3}).

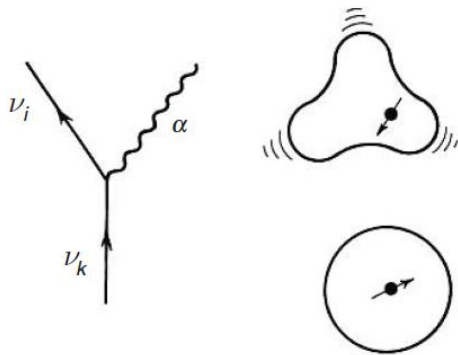


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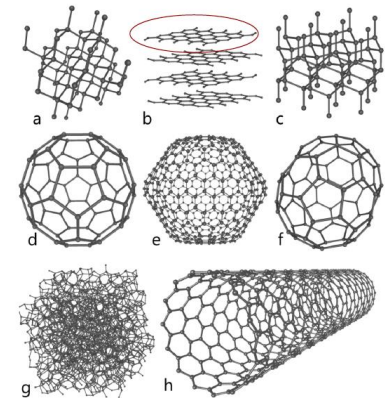
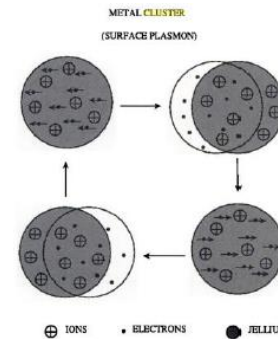
Particle-vibration coupling (PVC): general philosophy

- The basic idea is that in spherical nuclei there are **single-particle states** and (mainly surface) **collective vibrations**. The spectra result from their **interplay**. (Deformed nuclei: particle-rotation coupling).
- **Vibrations = phonons.**
- **Odd nuclei:**
core + 1 particle +
1 particle plus phonon ...



Electron-plasmon coupling

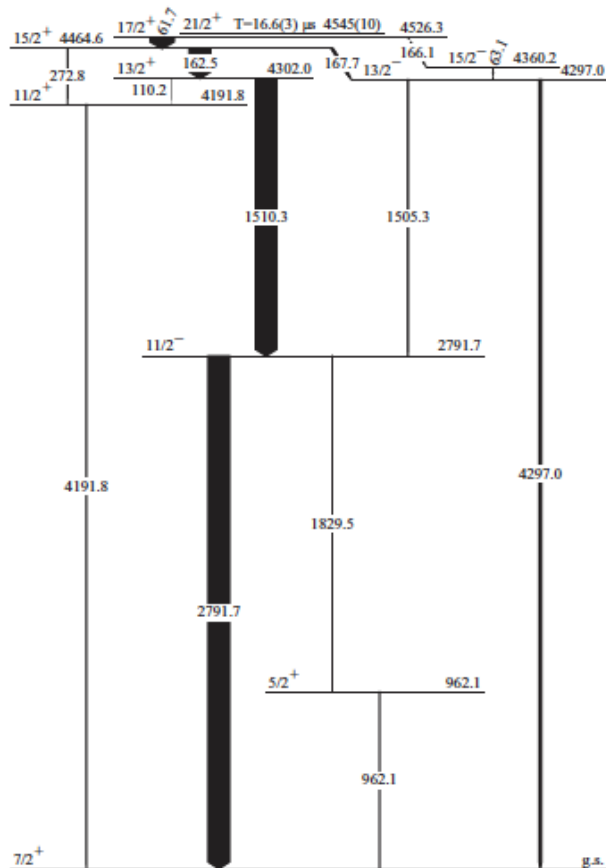
Phonons and Plasmons



(clusters, fullerenes)

Despite the importance of the region around ^{132}Sn , the information about **low-lying states of neighbouring nuclei** need still be completed.

^{133}Sb



- Recently new measurements (G. Bocchi *et al.*) have shed light on some **HIGHER SPIN** states (up to $25/2^+$) in ^{133}Sb .

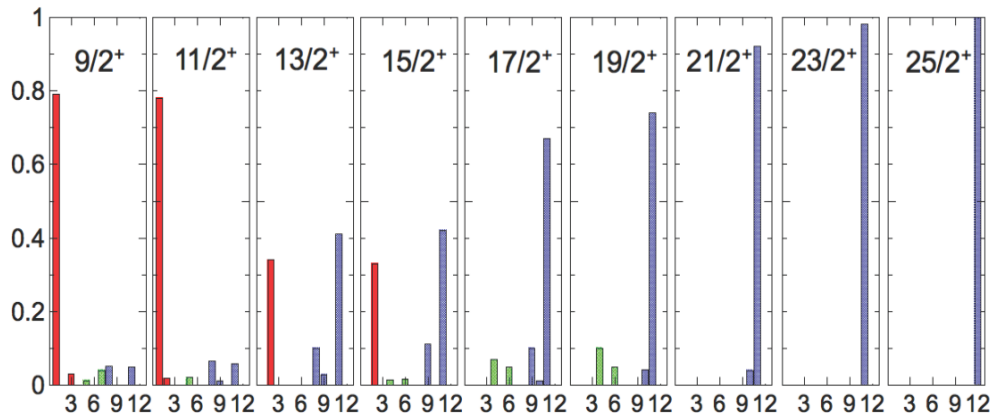
$$B(M1, 15/2^+ \rightarrow 13/2^+) = 0.24 \text{ W.u.}$$

$$B(M1, 13/2^+ \rightarrow 11/2^+) = 0.004 \text{ W.u.}$$

(ratio = 60).

- We have been able to explain this sudden change in a model that takes into account the aforementioned couplings and account for the change of the wave function of the states.





red: $\pi g_{9/2} \otimes 2^+, 4^+$
blue: $\pi g_{9/2} \nu h_{11/2}^{-1} \nu f_{7/2}$

This nature is reflected in the M1 transition probabilities.

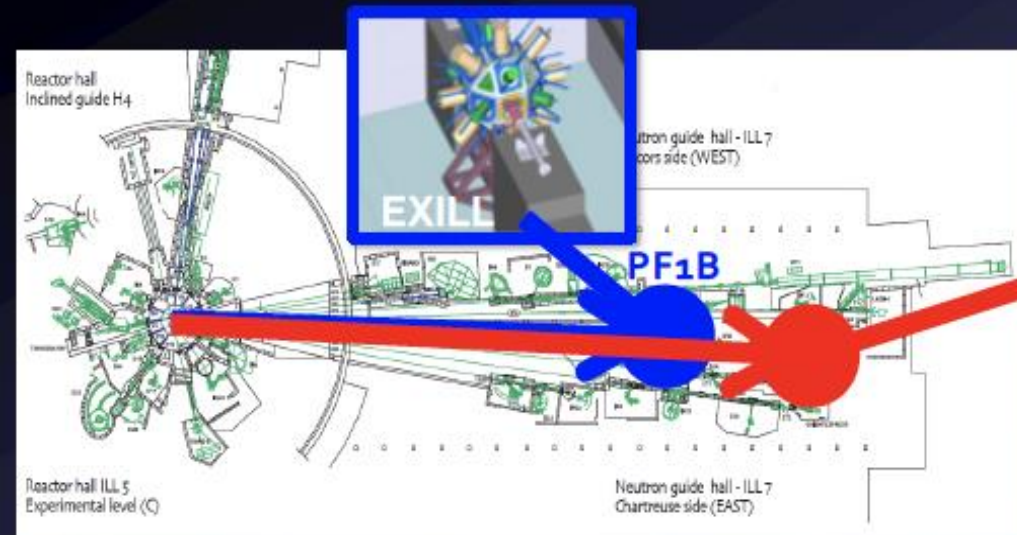
The wave functions of $15/2^+$ and $13/2^+$ are dominated by $g_{9/2}$, $h_{11/2}^{-1} f_{7/2}$, so the $B(M1)$ transition is made up with s.p. amplitudes. $B(M1)_{th} = 0.021 \text{ W.u.}$

In the case of the transition $13/2^+ \rightarrow 11/2^+$, the final state has phonon component so there is a mismatch in the components and $B(M1)$ is quenched, $B(M1)_{th} = 0.001 \text{ W.u. Ratio} = 20.$



Competitive Instrumentation for GAMMA Spectroscopy

Large Germanium Arrays



The EXILL Campaign (2012-2013)

2 Reactor Cycles \approx 100 days > 95% DATA TAKING

The FIPPS Permanent Setup (since 2016)

International Collaboration with 18 Institutions

Courtesy: S. Leoni



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Thank you!



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Backup slides

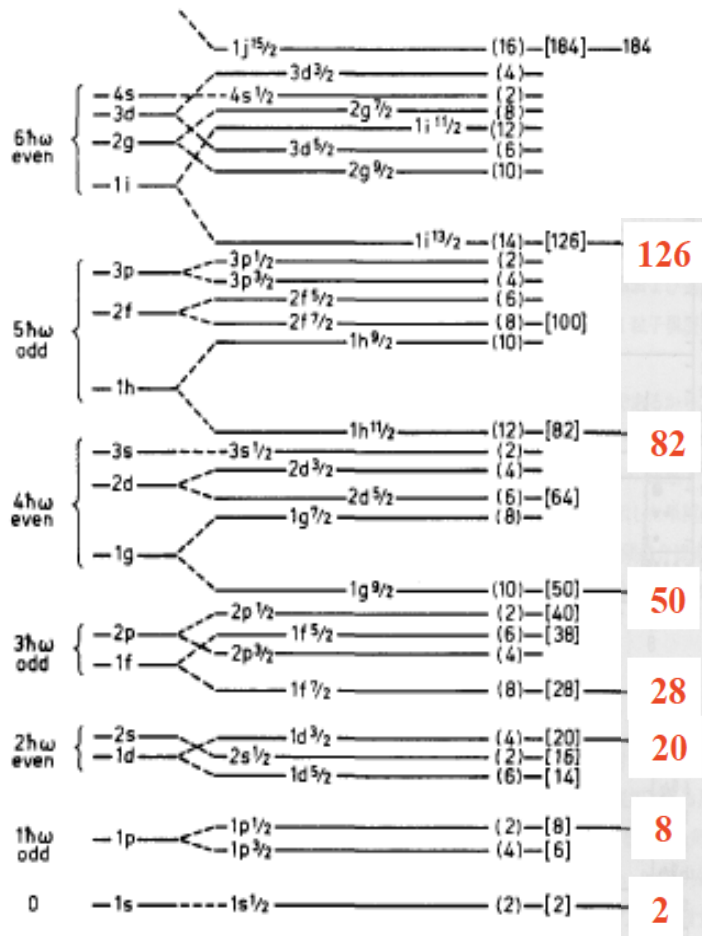


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The nuclear independent particle model

≈ MeV (levels from about -50 MeV)



Many experimental evidences point to the fact that nucleons move in nuclei, to a first approximation, as **independent** particles.

Examples: evidence of shells, ground-state of nuclei around closed shells (¹⁷O with Z=8, N=9 has $J^\pi=5/2^+$) ...



M.G. Mayer,
J.H.D. Jensen



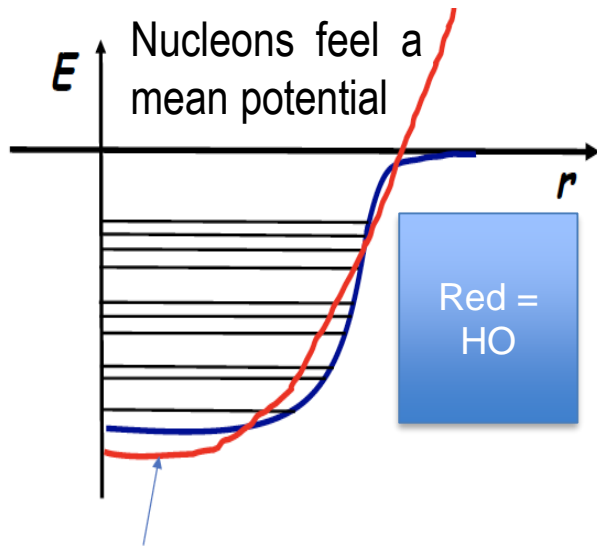
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From mean-field approximation to DFT

Strategies:

1. Start from a two-body (three-body) effective force and define $H = T + V_{\text{eff}}[\rho]$. Write the expectation value on a general Slater determinant.
“DFT is an exactification of Hartree-Fock” (W. Kohn).
2. Write directly the Energy Density Functional (EDF).



$$E = \langle \Psi | \hat{H} | \Psi \rangle \approx \langle \Phi | \hat{H}_{\text{eff}} | \Phi \rangle = E[\hat{\rho}]$$

$|\Phi\rangle$ Slater determinant



The Hohenberg-Kohn theorem (HK)

The original theorem and its proof can be found in P. Hohenberg, W. Kohn, Phys. Rev. 136, B864 (1964)¹. We have in mind a system of **interacting fermions** ($H = T + V$) in some **external potential** V_{ext} .

a) There **exist a functional of the fermion density**

$$E_{V_{\text{ext}}}[\rho] = \langle \Psi | T + V + V_{\text{ext}} | \Psi \rangle = F[\rho] + \int d^3r V_{\text{ext}}(r)\rho(r)$$

and the part denoted by F is universal (for nuclei, it would be the only part).

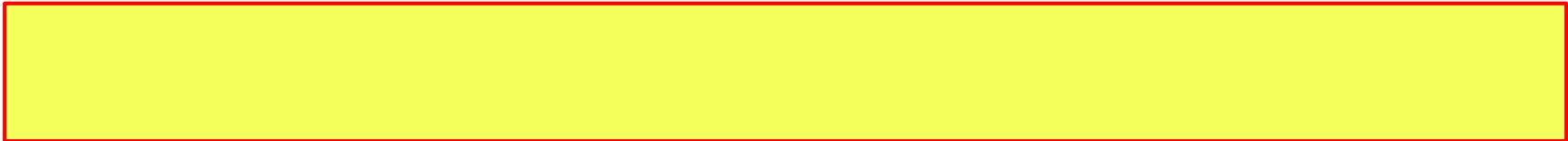
b) It holds:

$$\min_{\Psi} \langle \Psi | T + V + V_{\text{ext}} | \Psi \rangle = \min_{\rho} E_{V_{\text{ext}}}[\rho]$$

or, in other words, at least in principle **this functional has a minimum at the exact ground-state density where it assumes the exact energy as a value.**

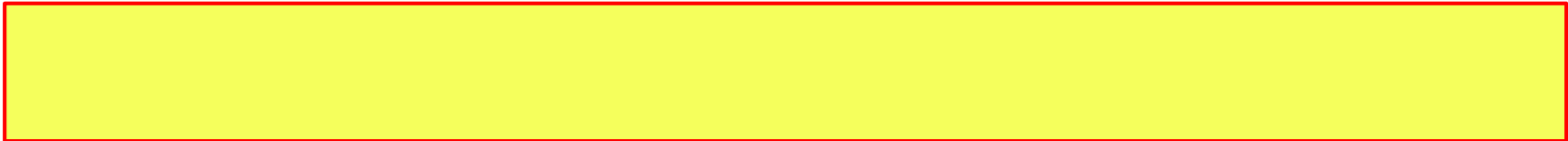
¹ More than 20,000 citations





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A realization: the Kohn-Sham scheme

We assume that the density can be expressed in terms of **single-particle orbitals**, and that the kinetic energy has the simple form:

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r}) \quad T = \sum_i \int d^3r \phi_i^*(\vec{r}) \left(-\frac{\hbar^2 \nabla_i^2}{2m} \right) \phi_i(\vec{r})$$

We have said that the energy must be minimized, but we add a constraint associated with the fact that we want **orbitals that form an orthonormal set** (Lagrange multiplier)

$$E - \sum_i \varepsilon_i \int d^3r \phi_i^*(\vec{r})\phi_i(\vec{r}) = T + F[\rho] + \int d^3r V_{\text{ext}}(\vec{r})\rho(\vec{r}) - \sum_i \varepsilon_i \int d^3r \phi_i^*(\vec{r})\phi_i(\vec{r})$$

The variation of this quantity, $\delta(\dots) = 0$ produces a Schrödinger-like equation:

$$\left(-\frac{\hbar^2 \nabla_i^2}{2m} + \frac{\delta F}{\delta \rho} + V_{\text{ext}} \right) \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r})$$

$$h\phi_i = \varepsilon_i \phi_i$$



The good, the bad and the ugly !

- The HK theorem has been **generalised** in (almost all) possible ways: degenerate ground-state, magnetic systems (**m** or spin densities), finite temperature, relativistic case ... (the list might be not exhaustive).
- **In all cases one then build the energy functional **E** and tries to find a minimum.**
- Kohn-Sham is a widely used scheme.
- Several algorithms.
- Then, all quantities are in principle given (!).
- **The REAL weak point is that the various proofs of HK theorems do not give any clue on HOW to build the functional **F**.**
- **There are many realizations of such theory and no obvious route for systematic improvement.**

One must use the functional derivative:

$$F[\rho] = \int d^3r \rho(r) f(r) \Rightarrow \frac{\delta F}{\delta \rho(r)} = f(r)$$



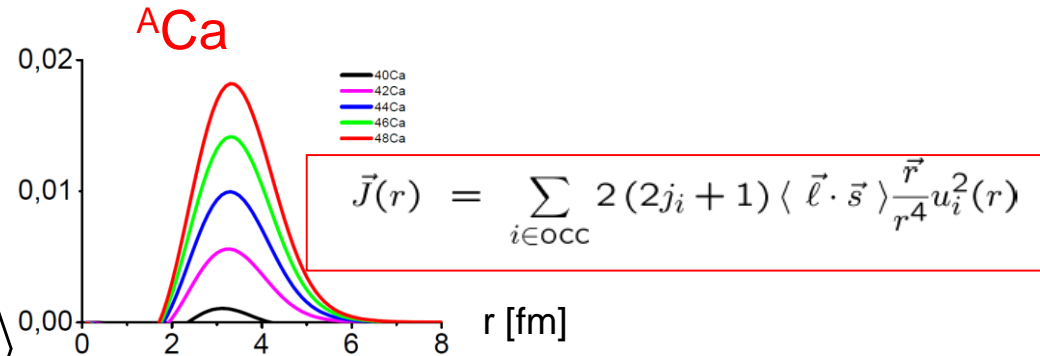
Realistic functionals

- One has to consider **several possible densities** (including spin densities, isospin densities, gradients ...).

$$\vec{\nabla} \rho$$

$$\tau = \sum_i |\vec{\nabla} \phi_i|^2$$

$$\vec{J} = \sum_{i, \sigma, \sigma'} \phi_i^\dagger \vec{\nabla} \phi_i \times \langle \sigma' | \vec{\sigma} | \sigma \rangle$$



- **Functionals will include all possible scalars made up with these quantities that respect the symmetries of the systems.**



(translations, Galilean boosts, rotations, parity and time-reversal)

- There exist relativistic functionals.



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The Skyrme force

attraction

$$\begin{aligned}\hat{v}_{\text{Sk}}(\mathbf{r}_{12}) = & \underbrace{t_0(1 + x_0 \hat{P}_\sigma) \delta(\mathbf{r}_{12})}_{\text{attraction}} + \frac{1}{2} \underbrace{t_1(1 + x_1 \hat{P}_\sigma) (\hat{k}^{\dagger 2} \delta(\mathbf{r}_{12}) + \delta(\mathbf{r}_{12}) \hat{k}^2)}_{\text{attraction}} \\ & + \underbrace{t_2(1 + x_2 \hat{P}_\sigma) \hat{k}^\dagger \cdot \delta(\mathbf{r}_{12}) \hat{k}}_{\text{attraction}} + \frac{1}{6} \underbrace{t_3(1 + x_3 \hat{P}_\sigma) \delta(\mathbf{r}_{12}) \rho^\alpha \left(\frac{r_1 + r_2}{2} \right)}_{\text{short-range repulsion}} \\ & + iW_0(\hat{\sigma}_1 + \hat{\sigma}_2) \cdot \hat{k}^\dagger \times \delta(\mathbf{r}_{12}) \hat{k}.\end{aligned}$$

short-range repulsion

$$\mathbf{k} = \frac{i}{2} (\vec{\nabla}_1 - \vec{\nabla}_2)$$

- There are velocity-dependent terms which mimic the finite-range. They are related to m^* .
 - The last term is a zero-range spin-orbit.
 - In total: **10 free parameters** to be fitted (typically).



Time-dependent DFT

$$h\phi_i = \varepsilon_i\phi_i$$

In the time-dependent case, one can solve the evolution equation for the density directly:

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

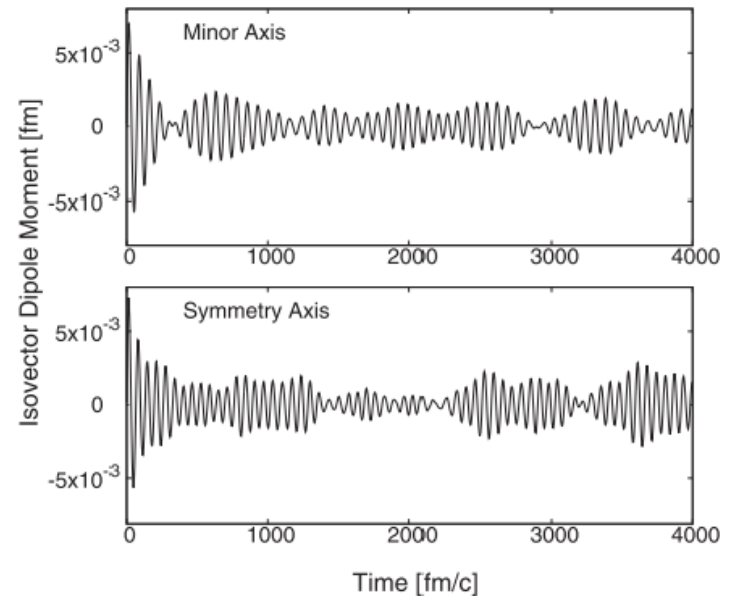
$$\rho(t=0) \neq \rho_{\text{g.s.}}$$

$$\rho(t = \Delta t) = U(t = 0, t = \Delta t)\rho(t = 0)$$

$$U = e^{-i\frac{\Delta t}{\hbar} \cdot h}$$

Often the equation for the density is linearized and solved on a basis (**Random Phase Approximation or RPA**).

From: P. Stevenson (U. Surrey)

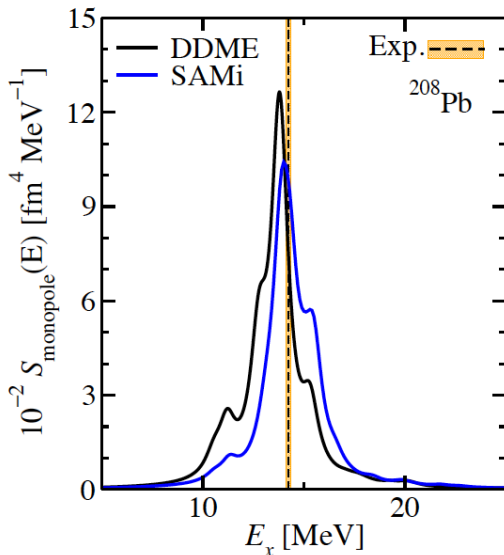


The FT will give the energy of the mode(s).



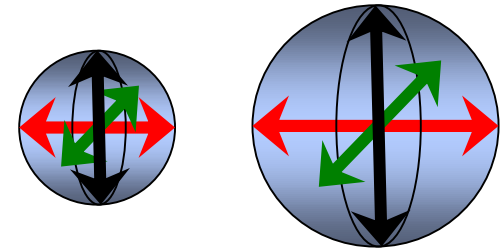
The Giant Monopole Resonance and EoS

One further example of study which is not carried out for mere “academic purposes”, but to shed light on more general properties of nature...



Breathing mode: in this case its energy is correlated with the **compressibility** of nuclear matter.

$$\chi \equiv -\frac{1}{\Omega} \left(\frac{\partial P}{\partial \Omega} \right)^{-1}$$



We better consider the density as a variable.

$$\rho = \frac{A}{\Omega}$$

Incompressibility:

$$\chi^{-1} = \rho^3 \frac{d^2}{d\rho^2} \left(\frac{E}{A} \right)$$

$$K_\infty = 9\rho_0^2 \frac{d^2}{d\rho^2} \left(\frac{E}{A} \right)_{\rho=\rho_0}$$

(around 240 MeV)

SN1987a



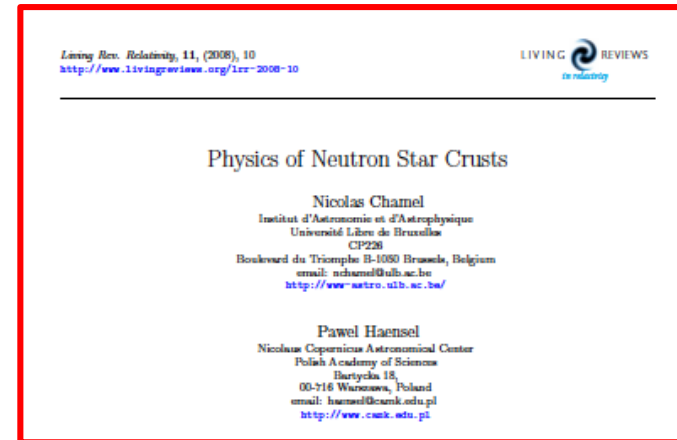
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Neutron stars

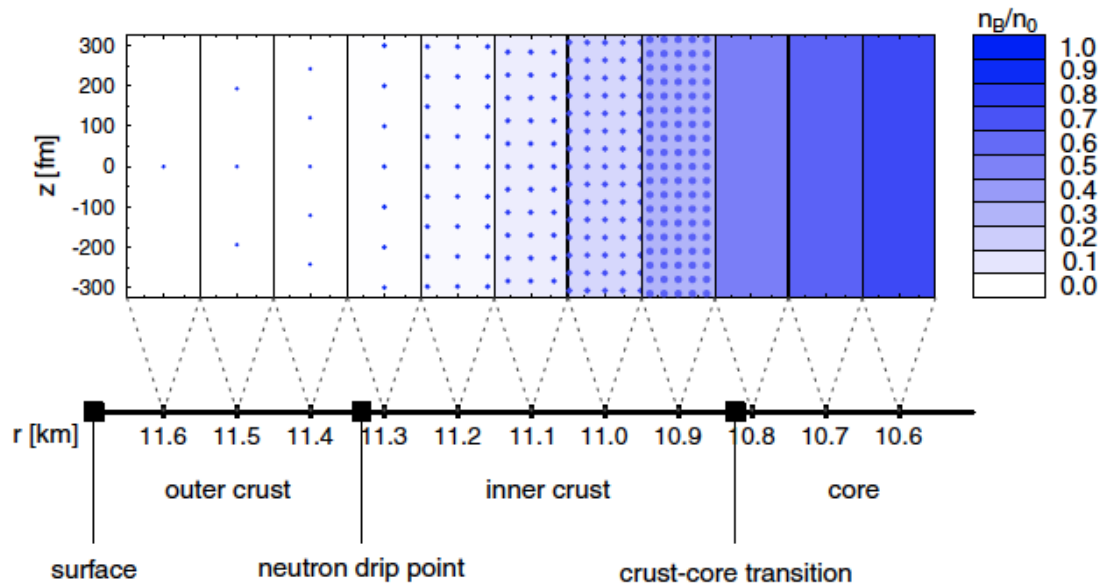
$$B(N, Z) = a_V A - a_S A^{2/3} - a_A \frac{(N - Z)^2}{A} - a_C \frac{Z^2}{A^{1/3}} + \delta + \frac{3}{5} \frac{GM^2}{R} + \frac{3}{5} \frac{Gm^2 A^2}{r_0 A^{1/3}}$$

- A bound system of neutrons can exist due to the gravitational force if the number of neutrons is large enough ($\approx 10^{55}$ - 10^{56}).
- Neutron stars observed much later than they were postulated.
- Now some properties are observed (masses and, to a lesser extent: radii, magnetic field, thermal properties...).



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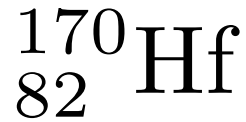
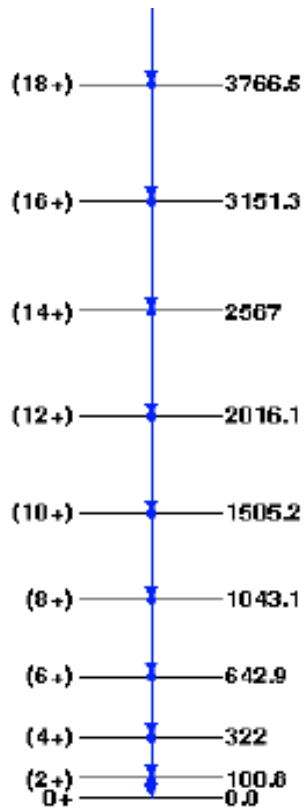
M. Oertel, *et al.*, Rev. Mod. Phys. 89, 015007 (2017)



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Symmetry breaking and restoration



$$E = \frac{\hbar^2}{2\mathcal{I}} J(J + 1)$$

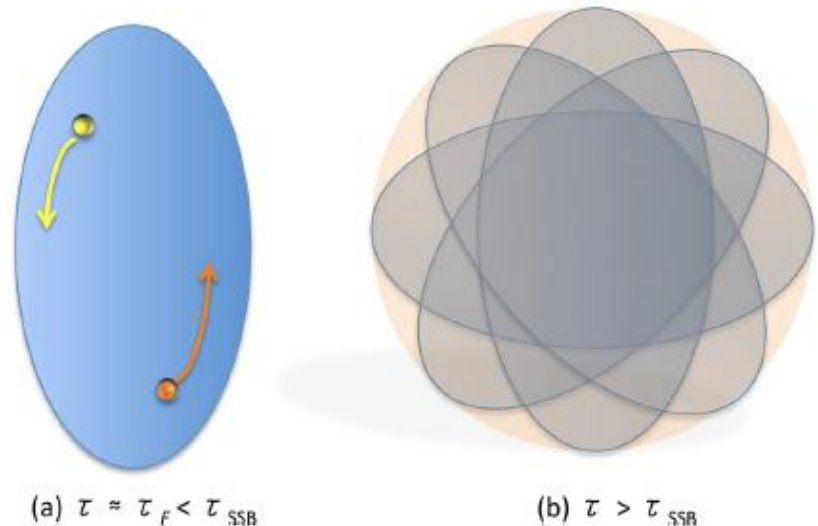
$$\tau_{\text{SSB}} \sim \frac{\hbar}{E}$$

$$\hbar = 6.6 \cdot 10^{-22} \text{ MeV} \cdot \text{s}$$

Rotational motion restores the symmetry in the lab system.

This may happen on a time scale which is significantly larger than

$$\tau_F \sim 10^{-22} \text{ s}$$



From: T. Nakatsukasa



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