Ab initio methods for nuclei

Lecture I

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Outline

★ Lecture I: Nuclear Many-Body Theory
  - Disclaimer
  - Basic facts on nuclear forces
  - Untying the *Gordian knot* of Nuclear Physics
  - The nuclear hamiltonian
  - Introduction to Nuclear Many-Body Theory (NMBT)

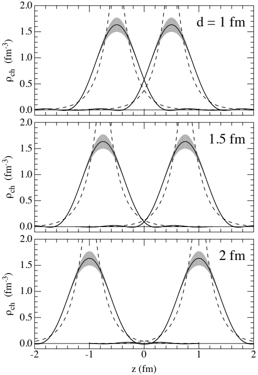
★ Lecture II: Nucleon Green's function and nuclear response at low to moderate momentum transfer

★ Lecture III: Electron and neutrino cross section in the impulse approximation and beyond

Disclaimer

- ★ Bottom line: there is no such thing as a *ab initio* method to describe the properties of atomic nuclei.
- ★ In the low-energy regime, the fundamental theory of strong interactions (QCD) is nearly intractable already at the level required for the description of hadrons, let alone nuclei

- ★ Nuclei are described in terms of *effective degrees of freedom*, protons and neutrons, and *effective interactions*, mainly meson exchange processes
- ★ As long as their size is small compared to the relative distance, treating nucleons as individual particles appears to be reasonable



The *paradigm*†

- ⋆ Nucleons behave as non relativistic particles, the dynamics of which are described by the hamiltonian

$$H = \sum_{i=1}^{A} \frac{\mathbf{k}_i^2}{2m} + \sum_{i<j=1}^{A} \mathrm{v}_{ij} + \ldots \ ,$$

  where v_{ij} is nucleon-nucleon (NN) interaction potential, and the ellipses refer to the possible occurrence of forces involving more thah two nucleons (to be discussed at a later stage)

- ⋆ The main qualitative features of the potential v_{ij} can be deduced from nuclear systematics (binding energies, charge-density distributions, energy spectra …)

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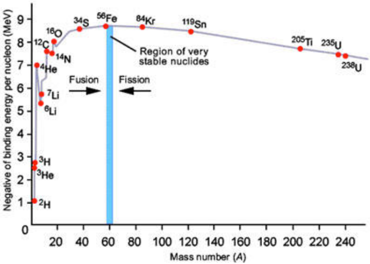
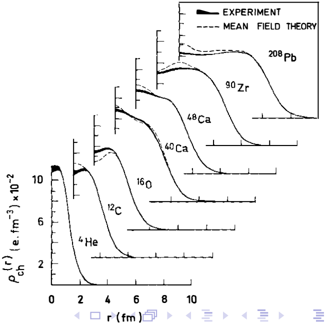
†Paradigm: a phylosophical or theoretical framework of any kind (Merriam-Webster).

Binding energies and charge-density distributions

- ⋆ The observation that the nuclear binding energy per nucleon is roughly the same for $A > 20$, its value being ~ 8.5 MeV , suggests that the range of the NN interaction is short compared to the nuclear radius.



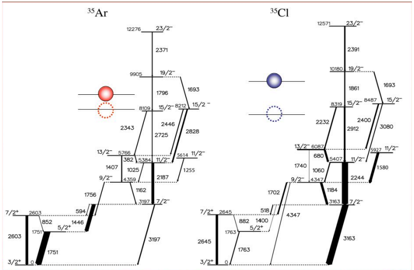
- ⋆ The observation that the charge-density in the nuclear interior is constant and independent of A indicates that the NN forces become strongly repulsive at short distance



Isotopic invariance

★ The spectra of mirror nuclei, e.g. $^{35}_{18}$Ar and $^{35}_{17}$Cl are identical, up to small electromagnetic corrections

★ Nuclear forces exhibit *charge independence*, which is a manifestation of a more general property: *isotopic invariance*



★ Neglecting the small mass difference, nucleons can be seen as two states of the same particle, the nucleon, specified by their *isospin*, $\tau_3 = \pm 1/2$.

★ The force acting between two nucleons depends on the total isospin of the pair, $T = 0$ or 1, but not on its projection T_3.

Untying the Gordian‡ knot of nuclear physics

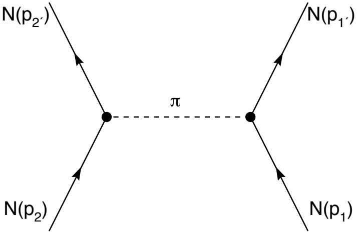
- ★ In principle, the form of the potential may be accurately determined through a fit to the large database of nuclear properties.
- ★ The calculations needed to obtain these quantities necessarily involve approximations, casting a strong bias on the underlying models of nuclear interactions.
- ★ The inextricable tie between the uncertainty associated with the nuclear hamiltonian and that arising from the solution of the nuclear many-body problem can be severed determining the nuclear hamiltonian from the properties of *exaxtly solvable* few-nucleon systems.

‡A metaphor for an apparently intractable problem solved by thinking "out of the box".

The NN force: Yukawa's theory (AD 1935)

- ★ NN interaction mediated by a particle of mass $\mu \sim 1\ \mathrm{fm}^{-1} = 200\ \mathrm{MeV}$, to be later identified with the π-meson, or pion

- ★ The pion, discovered in 1947, is a pseudoscalar (spin-parity 0^-) particle of mass $m_\pi \approx 140$ MeV
- ★ The three charge states of the pion, $\pi^\pm$ and π^0, form the isospin triplet $\boldsymbol{\pi}$
- ★ Simplest πN interaction lagrangian compatible with the observation that NN interactions conserve parity



$$\mathcal{L}_Y = ig\overline{N}\gamma^5 \boldsymbol{\tau} N \boldsymbol{\pi}$$

$$N = \begin{pmatrix} p \\ n \end{pmatrix} \ , \quad \boldsymbol{\pi} = \begin{pmatrix} (\pi^+ + i\pi^-)/\sqrt{2} \\ (\pi^+ - i\pi^-)/\sqrt{2} \\ \pi^0 \end{pmatrix} .$$

The one-pion-exchange (OPE) potential

- ⋆ Potential extracted from the non relativistic reduction of the NN amplitude, at 2nd order in $\mathcal{L}_Y$

$$
\begin{aligned}
\mathrm{v}_\pi &= \frac{g^2}{4m^2}\,(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(\boldsymbol{\sigma}_1\cdot\boldsymbol{\nabla})(\boldsymbol{\sigma}_2\cdot\boldsymbol{\nabla})\,\frac{\mathrm{e}^{-m_\pi r}}{r} \\
&= \frac{g^2}{(4\pi)^2}\,\frac{m_\pi^3}{4m^2}\,\frac{1}{3}(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)\left\{\left[(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)+S_{12}\left(1+\frac{3}{x}+\frac{3}{x^2}\right)\right]\frac{\mathrm{e}^{-x}}{x}\right. \\
&\left. -\ \frac{4\pi}{m_\pi^3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\delta^{(3)}(\mathbf{r})\right\}\ ,
\end{aligned}
$$

$$
S_{12}=\frac{3}{r^2}(\boldsymbol{\sigma}_1\cdot\mathbf{r})(\boldsymbol{\sigma}_2\cdot\mathbf{r})-(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\ ,
$$

- ⋆ Note that the potential is *spin dependent* and *non sperically symmetric*
- ⋆ For $g^2/4\pi\approx 14$ the above potential provides a reasonable description of NN scattering in states of high angluar momentum, driven by long-range interactions

Phenomenological potential models

- ⋆ Phenomenological potentials describing the *full* NN interaction can be written in the form

$$\mathrm{v} = \mathrm{v}_S + \mathrm{v}_I + \tilde{\mathrm{v}}_\pi$$

where $\tilde{\mathrm{v}}_\pi$ is the OPE potential, stripped of the δ-function contribution

- ⋆ State-of-the-art NN potential models include momentum-dependent and charge-symmetry breaking terms. The widely used ANL v_{18} potential is written in the form

$$\mathrm{v}_{12} = \sum_{p=1,18} \mathrm{v}^{(p)}(r) O_{12}^{(p)}$$

$$O_{12}^{(p)} = [\mathbb{1}, (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2), S_{12}, \mathbf{L}\cdot\mathbf{S}, \mathbf{L}^2, \mathbf{L}^2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2), (\mathbf{L}\cdot\mathbf{S})^2] \otimes [1, (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)]$$

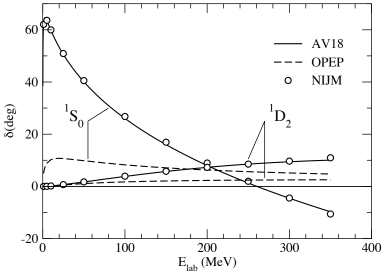
$$[\mathbb{1}, (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2), S_{12}] \otimes T_{12}\ , \ \text{and} \ (\tau_{z1} + \tau_{z2})$$

$$T_{12} = \frac{3}{r^2}(\boldsymbol{\tau}_1 \cdot \mathbf{r})(\boldsymbol{\tau}_2 \cdot \mathbf{r}) - (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$

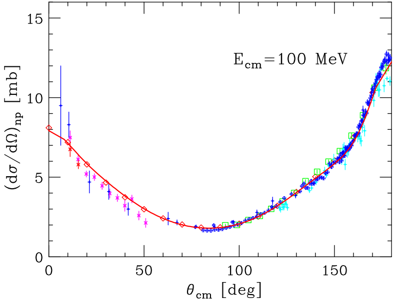
Phenomenological approach (continued)

- ⋆ The phenomenological potentials reproduce the two-nucleon data, for both bound and scattering states, by construction

- ⋆ Phase shifts extracted from NN scattering data

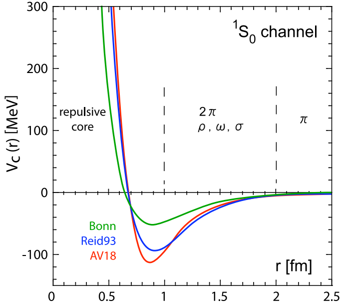


- ⋆ Differential cross section in the proton-neutron channel

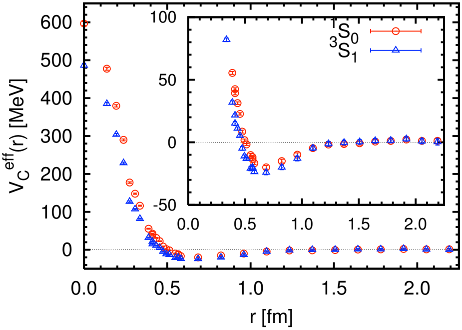


The NN potential in the $^1S_0$ channel

★ Phenomenological models



★ Lattice QCD, m_π = 530 MeV



★ Chiral perturbation theory provides an alternative scheme, allowing to derive the two- and three-nucleon potentials within a framework preserving the symmetries of QCD.

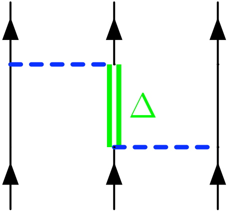
Three-nucleon interactions

- ⋆ Interactions involving more two nucleons arise as a consequence of the internal structure of the participating particles

- ⋆ The main contribution to the three nucleon forces comes from the Fujita-Miyazawa mechanism
- ⋆ Phenomenological three-nucleon potentials, written in the form

$$V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{N}$$

are determined through a fit to the properties of the three-nucleon system

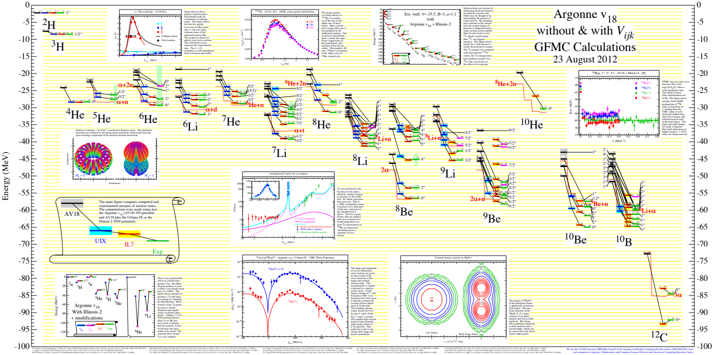


The nuclear many-body problem

★ The starting point for the description of nuclear properties within the Nuclear Many-Body Theory is the solution of the Schrödinger equation

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

★ Quantum Monte Carlo results are available for $A \leq 12$.



- In principle, more complex calculations (i.e. involving different observables and heavier nuclei) may be performed in perturbation theory, setting

$$H = H_0 + H_I \ ,$$

H_0 being the hamiltonian describing A non interacting nucleons.

- Problem: due to the nature of the NN potential, the matrix element of the perturbaton between stets belonging to the base of eigenstates of H_0

$$\langle n_0 | H_I | m_0 \rangle \quad , \quad H_0 | n_0 \rangle = \mathcal{E}_n | n_0 \rangle$$

turn out to be *large*. Perturbative expansions are useless.

- Two possible solutions:
  - Redefine the perturbing hamiltonian
  - Redefine the basis

Isospin-symmetric nuclear matter

- ⋆ Isospin-symmetric nuclear matter (SNM) can be thought of as a giant nucleus, with equal numbers of protons and neutrons interacting through nuclear forces only.
- ⋆ The understanding of SNM, besides being a useful intermediate step towards the description of real nuclei, is needed to develop realistic models of neutron star matter.
- ⋆ The calculation of the properties of SNM is greatly simplified by translational invariance
- ⋆ Basis states

$$|n_0\rangle = \frac{1}{\sqrt{A!}} \det\{\varphi_{\mathbf{k}\sigma\tau}(\mathbf{r})\} \quad , \quad \varphi_{\mathbf{k}\sigma\tau}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{\mathbf{k}\cdot\mathbf{r}} \, \chi_\sigma \eta_\tau \ ,$$

where V is the normalisation volume, while χ and η are the Pauli spinors belonging to the spin and isospin space, respectively.

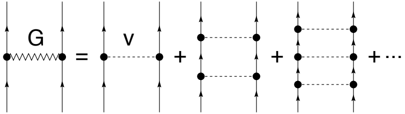
- ⋆ In the ground state the momenta of the occupied states fulfill

$$|\mathbf{k}| < k_F = (3\pi^2 \rho/2)^{1/3} \quad , \quad \rho = A/V$$

G-matrix perturbation theory

- ⋆ Replace the bare NN potential with the $G-matrix$, describing NN scattering in the nuclear medium

$$\text{v} \to G(e) = \text{v} - \text{v}\,\frac{Q}{e}\,G = \text{v}\,\Omega$$



- ⋆ The expansion in powers of matrix elements of the operator $\zeta = 1 - \Omega$ turns out to be convergent
- ⋆ Rate of convergence not fully established
- ⋆ Treatment of three-nucleon forces involves non trivial problems

Correlated Basis Function (CBF) perturbation theory

- ⋆ Replace the basis states of the non interacting system with the set of correlated states

$$|n\rangle = \frac{F|n_0\rangle}{\langle n_0|F^\dagger F|n_0\rangle}^{1/2}$$

$$F = \mathcal{S}\,\Pi_{j>i}\, f_{ij} \quad , \quad f_{ij} = \sum_p f^{(p)}(r_{ij}) O_{ij}^{(p)} \quad , \quad [f_{ij}, f_{jk}] \neq 0$$

- ⋆ Perturbing hamiltonian defined in terms of matrix elements in the correlated basis

$$H = H_0 + H_I$$

$$\langle m|H_0|n\rangle = \delta_{mn}\langle m|H|n\rangle \quad , \quad \langle m|H_I|n\rangle = (1-\delta_{mn})\langle m|H|n\rangle$$

- ⋆ If the correlated states have large overlaps with the true eigenstates of the hamniltonian, the perturbative expansion in powers of H_I is rapidly convergent

Cluster expansion and FHNC summation scheme

- ⋆ The calculation of matrix elements of many-body operators between correlated states involves prohibitive difficulties
- ⋆ The cluster expansion formalism (consider the ground state expectation value of the hamiltonian, as an exmple)

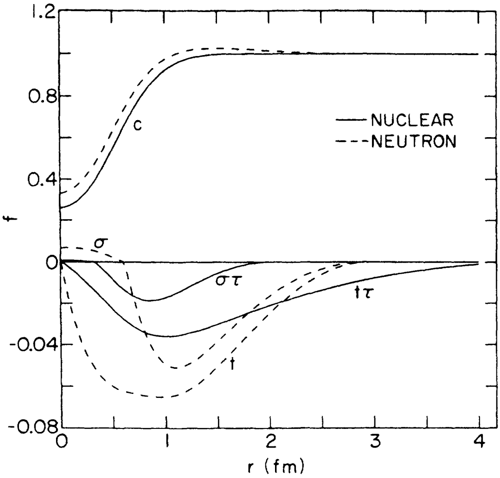
$$\langle 0|H|0\rangle = \frac{k_F^2}{2m} + \sum_n (\Delta E)_n$$

$(\Delta E)_n$ is the contribution arising from subsystem (clusters) consisting of n nucleons

- ⋆ The terms of the cluster expansion are represented by diagrams, that can be classified according to their topological structure and summed to all orders solving a set of integral equations, called Fermi-Hyper-Netted-Chain (FHNC) equations

- ⋆ The shapes of the correlation functions $f^{(p)}(r)$ are determined solving a set of Euler-Lagrange equations, resulting from the minimization of the hamiltonian expectation value in the correlated ground state

$$E_V = \min \langle 0|H|0\rangle \geq E_0$$



Application of CBF perturbation theory

- ⋆ CBF has been widely employed to study both structure and dynamics of nuclear matter and nuclei: the available results (to be discussed in the next lectures) include
  - Dynamic response to scalar and electromagnetic interactions at low to moderate momentum transfer ($q \lesssim 400$ MeV)
  - Green's functions
  - Electron and neutrino cross sections in the impulse approximation (IA) regime ($q \gtrsim 600$ MeV)

Summary of Lecture I

- ⋆ In spite of the fact that no truly *ab initio* approach is available, a consistent description of a variety of nuclear properties can be obtained from approaches based on effective degrees of freedom and effective interactions.
- ⋆ Highly realistic nuclear hamiltonian can be derived from the analysis of the properties of *exactly solvable* few-nucleon systems.
- ⋆ The formalism of many-body theory has reached the degree of maturity required for the treatment of nuclear structure and dynamics based on realistic hamiltonian.