Nuclear structure II:
Light and medium nuclei

Stefano Gandolfi

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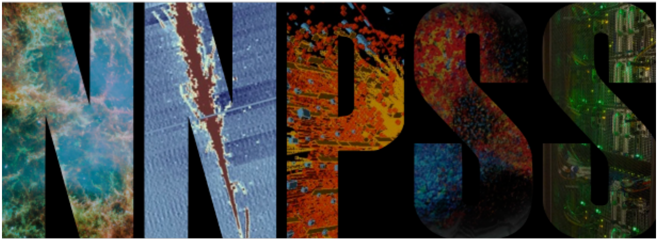

National Nuclear Physics Summer School
Massachusetts Institute of Technology (MIT)
July 18-29, 2016

Fundamental questions in nuclear physics

Physics of nuclei:

- How do nucleons interact?
- How are nuclei formed? How can their properties be so different for different A?
- What's the nature of closed shell numbers, and what's their evolution for neutron rich nuclei?
- What is the equation of state of dense matter?
- Can we describe simultaneously 2, 3, and many-body nuclei?

Many-body methods

First: How to solve the many-body Schroedinger equation?

Many methods (with pros. and cons.) available on the market.
A very incomplete list:

- Quantum Monte Carlo methods, VMC, GFMC, AFDMC, lattice EFT
- Coupled cluster (CC)
- No core shell model (NCSM), and importance truncated (IT)-NCSM
- Many body perturbation theory (MBPT)
- In-medium Similarity Renormalization Group (IM-SRG)

... and several techniques used to make the Hamiltonian softer:

- Lee-Suzuki
- Similarity Renormalization Group (SRG)
- low momentum potentials (V_{low-k})

Many of these methods are also used in other fields.

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Let me spend few slides on my favorite ones: **VMC, GFMC, AFDMC**

Three slides on Monte Carlo integration (1/3)

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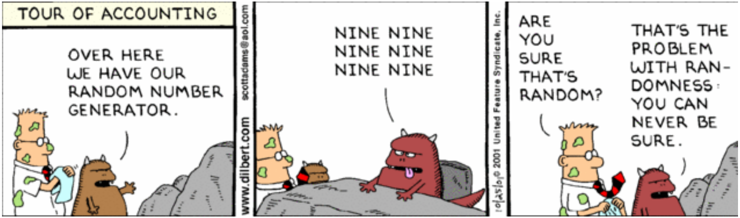

Three slides on Monte Carlo integration (2/3)

Suppose that we want to calculate some integral of dimension D. The easiest thing to do is a sum over discrete intervals h, something like

$$I = \int_a^b dx_1 \ldots \int_a^b dx_D f(x_1 \ldots x_D) \approx h^D \sum f(x_1 \ldots x_D)$$

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$$N = \epsilon^{-D}$$

so, for $\epsilon = 0.1$ and a system with 20 particles ($D = 60$) we have to sum $N = 10^{60}$ points.

With the best available supercomputers the time needed is greater than the age of the universe!

Let's have random numbers x distributed with probability $P(x)$ with

$$P(x) \geq 0\,, \qquad \text{and} \qquad \int P(x)dx = 1\,.$$

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Central limit *theorem:* if $N \to \infty$ and for any $P(x)$, we have that

$$P(S_N) = \frac{1}{\sqrt{2\pi\sigma_N}} e^{-\frac{(S_N - <f>)^2}{2\sigma_N}}$$

where

$$<f>= \int f(x)P(x)dx\,, \qquad \sigma_N = \frac{1}{N-1}\int f^2(x)P(x)dx - <f>^2\,.$$

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Integrals can be solved by sampling points distributed with $P(x)$:

$$\int F(x)dx = \int \frac{F(x)}{P(x)}P(x)dx = \int f(x)P(x)dx$$

Variational Monte Carlo

We want to solve

$$E_0 \leq E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int dr_1 \ldots dr_N \, \psi^*(r_1 \ldots r_N) H \psi(r_1 \ldots r_N)}{\int dr_1 \ldots dr_N \, \psi^*(r_1 \ldots r_N) \psi(r_1 \ldots r_N)}$$

$$= \frac{\int dR \, P(R) \frac{H\psi(R)}{\psi(R)}}{\int dR \, P(R)}$$

where $P(R) = \psi^*(r_1 \ldots r_N)\psi(r_1 \ldots r_N)$.

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where $P(R) = \psi^*(r_1 \dots r_N)\psi(r_1 \dots r_N)$. Variational wave function:

$$|\Psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] \left[\prod_{i<j<k} f_c(r_{ijk})\right] \left[1 + \sum_{i<j,p} \prod_k u_{ijk} f_p(r_{ij}) O_{ij}^p\right] |\Phi\rangle$$

where O^p are spin/isospin operators, f_c, u_{ijk} and f_p are obtained by minimizing the energy. About 30 parameters to optimize.

$|\Phi\rangle$ is a mean-field component.

Quantum Monte Carlo (1/3)

Propagation in imaginary time:

$$H\,\psi(\vec{r}_1\ldots\vec{r}_N)=E\,\psi(\vec{r}_1\ldots\vec{r}_N)\qquad \psi(t)=e^{-(H-E_T)t}\psi(0)$$

Ground-state extracted in the limit of $t\to\infty$:

$$\psi(t)=e^{-(H-E_T)t}\psi(0)=\sum_n e^{-(H-E_T)t}\phi_n=\sum_n e^{-(E_n-E_T)t}\phi_n\to c_0\phi_0$$

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then:

$$\langle R'|\psi(t)\rangle = \int dR\,G(R,R',t)\langle R|\psi(0)\rangle$$

where $G(R,R',t)$ is the propagator of the Hamiltonian.

Quantum Monte Carlo (2/3)

Let's define the propagator as the matrix element between two points in the volume:

$$G(R,R',t)=\langle R'|e^{-(H-E_T)t}|R\rangle$$

The expression above is very difficult to calculate. What is easy instead is:

$$G(R,R',t)\approx\prod_n G(R_n,R_{n-1},\Delta t)\approx\left[e^{-T\Delta t}e^{-V\Delta t}\right]^n$$

and $\langle R'|e^{-T\Delta t}e^{-V\Delta t}|R\rangle$ is easy to sample.

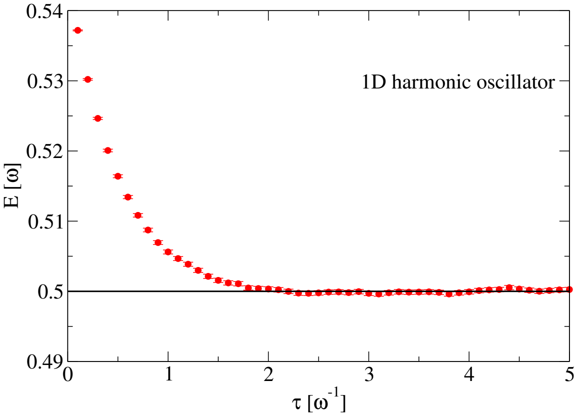
Then we need to iterate the integral in previous slide many times to reach the limit $t\to\infty$.

Other more details (importance sampling, sign problem, ...), ask if interested!

Ground–state obtained in a **non-perturbative way.** Systematic uncertainties within 1-2 %.

Quantum Monte Carlo (3/3)

An example: 1D harmonic oscillator, projection in imaginary time.
Energy as a function of the imaginary time τ:



Ground-state resolved!

Recap:

- Hamiltonian: phenomenological, AV8$'$ and AV18 + three-body forces, or chiral EFT (local versions), Gezerlis *et al.* PRL 111,032501 (2013), PRC 90, 054323 (2014), Lynn *et al.* PRL 116, 062501 (2016).
- Many body machinery: GFMC and AFDMC, Carlson *et al.* RMP 87, 1067 (2015).

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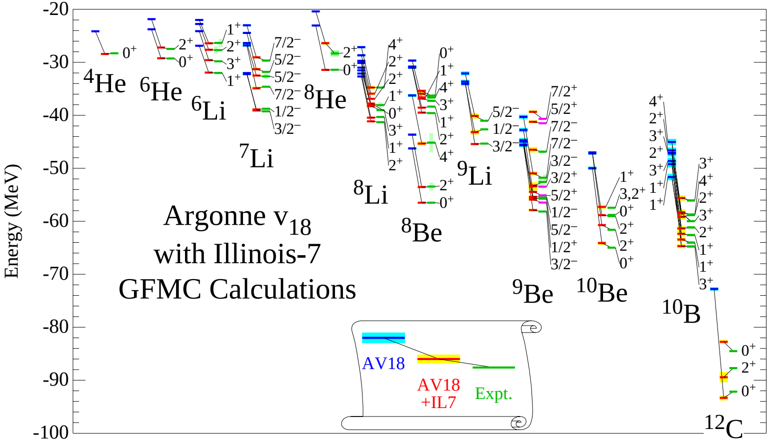
LET'S DO PHYSICS!!!

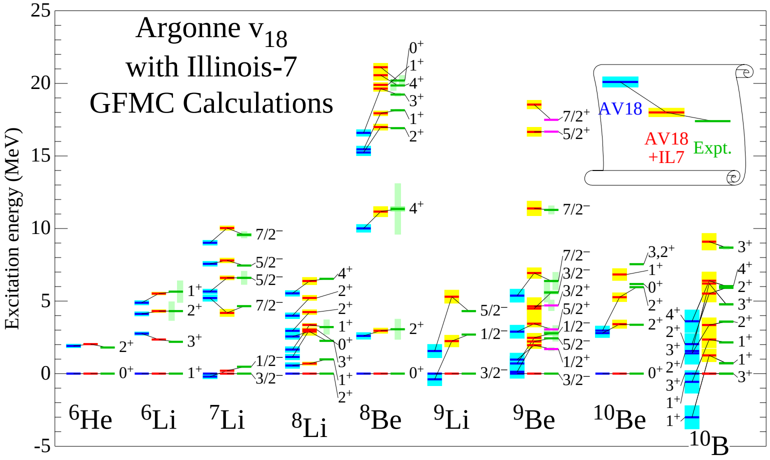
Light nuclei spectrum computed with GFMC



Carlson, *et al.*, Rev. Mod. Phys. 87, 1067 (2015)

Note the importance of three-body force!

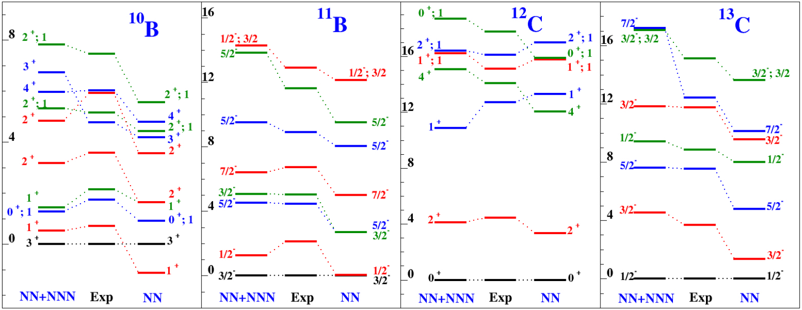
Light nuclei excited states computed with GFMC



Carlson, *et al.*, Rev. Mod. Phys. 87, 1067 (2015)

Again, three-body force essential in many cases!

NCSM calculation

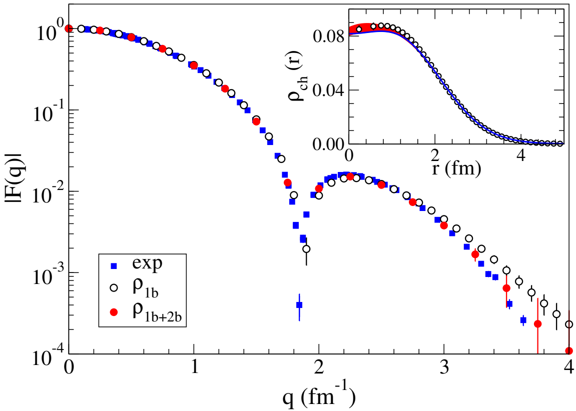


P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, PRL 99, 042501(2007)

Hamiltonian: NN at N^{3}LO (Entem, Machleidt) and NNN at N^{2}LO (Navratil)

Charge form factor of ^{12}C

$$|F(q)| = \langle \psi | \rho_q | \psi \rangle \qquad \rho_q = \sum_i \rho_q(i) + \sum_{i<j} \rho_q(ij)$$



Lovato, Gandolfi, Butler, Carlson, Lusk, Pieper, Schiavilla, PRL (2013)

Energy, rms radii, and magnetic moment of light nuclei

	E (MeV)		r_p $[r_n]$ (fm)			μ (μ_N)	
$^AZ(J^\pi;T)$	GFMC	exp.	GFMC		exp.	GFMC	exp.
^{2}H$(1^+;0)$	-2.225	-2.2246	1.98		1.96	0.8604	0.8574
^{3}H$(\frac{1}{2}^+;\frac{1}{2})$	-8.47(1)	-8.482	1.59	[1.73]	1.58	2.960(1)	2.979
^{3}He$(\frac{1}{2}^+;\frac{1}{2})$	-7.72(1)	-7.718	1.76	[1.60]	1.76	-2.100(1)	-2.127
^{4}He$(0^+;0)$	-28.42(3)	-28.30	1.43		1.462(6)		
^{6}He$(0^+;1)$	-29.23(2)	-29.27	1.95(3)	[2.88]	1.93(1)		
^{6}Li$(1^+;0)$	-31.93(3)	-31.99	2.39		2.45(4)	0.835(1)	0.822
^{7}He$(\frac{3}{2}^-;\frac{3}{2})$	-28.74(3)	-28.86	1.97	[3.32(1)]			
^{7}Li$(\frac{3}{2}^-;\frac{1}{2})$	-39.15(3)	-39.25	2.25	[2.44]	2.31(5)	3.24(1)	3.256
^{7}Be$(\frac{3}{2}^-;\frac{1}{2})$	-37.54(3)	-37.60	2.51	[2.32]	2.51(2)	-1.42(1)	-1.398(15)
^{8}He$(0^+;2)$	-31.42(3)	-31.40	1.83(2)	[2.73]	1.88(2)		
^{8}Li$(2^+;1)$	-41.14(6)	-41.28	2.10	[2.46]	2.20(5)	1.48(2)	1.654
^{8}Be$(0^+;0)$	-56.5(1)	-56.50	2.40(1)				
^{8}B$(2^+,1)$	-37.51(6)	-37.74	2.48	[2.10]		1.11(2)	1.036
^{8}C$(0^+;2)$	-24.53(3)	-24.81	2.94	[1.85]			
^{9}Li$(\frac{3}{2}^-,\frac{3}{2})$	-45.42(4)	-45.34	1.96	[2.33]	2.11(5)	3.39(4)	3.439
^{9}Be$(\frac{3}{2}^-,\frac{1}{2})$	-57.9(2)	-58.16	2.31	[2.46]	2.38(1)	-1.29(1)	-1.178
^{9}C$(\frac{3}{2}^-,\frac{3}{2})$	-38.88(4)	-39.04	2.44	[1.99]		-1.35(4)	-1.391
^{10}Be$(0^+;1)$	-64.4(2)	-64.98	2.20	[2.44]	2.22(2)		
^{10}B$(3^+;0)$	-64.7(3)	-64.75	2.28		2.31(1)	1.76(1)	1.801
^{10}C$(0^+;1)$	-60.2(2)	-60.32	2.51	[2.25]			
^{12}C$(0^+;0)$	-93.3(4)	-92.16	2.32		2.33		

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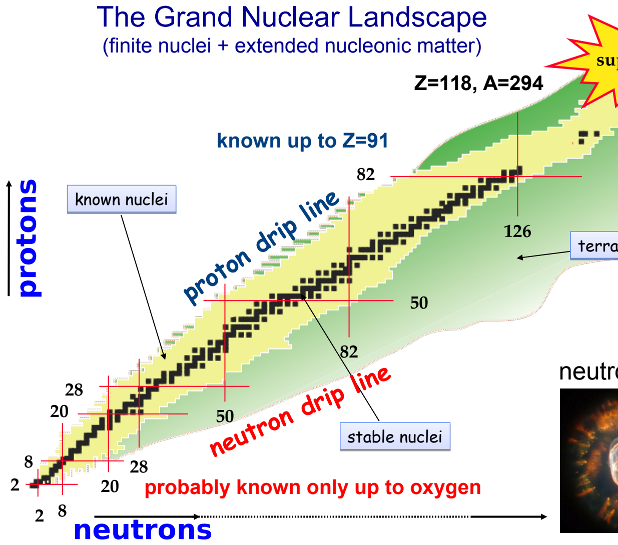
A bigger picture

Credit: Witek Nazarewicz



neutron stars

The nuclear shell model

Clear experimental evidence of magic numbers.

N or $Z = 2, 8, 20, 28, 50, 82, 126$

Signatures (incomplete list) of properties of magic nuclei:

- Nuclei very stable (long lasting)
- Large separation energy (energy needed to extract a nucleon)
- Neutron-capture cross-sections very low (nuclei like to stay in those configurations)

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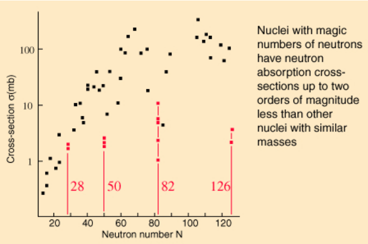

hyperphysics.phy-astr.gsu.edu

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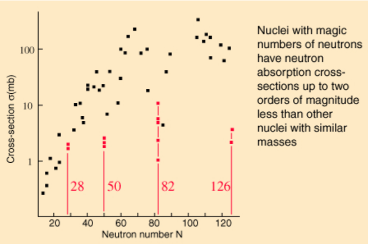

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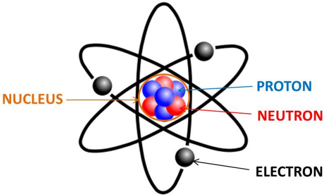
Another similarity in nature: atoms!



The nuclear shell model

Atoms:

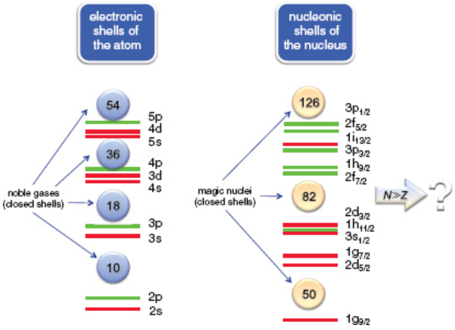
Closed shells: high ionization energy needed to remove an e^-

Potential: Coulomb among electrons, and between electrons and a point-like nucleus (plus spin-orbit)

Nuclei:

Magic nuclei: Large separation energy

Potential: Nuclear forces among nucleons and Coulomb repulsion between protons. "Self-bound"



The shell model

Let's assume:

- The potential acting on a single nucleon is generated from the other (A-1) nucleons
- The potential is proportional to the density, $V(r) \propto \rho(r)$
- Spherical symmetry: the w.f. can be factorized as $\psi(\vec{r}) = R_{nl}(r)\, Y_l^m(\theta, \phi)$

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Let's try with the Harmonic Oscillator potential:

$$E = \left(N + \frac{3}{2}\right)\hbar\omega = \left[2(n-l) + l + \frac{3}{2}\right]\hbar\omega$$

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Shells:

N	nl	states	total states
0	1s	2	2
1	1p	6	8
2	1d	10	18
2	2s	2	20
3	1f	14	34
3	2p	6	40
4	1g	18	58
4	2d	10	68
4	3s	2	70
...	...	...	...

Observed shell numbers: 2,8,20,28,50,82

$$E = \left(N + \frac{3}{2}\right)\hbar\omega = \left[2(n-l) + l + \frac{3}{2}\right]\hbar\omega$$

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What about the others???

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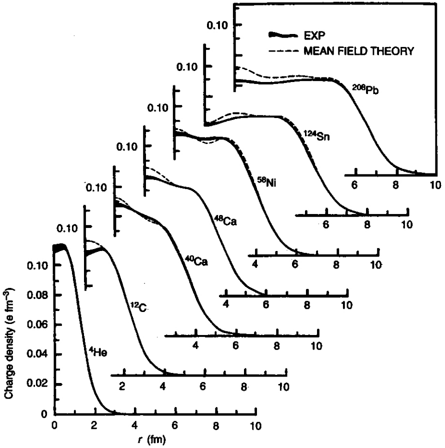
Nuclear densities

Observed and calculated charge densities:



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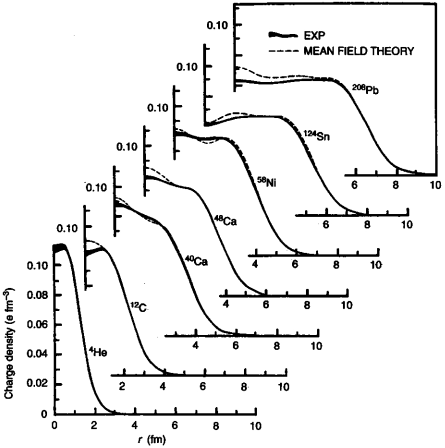

"Flat" region needed in the center for medium and large nuclei.

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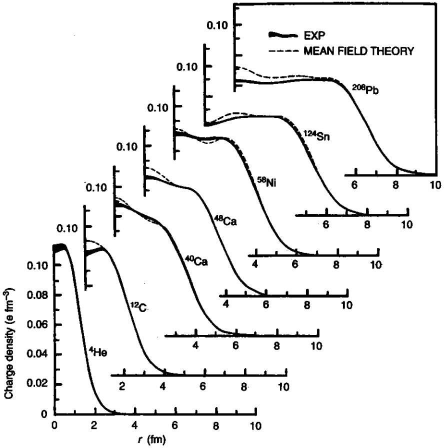


"Flat" region needed in the center for medium and large nuclei.

Harmonic Oscillator **qualitatively** good only for small nuclei!

Wood-Saxon potential:

density described by the Fermi-distribution:

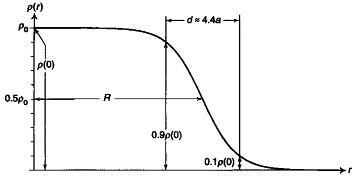
$$v(r) = \frac{-V_0}{1 + e^{(r-R)/a}}$$

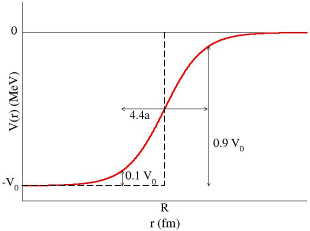
typical values:

$V_0 \simeq 50\text{MeV}$,

$R \simeq 1.27\text{fm}A^{1/3}$,

$a \simeq 0.67\text{fm}$.





Wood-Saxon potential and spin-orbit coupling

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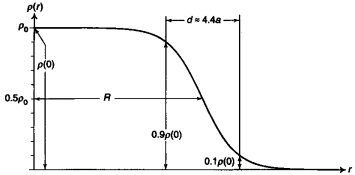
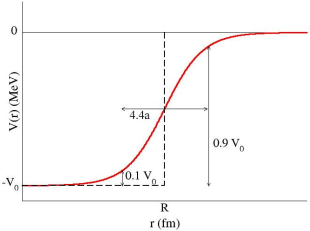
$\rightarrow$ L-S coupling:

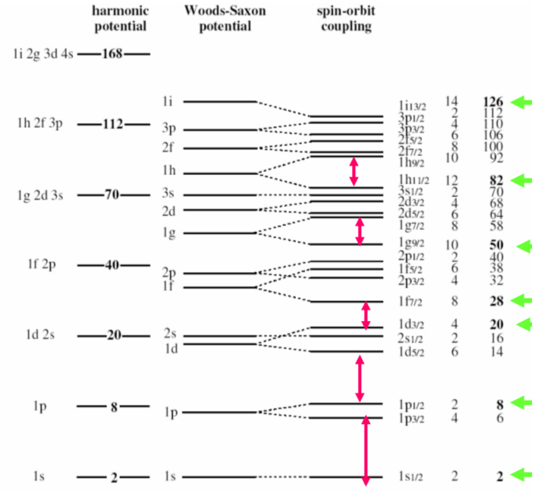
the energy levels of nuclei strongly depend to the spin S.

$$\vec{J} = \vec{L} + \vec{S}, \qquad (\text{cf. atoms } \vec{j} = \vec{l} + \vec{s})$$





Magic numbers finally explained!



Observed shell numbers: 2,8,20,28,50,82,126!

Wigner, Geoppert-Mayer, Jensen, Nobel Prize in 1963.

Magic numbers

Magic numbers explain a lot of stable configurations, high separation energies, low cross-sections, quadrupole deformations, etc.

End of the story??? Of course not!

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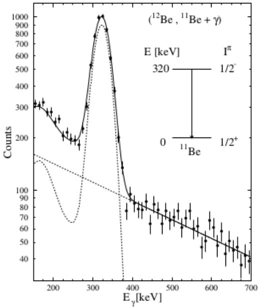
$Z = 4$, $N = 8$ $(1s_{1/2}, 1p_{3/2}, 1p_{1/2})$
Experimentally it has been demonstrated that there is a strong $2s_{1/2}$ component in the ground state *and hence the breakdown of the N=8 shell closure*.

Navin et al., PRL 85, 266 (2000).



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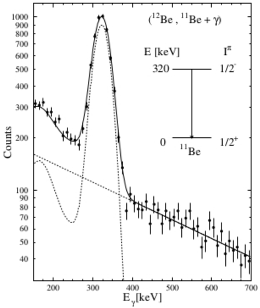

There are many other examples where magic numbers disappear for particular Z or N. Also some evidence of new magic numbers!

The drip line

From Wikipedia:

> *The nuclear drip line is the boundary delimiting the zone in which atomic nuclei lose stability due to the transmutation of neutrons, causing an isotope of one element to mutate into an element with one more proton.*

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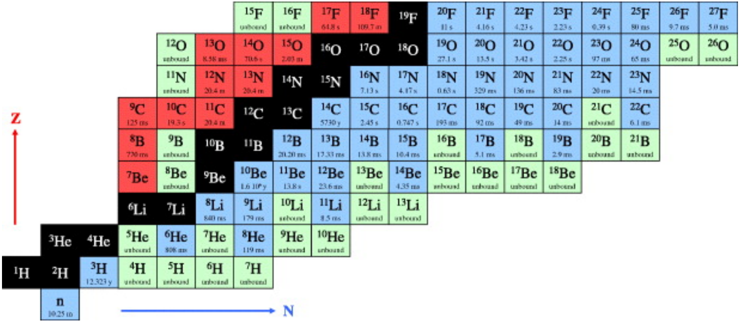
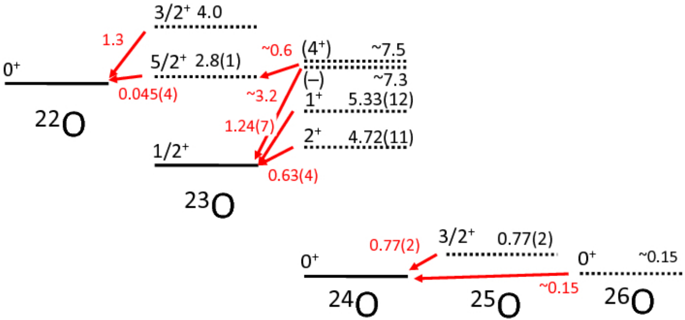


Example, Z=8 (Oxygen) drip line:



M. Thoennessen, et al., Acta Phys. Pol. B 44, 543 (2013)

The Oxygen dripline

Effect of three-body forces to the drip line of Oxygen:

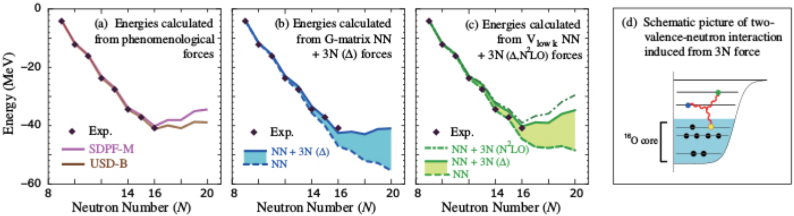
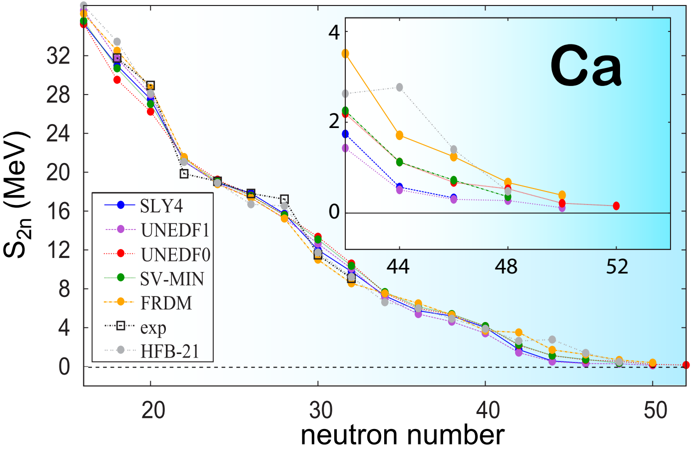


FIG. 4 (color online). Ground-state energies of oxygen isotopes measured from ^{16}O, including experimental values of the bound 16–24 O. Energies obtained from (a) phenomenological forces SDPF-M [13] and USD-B [14], (b) a G matrix and including FM $3N$ forces due to Δ excitations, and (c) from low-momentum interactions $V_{\text{low }k}$ and including chiral EFT $3N$ interactions at N^2LO as well as only due to Δ excitations [25]. The changes due to $3N$ forces based on Δ excitations are highlighted by the shaded areas. (d) Schematic illustration of a two-valence-neutron interaction generated by $3N$ forces with a nucleon in the ^{16}O core.

Otsuka, et al., PRL, 105, 032501 (2010).

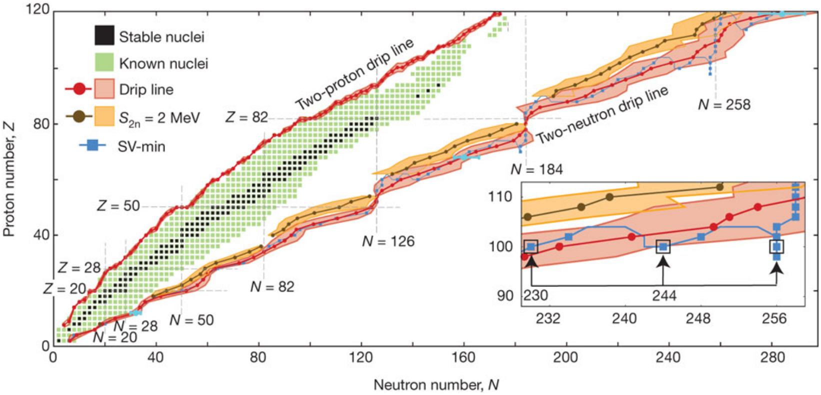
Example, theoretical prediction of Z=20 (Calcium) drip line:



Forssén, et al., Phys. Scr. T152, 014022 (2013).

The bigger picture

Theoretical prediction of nuclear drip lines:



Erler, et al., Nature 486, 509 (2012).

Facility for Rare Isotope Beams: Program

Properties of atomic nuclei

- Develop a predictive model of nuclei and their interactions
- Detailed study of nuclear structure relevant to symmetries tests (DBD, etc.)

Astrophysics: Nuclear processes in the cosmos

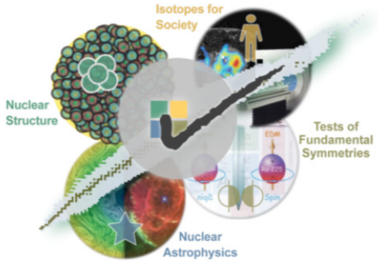
- Origin of the elements, chemical history
- Explosive environments: novae, supernovae, X-ray bursts …
- Properties of neutron stars

Fundamental Symmetries

- Effects of symmetry violations are amplified in certain nuclei
- Example: Enhanced EDM searches

Societal applications and benefits

- Medicine, energy, material sciences, …



FRIB Facility for Rare Isotope Beams
U.S. Department of Energy Office of Science
Michigan State University

Sherrill - Fundamental Symmetry Tests with Rare Isotopes 2014, Slide 4

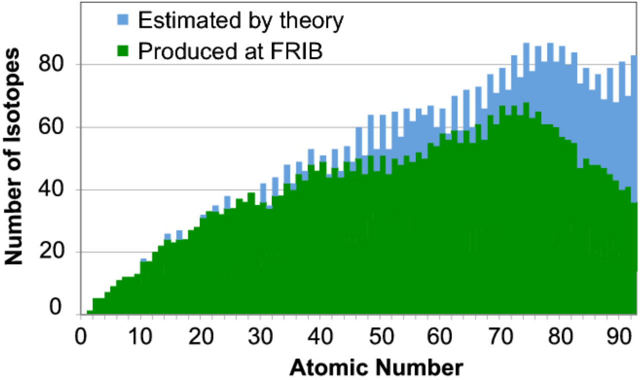
Brad Sherrill for the FRIB project team

How many nuclei?

How many protons and neutrons can form a bound nucleus?

Theory predictions: 6,900$\pm$500 nuclei with $Z < 120$ are bound.

FRIB expected limits:



Balantekin, et al., Mod. Phys.Lett. A29, 1430010 (2014).

Summary of this lecture:

- Many-body methods (QMC)
- Role of three-nucleon force in light nuclei
- Close shell numbers
- Nuclear dripline

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End for today...