Basic nuclear interactions and their link to nuclear processes in the cosmos and on earth

Theoretical historical introduction

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Rewriting nuclear physics textbooks
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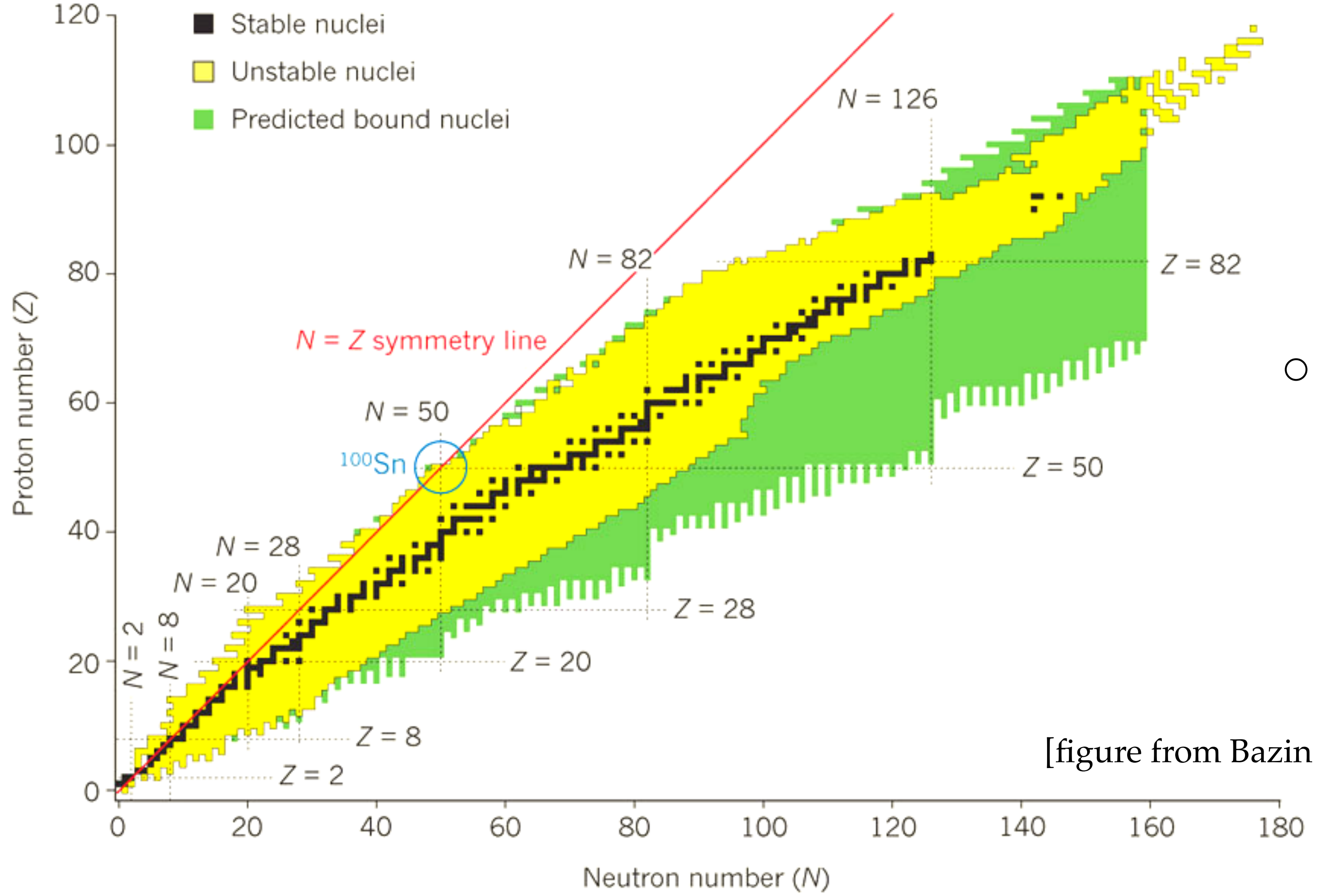
Basic facts about nuclei

○ 254 stable isotopes, ~3000 synthesised in the lab

○ Heaviest synthesised element Z=118



[figure from Bazin 2012]

○ Light/mid-mass elements produced in stellar fusion

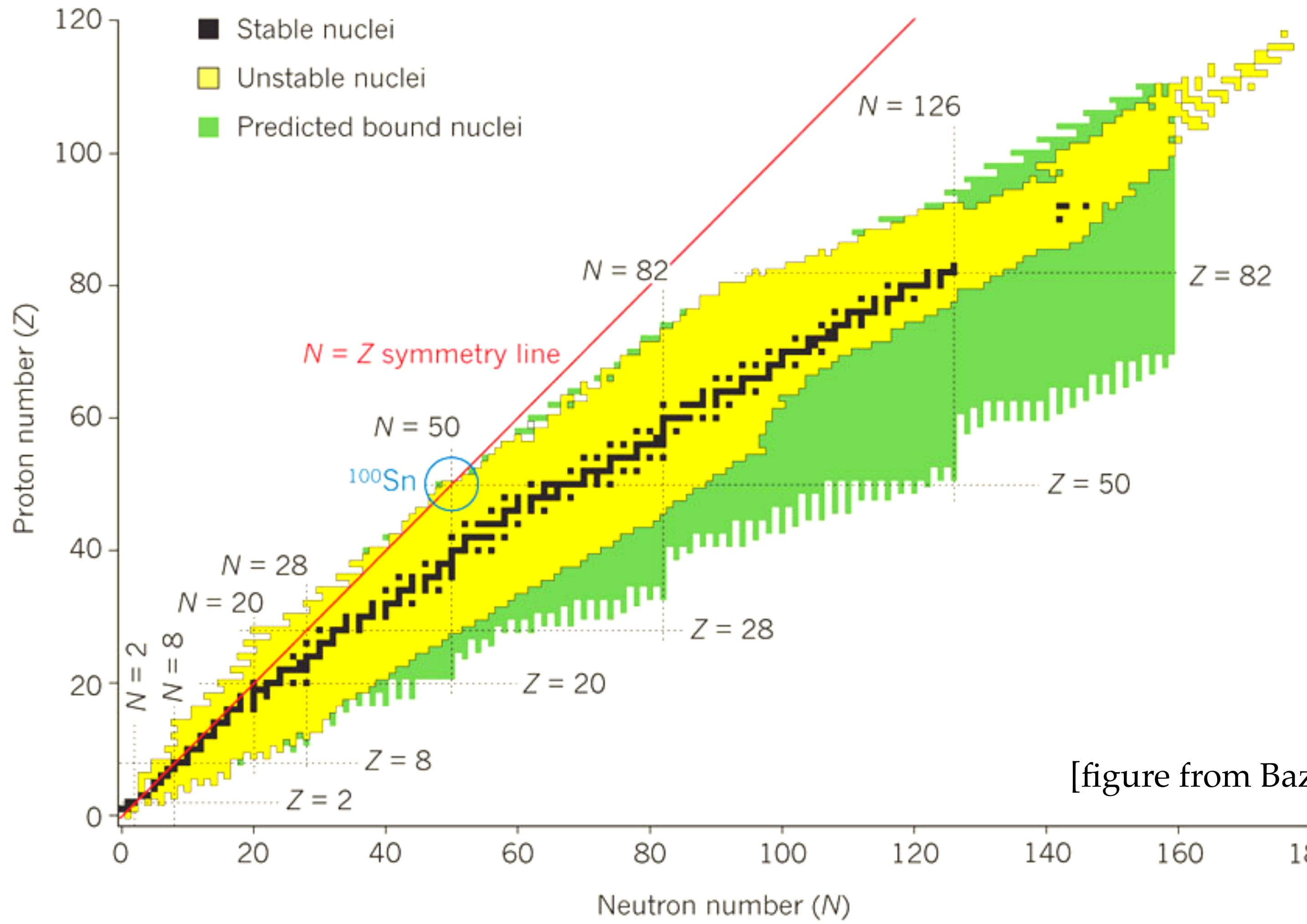
○ Neutron **drip-line** known up to Z=8 (16 neutrons)

○ Over-stable magic nuclei (2, 8, 20, 28, 50, 82, …)

Basic questions about nuclei

- ○ 254 stable isotopes, ~3000 synthesised in the lab
- ○ **How many** bound nuclei exist? (~6000-7000?)

- ○ Heaviest synthesised element *Z*=118
- ○ **Heaviest possible** element? Enhanced stability near *Z*=120?



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- ○ Light/mid-mass elements produced in stellar fusion
- ○ How have heavy elements been produced?

- ○ Neutron **drip-line** known up to *Z*=8 (16 neutrons)
- ○ Where is the neutron drip-line beyond *Z*=8?

- ○ Over-stable magic nuclei (2, 8, 20, 28, 50, 82, …)
- ○ Are **magic numbers** the same for unstable nuclei?

Diversity of nuclear phenomena

Nucleus: bound (or resonant) state of Z protons and N neutrons

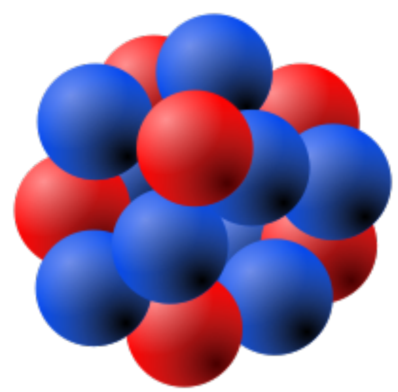
Several scales at play:

p & n momenta ~ $\mathbf{10^8}$ eV

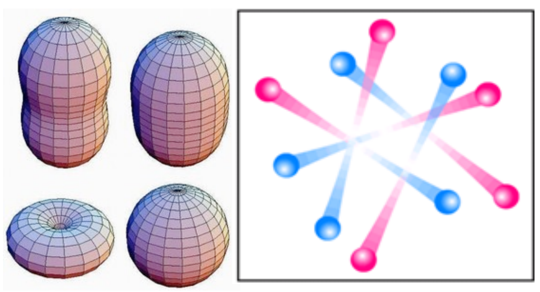
Separation energies ~ $\mathbf{10^7}$ eV

Vibrational excitations~ $\mathbf{10^6}$ eV

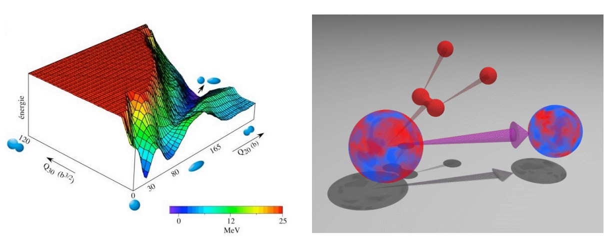
Rotational excitations ~ $\mathbf{10^4}$ eV



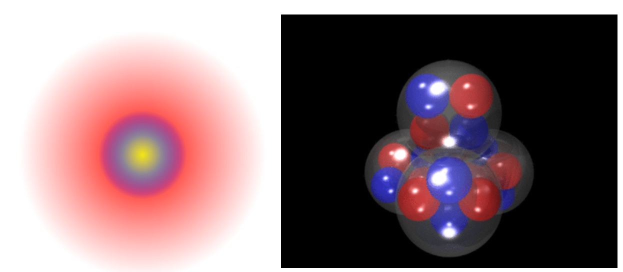
Ground state
Mass, size, superfluidity, …



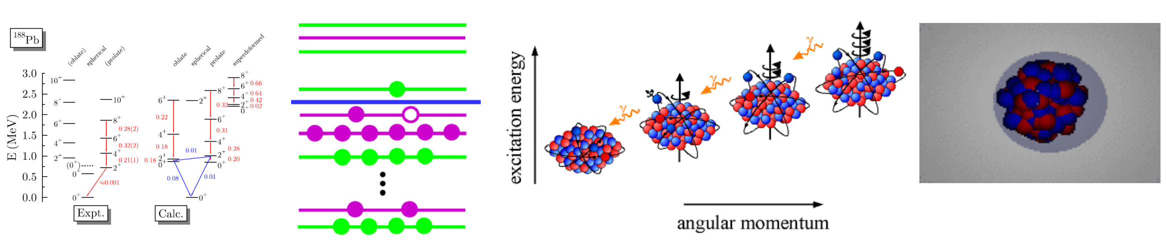
Radioactive decays
β, 2β, α, p, 2p, fission, …



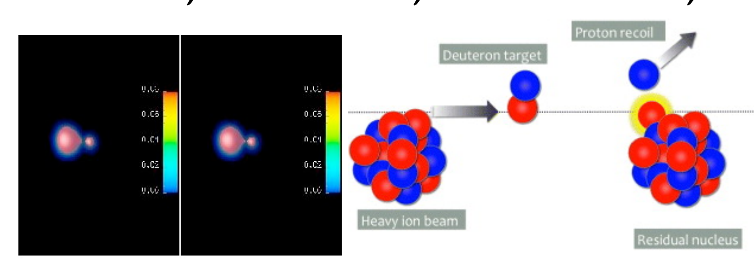
Exotic structures
Clusters, halos, …



Spectroscopy
Excitation modes



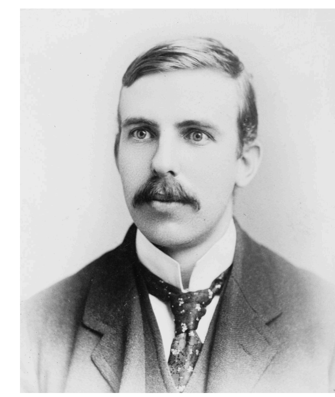
Reaction processes
Fusion, transfer, knockout, …



Historical preamble

1896 Becquerel discovers radioactivity

1898 Pierre & Marie Curie find α, β and γ rays



1911 Rutherford proposes the atomic nucleus

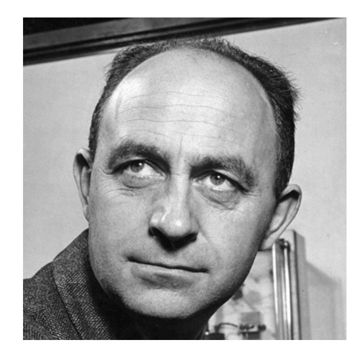
1919 Rutherford identifies the hydrogen nucleus as the proton

1929 Heitler & Herzberg show that ^{14}N is a boson

1931 Pauli proposes the neutrino

1932 Chadwick discovers the neutron

1933 Fermi proposes theory of weak interactions and β decay



Nuclear theory begins

Outline

Pre-1935 stuff (Radioactivity, Rutherford's experiment, discovery of the neutron, …)

1935 Semi-empirical mass formula (liquid drop)

2010's First lattice QCD calculations of NN potential & multi-baryon systems

Today

Liquid drop model & semi-empirical mass formula

⦿ Picture the nucleus as a (suspended) drop of (incompressible) liquid with surface tension

[Gamow, Bohr, Wheeler]

Liquid drop model

Competing processes give rise to nuclear binding

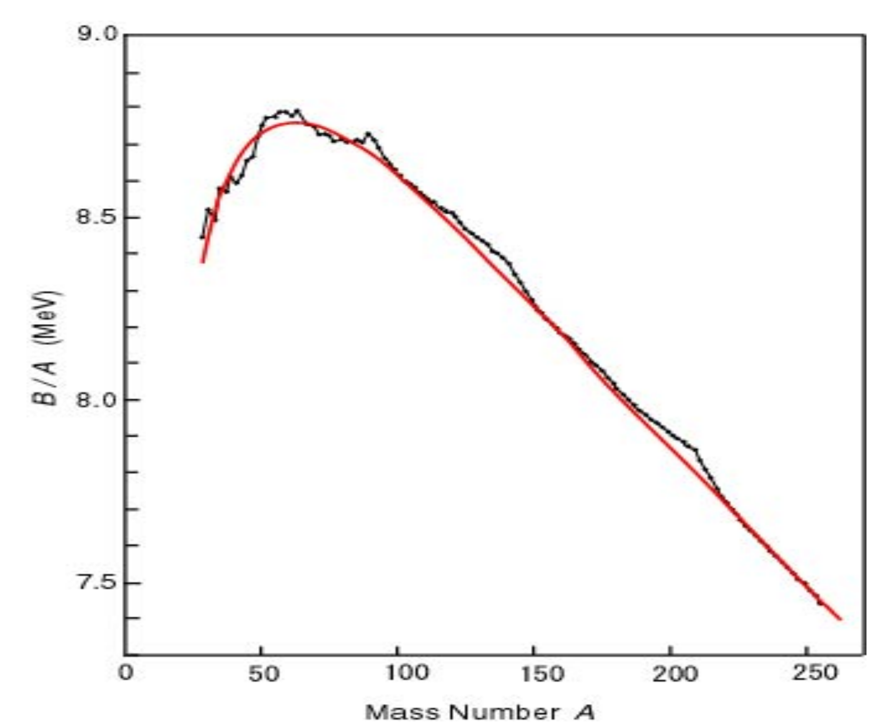
$A = Z + N$

$$\mathrm{BE}(Z,N) = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(N-Z)^2}{4A} - \frac{\delta}{A^{1/2}}$$

volume surface Coulomb N-Z asymmetry pairing

1935

[Weizsäcker, Bethe]



✓ Successful in explaining binding energy global trend

✗ Unsuccessful in explaining fine features, excitation spectra, …

Nuclear many-body problem

- Liquid drop model is semi-classical $\rightarrow$ we need fully quantum mechanical treatment

Nuclear many-body problem

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- **Which degrees of freedom?**
  - Quantised collective modes?
  - Protons and neutrons (≡ nucleons)? → usually the natural choice
  - What about quarks and gluons? (Full QCD treatment?)

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  - QCD: nuclear interactions as residual forces between bound states of quarks/gluons
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- **Provided we have nucleon forces, we need to solve a complicated quantum mechanical problem**
  - Many nucleons, but not enough to exploit statistical mechanics
  - Relativistic treatment? $\frac{\vec{p}}{m} \approx \frac{200 \text{ MeV}}{1000 \text{ MeV}} \implies \left(\frac{v}{c}\right)^2 < 0.1 \implies$ nucleon dynamics non relativistic

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↓ Typical strategy

1. Derive/build/model basic interactions between nucleons

2. Solve non-relativistic many-body Schrödinger equation

Structure vs reaction

- A-body Schrödinger eigenvalue equation $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$

Structure properties of nuclei with A=2, ~400

E.g. addition/removal energies

$$E_k^{\pm} \equiv \pm(E_k^{A\pm 1} - E_0^A)$$

Nuclear matter properties

E.g. equation of state

$$E/A\,(\rho, x, T)$$

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- Time-dependent Schrödinger equation $H|\Psi^{A+B\to C+D}(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi^{A+B\to C+D}(t)\rangle$

Reaction cross section

$$\sigma(A_k + B_l \to C_m + D_n)$$

Simplest reaction, but many other possibilities: more than two final products, more than two reactants (rare), particles other than nuclei (photons, neutrinos, …)

→ Are structure properties easily obtainable from the reaction process?

→ When we make approximations, are they at the same level for structure and reactions?

Ab initio vs effective approach

Ab initio **(= "from scratch") approach**

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

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A-body Hamiltonian

$$H = T + V^{2\mathrm{N}} + V^{3\mathrm{N}} + ... + V^{A\mathrm{N}}$$

Do we need all these terms??

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A-body wave-function

5 variables x *A nucleons*

Unfavourable scaling for large A!

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Effective approach

Two main options

- Reduce active Hilbert space → Interacting shell model
- Simplify $|\Psi_k^A\rangle$ → Energy density functional

$$H^{\mathrm{eff}}|\Psi^{\mathrm{eff}}\rangle = E|\Psi^{\mathrm{eff}}\rangle$$

Ab initio vs effective approach

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$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

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Simplify $|\Psi_k^A\rangle$ → Energy density functional

$$H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$$

- Which properties we aim at and which level of accuracy are we seeking?
- Applicability throughout the nuclear chart? → Universal/global vs local description
- Predictive power? → Estimate of theoretical error

Independent particle model & mean field

- If particles of a many-body system don't interact, then $H = \sum_i^A h_i$ (= 1-body only), and

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle \longrightarrow h_i|\phi_k^i\rangle = \varepsilon_k^i|\phi_k^i\rangle$$

→ From an A-body problem to A one-body problems

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→ From an A-body problem to A one-body problems

⊙ **Independent particles: nucleons move inside a (one-body) potential well or *mean field***

⊙ Does an independent-particle picture make any sense at all?

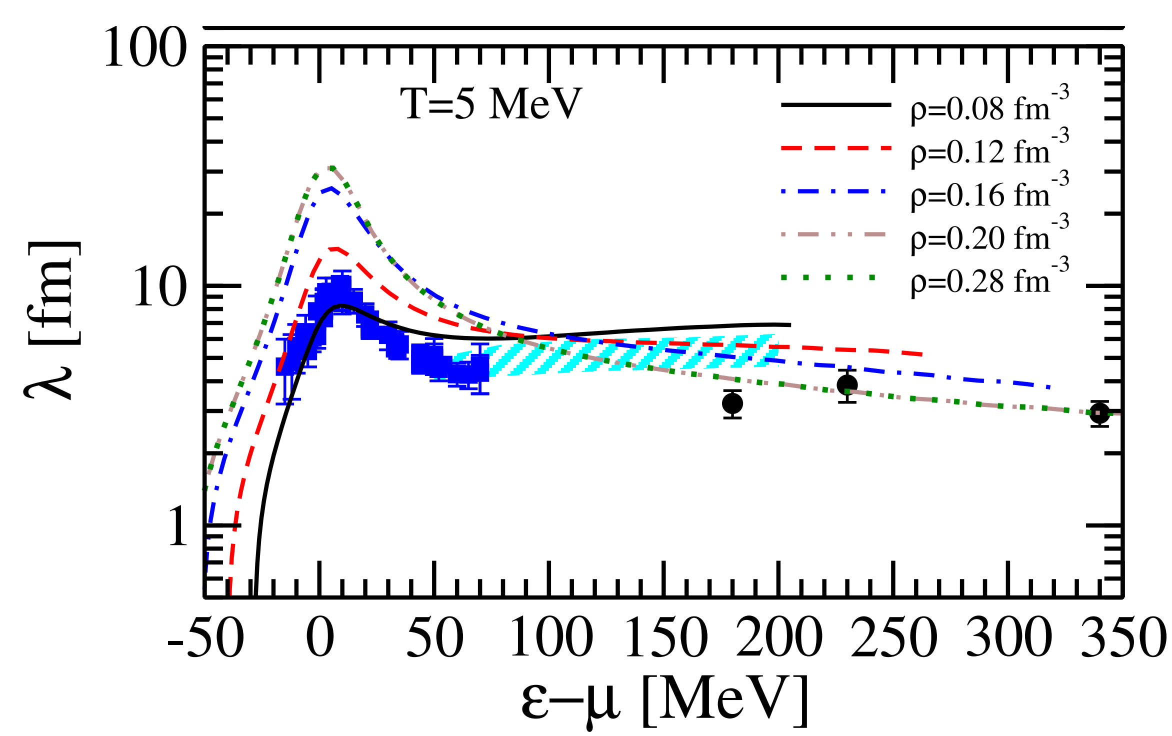
→ Inter-particle distance in nuclei ~ 2 fm

→ Range of nuclear interaction ~ 2 fm

Turns out that it does

✓ Fermi statistics helps out

✓ Large mean free path λ



[Rios & Somà 2012; Lopez *et al.* 2014]

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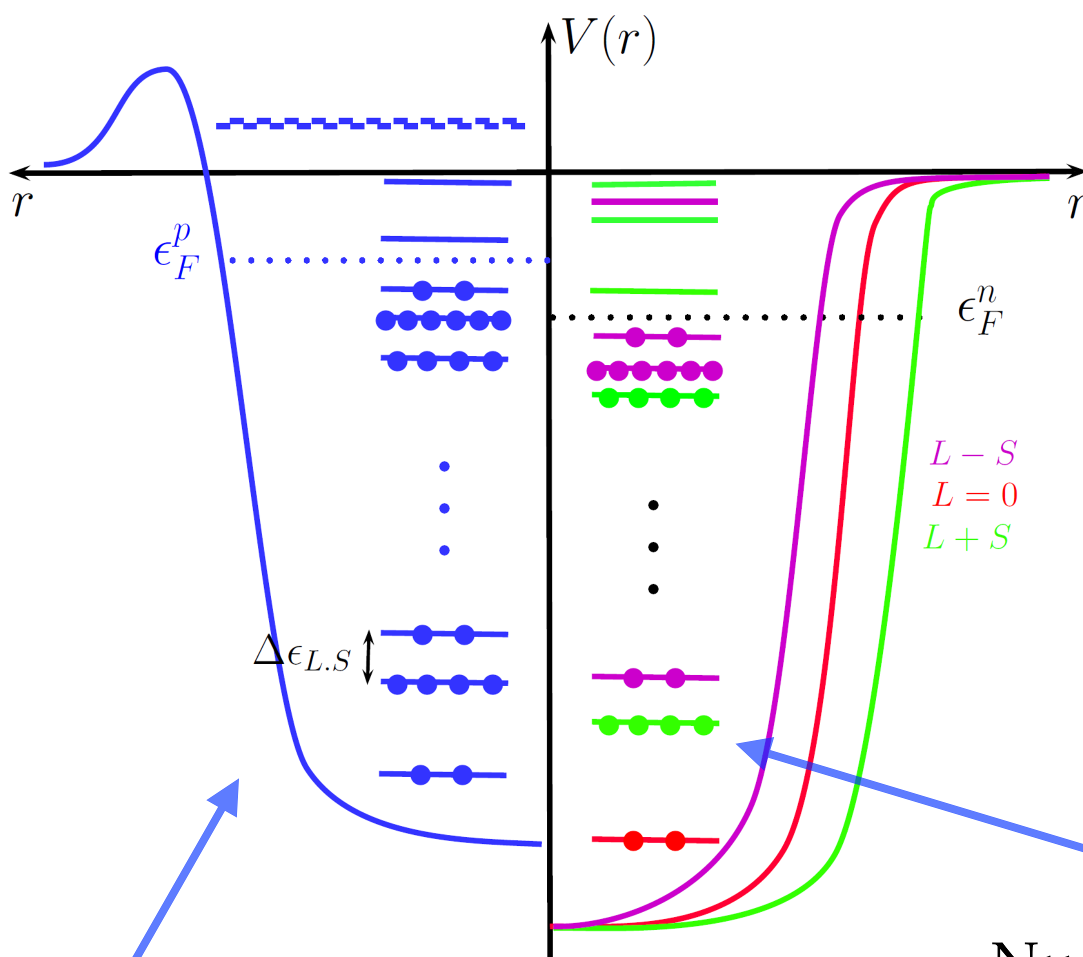


$$h_i = \frac{p_i^2}{2m} + V(r_i)$$

Commonly used are potentials of **Woods-Saxon** type

$$V(r_i) = -\frac{V_0}{1+\exp\left(\frac{r_i - R}{a}\right)}$$

Coulomb shifts proton potentials

Nucleons (which are fermions) are placed in energy levels according to Pauli principle

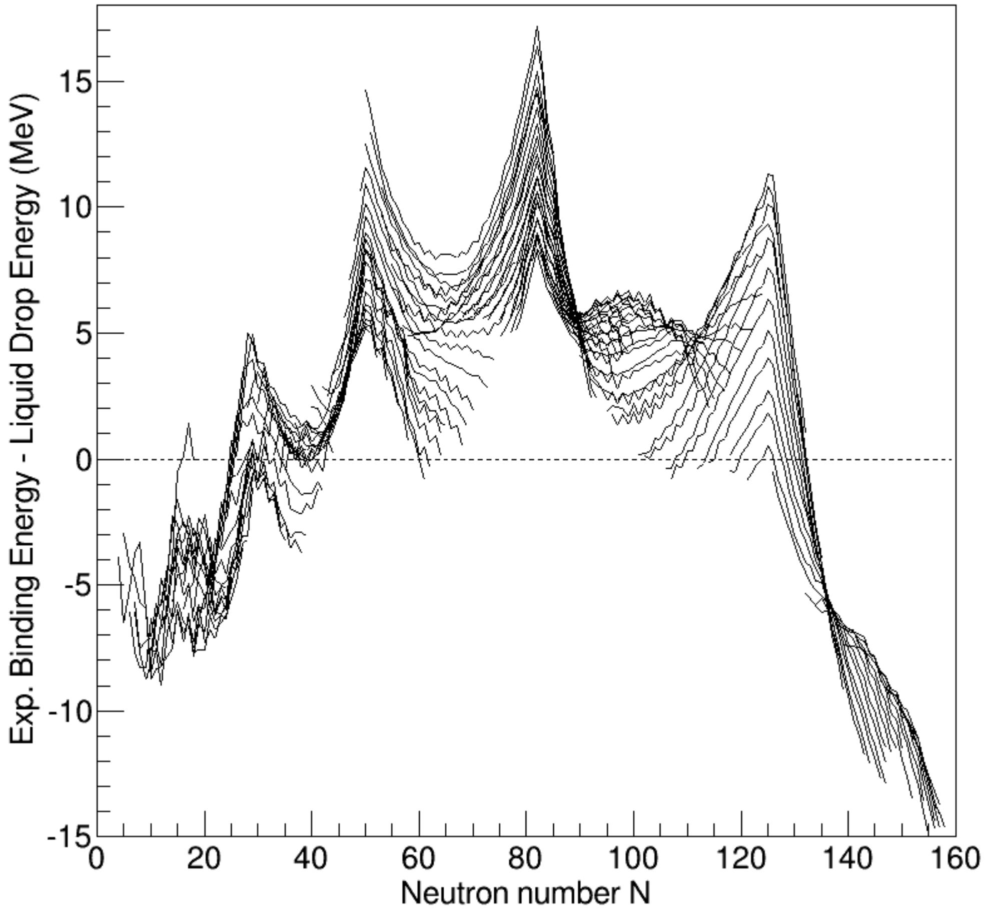
(Non-interacting) shell model

Measured binding energies

vs.

Liquid drop model predictions

Systematic deviations



- **What creates regular patterns?**
  - Nucleon shells? (cf. electrons in the atom)
  - Yet, no obvious common potential

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Measured binding energies
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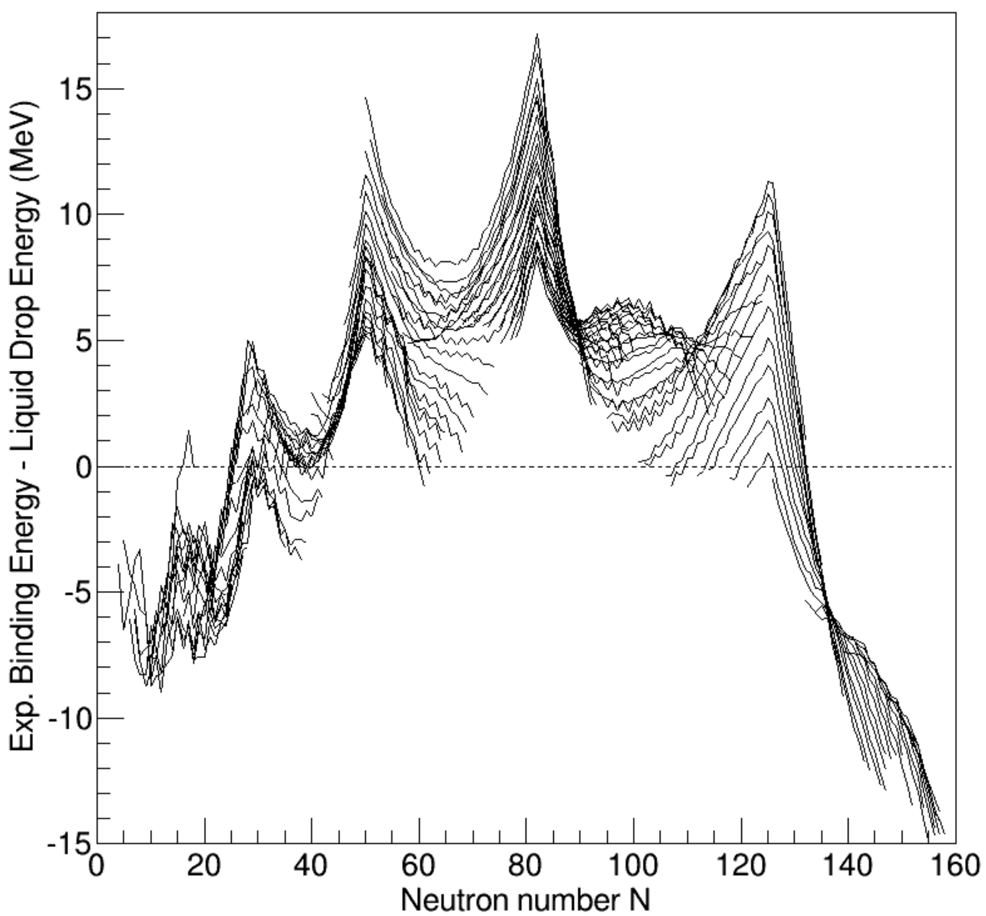

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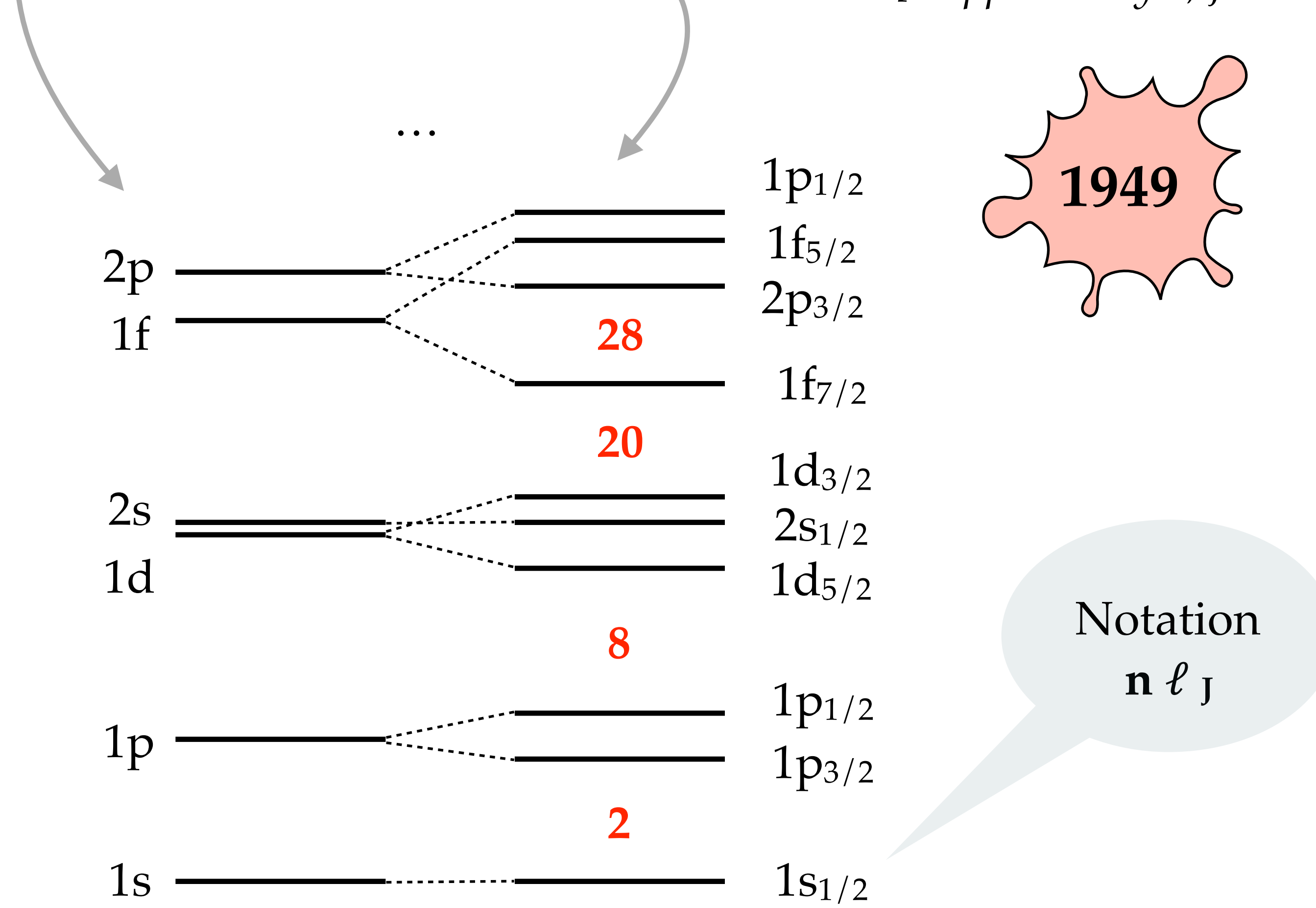
➪ **Idea: devise an effective one-body potential**

- ○ 1. Start with 3D spherical HO potential
- ○ 2. Add term proportional to ℓ^2 (centrifugal)
- ○ 3. Add a spin-orbit term $\ell \cdot s$

[Göppert-Mayer, Jensen]

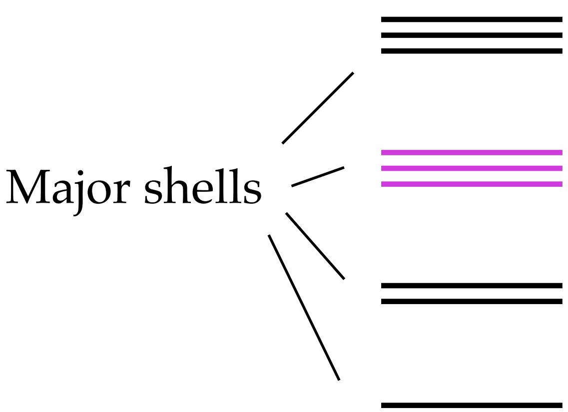


Magic numbers reproduced!

(Interacting) shell model

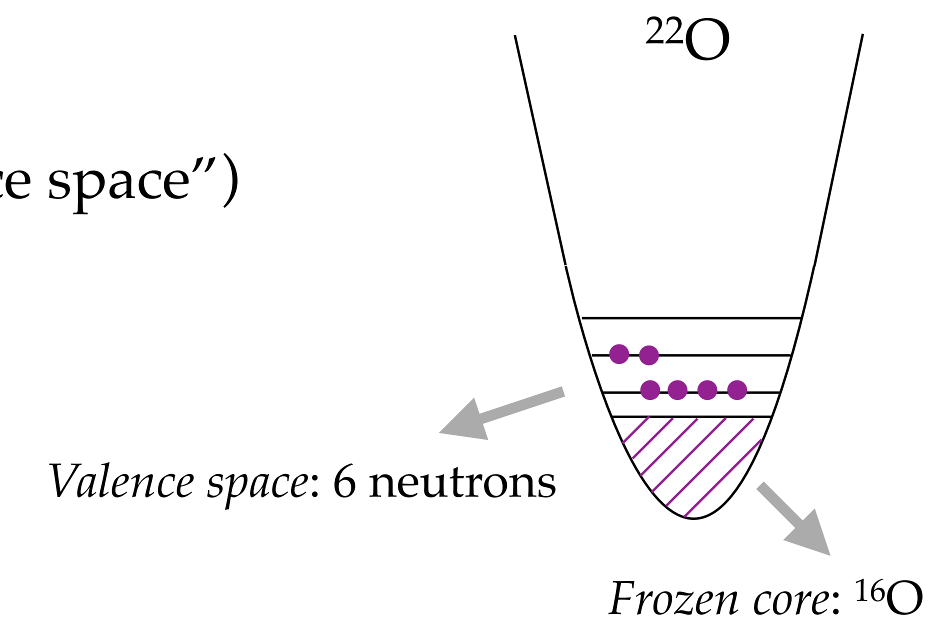
- Independent-particle shell model OK for closed shells/magic numbers
- In general, a correlated wave function is needed… but $H = H_{\text{IP-SM}} + H_{\text{res}}$ too costly to diagonalise

➪ **Idea: exploit "shells" and their energy separation**



1. Define an active Hilbert space ("valence space")
2. Build valence-space Hamiltonian H^{eff}
3. Diagonalise H^{eff} in the restricted space

1960's



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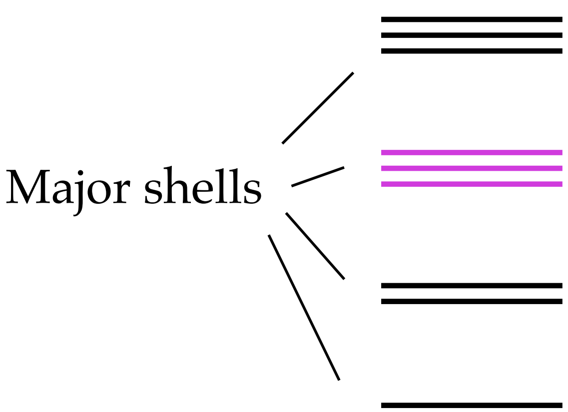

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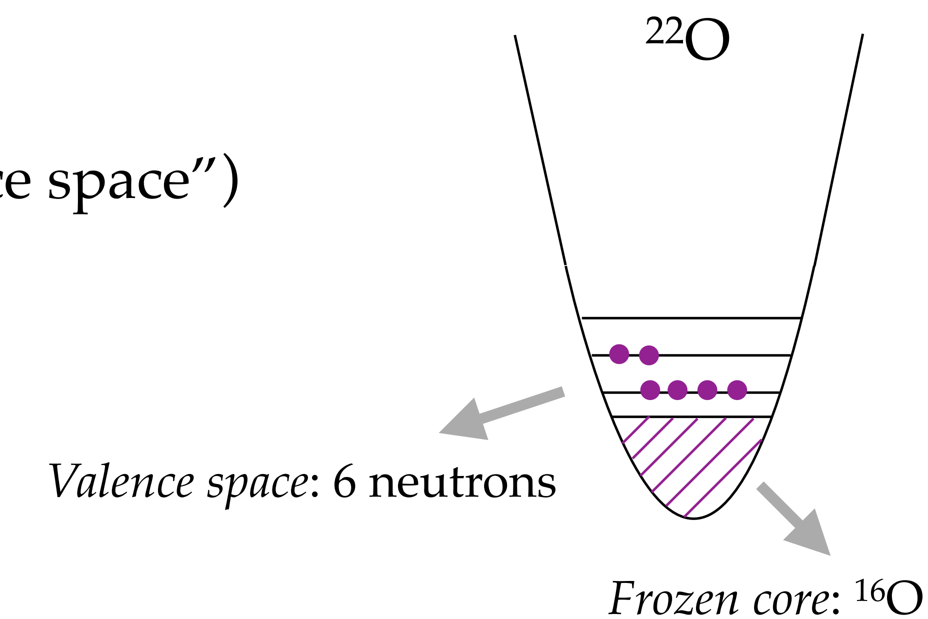
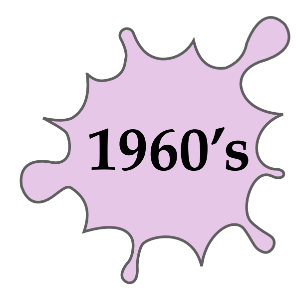




- How to build valence-space interactions?
  - **Ab initio**: use projection techniques to go from full to restricted Hilbert space
    - ✓ Universal and systematic → predictive power
    - ✗ Requires sophisticated many-body techniques → "fully ab initio" only very recently
  - **Phenomenologically**: (re)fit parameters of H^{eff} to data
    - ✓ Successful in reproducing fine spectroscopy → very good accuracy
    - ✗ H^{eff} depends on exp. data locally → validity of extrapolations not guaranteed

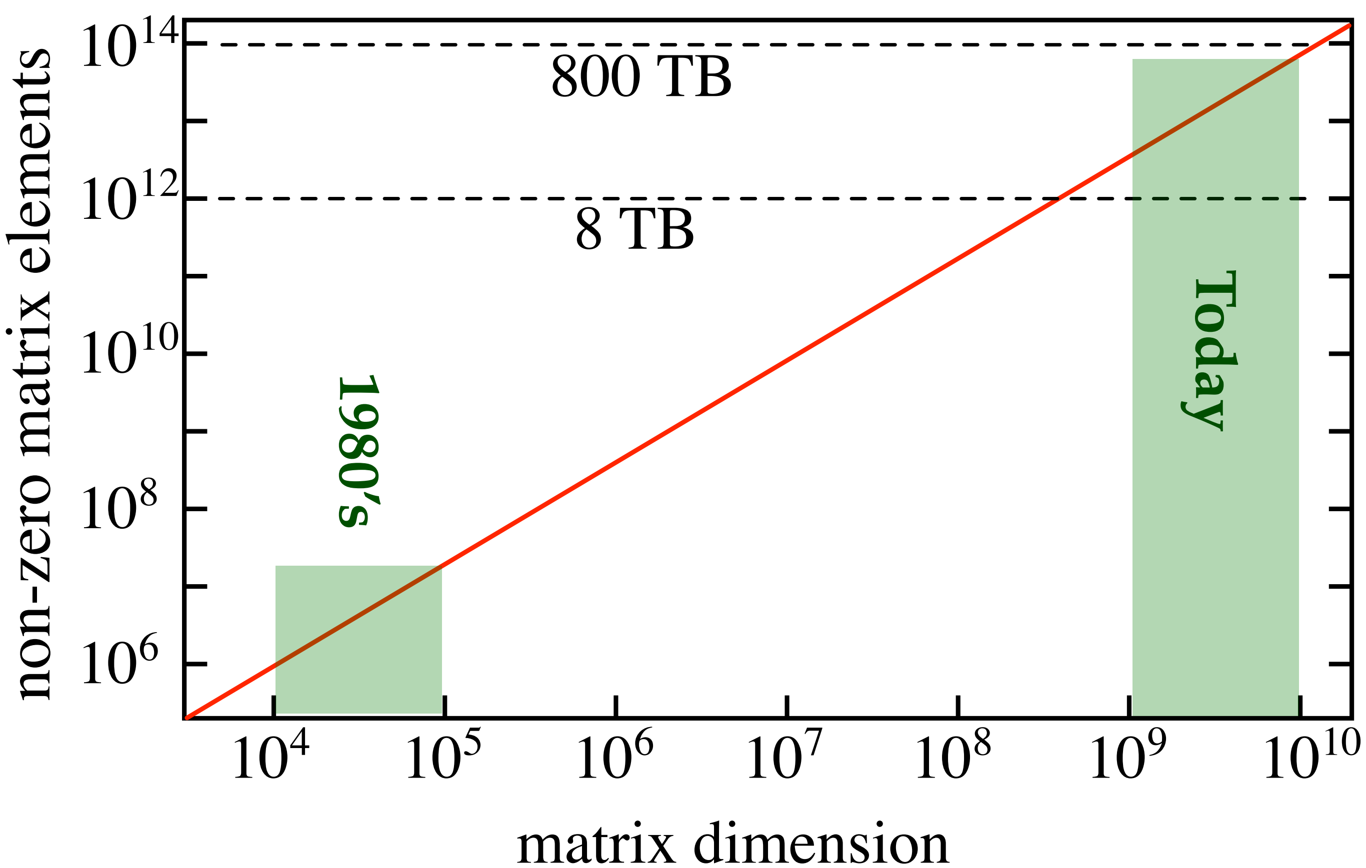
(Interacting) shell model

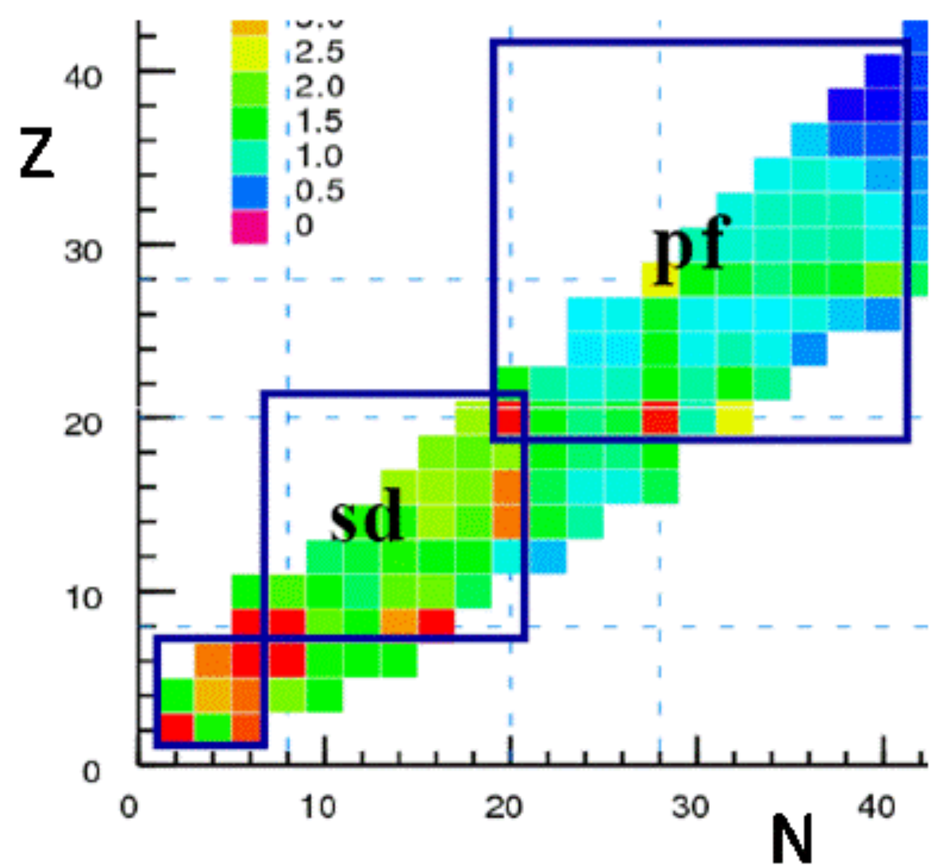
- Problem: as *A* increases, dimensions of relevant valence spaces increase
- Computational aspects of the method rather challenging
  - Progress in algorithms + computational resources have pushed the limits of applicability
  - First calculations (1960's): matrix dimensions 10^2 → today: matrix dimensions 10^9-10^{10}

➪ **Main limitation: aggregate memory**

- 10^{14} nonzero matrix elements → 800 TB
- Progress relies on "Moore's law"

Applicability: A < 80-100





Energy density functionals

➪ **Idea: work with a simplified many-body wave-function** $|\phi_k^A\rangle$

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle \longrightarrow H_{\text{eff}}|\phi_k^A\rangle = E_k^A|\phi_k^A\rangle$$

Correlations incorporated in H_{eff}

Simplest possible: independent particles

⊙ **Original** approach: Hamiltonian-based

- ○ Hartree-Fock theory → mean-field potential built self-consistently from a *NN* interaction

⊙ **Modern** approach: energy as a functional of (one-body) densities (+ currents)

- ○ First density-dependent Hamiltonian, then more general functional of one-body density

⊙ For both, parameters are fitted to data

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- **Modern** approach: energy as a functional of (one-body) densities (+ currents)
  - First density-dependent Hamiltonian, then more general functional of one-body density
- For both, parameters are fitted to data
- Relies on symmetry breaking and restoration

Physical solution must have good symmetries → one must restore them in the end

Wave function has lost some of the symmetries of the Hamiltonian, but energy is closer (w.r.t. symmetry-conserved case) to the exact one !

✓ Symmetry-broken HF calculations provide fair description and have low computational cost

✗ Restoring symmetries needed for refined results but may become very costly

Energy density functionals

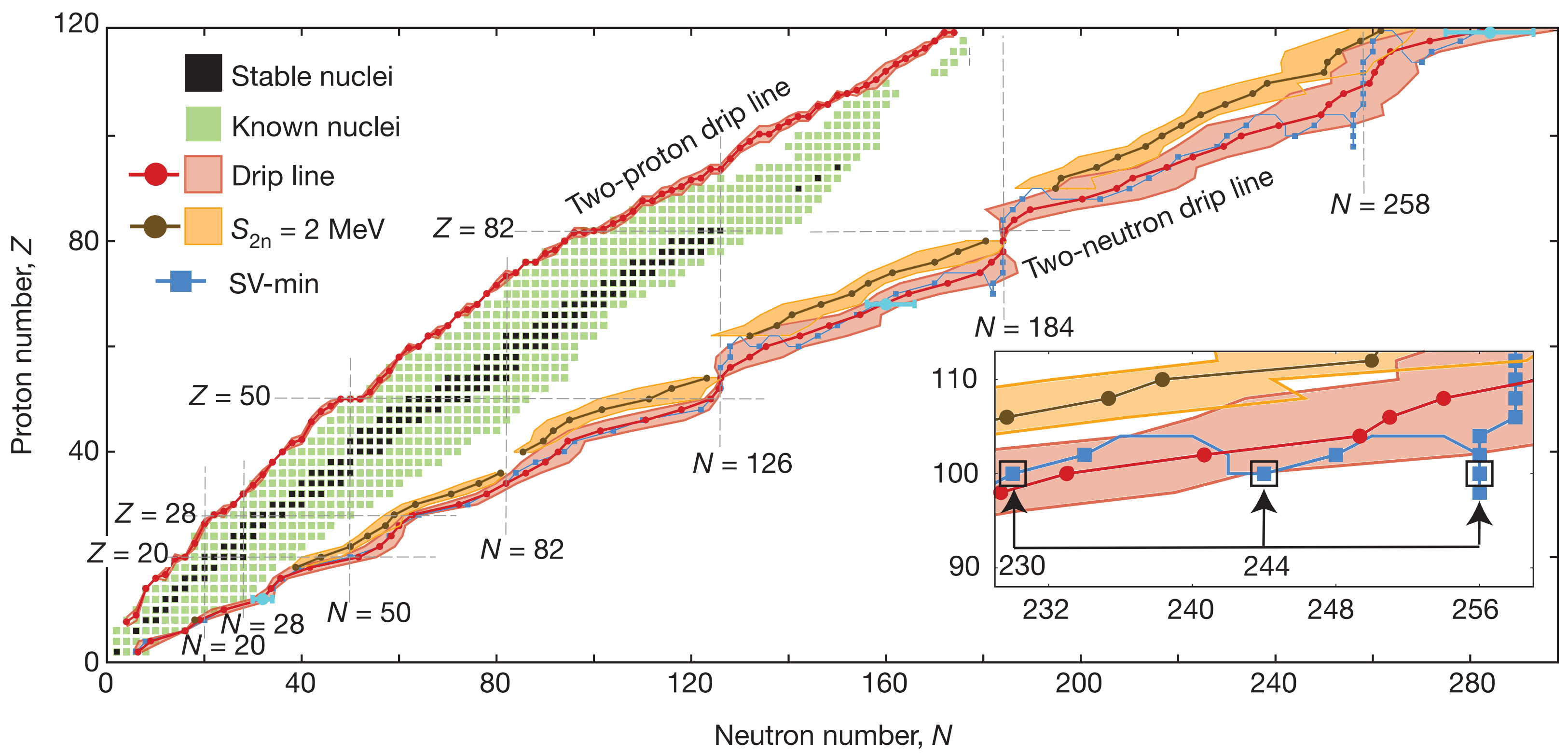
- Several implementations developed over the years
  - Non-relativistic: Skyrme (1972+) and Gogny (1975+)
  - Relativistic: (1986+)

✓ Favourable scaling → **only method applicable to all nuclei**

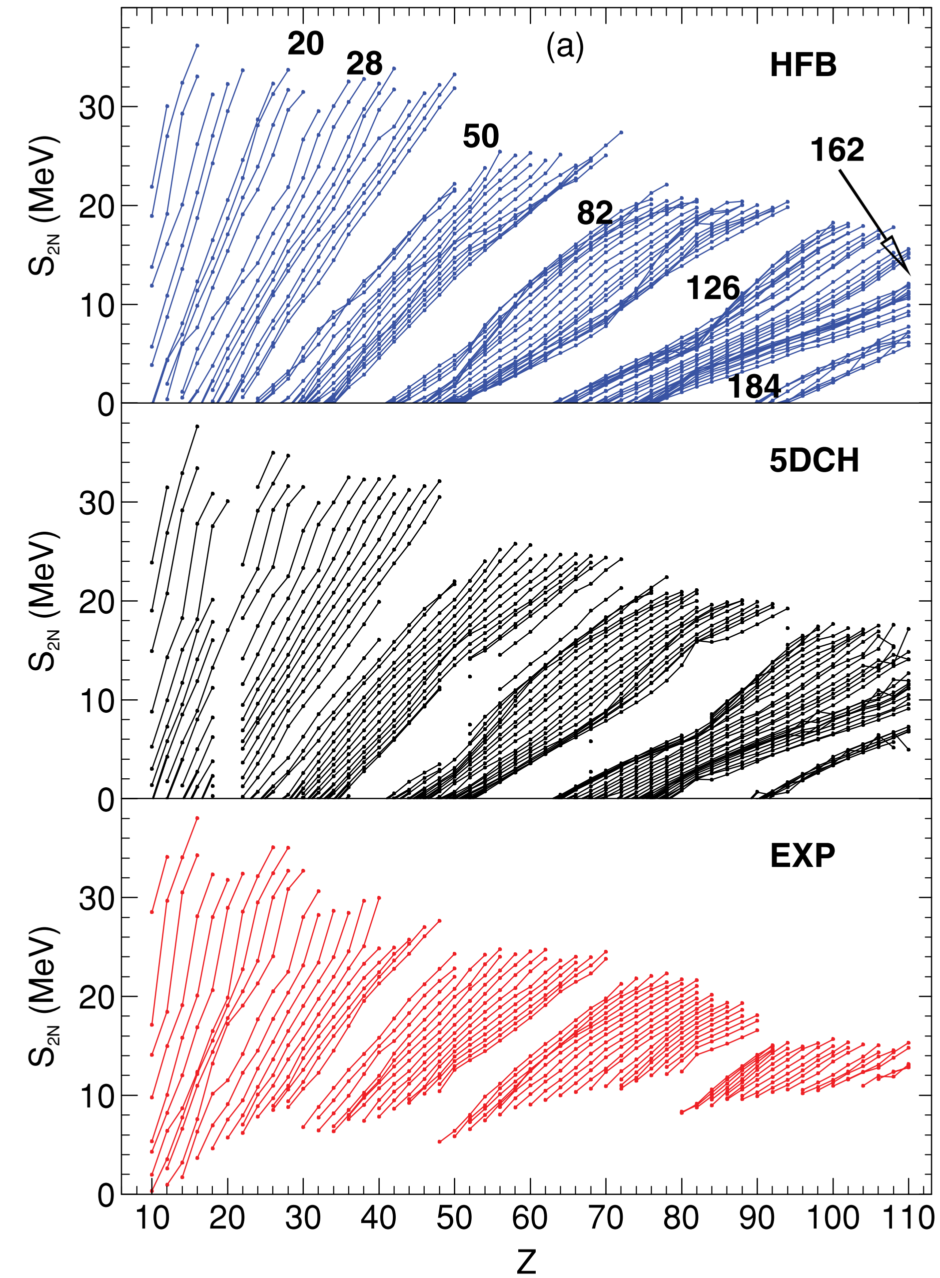
✓ Can tackle efficiently nuclear matter

✗ Lack of systematic character

✗ Validity of extrapolations not guaranteed



[Erler *et al.* 2012]



[Delaroche *et al.* 2010]

Historical recap #1

Pre-1935 stuff (Radioactivity, Rutherford's experiment, discovery of the neutron, …)

1935 Semi-empirical mass formula (liquid drop)

1949 Non-interacting shell model

1960's Valence-space interaction (= interacting shell model)

1970's Energy density functionals

Today

Basic structure of NN interaction

- Hamiltonian for the 2-nucleon system $H = T + V_{NN} + V_{\mathrm{em}}$ → Coulomb (+ small corrections)

- Most general form $V_{NN} = V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{p}_1, \boldsymbol{p}_2, \sigma_1, \sigma_2, \tau_1, \tau_2)$

  positions ($\boldsymbol{r}_1, \boldsymbol{r}_2$), momenta ($\boldsymbol{p}_1, \boldsymbol{p}_2$), spins ($\sigma_1, \sigma_2$), isospins ($\tau_1, \tau_2$)

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  positions / momenta / spins / isospins

- Symmetry-constrained form
  - Continuous symmetries (translation in time/space, rotation in space+spin, Galilean invariance)
  - Discrete symmetries (parity, time reversal, baryon+lepton number conservation)
  - Isospin:

charge symmetry	*charge independence*
p ↔ n ⟹ pp ↔ nn	pp ↔ pn ↔ nn
(→ spectra of mirror nuclei)	(→ pp vs. np scattering lengths)

$$V_{NN} = V_1(\boldsymbol{r}, \boldsymbol{p}, \sigma_1, \sigma_2) + V_\tau(\boldsymbol{r}, \boldsymbol{p}, \sigma_1, \sigma_2)\, \tau_1 \cdot \tau_2$$

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$$
$$\boldsymbol{p} = \boldsymbol{p}_1 - \boldsymbol{p}_2$$

each one with 3 parts:

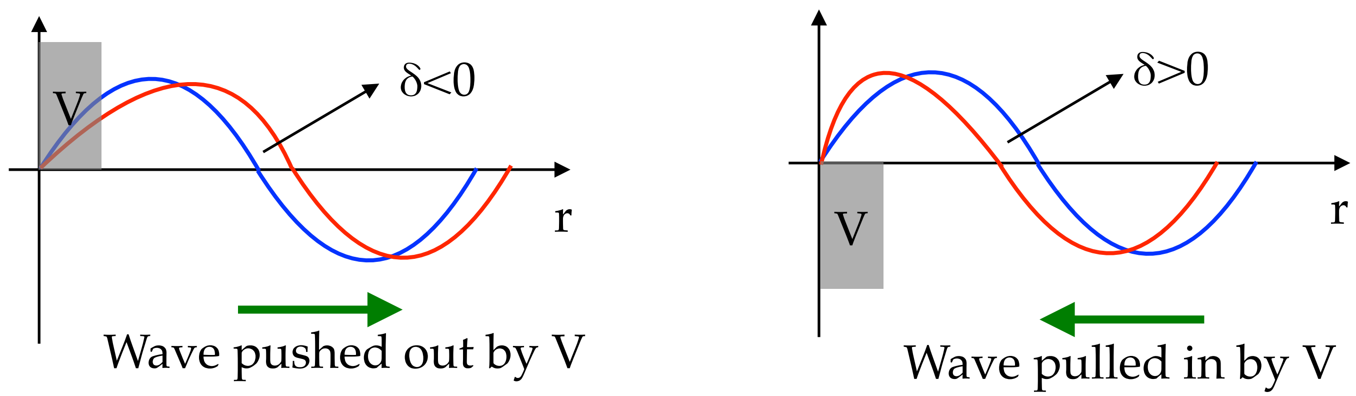
spin-scalar + **spin-vector** + **spin-tensor**

Basic properties of NN interaction

⊙ Nucleon-nucleon scattering

○ Interaction leads to a change in the phase of the scattered wave → **scattering phase shifts δ**

Repulsive



Attractive

Basic properties of NN interaction

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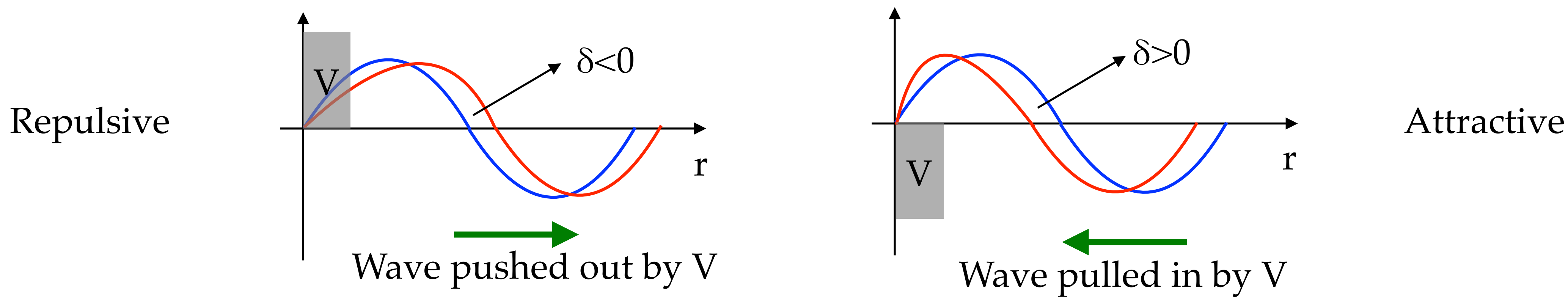


- Scattering is analysed in **partial waves**

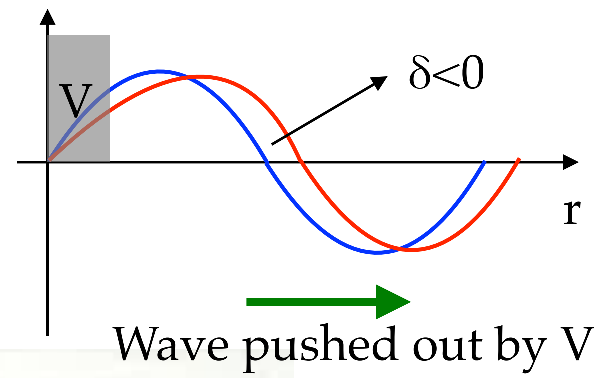
Total momentum is conserved $\vec{J} = \vec{L} + \vec{S} \implies |L - S| \leq J \leq |L + S|$

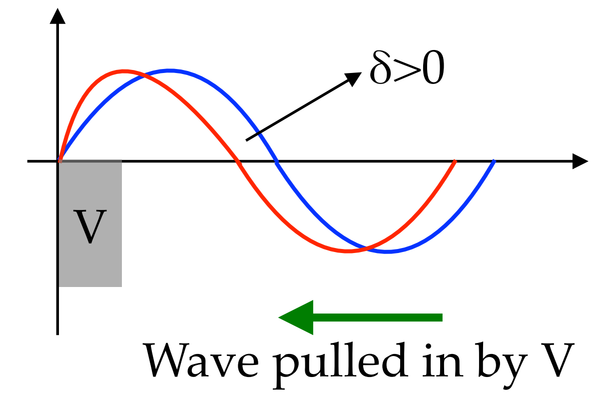
$$\vec{S} = \vec{s_1} + \vec{s_2} \implies S = 0, 1 \implies J = \begin{cases} L & \text{for } S = 0 \\ |L-1|, L, L+1 & \text{for } S = 1 \end{cases}$$

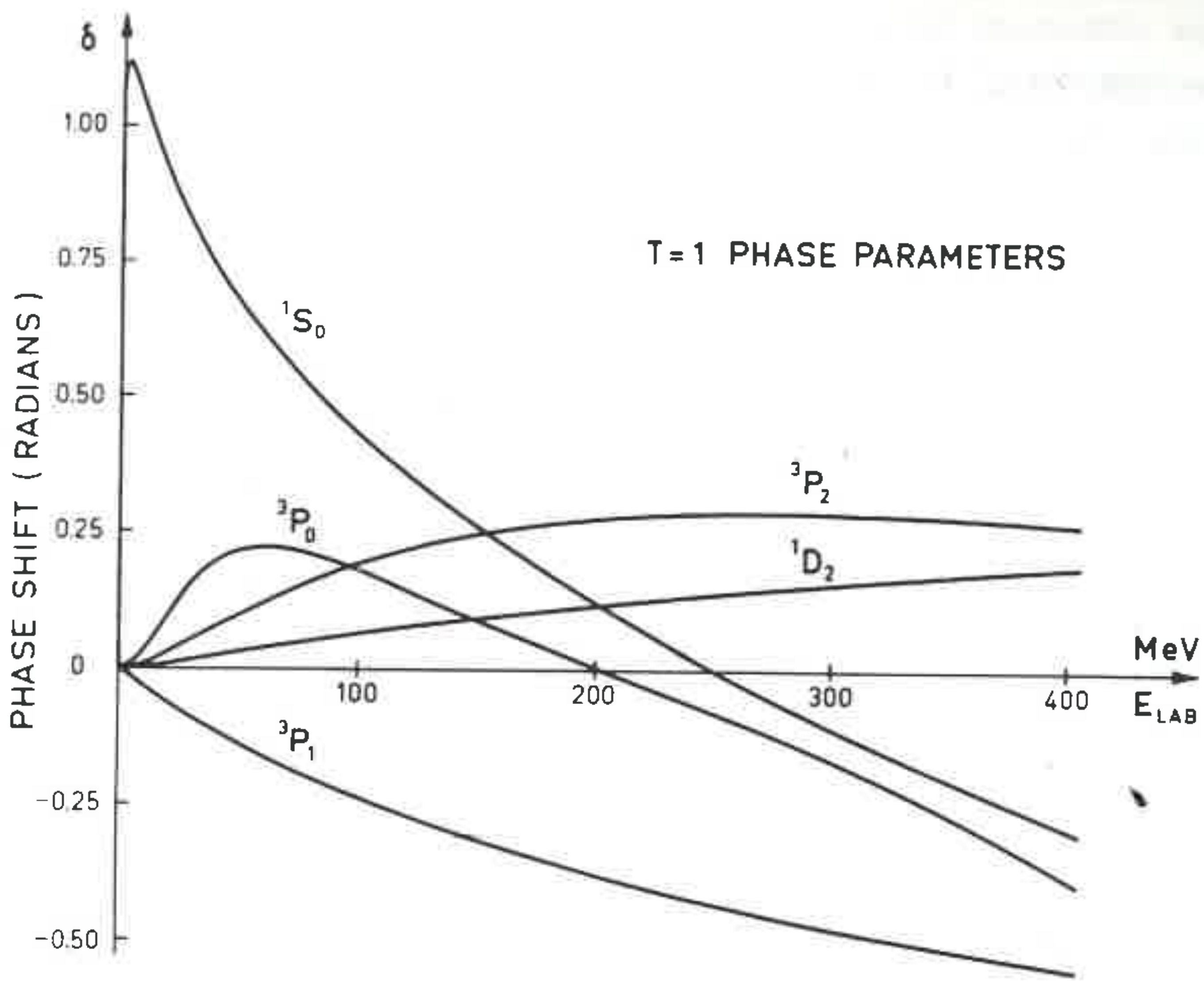
Spectroscopic notation $^{2S+1}L_J$

Basic properties of NN interaction

- **Nucleon-nucleon scattering**
  - Example of phase shifts







$$^{2S+1}L_J$$

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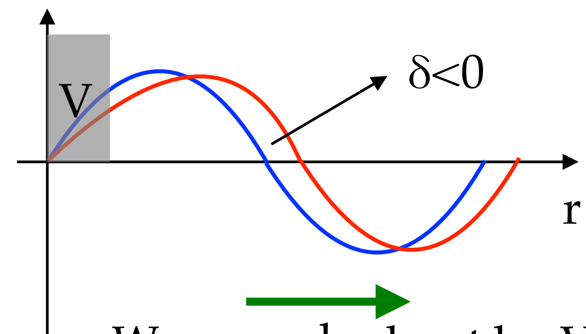
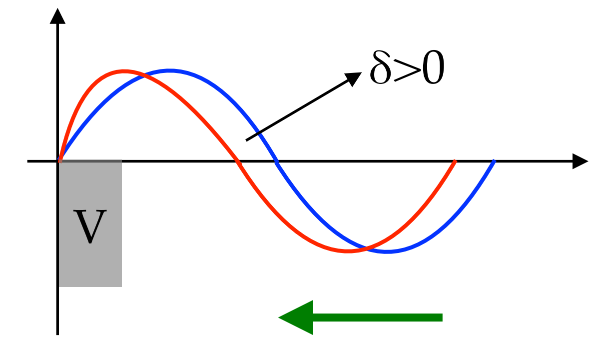


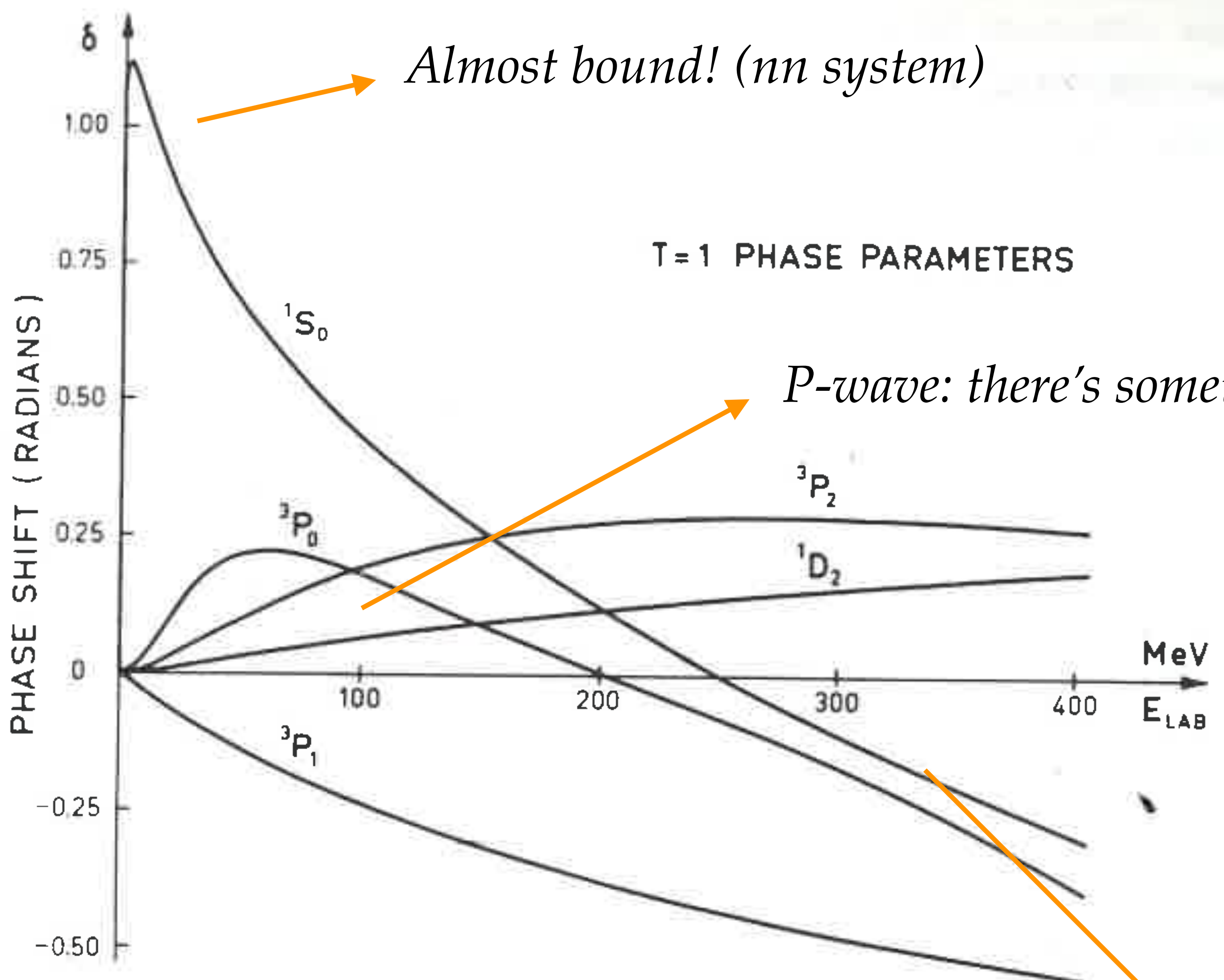
Wave pushed out by V



Wave pulled in by V

$^{2S+1}L_J$

Almost bound! (nn system)



P-wave: there's something more than central → spin orbit

S-wave: becomes repulsive at small distances

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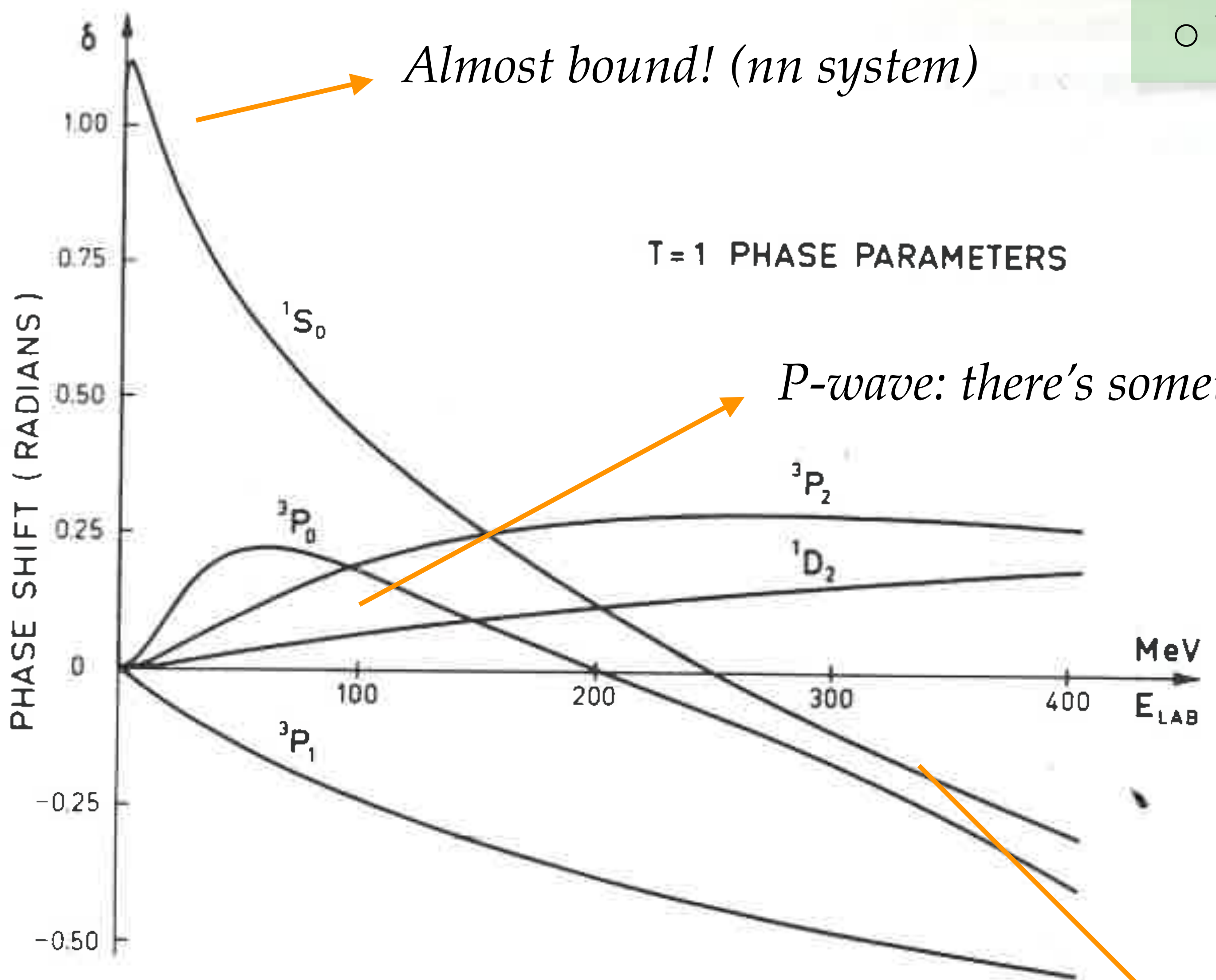


P-wave: there's something more than central → spin orbit

S-wave: becomes repulsive at small distances

- **Deuteron properties:**
  - Non-zero quadrupole moment → tensor
  - Loosely bound system

Yukawa potential

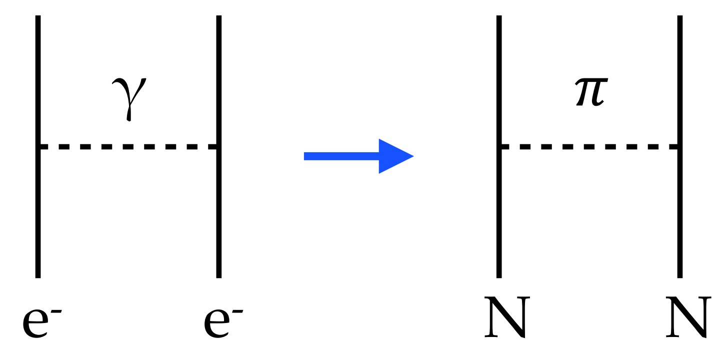
What was known:

- ○ Coulomb interaction between charged particles (infinite range)
- ○ Nuclear interaction is short range ~ 2 fm

➪ **Idea: nuclear force mediated by massive spin-0 boson** (the "mesotron" → later, pion)

[Yukawa, Proca]

1935



Yukawa potential

$$V(r) \propto \frac{e^{-mr}}{r}$$

m ~ 100 MeV ← r ~ 2 fm

Range ~ Compton wavelength of exchanged boson ~ 1/m

- ⦿ One-pion exchange describes long-range attraction between nucleons
  - ○ Works so well that, as of today, it is part of most sophisticated potential models!
- ⦿ However, not the full story. Short-range part?
  - ○ 1950's: Multi-pion exchange: disaster
  - ○ 1960's: More mesons discovered → multi-pion resonances ≈ exchange of heavier mesons

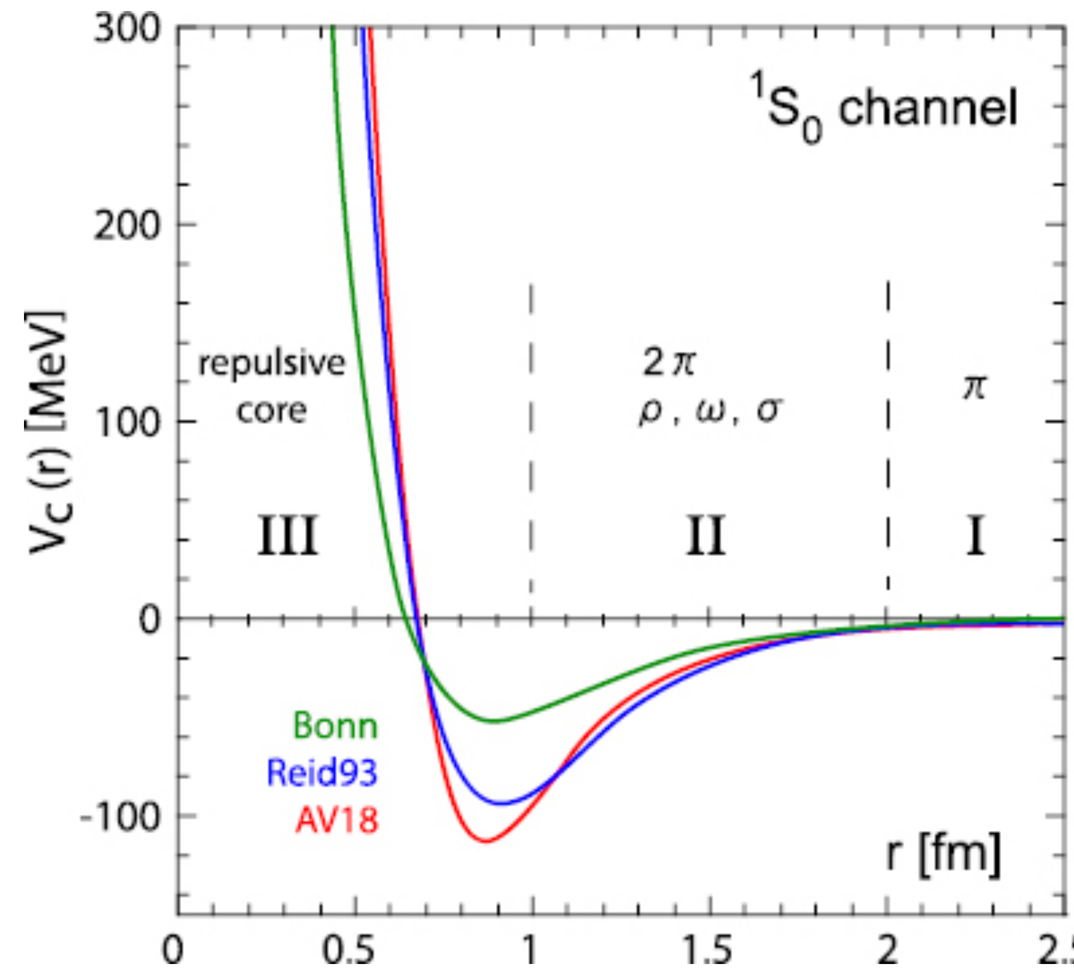
One-boson-exchange potentials

1970's

- Meson with larger masses (ρ , ω, σ) can model ranges smaller than $1/m_\pi$
  - Different spin/isospin structures generated
  - Parts sometimes phenomenological (or the whole, e.g. Av18)

➪ **Strategy:**

1. Construct the operatorial structure
   - Radial functions
   - Spin/tensor/isospin operators)
2. Fit coupling constants to data
   - NN scattering
   - Deuteron properties



- Experimental side: more and more precise *NN* data
- Theoretical side: more sophisticated potentials → $\chi^2 \approx 2$ in the 1980's, $\chi^2 \approx 1$ in the 1990's

What about nuclear structure calculations?

Historical recap #2

Pre-1935 stuff (Radioactivity, Rutherford's experiment, discovery of the neutron, …)

1935 Semi-empirical mass formula (liquid drop)

1935 Yukawa potential

1949 Non-interacting shell model

1960's Valence-space interaction (= interacting shell model)

1970's Energy density functionals

1970's One-boson exchange potentials

1980's High precision one-boson exchange potentials

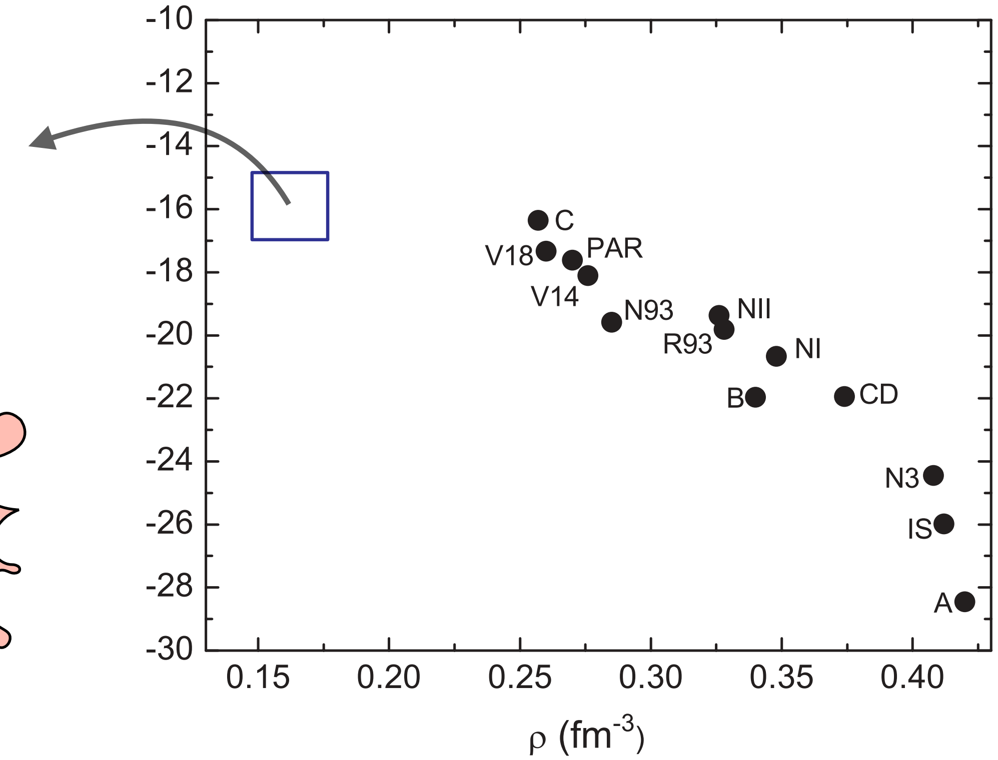
Today

Three-nucleon forces

- Calculations with accurate ($\chi^2 = 1$) OBE potentials show deficiencies in systems with $A>2$
  - Lightest nuclei do not match experiment
  - Saturation point of nuclear matter is not reproduced

Three-nucleon forces must be considered

1980's



[Li *et al.* 2006]

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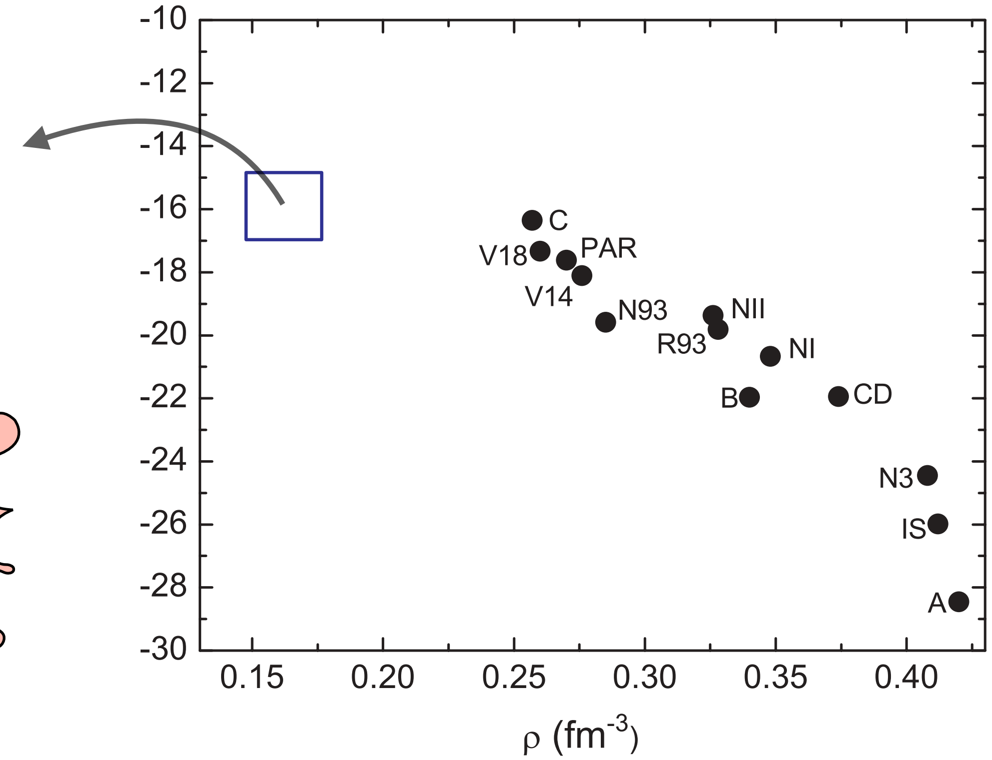


[Li *et al.* 2006]

Three-nucleon forces must be considered

1980's

➪ **Fundamental reason**: nucleons are composite particles, but we treat them as structureless

- Certain processes, e.g. involving nucleon excitations, can not be described as 2-body

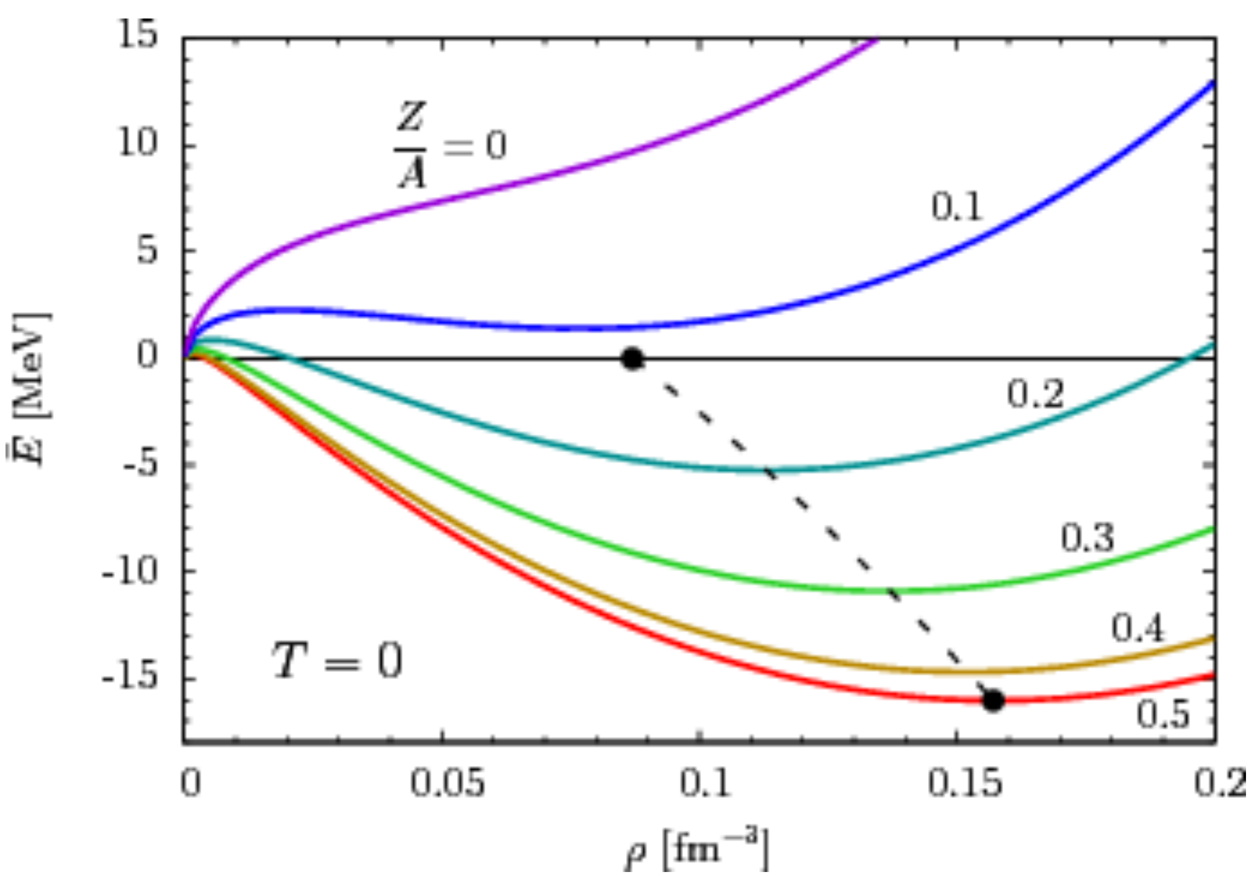
[Fujita, Miyazawa]

- Three-nucleon forces are added mostly phenomenologically to OBE potentials

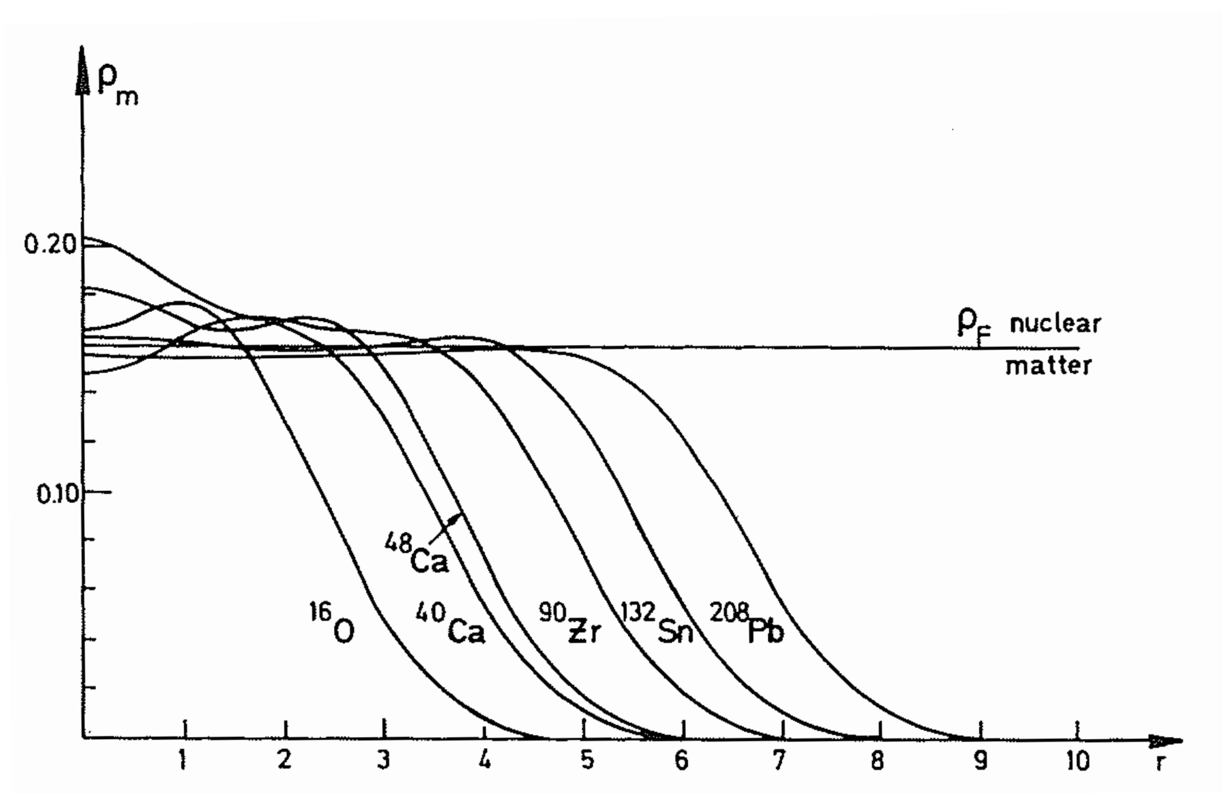
Extended nuclear matter

- Nuclear matter as a theoretical laboratory to test interactions & many-body methods
  - **Homogeneous system** of nucleons interacting via strong interactions (Coulomb switched off)
  - Thermodynamic limit ($A \to \infty$, $\mathcal{V} \to \infty$, $\rho = A/\mathcal{V}$ constant)
  - Pure neutron matter is simpler and provides constraints for astrophysical systems
  - Isospin-symmetric nuclear matter relates to bulk properties of nuclei

Equation of state of nuclear matter



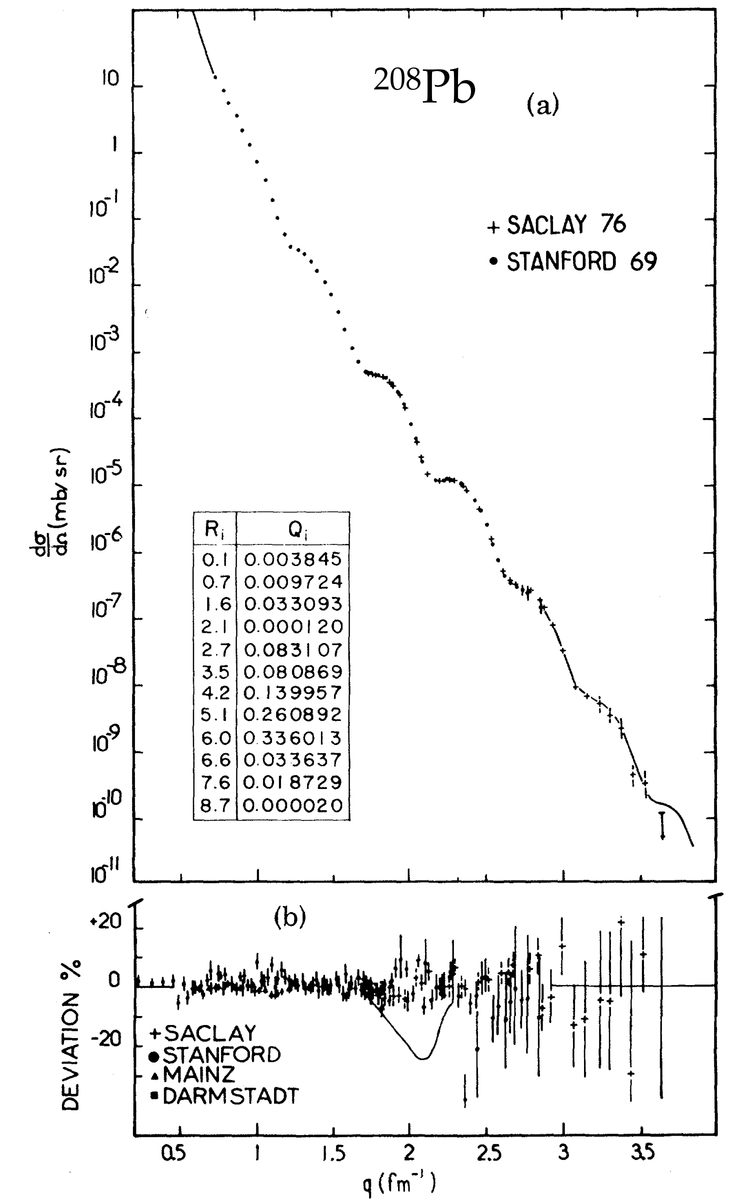
Density distributions of nuclei



[Heyde 1998]

Electron scattering off nuclei

- Electrons constitute an optimal probe to study atomic nuclei
  - Point-like → excellent spatial resolution
  - EM weak and theoretically well constrained
- Accélérateur Linéaire @ Saclay (ALS)
  - Electron accelerator (1969-1990)
  - Refined data on tens of stable nuclei

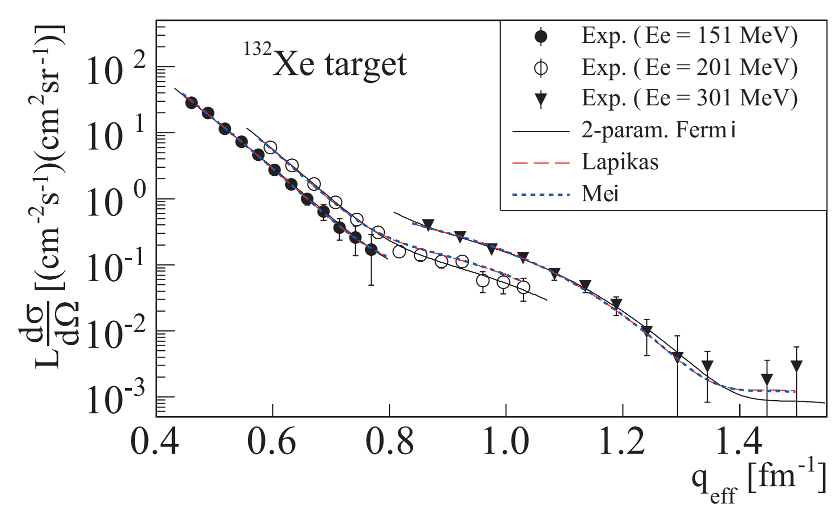


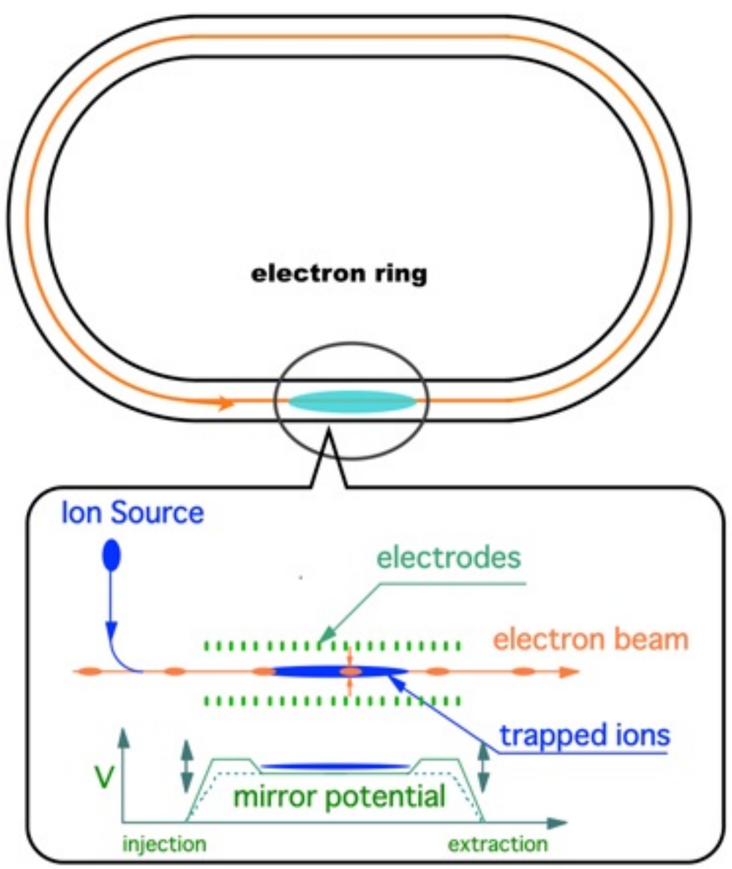
R_i	Q_i
0.1	0.003845
0.7	0.009724
1.6	0.033093
2.1	0.000120
2.7	0.083107
3.5	0.080869
4.2	0.139957
5.1	0.260892
6.0	0.336013
6.6	0.033637
7.6	0.018729
8.7	0.000020

13 orders of magnitude!

[Frois *et al*. 1977]

[Tsukada *et al*. 2017]

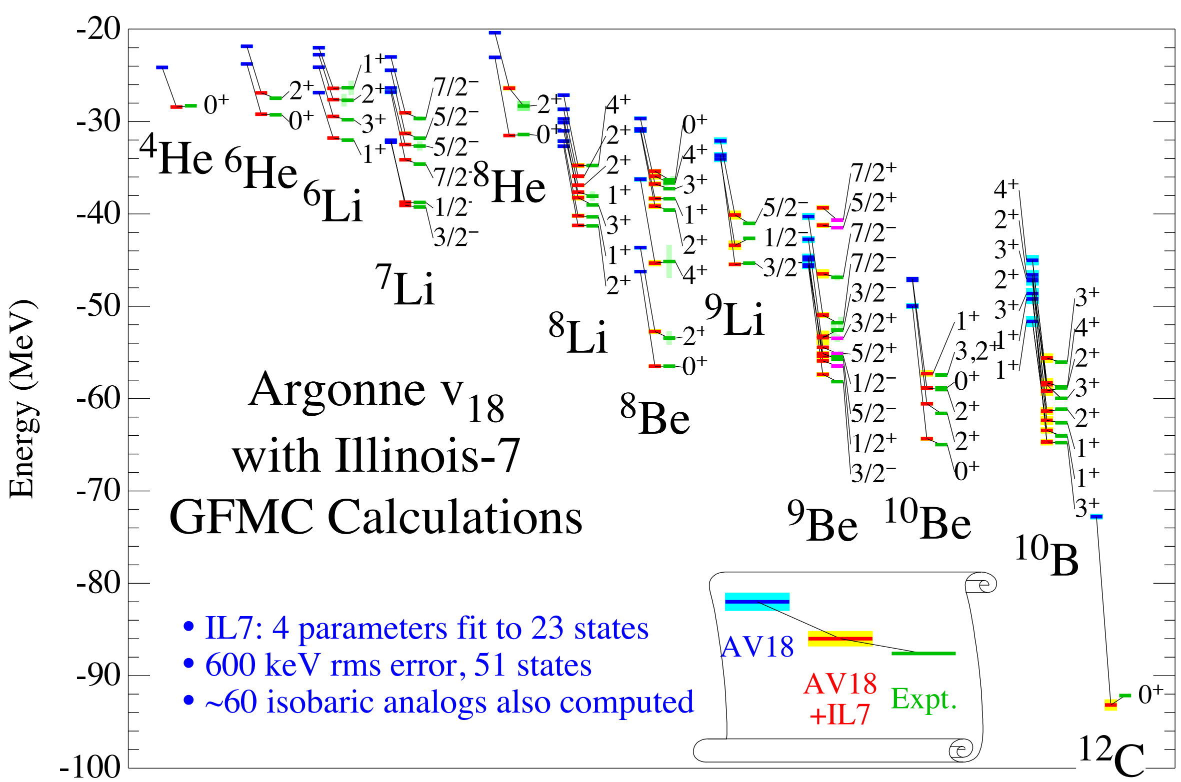




➪ **Electron scattering off unstable nuclei?**
- Challenge for the future
- First physics experiments in 2017 with SCRIT @ RIKEN

First ab initio calculations

- **1990's: Green function Monte Carlo approach**
  - ○ MC techniques to sample many-body wave function in coordinate, isospin and spin space
- **2000's: No-core shell model approach**
  - ○ Diagonalisation of the Hamiltonian in a finite-dimensional space (but with no core!)



Nuclei simulated from scratch!

Closed the gap between elementary nucleon-nucleon interactions and properties of nuclei

[Pieper & Wiringa 2001]

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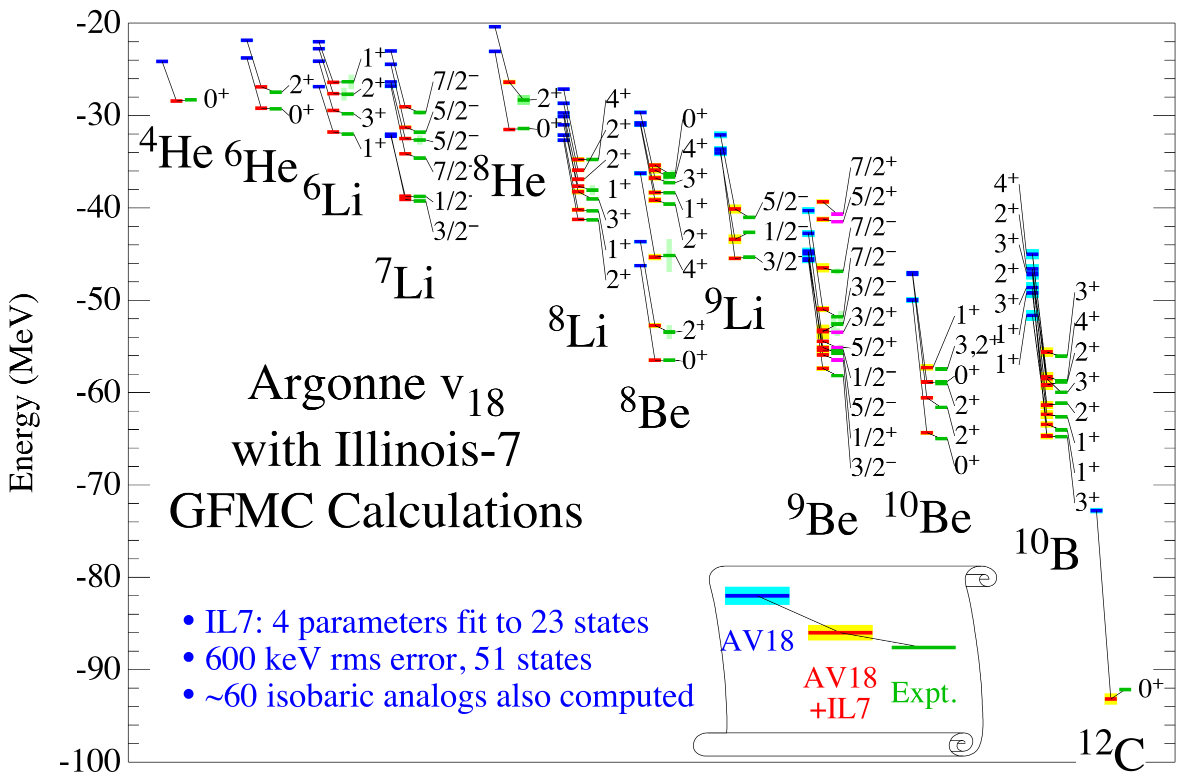

Nuclei simulated from scratch!

Closed the gap between elementary nucleon-nucleon interactions and properties of nuclei

[Pieper & Wiringa 2001]

✗ Computational effort increases exponentially / factorially with nucleon number

✗ Necessity of treating three-nucleon forces makes it more severe

→ Approach currently limited to light nuclei

Resolution scale of nucleon-nucleon interactions

⦿ **Two main problems with OBE potentials**

1. Substantial part remains phenomenological (in particular 3N sector)

2. Strong repulsive short-range component (“hard core”)

   ○ Induces strong correlations in the wave function

   ○ Large bases needed to converge → applicability limited to light nuclei

Hard core ↔ Strong coupling between low and high momenta ↔ High resolution

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Hard core ↔ Strong coupling between low and high momenta ↔ High resolution

Do we really need such high resolution to compute properties of nuclei?

ρ , ω, σ masses $>$ 700 MeV spatial distances $<$ 0.5 fm cf. nucleon radius ~ 0.8 fm	↔	pion mass ~ 140 MeV av. nucleon momenta ~ 200 MeV	↔	observables ~ 0.1-10 MeV

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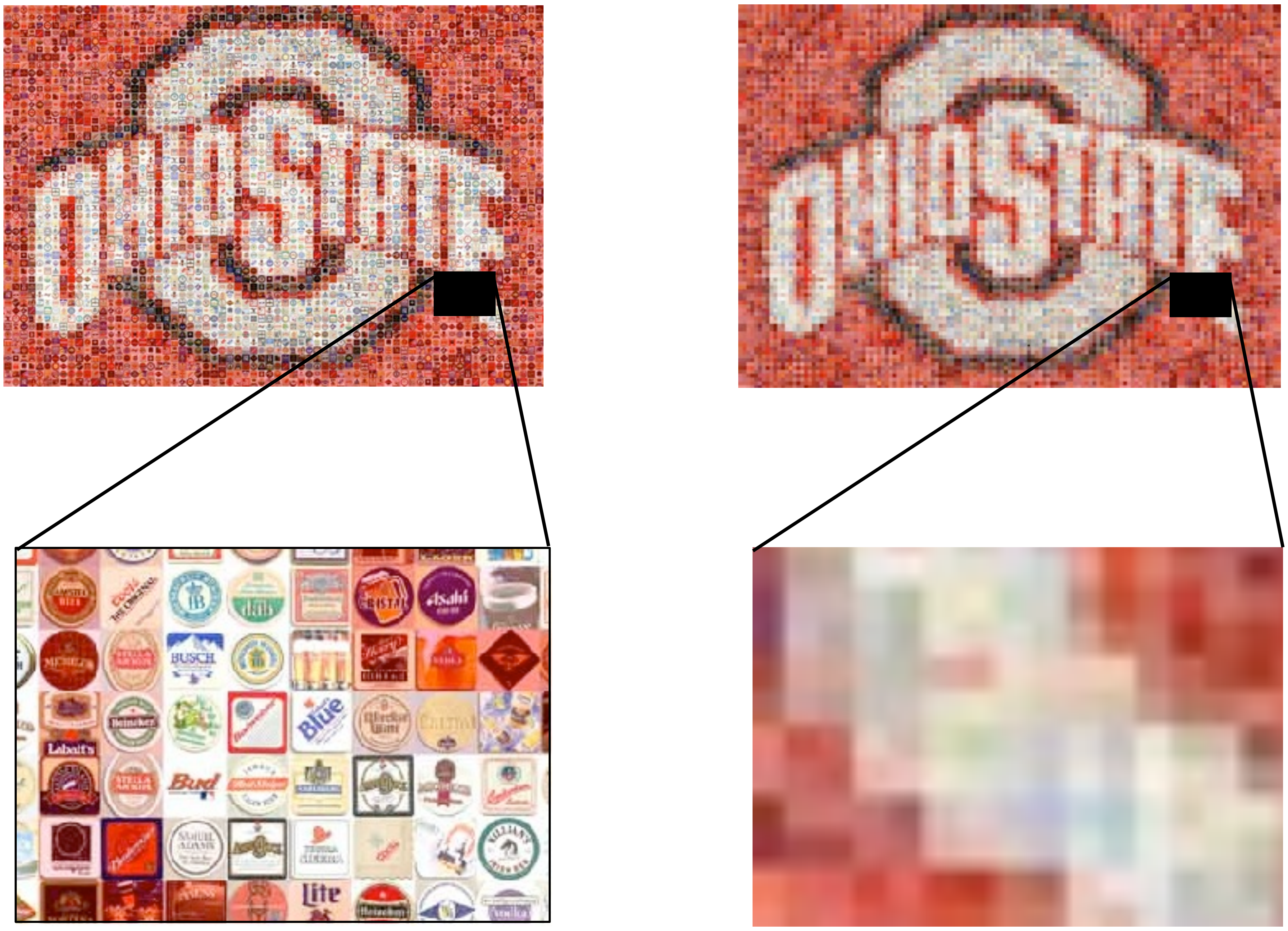
➪ **Conceptual breakthrough**: apply Effective Field Theory to build nuclear potentials

➪ **Technical breakthrough**: apply Renormalisation Group techniques to transform nuclear potentials

Resolution scale of nucleon-nucleon interactions

[figures from K. Hebeler]

Resolution scale of nucleon-nucleon interactions



[figures from K. Hebeler]

Effective field theory

- **The principles**

[Weinberg, van Kolck, ..]

1990's

1. Use separation of scales to define d.o.f & expansion parameter

   Typical momentum at play ← $\frac{Q}{M}$ → High energy scale (not included explicitly)

2. Write all possible terms allowed by symmetries of underlying theory (QCD)

3. Order by size all possible terms $\rightarrow$ systematic expansion (= "power counting")

4. Truncate at a give order and adjust coupling constants (use underlying theory or data)

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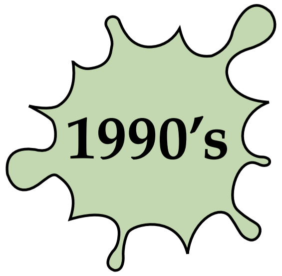

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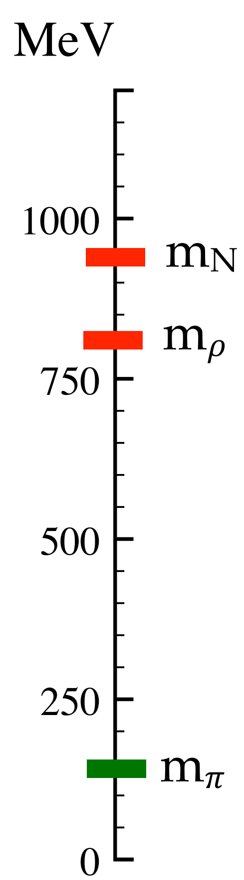

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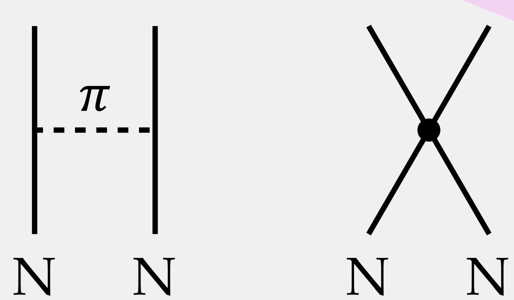
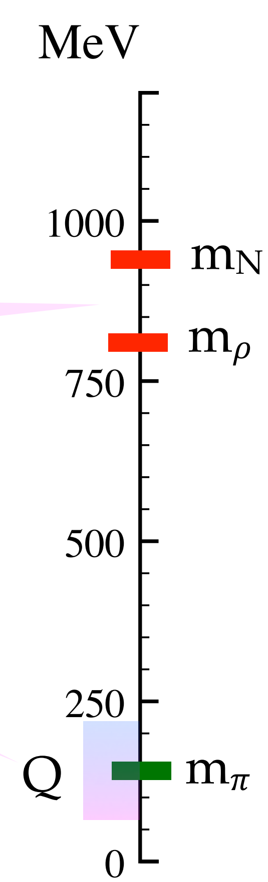
Chiral EFT

➪ Expand around Q ~ m_π

High-energy via contact interactions

Keep pion dynamic explicit





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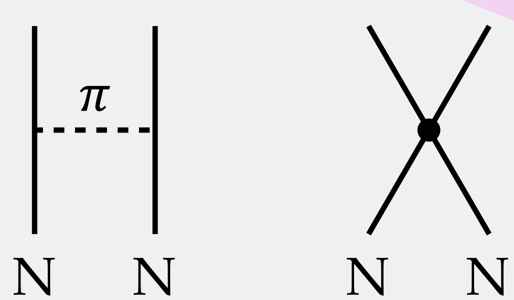
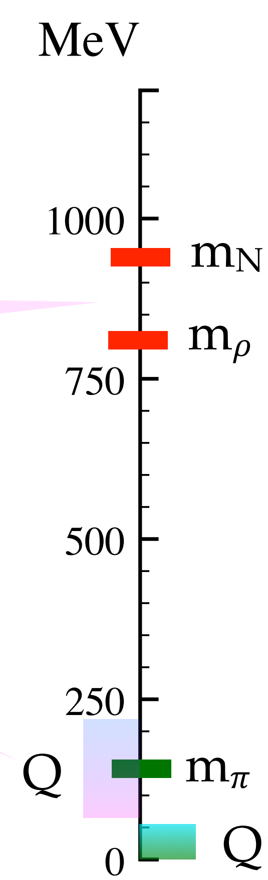
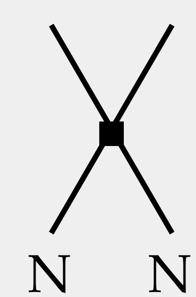




Pionless EFT

➪ Expand around Q ~ 0

Integrate out pions too
→ only contact terms



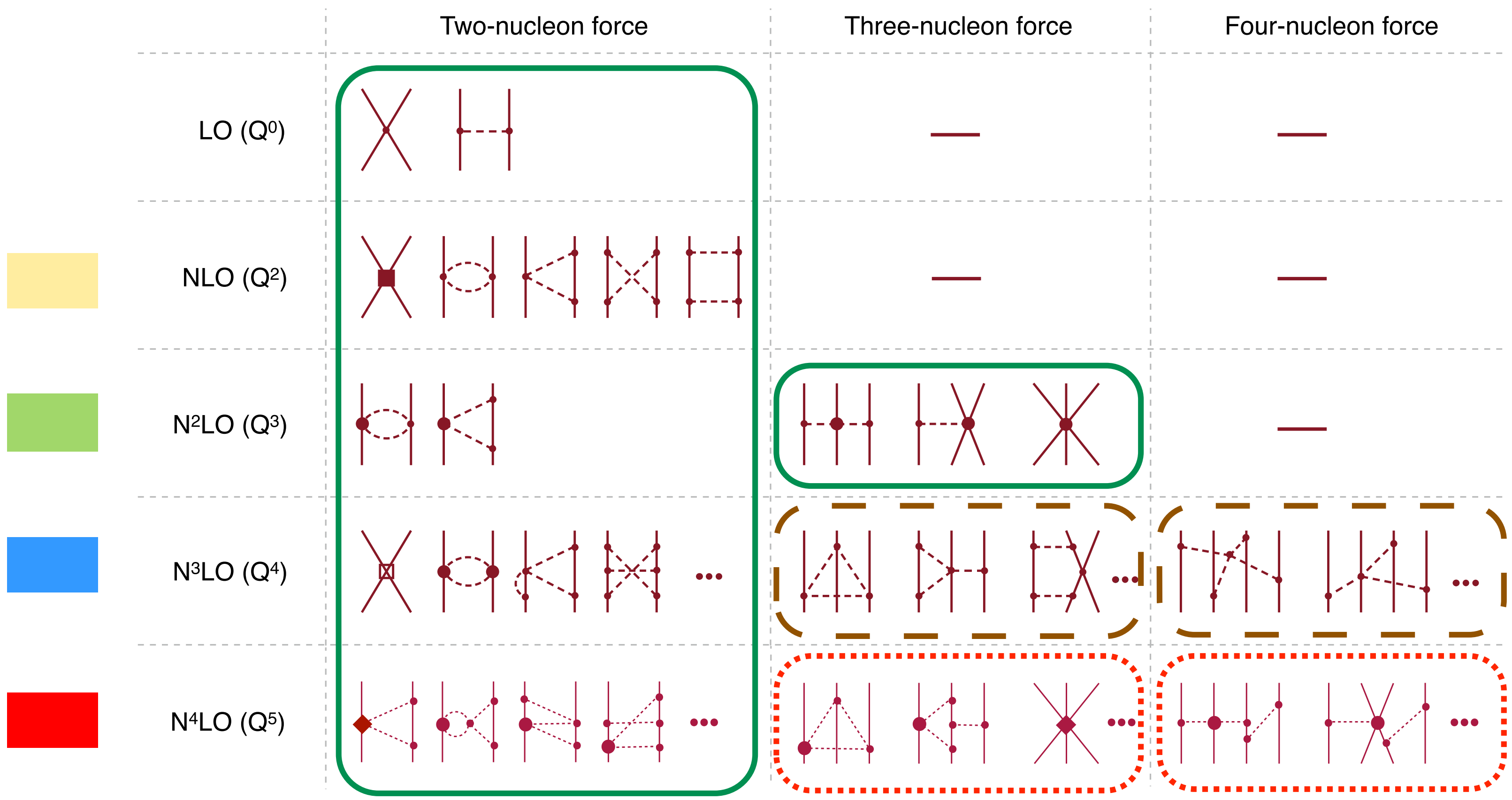
Chiral effective field theory

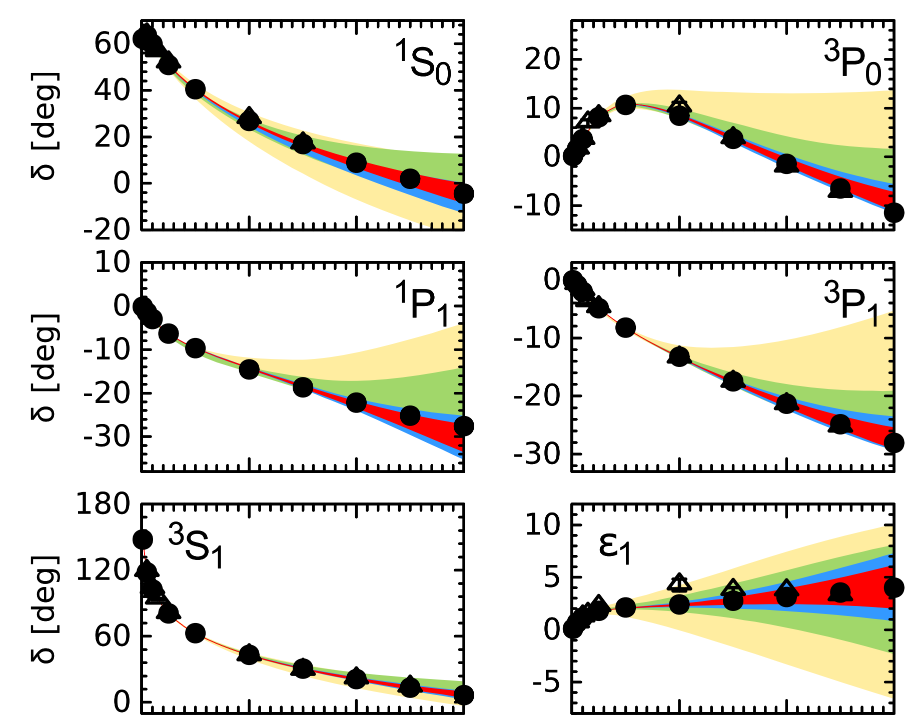
✓ **Systematic** framework to construct *A*N interactions (*A*=2, 3, …)

✓ A **theoretical error** can be assigned to each order in the expansion

⦿ Is the chiral expansion converging quickly enough?

→ If not, the approach becomes unfeasible





[Meißner 2016]

⦿ Goal: apply to the many-nucleon system (and propagate the theoretical error!)

Solving the many-body Schrödinger equation

⦿ **Basis truncation**

- Representation of the many-body wave function
- Infinite in principle, finite in practise → need to be large enough to contain relevant physics
- **The weaker the high-momentum components in H, the smaller the basis to converge**

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⦿ **Expansion around a reference state**

- One particular configuration can be solution of an auxiliary problem (with Hamiltonian H_0)
- Express total Hamiltonian as $H = H_0 + H_1$
- Expand exact wave function around that "reference state" → approximate ab initio

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⦿ **Many-body truncation**

- Order "by size" contributions from all different configurations
- Keep only the most important ones → approximate ab initio
- **The weaker the high-momentum components in H, the more you can truncate**

Approximate ab initio methods

⦿ **Trade exactness of the solution for more favourable scaling with A**

○ Express the problem in perturbation → truncate → resum (non perturbative)

○ Three main methods:

1. Self-consistent Green's function theory (SCGF)

○ Rewrite many-body Schrödinger equation in terms of G and Σ → Dyson equation

$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

2. Coupled-cluster theory (CC)

○ Computes the similarity-transformed normal-ordered Hamiltonian

$$\overline{H} \equiv e^{-T} H_N e^{T} \qquad\qquad E = \langle \phi | \overline{H} | \phi \rangle$$

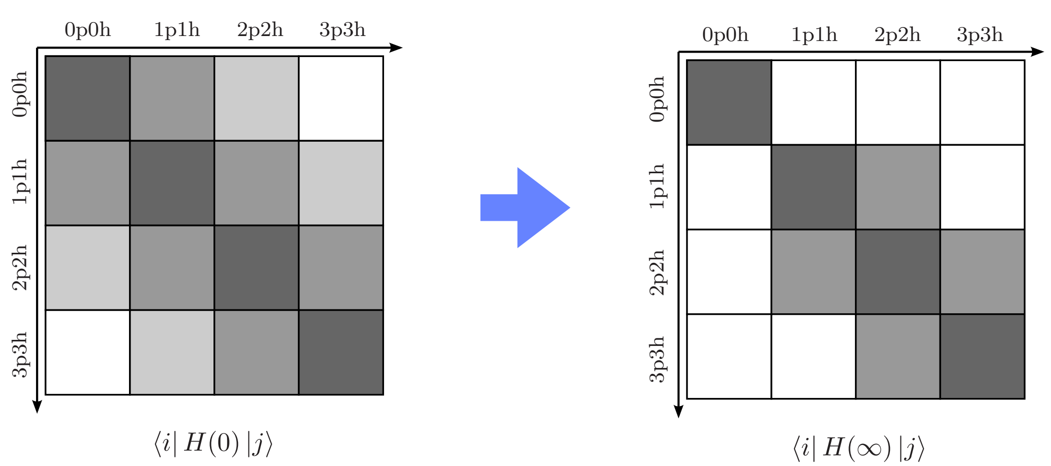
3. In-medium similarity renormalisation group (IM-SRG)

○ Employs a continuous unitary transformation of H to decouple g.s. from excitations

Flow equation

$$\frac{d}{ds} H(s) = [\eta(s),\, H(s)]$$

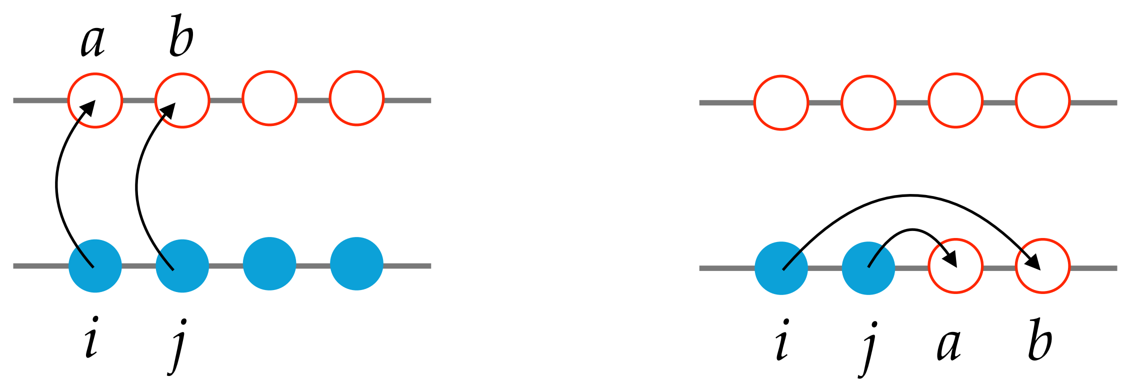
truncated at rank n at each step



Approximate ab initio methods

- Approximate/truncated methods capture correlations via an expansion in **ph excitations**
- Open-shell nuclei are **(near-)degenerate** with respect to ph excitations

closed-shell



open-shell

○ E.g. consider MBPT(2) $\Delta E^{(2)} = \frac{1}{4} \sum_{abij} \langle ij|\hat{v}|ab\rangle \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$

when $\epsilon_i + \epsilon_j = \epsilon_a + \epsilon_b$ the expansion breaks down

- Way out: formulate the expansion around a **symmetry-breaking** reference state
  - ○ Symmetry-breaking solution allows to **lift the degeneracy**
  - ○ GF theory extended to particle-number breaking scheme (Gorkov formalism) [Gorkov 1958]
  - ○ Implementation for semi-magic nuclei developed in Saclay & Surrey [Somà, Duguet & Barbieri 2011]
  - ○ Symmetries must be eventually restored

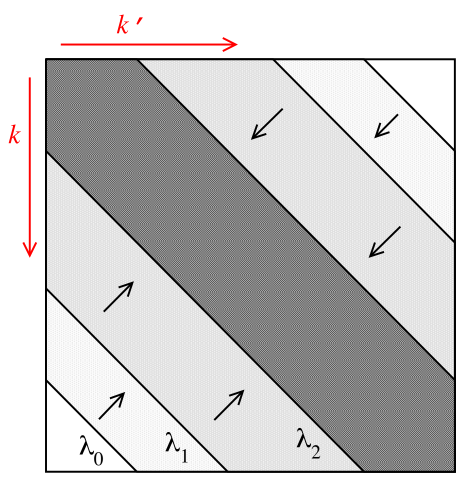
Similarity renormalisation group

➪ Can we make the couplings between low and high momenta even weaker?

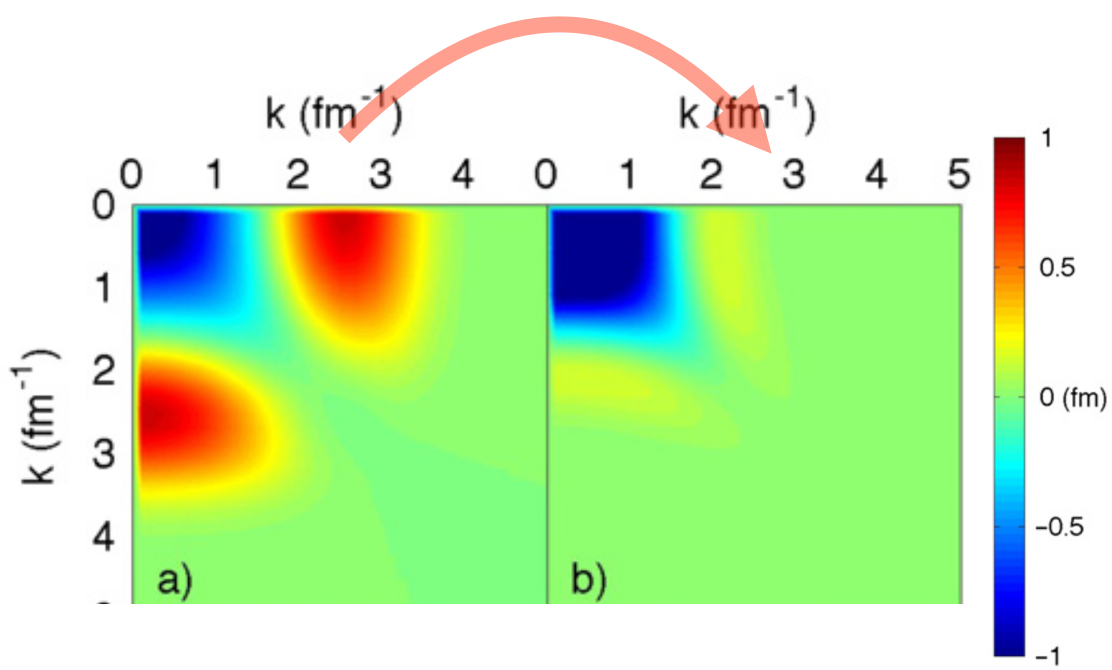
→ After all, any unitary transformation on H leaves observables unchanged!

Similarity Renormalisation Group (SRG) techniques for 2N and 3N forces

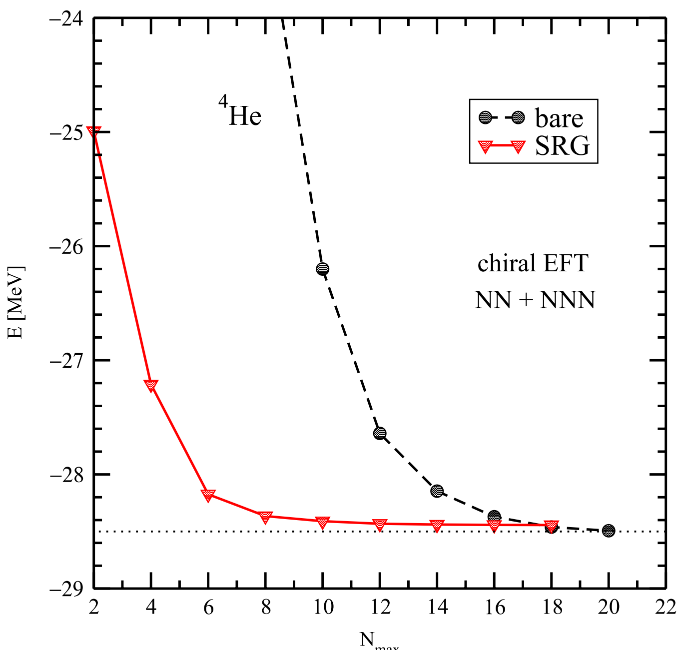
= Unitary transformation to further **lower the resolution scale** of the original Hamiltonian



V_{SRG}



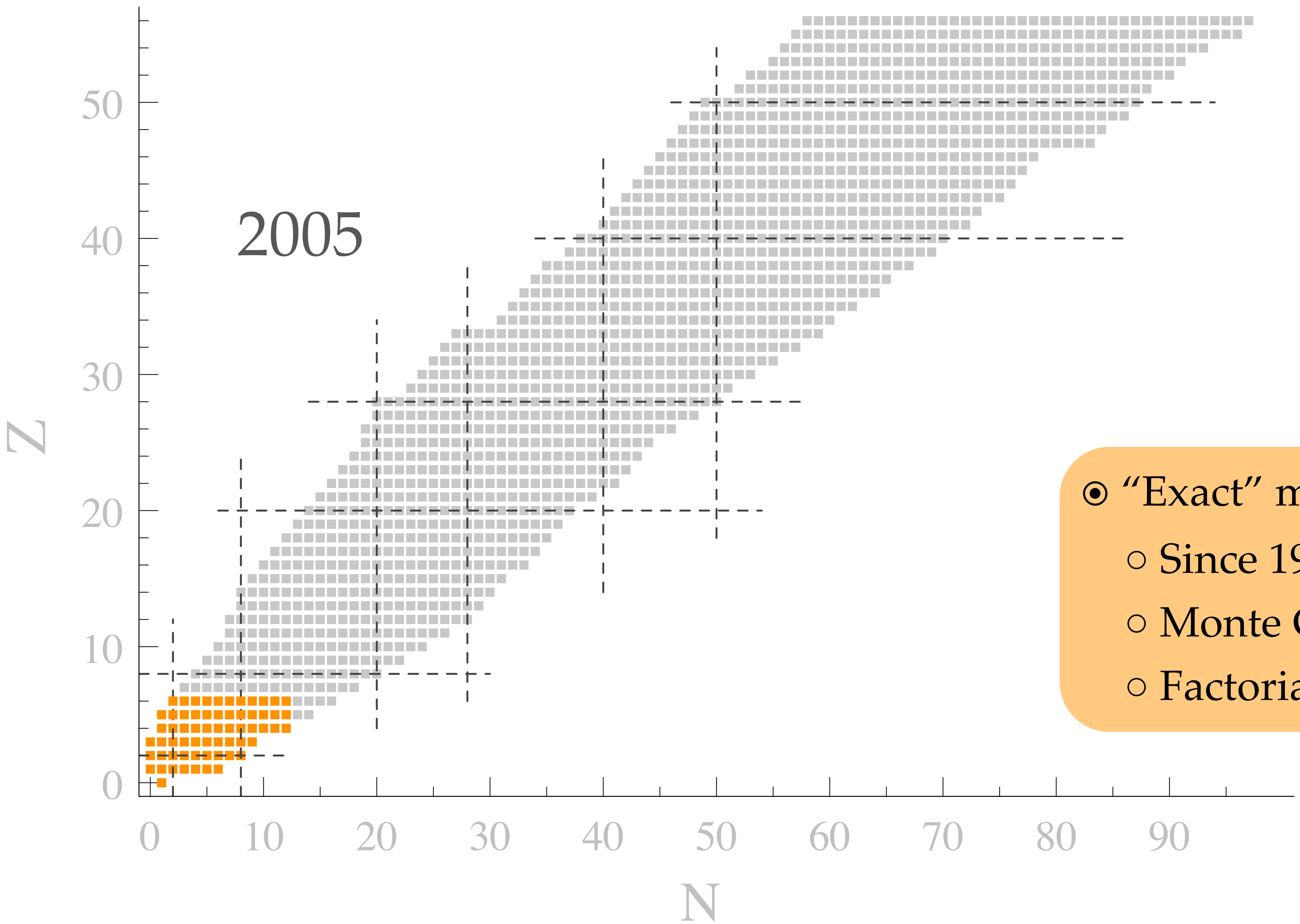
[Bogner, Furnstahl & Schwenk 2010]



[Jurgenson, Navratil & Furnstahl 2013]

✗ **No free lunch**: unitary transformation generates 3- and many-body forces

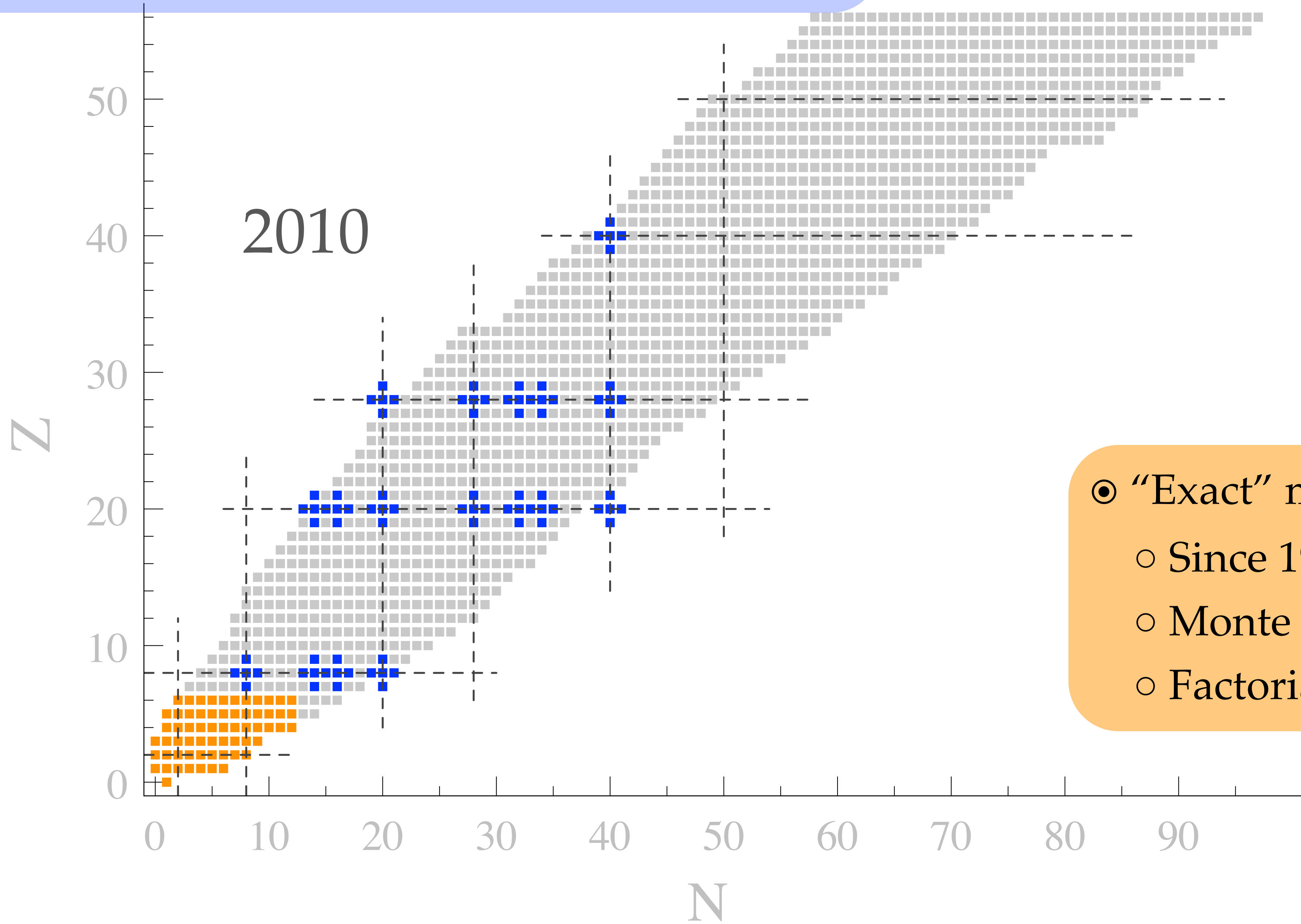
Evolution of ab initio nuclear chart



- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

Evolution of ab initio nuclear chart

- Approximate methods for closed-shells
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling



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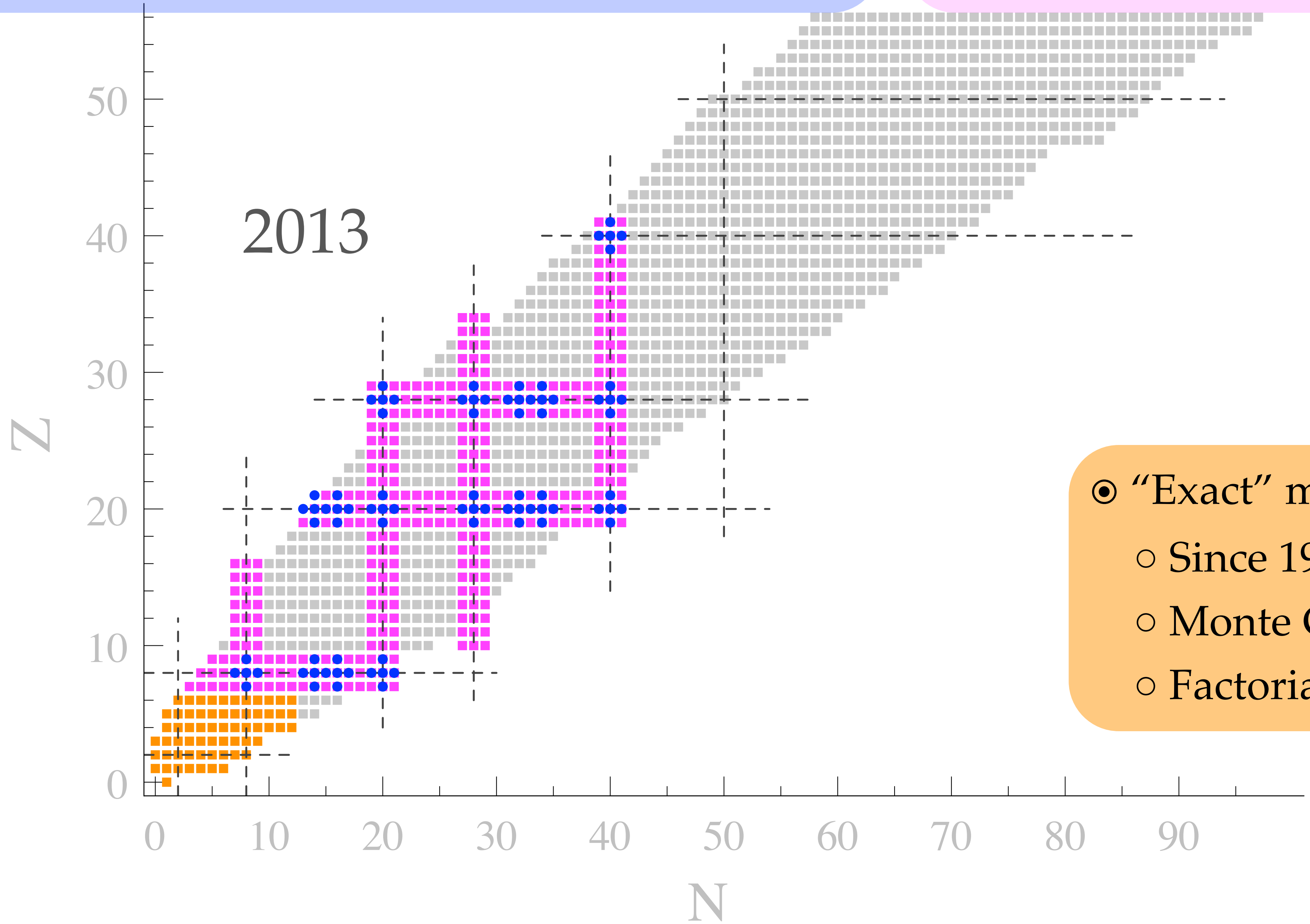
- Approximate methods for open-shells
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling

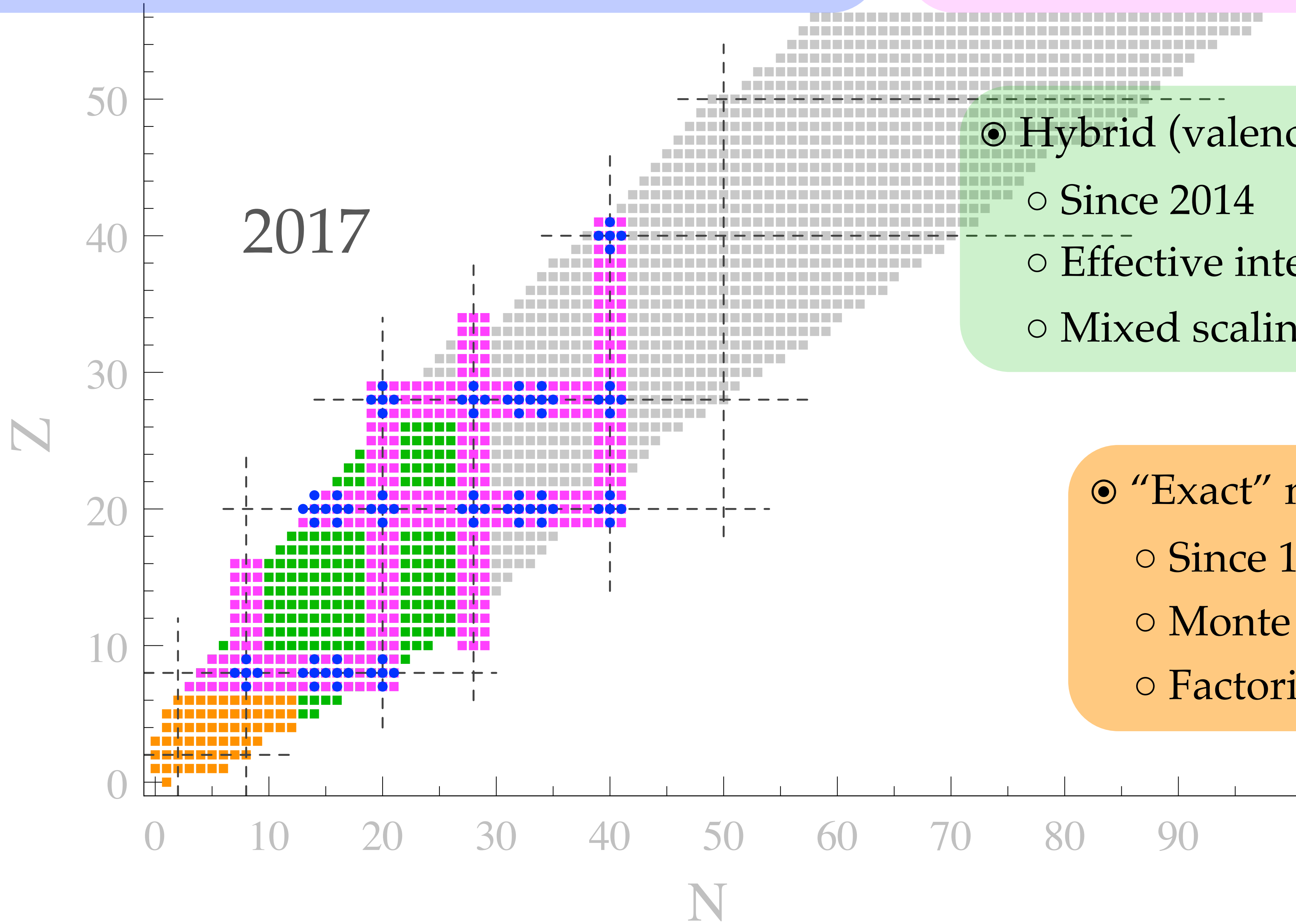


- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

Evolution of ab initio nuclear chart

- Approximate methods for closed-shells
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling

- Approximate methods for open-shells
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling



- Hybrid (valence-space) methods
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

The potential "bubble nucleus" Si34

⦿ **Unconventional depletion** ("bubble") in the centre of ρ_{ch} conjectured for certain nuclei

⦿ **Purely quantum mechanical effect**

- ○ $\ell = 0$ orbitals display radial distribution peaked at $r = 0$
- ○ $\ell \neq 0$ orbitals are instead suppressed at small r
- ○ Vacancy of s states ($\ell = 0$) embedded in larger-ℓ orbitals might cause central depletion

⦿ **Ab initio Green's function calculations**

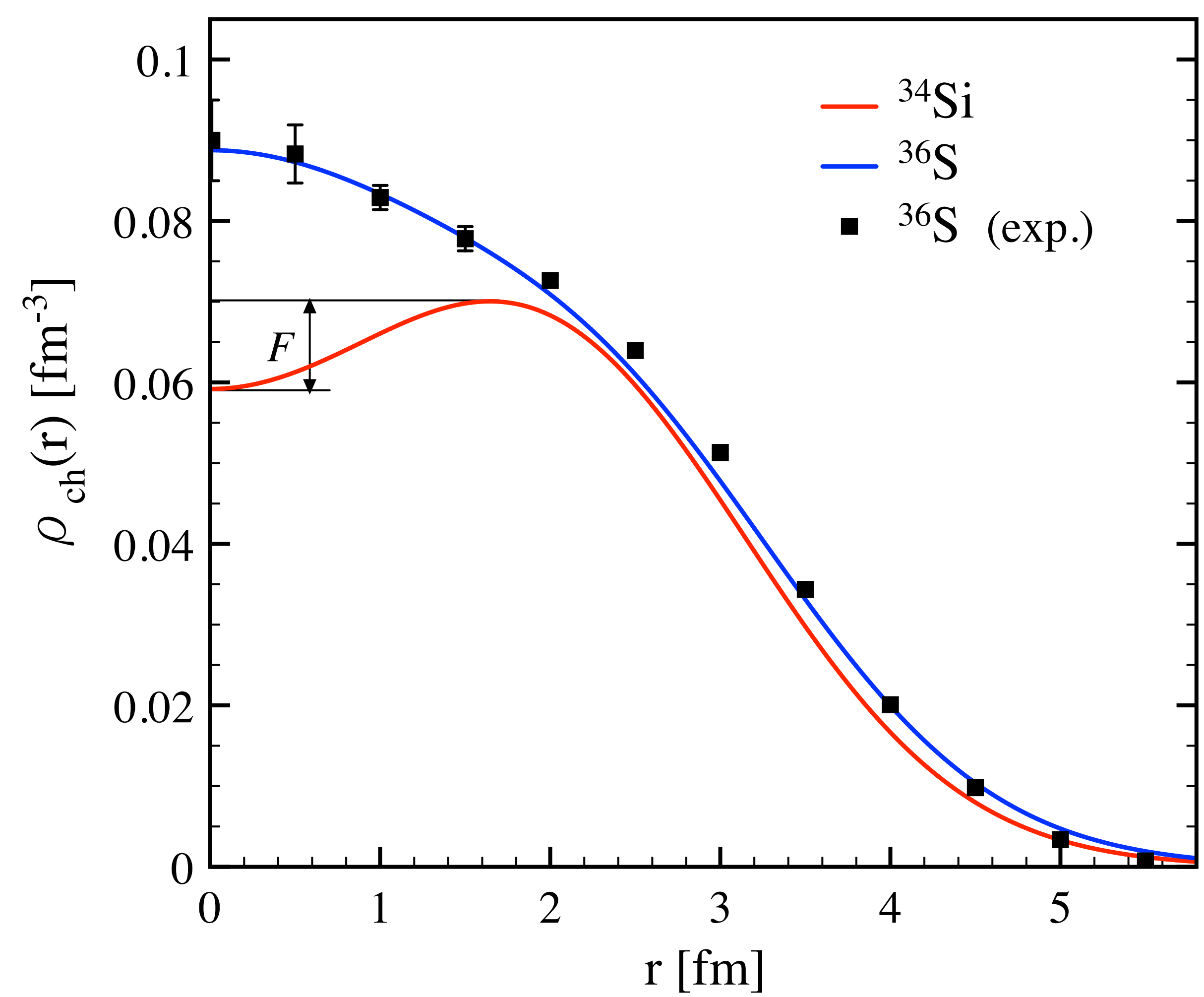
- ○ Input: NN+3N interactions from ChEFT
- ○ Output: BE, radii, densities, spectra, …

✓ Computed density of ^{36}S agrees with data

✓ Computed density of ^{34}Si shows bubble

➪ Density measurement of (unstable) ^{34}Si?

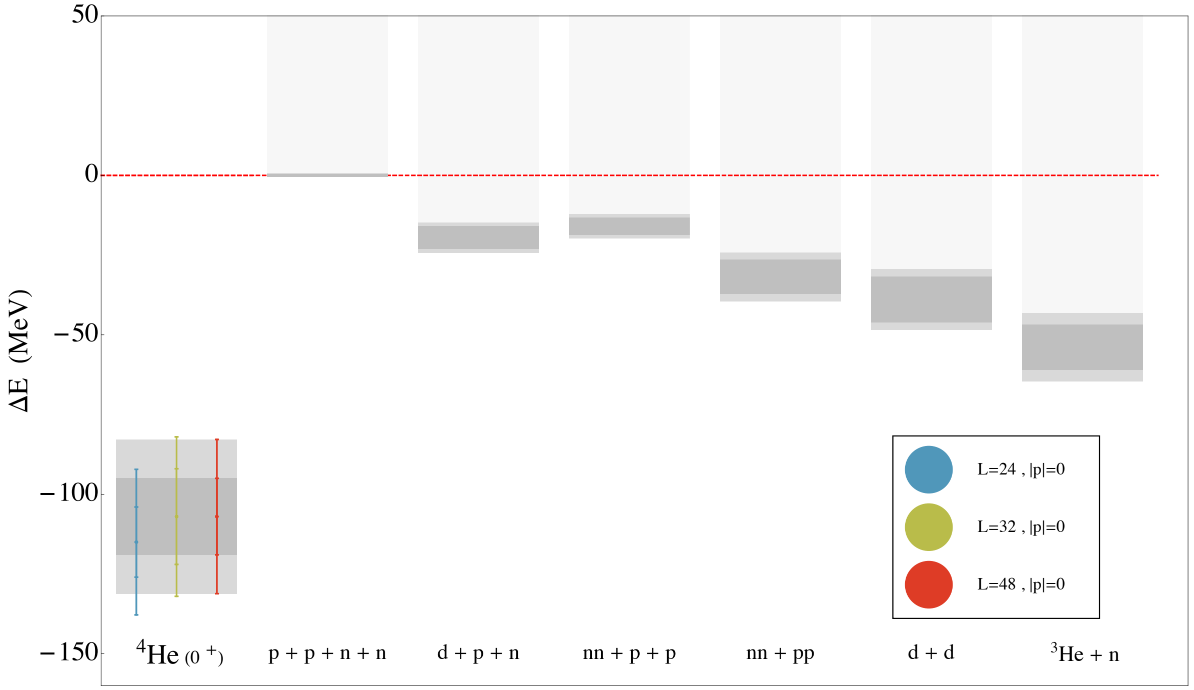
[Duguet, Somà *et al.* 2017]



Lattice QCD

- At low-energy, QCD is non-perturbative → calculations possible only on the lattice
  - Calculation of hadron masses very successful
  - Multi-baryon systems? Atomic nuclei?
- Two different routes are currently followed

➪ Direct calculation of nuclei

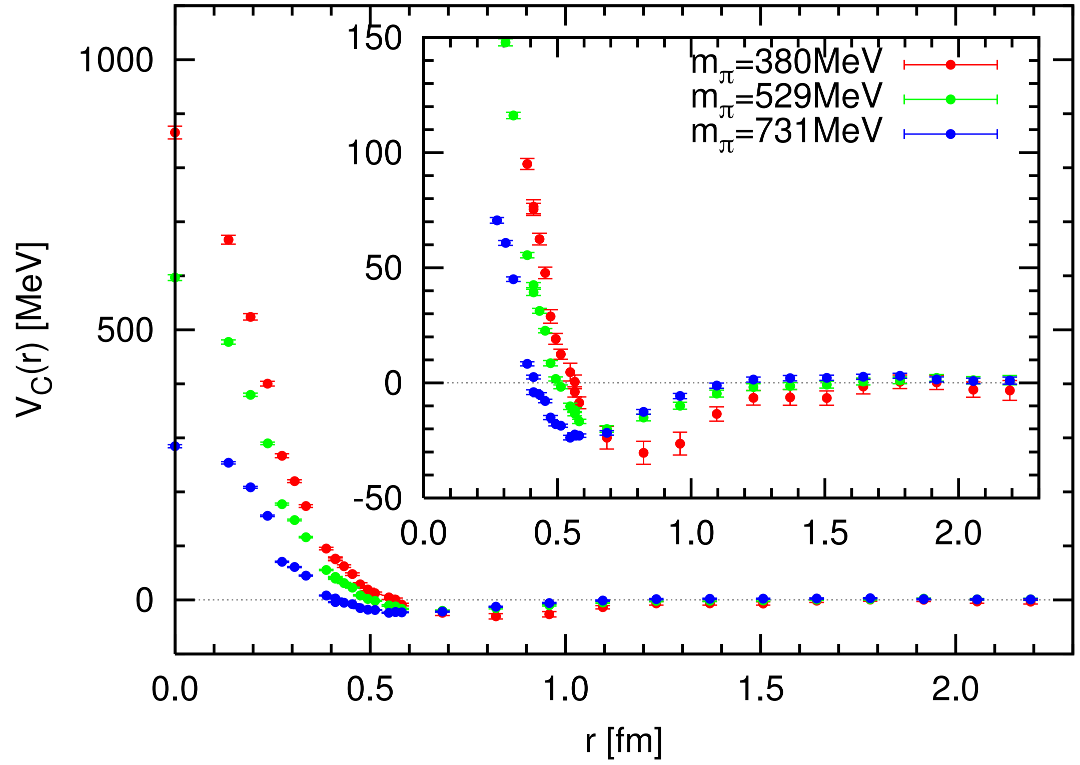


[Beane *et al.* 2012]

Excitation energy << QCD scales

✗ High statistic data required

➪ Calculation of nucleon-nucleon potential



[Ishi, Aoki & Hatsuda 2007]

Model-dependent extraction

✗ 3-body part problematic

Historical recap #3

Pre-1935 stuff (Radioactivity, Rutherford's experiment, discovery of the neutron, …)

1935 Semi-empirical mass formula (liquid drop)

1935 Yukawa potential

1949 Non-interacting shell model

1960's Valence-space interaction (= interacting shell model)

1970's Energy density functionals

1970's One-boson exchange potentials

1980's High precision one-boson exchange potentials

1990's First ab initio calculations

1990's Effective field theory applied to nuclear forces

2000's Approximate ab initio (= "many-body") methods developed

2010's Renormalisation group techniques applied to nuclear forces

2010's Massively-parallelised simulations of medium-mass nuclei

2010's First lattice QCD calculations of NN potential & multi-baryon systems

Today

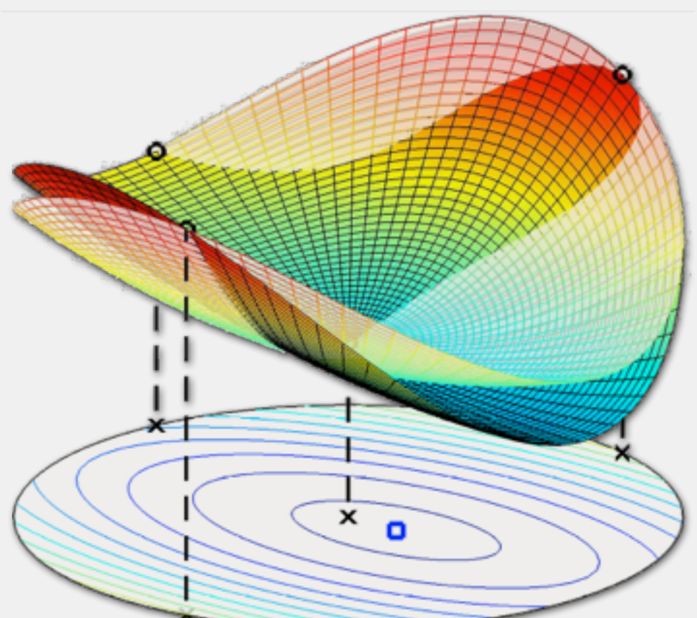
Computational challenges

Curie @ CCRT / CEA, France

- Progress relies on increasing computational resources
  - Numerical codes heavily parallelised
  - Collaboration with computer scientists necessary
  - Yearly allocations of the order of 10-100M CPU hours

Building of NN/3N interactions

Costly multi-parameter fits

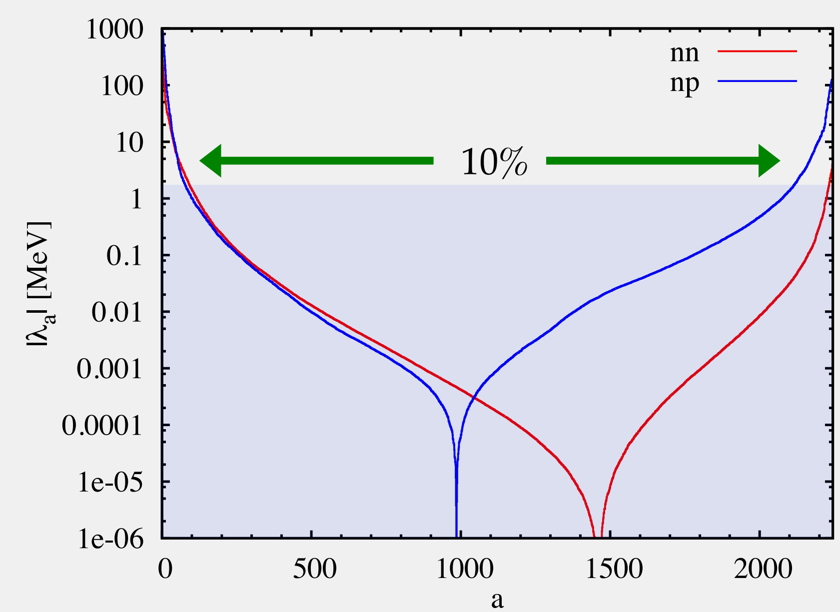


[figure from C. Forssén]

➪ Machine learning techniques

Ab initio three-body forces

Number of matrix elements explodes



[Lesinski 2011]

➪ Algorithms / tools from "big data"

Theoretical challenges

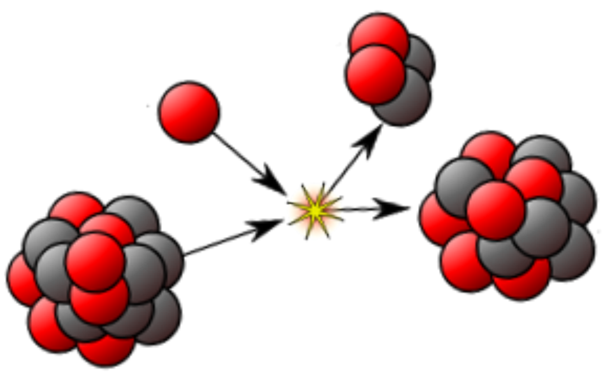
◉ **Bridge structure and reactions**

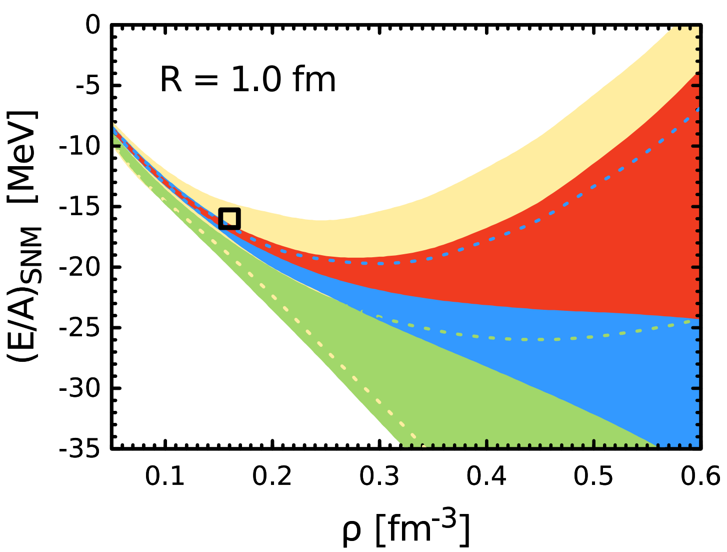
○ Theoretical tools to deal with continuum

○ Nucleon-nucleus interaction?

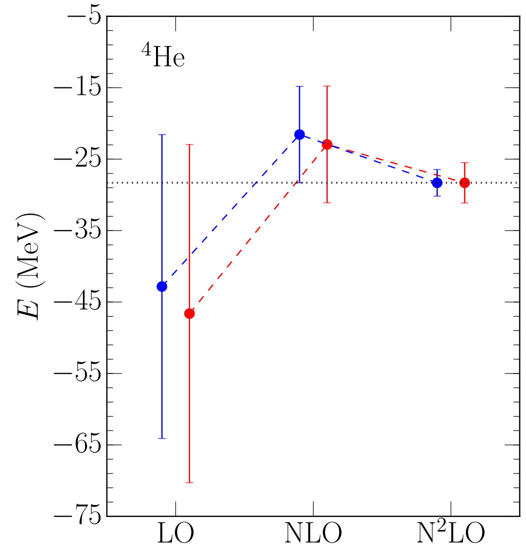
○ Reaction approaches ↔ model dependence?

○ Structure consistently "extracted" and computed?





[Hu *et al.* 2017]



[Lynn *et al.* 2017]

◉ **Theoretical errors**

○ Systematic errors hardest to estimate

○ Crucial where no data is / will be available

○ EFTs offer tools to quantify our ignorance

○ Challenge: EFT + nuclear many-body problem