Nuclear Structure Theory (lecture I)

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Outline of the lectures

- Lecture 1: General concepts. What is nuclear structure theory? *Ab initio*, shell-model.
- Lecture 2: Density Functional Theory. Applications. Spherical, deformed and “soft” nuclei.
- Lecture 3: Collective and single-particle spectroscopy.

Two important points:

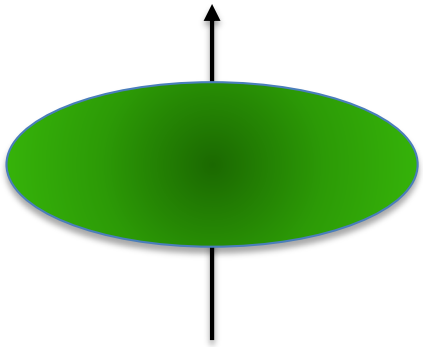
- Please, do interrupt – particularly, if you feel that without a prompt clarification you will not profit from the rest of the lecture !
- A few codes that may help are available – I will provide you with a link later on.

Let's start

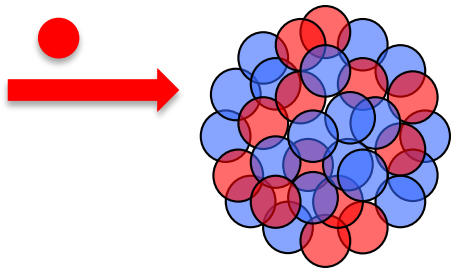
The goal of nuclear structure theory is to explain what is observed, starting from a theory, or a model, that considers appropriate degrees of freedom (as a rule, point-like nucleons) and treats them consistently with quantum mechanics and its symmetries.

Is there a single, or a standard, nuclear model? **NO!**

This is, most likely, unavoidable.



43 keV rotation in U:
$t \approx 10^{-20}$ s



proton at 400 MeV:
$t \approx 10^{-23}$ s
λ_{DB} = 1.3 fm

Perhaps we can say that all models lie under the EFT ``umbrella''.

Reductionism? Unfeasible...

QCD, the basic theory of the strong interaction, is **not perturbative** at low energy (cannot be solved by summing Feynman diagrams).

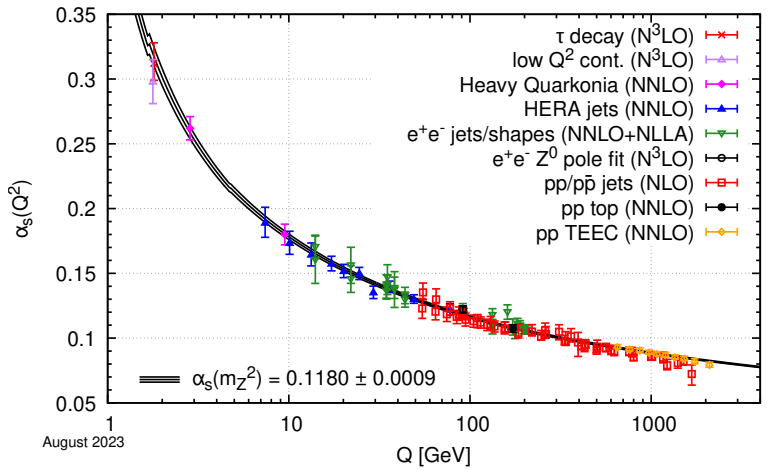
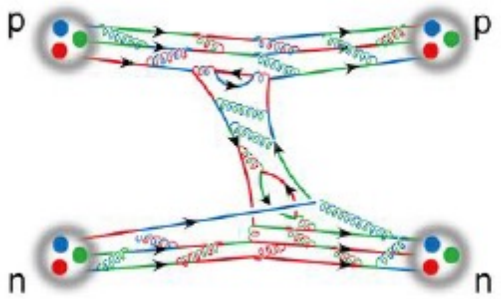


Figure from:
https://pdg.lbl.gov/2023/reviews/rpp2023-rev-qcd.pdf

QCD can, in principle, be solved on a **lattice** (i.e., the space-time is discretized).

However, these calculations are **not giving stable and realistic results at the nuclear physics scale.**



No bound two- or three-nucleon system.
BE (^{4}He) around 5 MeV.
T. Inoue *et al.*, PRL 111, 112503 (2013)
Cf. also C. Drischler *et al.*, PPNP 121, 103888 (2021)

How to not get lost

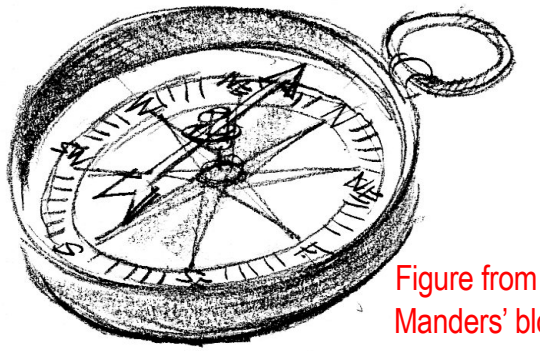
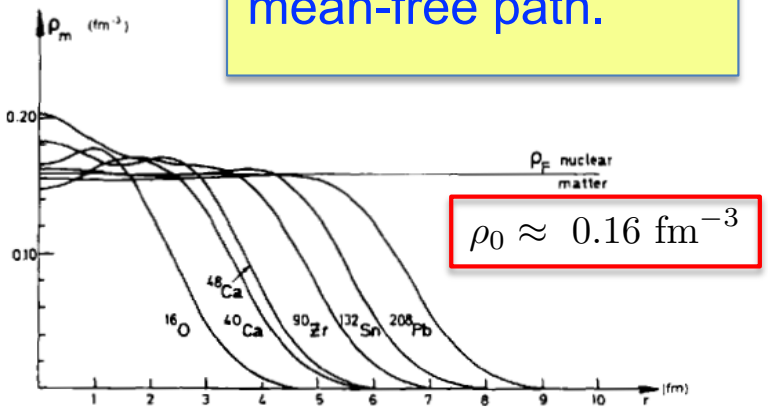


Figure from J. Manders' blog

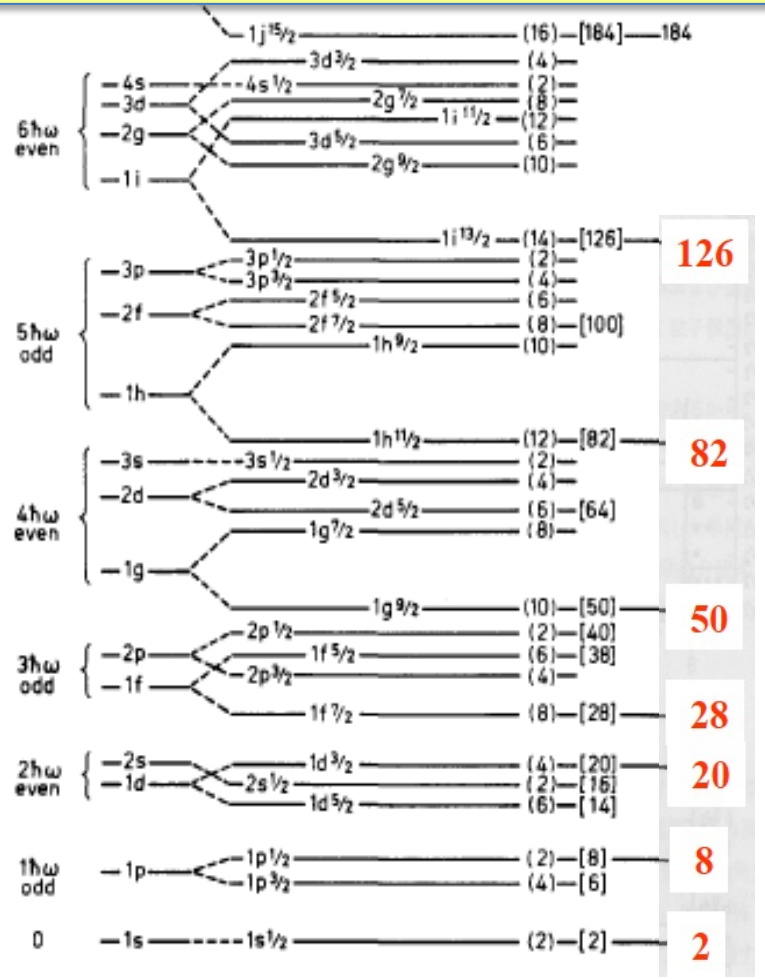
Many experimental evidences point to the fact that nucleons move in nuclei, to a first approximation, as **independent** particles.

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

Nuclei are "dilute". Nucleons have large mean-free path.



$$\rho_0 \approx 0.16 \text{ fm}^{-3}$$



Cf. the lecture(s) by Sean

How to not get lost

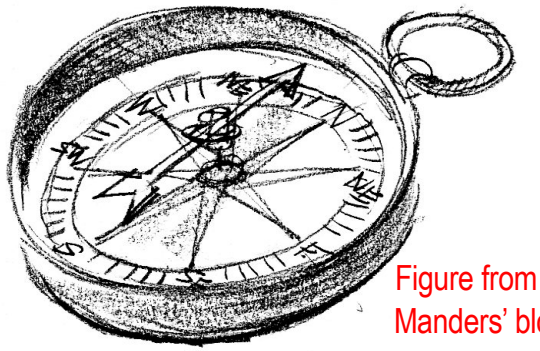
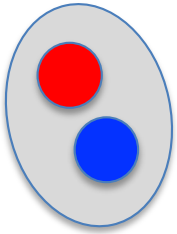


Figure from J. Manders' blog

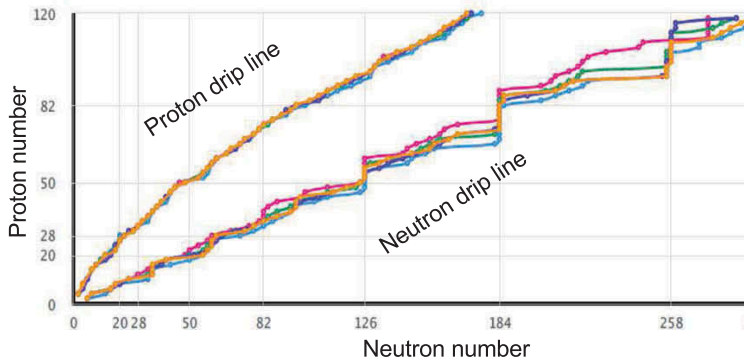


V_{pn} much stronger than V_{nn}, V_{pp}.

Exercise: reconcile this fact with the fact that V commutes with isospin.
Hint: use the Pauli principle.

Important role for the nuclear stability.

Drip lines: the loci where the separation energy changes its sign and the nuclei become unbound.



As a function of the neutron number, ^{24}O is the last bound O isotope (Z=8); **if we add just one proton and move to F (Z=9), we can bind seven more neutrons** as the last bound F isotope is ^{31}F!

There are several combinations of **nuclear Hamiltonians and many-body methods** to solve the nuclear problem.

Ab initio approaches

Configuration interaction/Shell model

Mean-field and DFT

...

The wording may not really convey the meaning.

What is really meant? What are the key ideas behind? What are the questions you should ask to the practitioners of these models?

$$H\Psi = E\Psi$$

$$H = T + V = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V_2(i,j) + \sum_{i<j<k} V_3(i,j,k)$$

How to not get lost

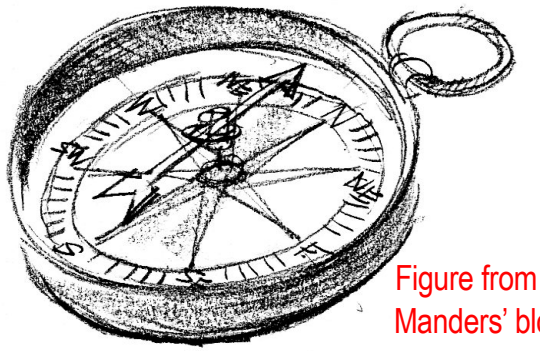


Figure from J. Manders' blog

$$E(\alpha) = \frac{\langle \Psi(\alpha)|H|\Psi(\alpha)\rangle}{\langle \Psi(\alpha)|\Psi(\alpha)\rangle}$$

$$E_0 = \min_\alpha E_\alpha$$

To a large extent, methods either are based on the **variational principle** or rely on **expansion (perturbative) techniques**.

$$H = H_0 + H_1$$

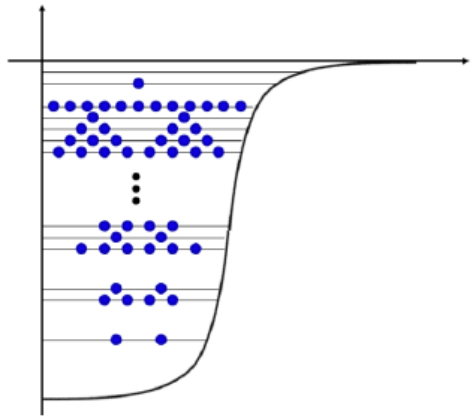
$$E^{(2)} = \sum_{k\neq 0} \frac{\langle 0|H_1|k\rangle^2}{E_0 - E_k}$$

Independent particles: the Slater determinant

A Slater determinant is the *N*-particle wave function that is associated with *N* independent single-particle wave functions **(for fermions)**.

$$\Phi(x_1 \ldots x_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1(x_1) & \ldots & \phi_A(x_1) \\ \ldots & \ldots & \ldots \\ \phi_1(x_A) & \ldots & \phi_A(x_A) \end{vmatrix}$$

$$x \equiv (\vec{r}, \sigma, \tau)$$



2 particles: $\frac{1}{\sqrt{2}} [\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)]$

Exercise: if O_1, O_2, O_3 are 1-body, 2-body, 3-body operators, prove the following formulas: *(Tilde ~ means anti-symm)*

$$\langle \Phi | O_1 | \Phi \rangle = \sum_i \langle i | O_1 | i \rangle,$$

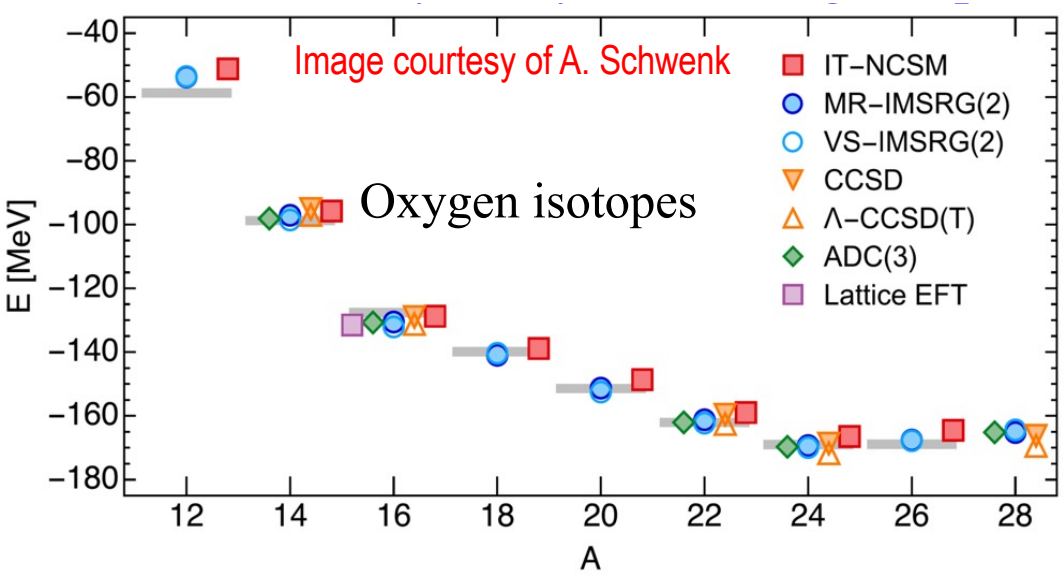
$$\langle \Phi | O_2 | \Phi \rangle = \frac{1}{2!} \sum_{ij} \langle ij | \tilde{O}_2 | ij \rangle,$$

$$\langle \Phi | O_3 | \Phi \rangle = \frac{1}{3!} \sum_{ijk} \langle ijk | \tilde{O}_3 | ijk \rangle.$$

Ab initio nuclear structure

Techniques to solve the many-body problem that are **exact, or systematically improvable, and can provide reliable estimates of the theoretical errors.**

Results are sensitive to the choice of the Hamiltonian.



- Quantum Monte Carlo (QMC)
- Lattice EFT
- In-medium similarity renormalization group (IMSRG)
- Coupled cluster (CC)
- Self-consistent Green's function (SCGF)
- No-core Shell Model (NCSM)

...

Ab initio, depending on the specific implementation, **has difficulties to handle heavy nuclei and highly excited states.**

Quantum Monte Carlo

Variational Monte Carlo (VMC)

$$E(\alpha) = \frac{\langle \Psi(\alpha)|H|\Psi(\alpha)\rangle}{\langle \Psi(\alpha)|\Psi(\alpha)\rangle} \qquad E_0 = \min_\alpha E_\alpha$$

Diffusion Monte Carlo (DMC)

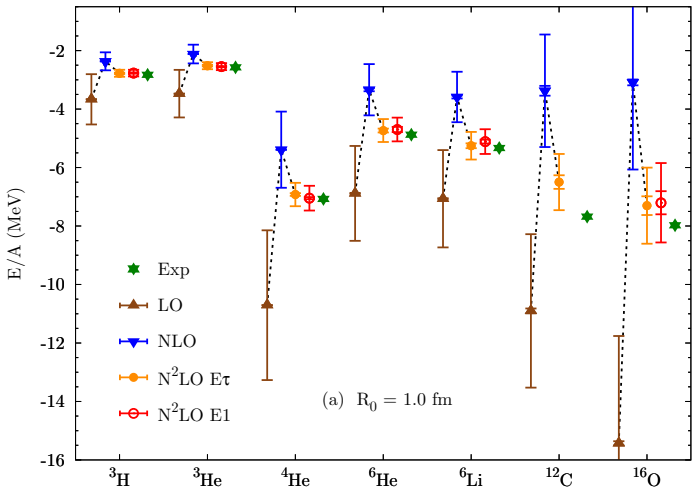
$$|\Psi_0\rangle = \lim_{\tau\to\infty} e^{-(H-E_T)\tau}|\Psi_{\rm trial}\rangle$$

$$|\Psi_{\rm trial}\rangle = \sum_{n\geq 0} c_n|\Psi_n\rangle \qquad e^{-(H-E_T)\tau}|\Psi_{\rm trial}\rangle = \sum_{n\geq 0} e^{-(E_n-E_T)\tau}c_n|\Psi_n\rangle$$

The MC aspect lies in the fact that integrals are evaluated with stochastic algorithms (Metropolis, Importance sampling...)

GFMC vs AFDMC: spin and isospin treated (not treated) explicitly

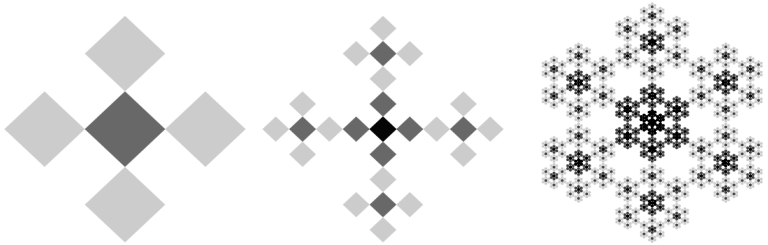
Computationally very demanding: only nuclear matter and light nuclei doable



D. Lonardoni et al., PRC 97, 044318 (2018)
J. Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)

SRG and IM-SRG

Renormalization Group (RG) refers to the formal investigation of the changes in a **physical system viewed at different scales**.



The ideas of RG can be used to simplify the nuclear many-body problem. In particular, IM-SRG aims to decouple the ground-state from the excited states.

Cf. R. Roth, lectures @ GGI
H. Hergert, Phys. Scripta 92, 023002 (2017)

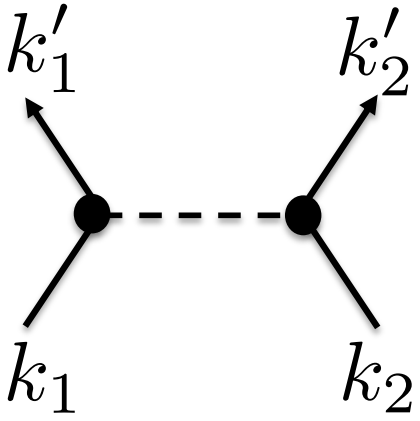
$$H(s) = U(s)H(0)U^\dagger(s)$$

$$\eta(s) \equiv \frac{dU}{ds}U^\dagger$$

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

$$H(s) \to H_{\text{diagonal}} \quad \text{if} \quad s \to \infty$$
$$\eta(s) = [H_{\text{diag.}}(s), H_{\text{off-diag.}}(s)]$$

Realistic case



$$k' = \frac{k_1' - k_2'}{2}$$

$$k = \frac{k_1 - k_2}{2}$$

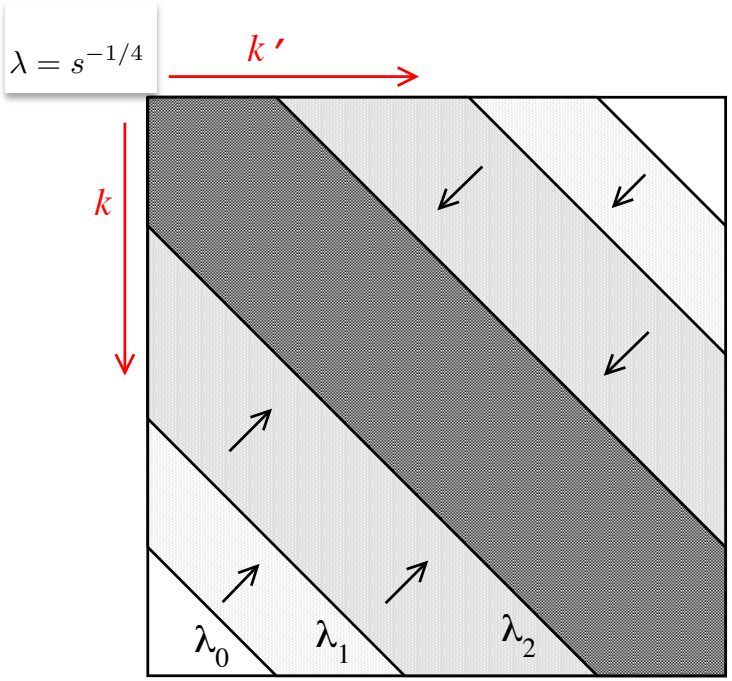
Exercise:

$$H(s) = \begin{pmatrix} E_1(s) & 0 \\ 0 & E_2(s) \end{pmatrix} + \begin{pmatrix} 0 & V(s) \\ V(s) & 0 \end{pmatrix}$$

$$E_\pm \equiv \frac{1}{2}\left(E_1 \pm E_2\right)$$

$$H(s) = E_+ + E_- \sigma_z + V\sigma_x$$

Solve by 2x2 diagonalization and then with SRG equations



Coupled cluster (CC)

Quite successful in **quantum chemistry**.

The ansatz for the wave function is given by **single (S) and double (D) excitations of a reference Slater determinant**:

$$|\Psi\rangle = e^{T}|\Phi\rangle$$

$$T = T_1 + T_2 + \dots$$

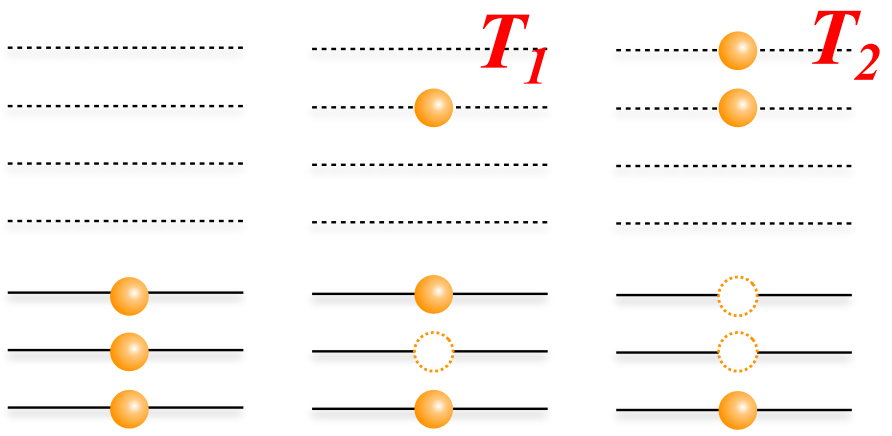
$$T_1 = \sum_{ph} t_{ph} a_p^\dagger a_h$$

$$T_2 = \sum_{php'h'} t_{php'h'} a_p^\dagger a_{p'}^\dagger a_h a_{h'}$$

The amplitudes *t* are the unknowns. They enter the Schrödinger equation.

Use of formulas for exponentiation.

Currently up to T_3.



Is there a unique Hamiltonian?

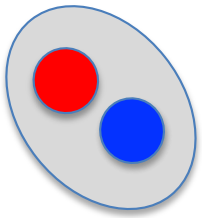
Which are the requirements that a Hamiltonian must have?

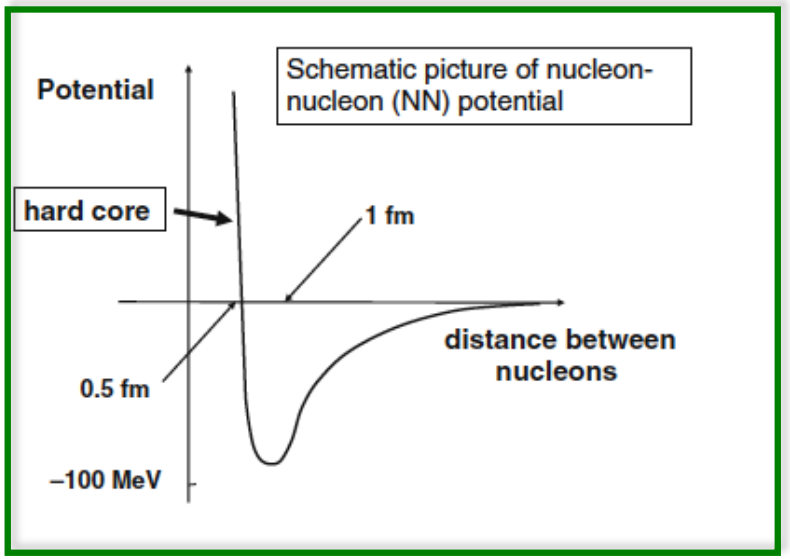
Answers depend on whom you ask ...

The NN interaction ("traditional" view)

- **Attractive** but with an **infinitely repulsive "hard-core"**
- **Short-range and strongly spin-dependent**. The S=1 (T=0) system, i.e. the deuteron, is bound while the S=0 (T=1) systems are not
- **Non-central components**:
  spin-orbit / tensor

$$\sim \vec{L}\cdot(\sigma_1+\sigma_2) \qquad \sim S_{12} \equiv \frac{3(\sigma_1\cdot r)(\sigma_2\cdot r)}{r^2} - \sigma_1\cdot\sigma_2$$





Notation : $\vec{l}_1,\ \vec{l}_2$ coupled to $\vec{L},\ \vec{s}_1,\vec{s}_2$ coupled to $\vec{S},$ same for $\vec{J}=\vec{L}+\vec{S}$ and isospin $\vec{T}$

Three-body force needed! Four-body?

Phenomenological potentials

Strategy: write down the **most general potential consistent with symmetries(*)** and fit its coefficients (for instance: Argonne potential).

See: https://www0.mi.infn.it/~colo/Didattica/Nucleare/2021_22/nuclphys3.pdf

Symmetries: TRANSLATION, GALILEAN BOOSTS, ROTATIONS, PARITY, TIME-REVERSAL, INTERCHANGE OF THE TWO PARTICLES.

$$V(1,2) = \sum \left[1,\ \sigma_1 \cdot \sigma_2,\ S_{12},\ L \cdot S,\ L^2,\ L^2\,(\sigma_1 \cdot \sigma_2),\ (L \cdot S)^2\right] \otimes \left[1,\ \tau_1 \cdot \tau_2\right]$$

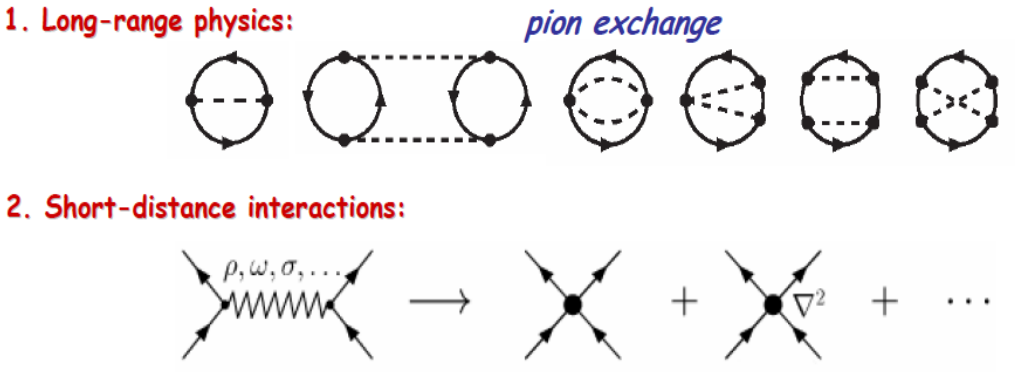
A number of very accurate *NN* potentials constructed in the 1990s reproduce the long-range one-pion-exchange part of the interaction and fit the large amount of empirical information about *NN* scattering data contained in the Nijmegen database (Stoks *et al.*, 1993b) with a $\chi^2/N_{data} \sim 1$ for lab energies up to ~ 350 MeV. These include the potentials of the Nijmegen group (Stoks *et al.*, 1994), the Argonne potentials (Wiringa and Pieper, 2002; Wiringa *et al.*, 1995) and the CD-Bonn potentials (Machleidt, 2001; Machleidt *et al.*, 1996). Of those potentials

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

(*) Exercise: try it

Chiral forces

- Based on the idea by S. Weinberg: a low-energy Lagrangian that has **all the terms consistent with the symmetries of QCD** will give correct results at that energy scale. Chiral symmetry can be assumed (quark masses ≈ 0).
- There is a breakdown scale (≈ GeV). The pion exchange between nucleons is kept, the heavy mesons are not.
- One needs a cut-off Λ.
- There are parameters to be adjusted.



	2N Force	3N Force	4N Force
LO $(Q/\Lambda)^0$			
NLO $(Q/\Lambda)^2$			
NNLO $(Q/\Lambda)^3$	+...		
N^{3}LO $(Q/\Lambda)^4$	+...	+...	+...

- Dependence on power counting scheme and order (LO, NLO, N^2LO, N^3LO).
- Sensitivity to the cut-off Λ.

WE'VE GOT ISSUES

J. Simonis et al., Phys. Rev. C 96, 014303 (2017)

$\lambda_{NN}/\Lambda_{3N}$

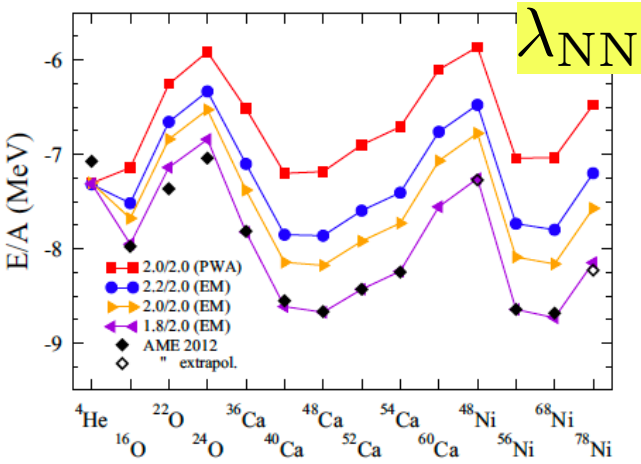


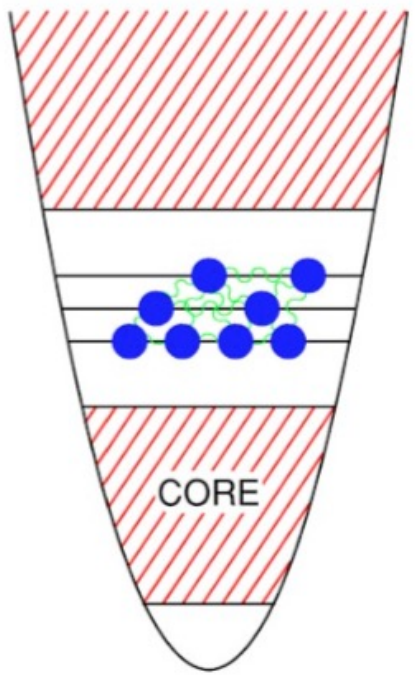
FIG. 5. Systematics of the energy per nucleon E/A of closed-shell nuclei from ^{4}He to ^{78}Ni calculated with the IM-SRG for the four Hamiltonians considered. The results are compared against experimental ground-state energies from the AME 2012 [40] (extrapolated for ^{48,78}Ni).

Ab initio is a wording that has no universally accepted meaning.

The answer to this question depends on the definition of '*ab initio*'. We here take this to be synonymous with 'first principles' and more restrictive than 'nonempirical'. A calculation or a method is *ab initio* if the only dimensional constants and parameters appearing in it are fundamental constants of nature, such as the electronic charge, spin and mass, Planck's constant, the vacuum dielectric constant, the proton charge, spin and mass, etc. In addition, we allow the presence of dimensionless numbers, such as the atomic numbers Z of the atoms in the system under study. Methods employing empirical parameters are clearly not *ab initio*. By this definition, any calculation making use only of quantities that appear in the basic

Shell model or Configuration Interaction

- Nucleons (A) distributed within a given set of orbitals (n) in all possible ways.
- Roughly combinatorial, but there are ways to restrict to good J and parity.
- Diagonalization of H on this basis.
- Analogous to CI for molecules.
- Recent progress has been made concerning the SM embedded in the **continuum**.
- Role of the core...



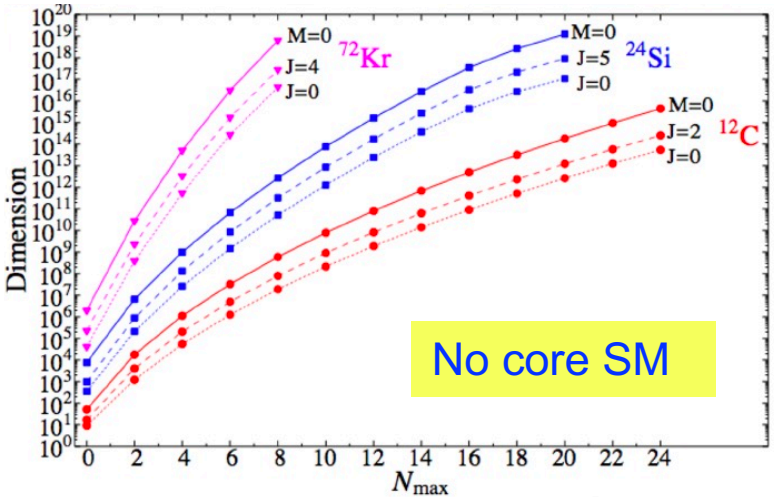
SM

Lecture/material from Sean

Shell model and no-core shell model

NCSM: **all nucleons are active**. One can employ a realistic Hamiltonian. In this respect, it is commonly included among the *ab initio* approaches.

SM: **only particles in active shells are considered**. The Hamiltonian must be "reduced" to the active space (cf. Lee-Suzuki). Moreover, in many cases empirical Hamiltonians are used.



ns4exp.mi.infn.it

KSHELL code (SM)

(limited resources, so that the choice of the model space and interaction is not free)

Implemented thanks to I. Moumene (Milano), G. Di Gregorio (Caserta), A. Gargano (Napoli)

Backup slides

$$E = \frac{\int \Psi^*(x_1 \dots x_N;\alpha) H \Psi(x_1 \dots x_N;\alpha)}{\int \Psi^*(x_1 \dots x_N;\alpha) \Psi(x_1 \dots x_N;\alpha)} \equiv \frac{\langle \Psi(\alpha)|H|\Psi(\alpha)\rangle}{\langle \Psi(\alpha)|\Psi(\alpha)\rangle}$$

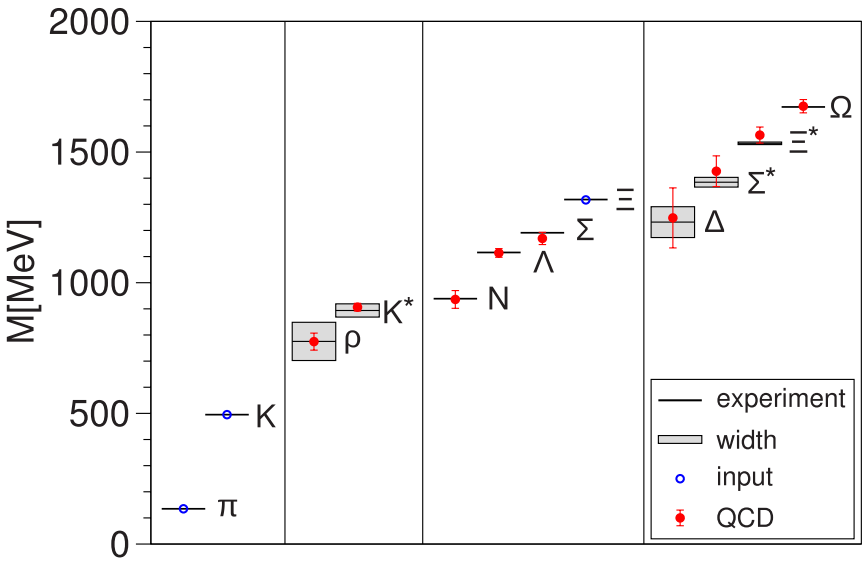
Variational principle: $$\frac{\partial E}{\partial \alpha} = 0$$

$$E_L \equiv \frac{1}{\Psi} H\Psi \qquad P(x;\alpha) \equiv \frac{|\Psi(x;\alpha)|^2}{\int \Psi^*(x;\alpha)\Psi(x;\alpha)}$$

$$E = \int P(x;\alpha) E_L$$

How do we sample the integrand:
Metropolis algorithm
Importance sampling
...

Lattice QCD for hadrons



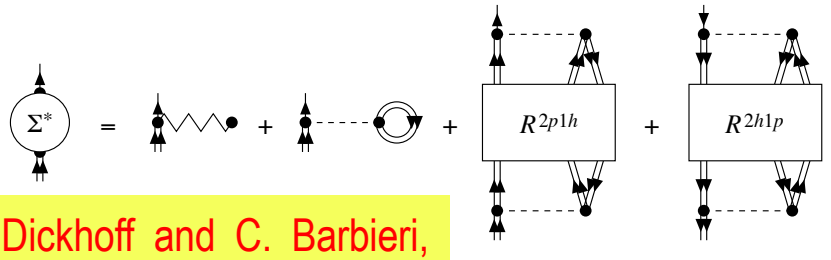
Dürr *et al.*, Science 322, 1224 (2008)

Lattice QCD not yet able to calculate nuclei

Self-consistent Green's function (SCGF)

The basic object is the **Green's function**, that represents the probability amplitude that a particle is found in state α at time t after having been introduced in the system at time t' in state β

$$g_{\alpha\beta}(t-t') \quad \rightarrow \quad g_{\alpha\beta}(\omega)$$



W.H. Dickhoff and C. Barbieri, PPNP 52, 377 (2004)

It obeys the **DYSON EQUATION:**

$$g_{\alpha\beta}(\omega) = g^{(0)}_{\alpha\beta}(\omega) + \sum_{\gamma\delta} g^{(0)}_{\alpha\gamma}(\omega)\Sigma_{\gamma\delta}(\omega)g_{\delta\beta}(\omega)$$

V. Somà, Frontiers in Physics(2020)

C. Barbieri, PRL 103, 202502 (2009)

The self-energy Σ :
approximated by a set of diagrams.