

Ab-initio methods for nuclei

Alessandro Lovato

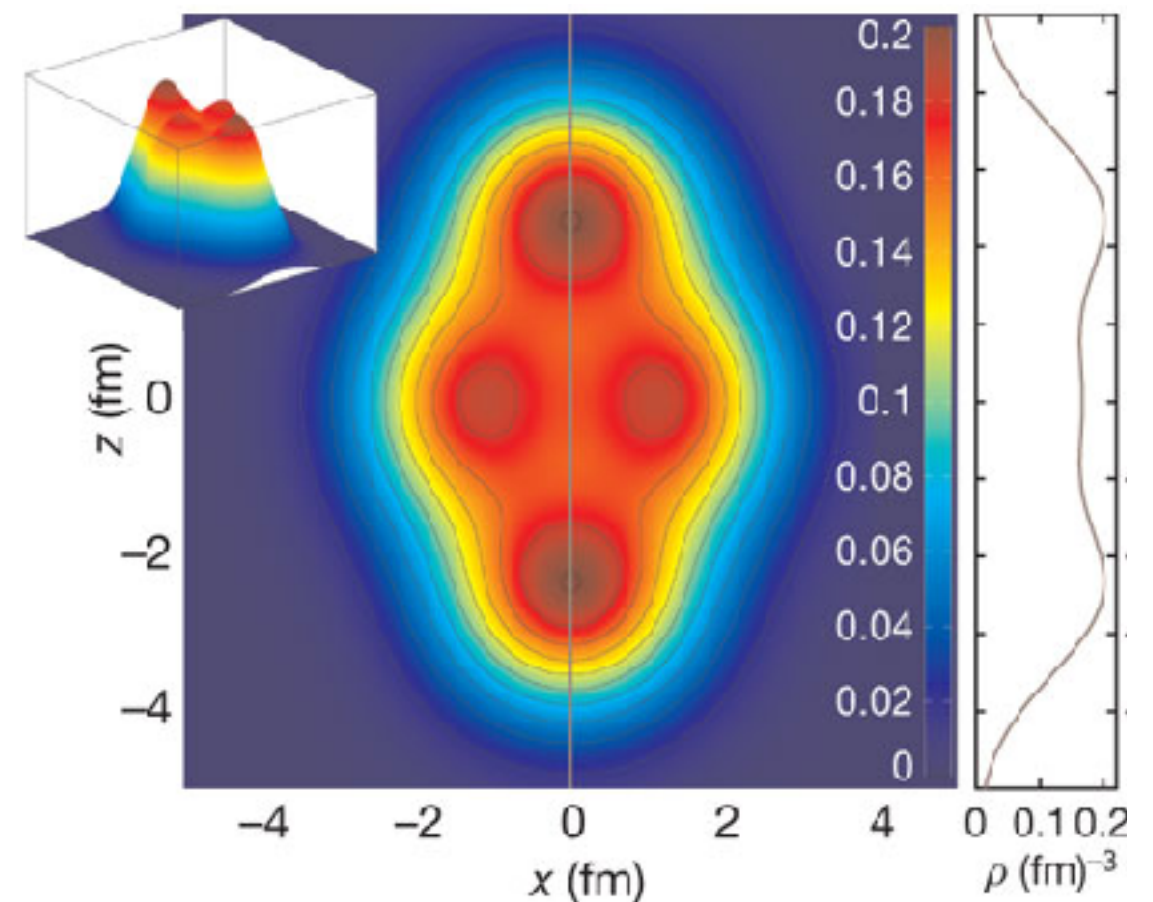
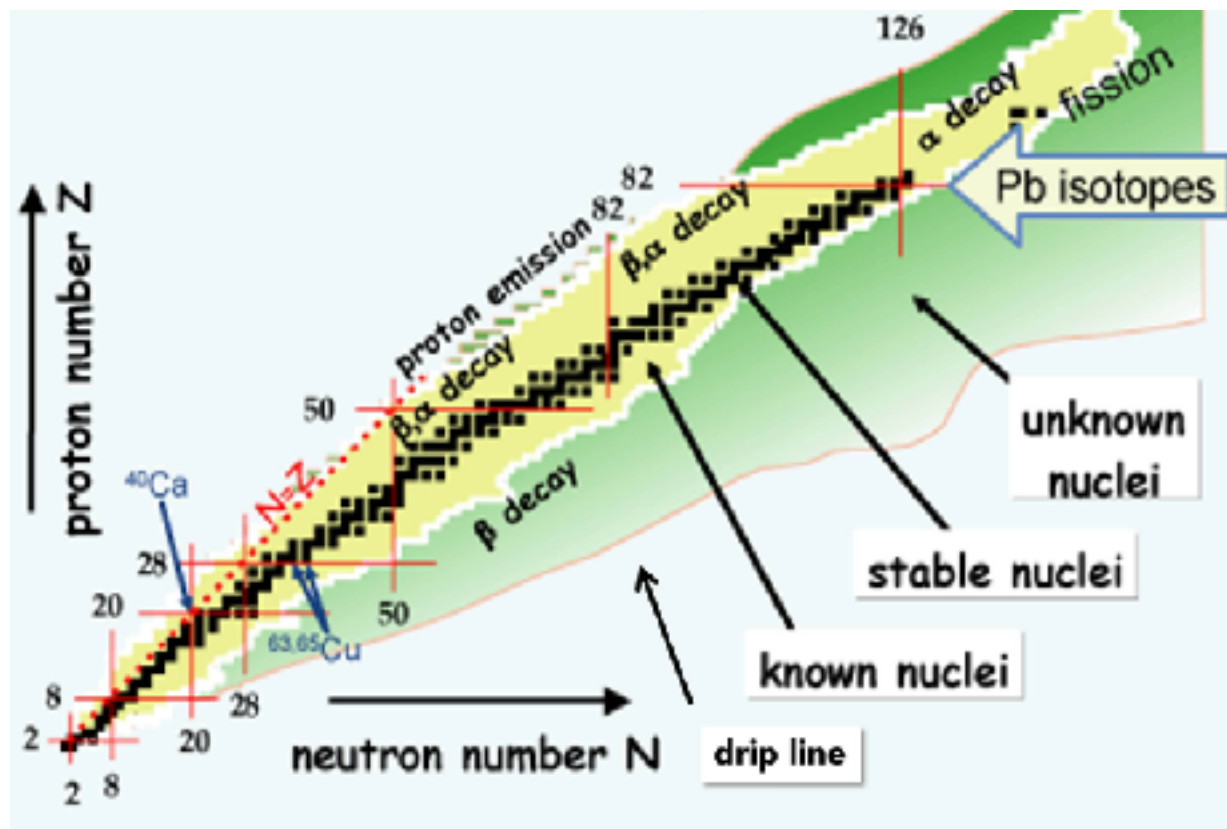


Chapter 1

Introduction

Ab-initio nuclear theory

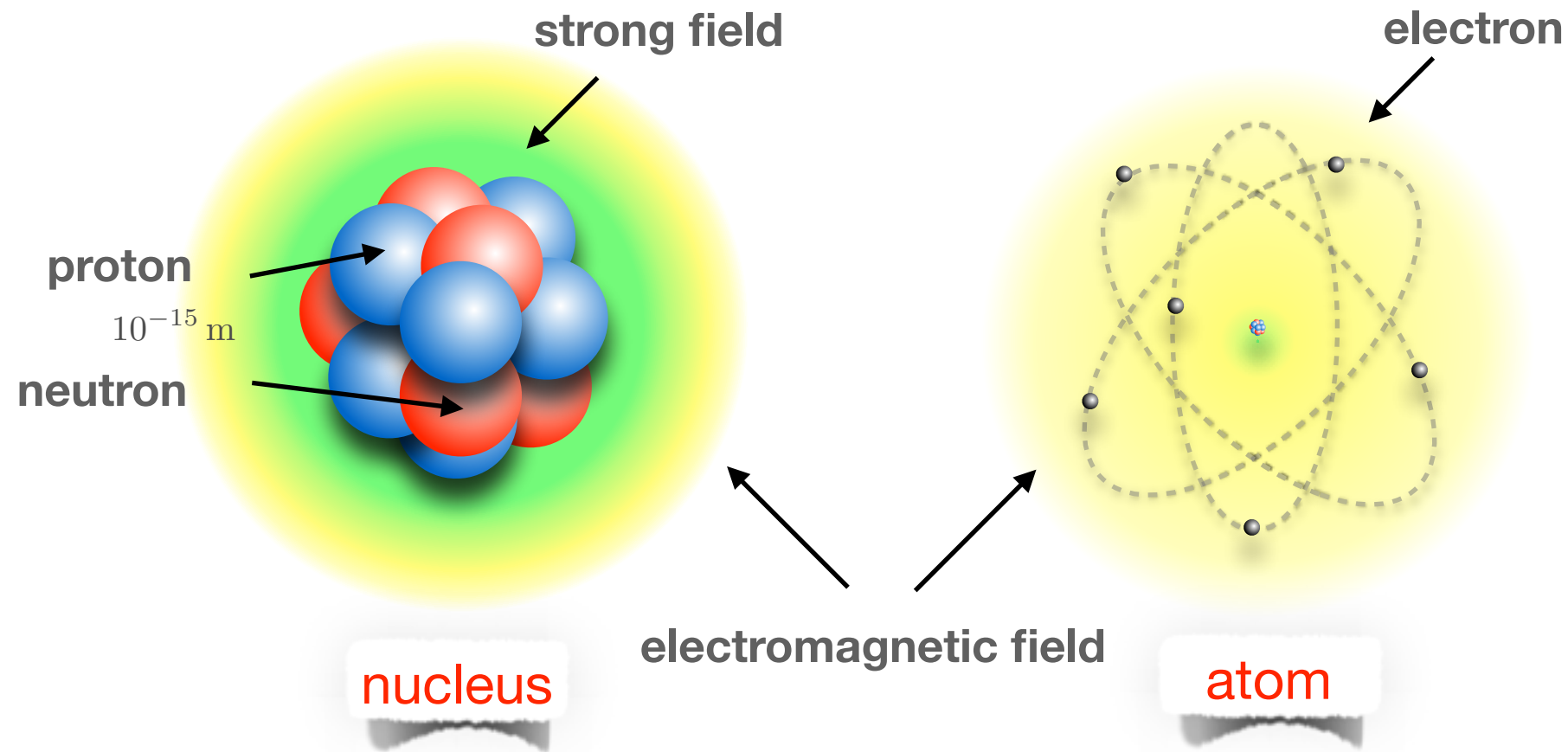
- Atomic nuclei are strongly interacting many-body systems exhibiting fascinating properties including: shell structure, pairing and superfluidity, deformation, and self-emerging clustering.



- Understanding their structure, reactions, and electroweak properties within a unified framework well-rooted in quantum chromodynamics has been a long-standing goal of nuclear physics.

Ab-initio nuclear theory

- Nuclei are self-bound system whose structure is dictated by strong and electromagnetic forces



- It is truly astonishing that the nuclear chart is fully determined by only five parameters: the up-, down- and strange-quark masses, the overall scale of the strong interactions and the electromagnetic coupling constant

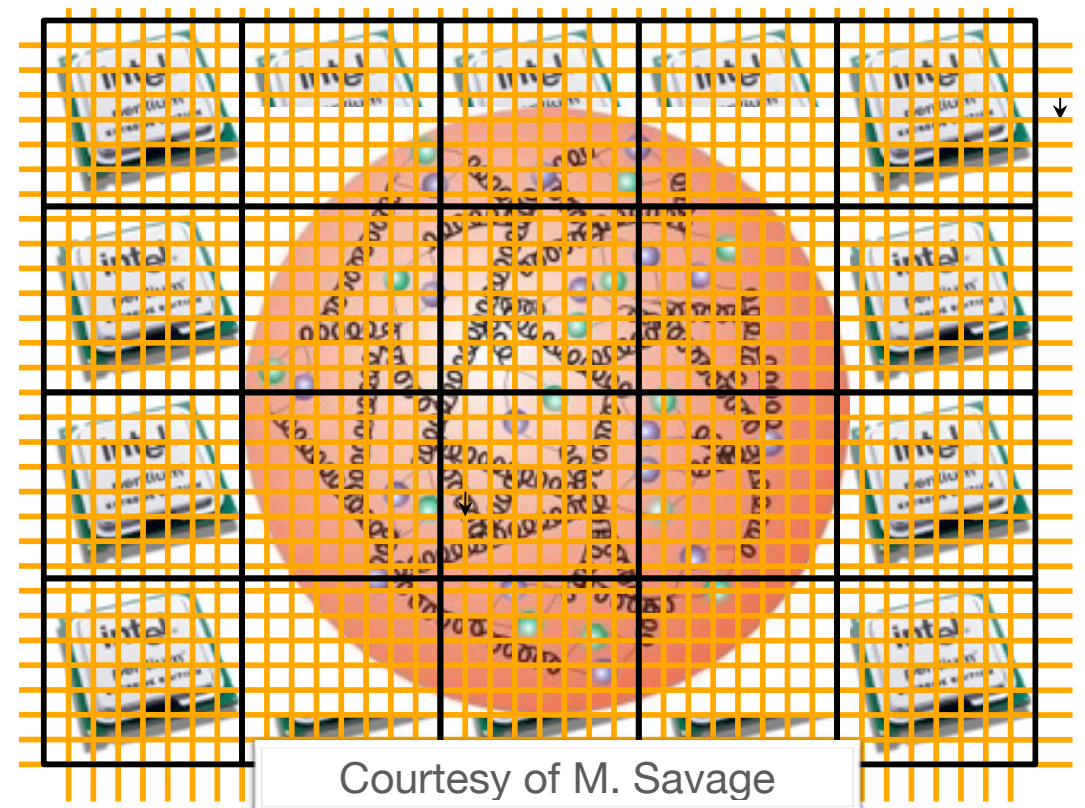
$$\mathcal{L}_{QCD} = \bar{q}(i\gamma_\mu D^\mu - \mathcal{M})q - \frac{1}{4}G_{\mu\nu}^a G^{a\mu\nu} \longrightarrow \left\{ \begin{array}{l} D_\mu = \partial_\mu - ig_s G_\mu^a T^a \\ \mathcal{M} = \text{diag}(m_u, m_d) \end{array} \right.$$

From QCD to nuclear physics

- Owing to its non-abelian character, QCD is strongly non-perturbative in its coupling constant at “large” distances.

- Lattice-QCD is the most reliable way of “solving” QCD in the low-energy regime, and it promises to provide a solid foundation for the structure of nuclei directly from QCD

- The applicability of Lattice-QCD is limited to few body systems, ($A < 4$), and to a nuclear physics in which the pion mass must be kept much higher than the physical one.



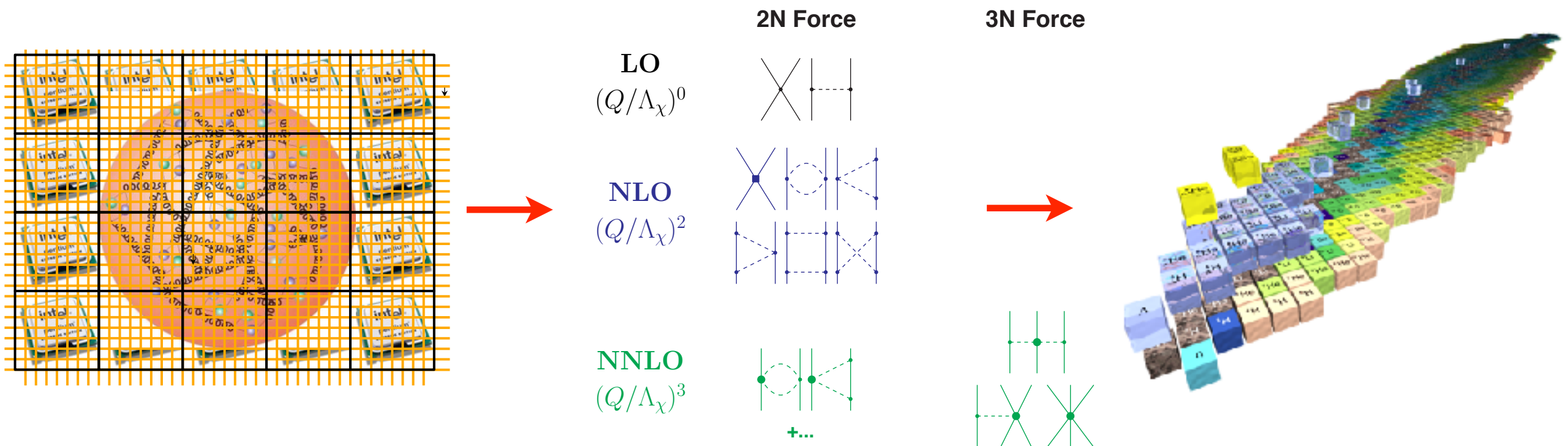
- Capitalizing on Lattice-QCD calculations at quark masses heavier than found in Nature, we try to understand whether Standard Model parameters might have to be finely tuned for nuclei to be stable: a problem as intriguing as that of the cosmological constant.
- Lattice-QCD inputs are essential when experimental data are scarce, as in the determination of the nucleon axial form factor, nucleon-hyperon, and three-neutron interactions

From QCD to nuclear physics

- At the energy regime relevant for the description of nuclei, quark and gluons are confined inside hadrons. Nucleons can be treated as point-like particles interacting through the Hamiltonian

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

- Effective field theories are the link between QCD and nuclear observables. They exploit the separation between the “hard” ($M \sim$ nucleon mass) and “soft” ($Q \sim$ exchanged momentum) scales

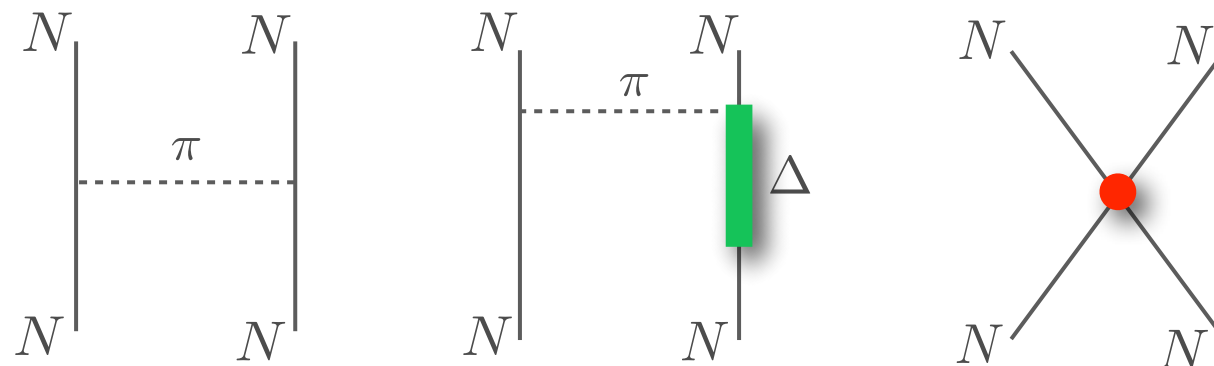


The nuclear Hamiltonian

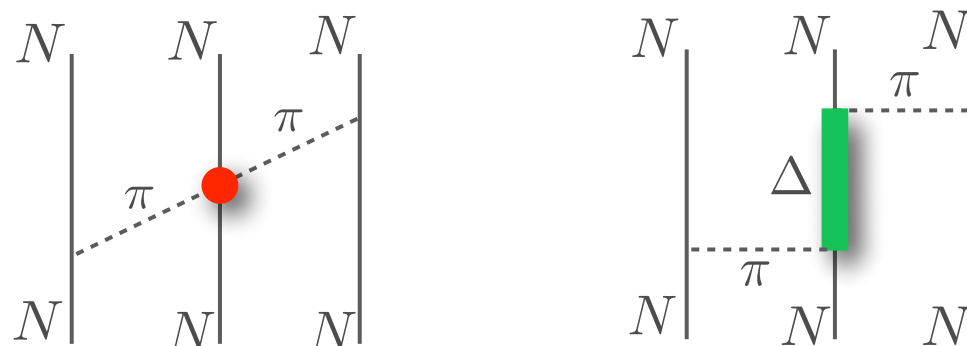
- Ab initio approaches are based on the non relativistic hamiltonian

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \dots$$

Realistic nucleon-nucleon potentials are controlled by ~4300 np and pp scattering data below 350 MeV of the Nijmegen database (Saori's lectures)



Three-nucleon interactions effectively include the lowest nucleon excitation, the $\Delta(1232)$ resonance, and other nuclear effects



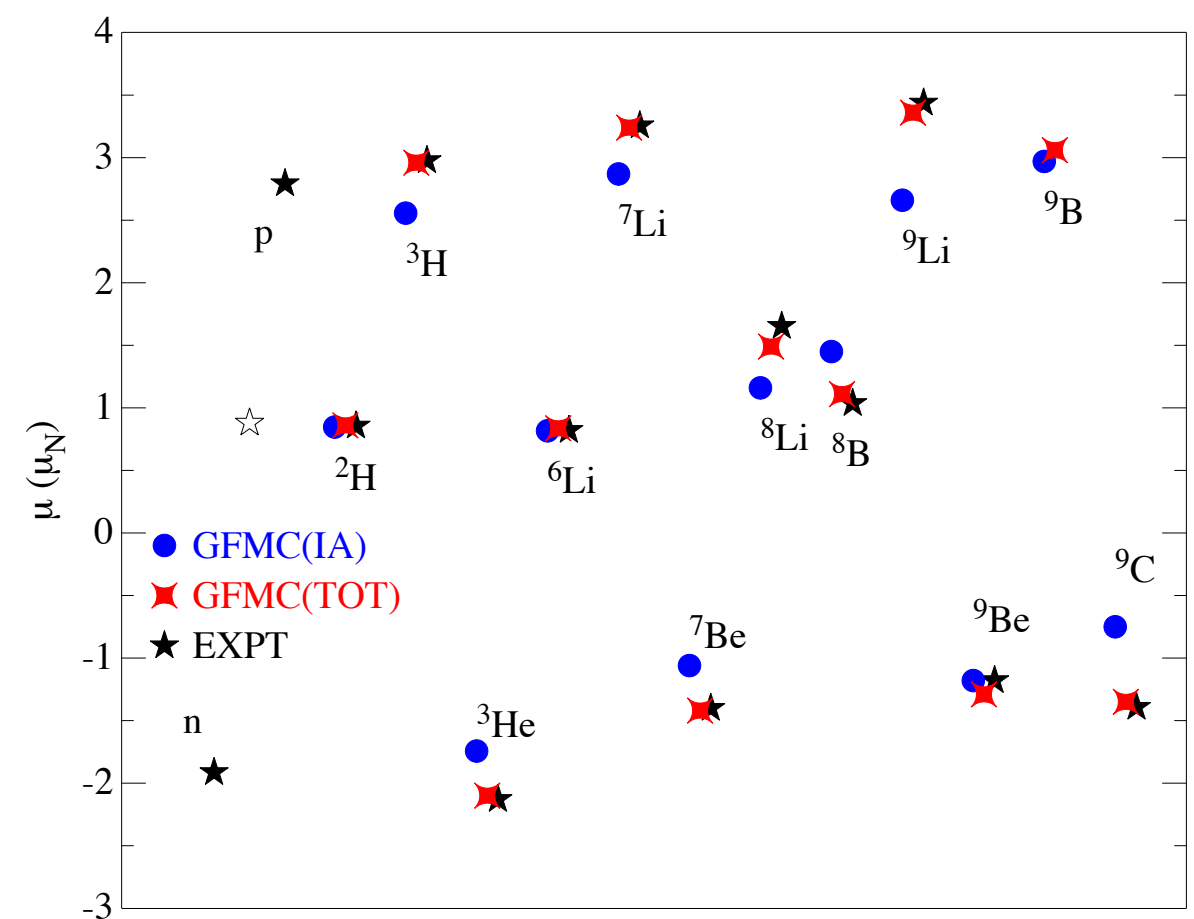
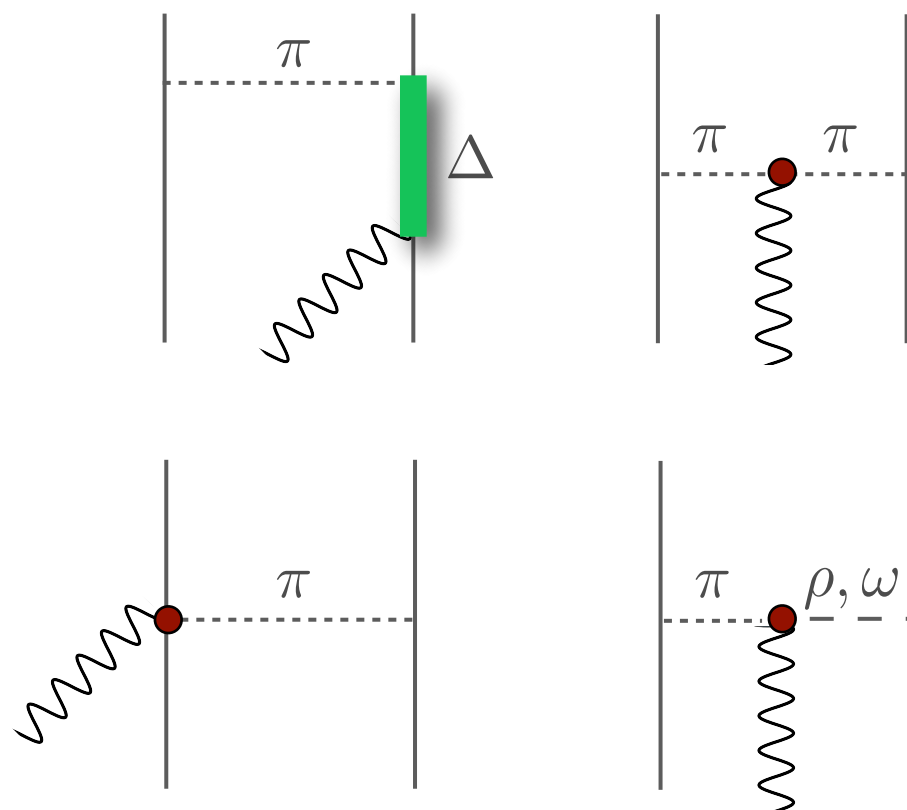
Nuclear currents

The nuclear electromagnetic current is constrained by the Hamiltonian through the continuity equation

$$\nabla \cdot \mathbf{J}_{\text{EM}} + i[H, J_{\text{EM}}^0] = 0$$

- The above equation implies that \mathbf{J}_{EM} involves two-nucleon contributions.

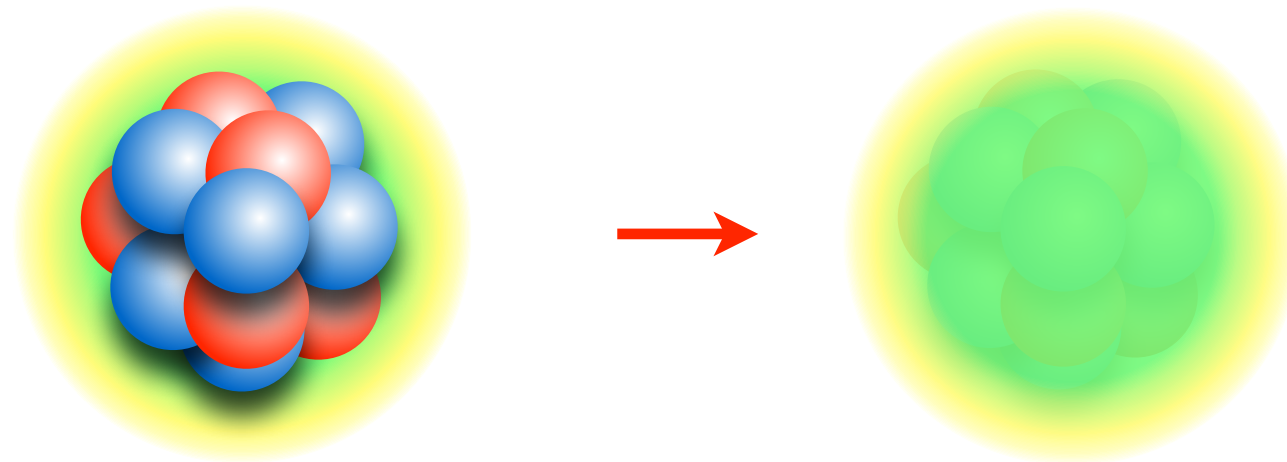
- They are essential for low-momentum and low-energy transfer transitions.



S. Pastore et al., PRC 87, 035503 (2013)






Introduction

- The Liquid Drop Model assumes that nuclei can be treated as drops of an incompressible liquid



- This model encompasses the saturation of nuclear forces, a consequence of their short-range nature
- The nuclear binding energy is given by the Weizsäcker formula

$$B(A, Z) = a_V A + a_S A^{2/3} + a_C \frac{Z^2}{A^{1/3}} + S_N \frac{(N - Z)^2}{A} + a_P \frac{(-1)^Z + (-1)^N}{2A^{1/2}}$$

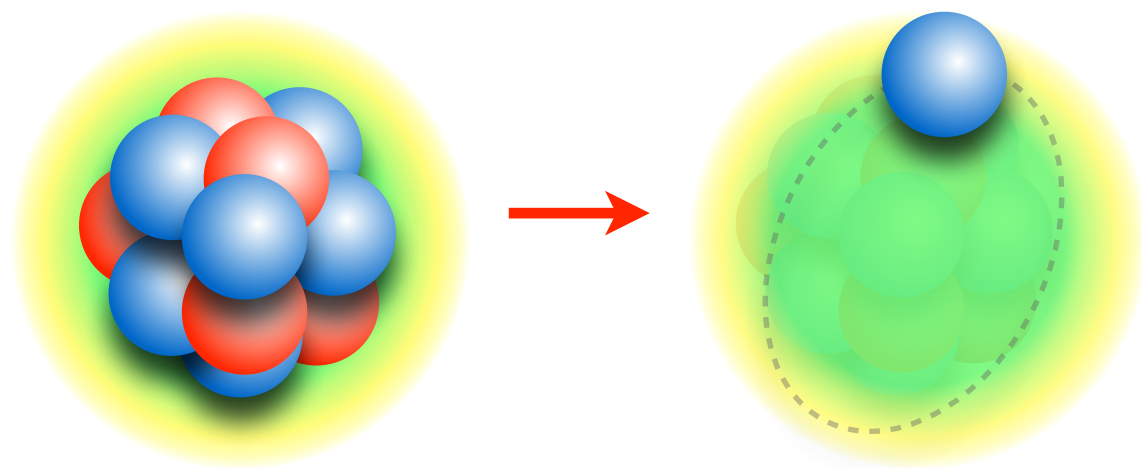
    

Volume Surface Coulomb Symmetry Pairing

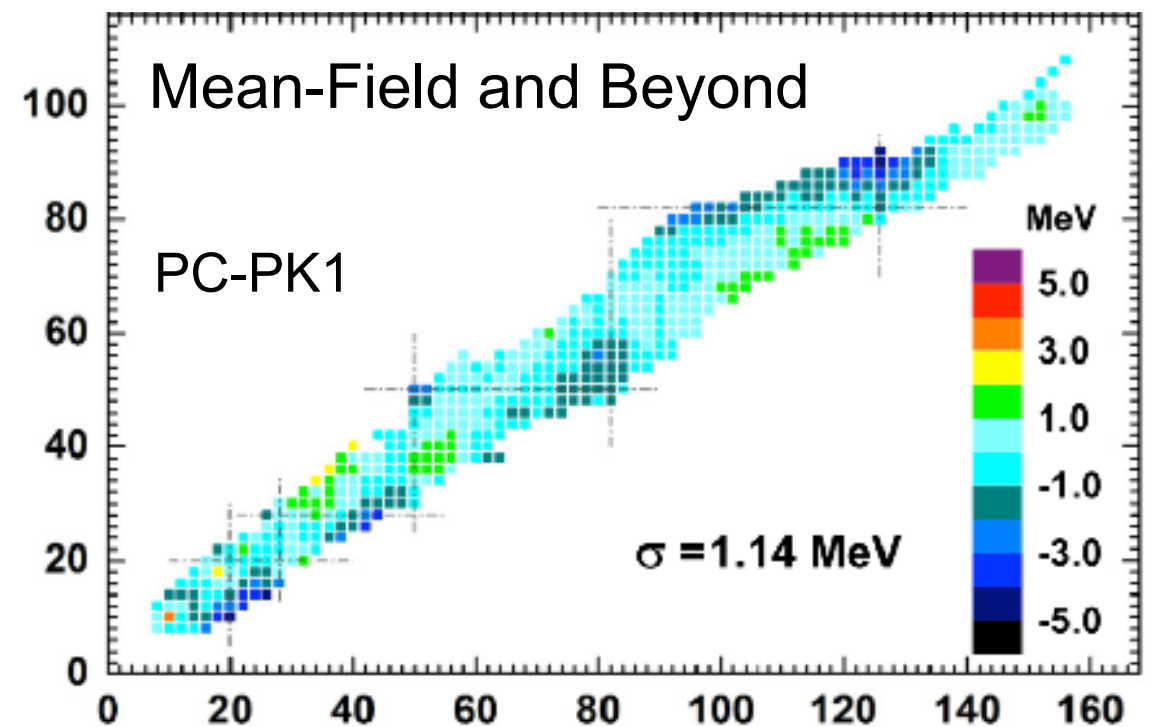
Mean field models

- Mean field theory: nucleons are independent particles subject to an average nuclear potential

$$\left[\sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} \right] \rightarrow \sum_i U_i$$



- The interaction is usually fitted on nuclear binding energies and charge radii of stable nuclei



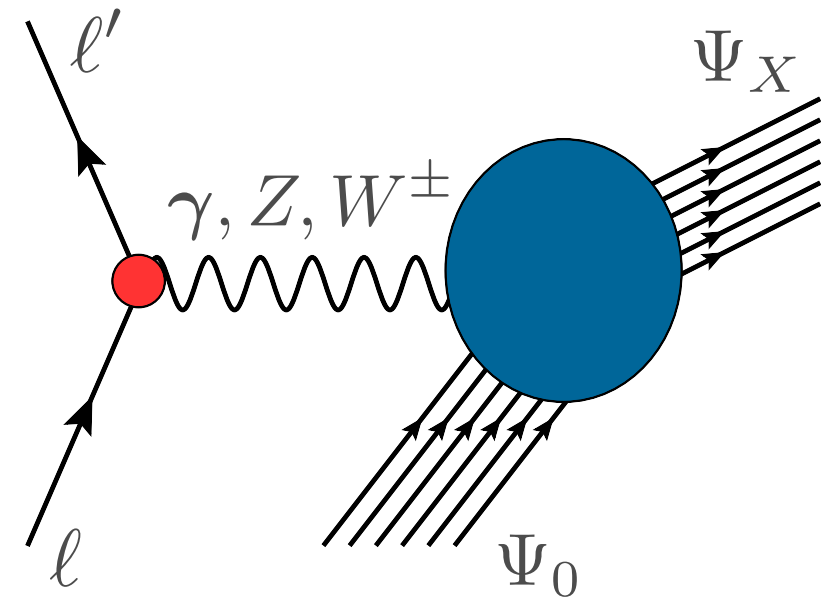
P. W. Zhao, et al. PRC 82, 054319 (2010)

- Despite being the tool of choice for describing large nuclei:
 - * Nucleon-nucleon scattering data and deuteron properties are ignored
 - * There is no clear way to derive effective currents
 - * The average procedure depends upon the (large) system of interest

Lepton-nucleus scattering

The inclusive cross section of the process in which a lepton scatters off a nucleus and the hadronic final state is undetected can be written as

$$\frac{d^2\sigma}{d\Omega_\ell dE_{\ell'}} = L_{\mu\nu} W^{\mu\nu}$$



- The leptonic tensor $L_{\mu\nu}$ is fully specified by the lepton kinematic variables. For instance, in the electron-nucleus scattering case

$$L_{\mu\nu}^{\text{EM}} = 2[k_\mu k'_\nu + k_\nu k'_\mu - g_{\mu\nu}(kk')]$$

- The Hadronic tensor contains all the information on target response

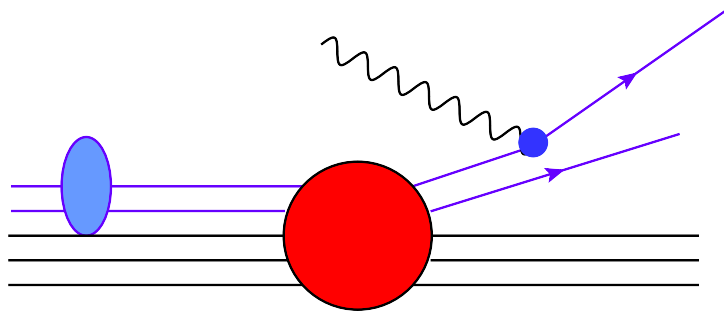
$$W^{\mu\nu} = \sum_X \langle \Psi_0 | J^{\mu\dagger}(q) | \Psi_X \rangle \langle \Psi_X | J^\nu(q) | \Psi_0 \rangle \delta^{(4)}(p_0 + q - p_X)$$

Note that the initial state does not depend on the momentum transfer!

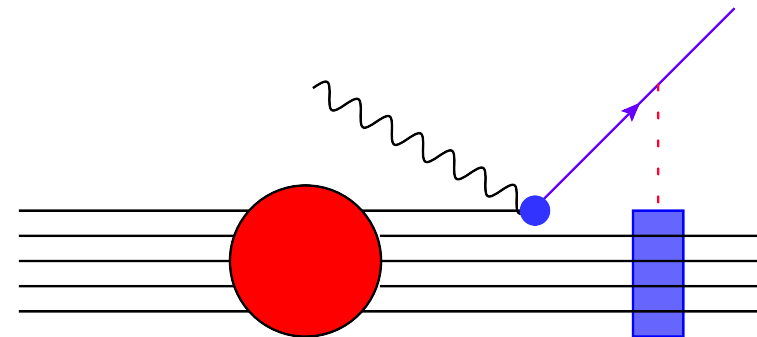
Two-body currents and nuclear correlations

Two-body meson exchange currents and nuclear correlations need to be fully accounted in the calculation of response functions

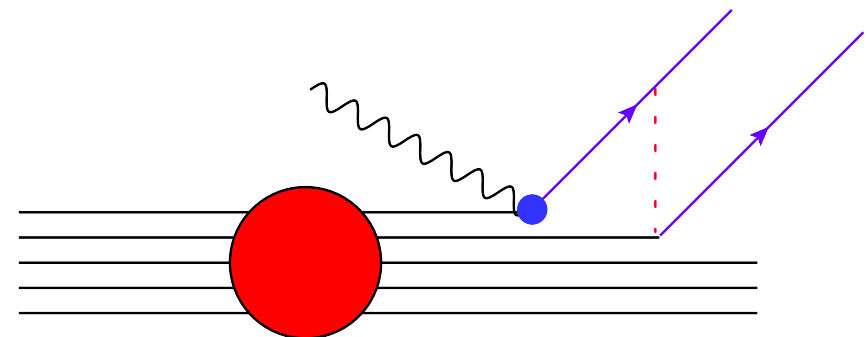
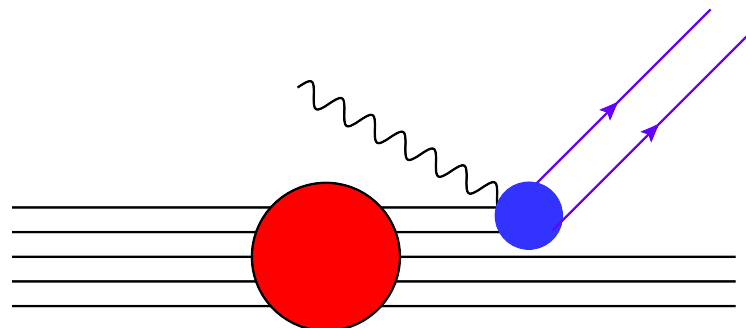
- Initial State Correlations



- Final State Interactions

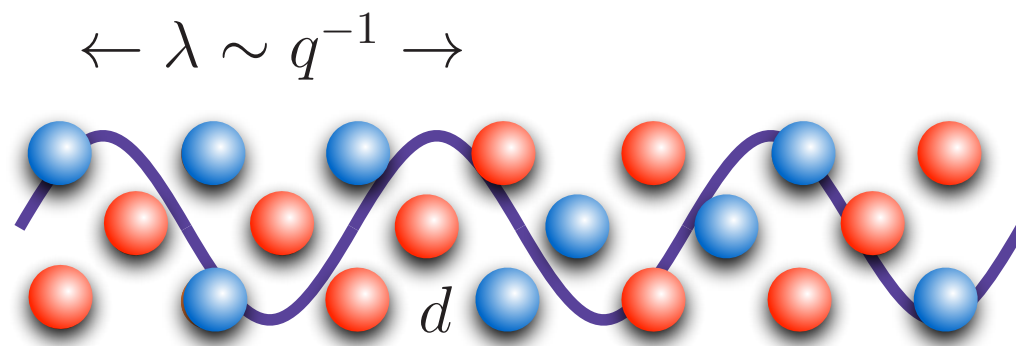


- Meson Exchange Currents



Lepton-nucleus scattering

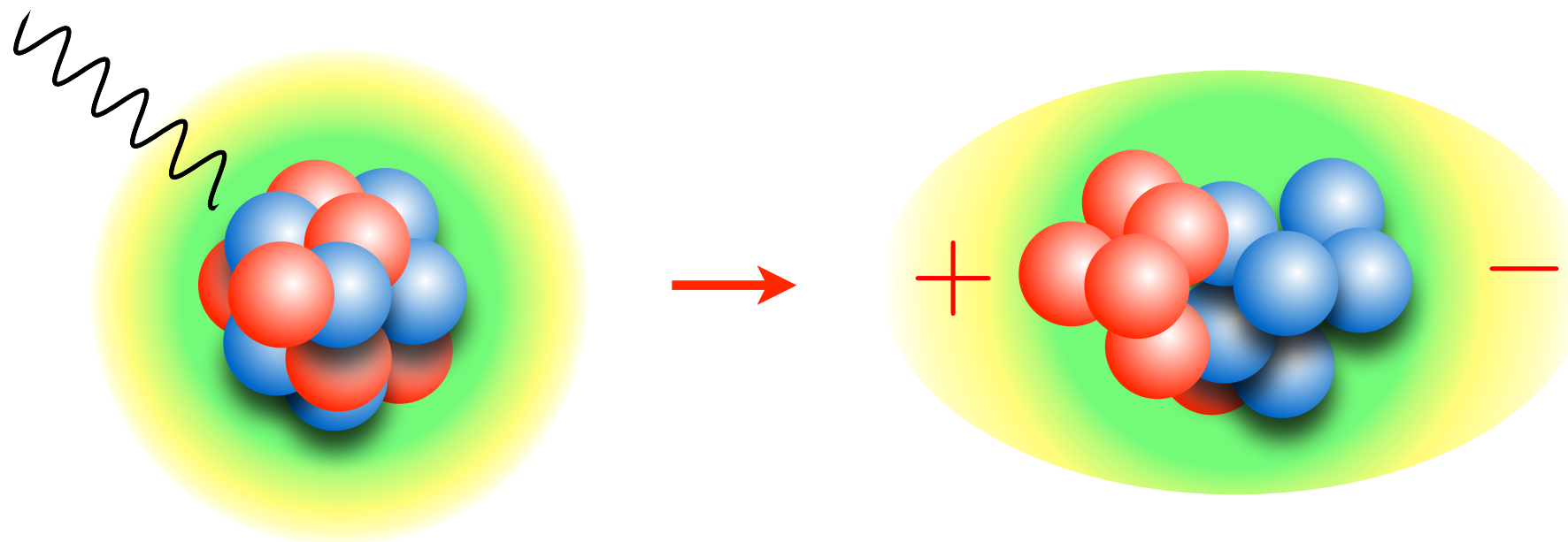
- At low momentum transfer the space resolution of the lepton becomes much larger than the average NN separation distance (~ 1.5 fm).
- In this regime the interaction involves many nucleons \longrightarrow long-range correlations



$$|\Psi_f\rangle = \sum c_{1p,1h}^f |\Psi_{1p1h}\rangle$$

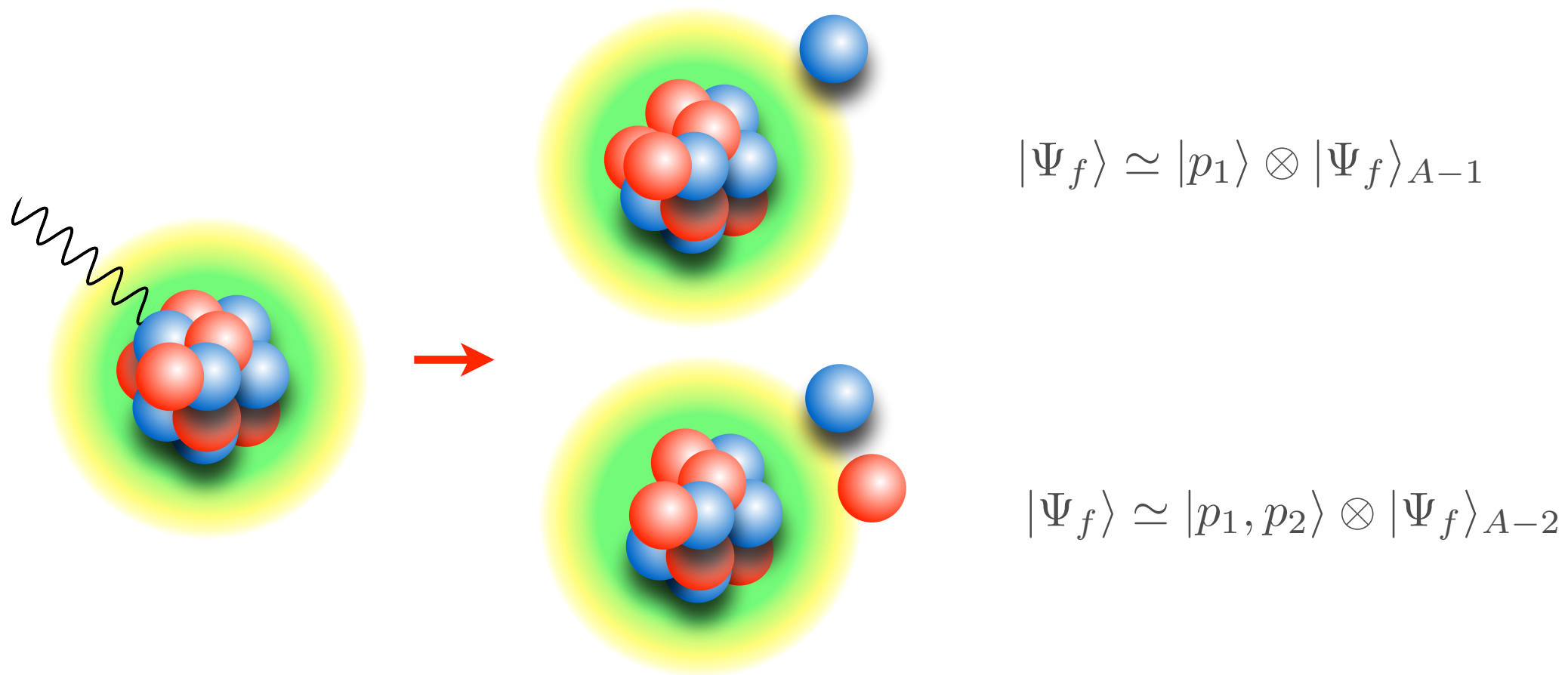
$$H^{\text{eff}} |\Psi_f\rangle = E_f |\Psi_f\rangle$$

- The giant dipole resonance is a manifestation of long-range correlations



Lepton-nucleus scattering

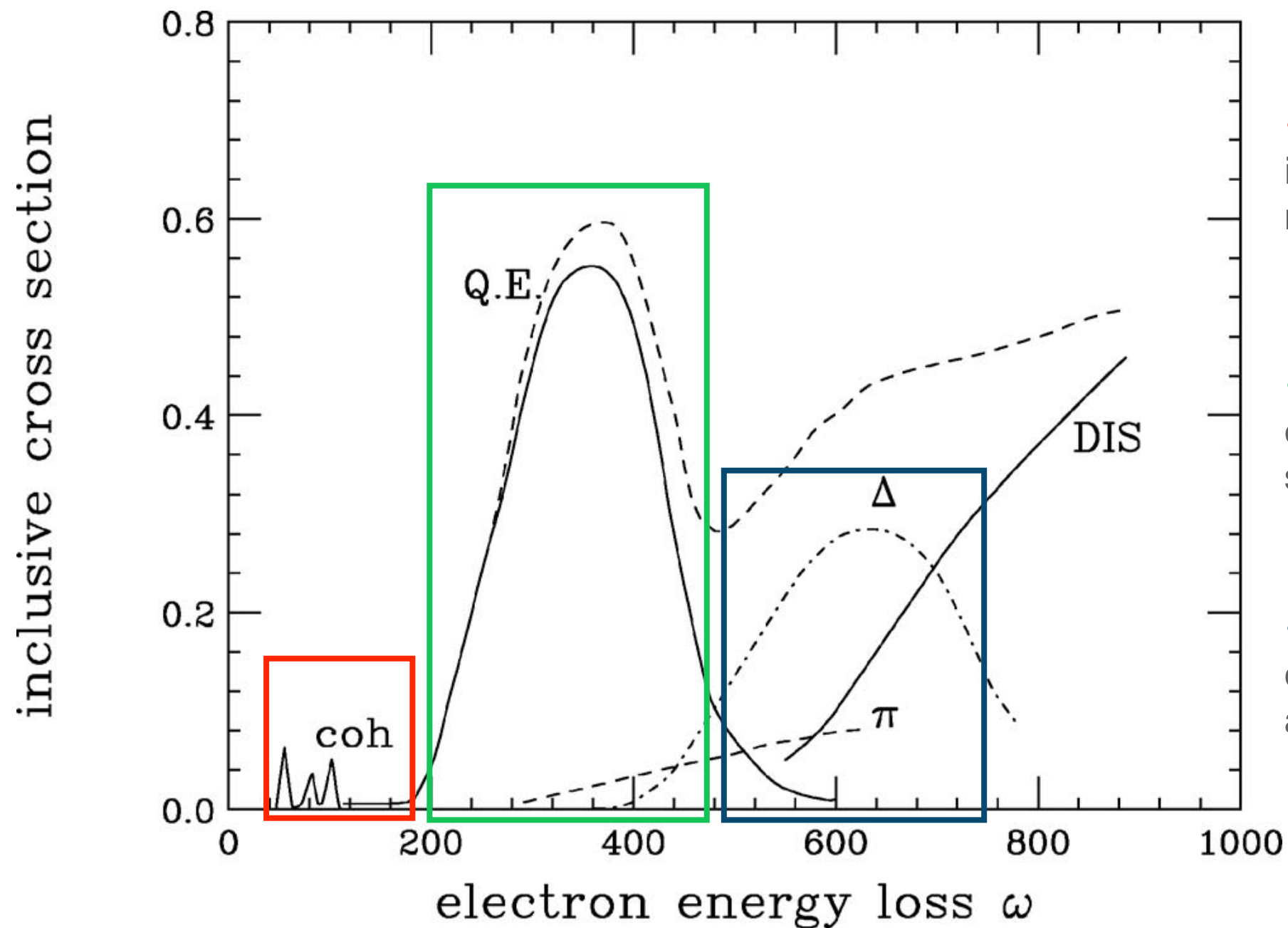
- At (very) large momentum transfer, scattering off a nuclear target reduces to the sum of scattering processes involving bound nucleons \longrightarrow short-range correlations.



- Relativistic effects play a major role and need to be accounted for along with nuclear correlations (Non trivial interplay between them)
- Resonance production and deep inelastic scattering also need to be accounted for

Electron-nucleus scattering

Schematic representation of the inclusive cross section as a function of the energy loss.



- Elastic scattering and inelastic excitation of discrete nuclear states.
- Broad peak due to quasi-elastic electron-nucleon scattering.
- Excitation of the nucleon to distinct resonances (like the Δ) and pion production.

Why quantum Monte Carlo?

In the non-relativistic regime, typically corresponding to $|\mathbf{q}| \lesssim 500 \text{ MeV}$, both the initial and the final state of the hadronic tensor are eigenstates of the nonrelativistic nuclear hamiltonian

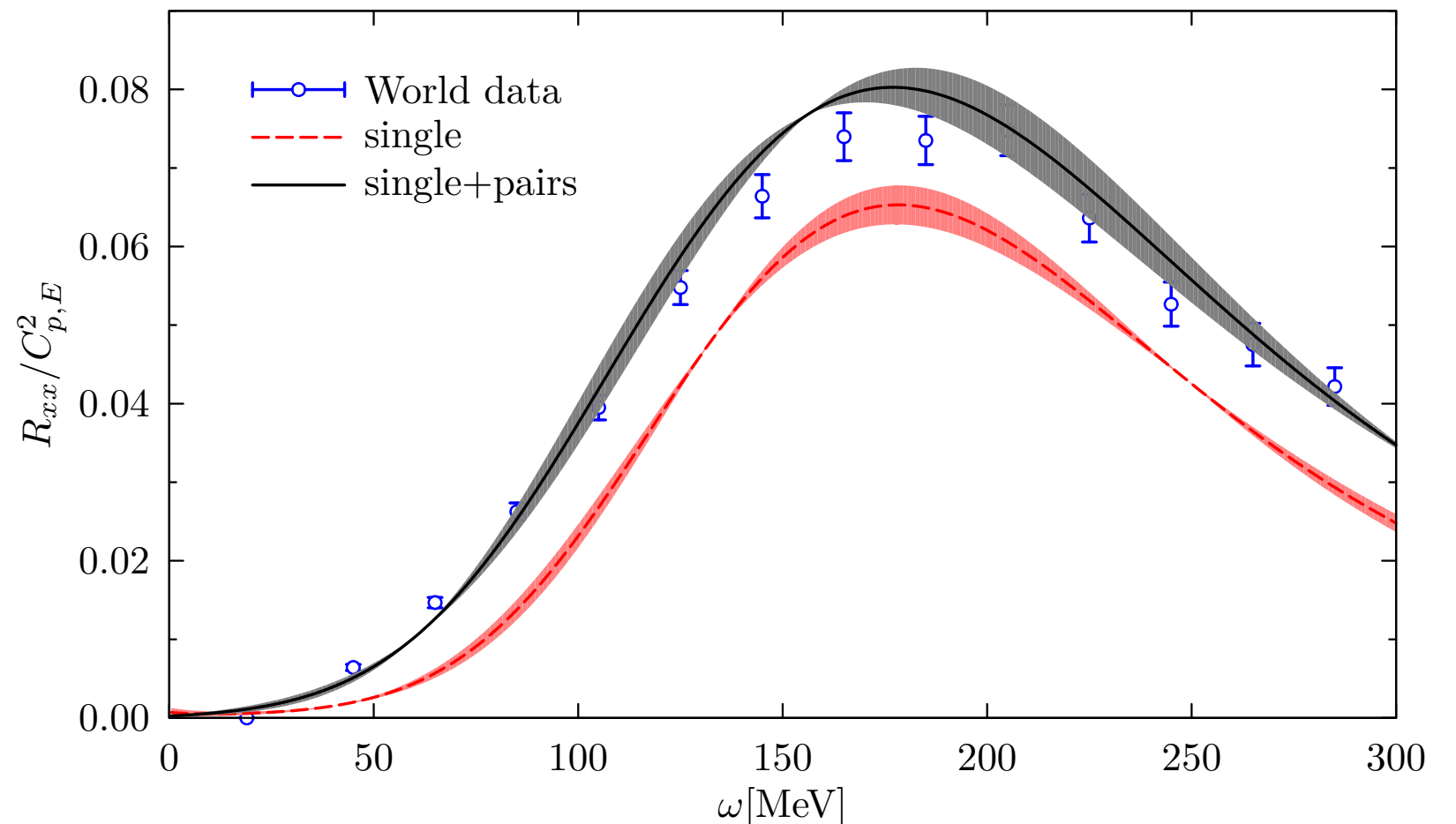
$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

$$H|\Psi_X\rangle = E_X|\Psi_X\rangle$$

As for the electron scattering on ^{12}C

$$|\Psi_X\rangle = |^{11}\text{B}, p\rangle, |^{11}\text{C}, n\rangle, |^{10}\text{B}, pn\rangle, |^{10}\text{Be}, pp\rangle \dots$$

QMC calculation of the nuclear response from threshold up to the quasi-elastic region (for nuclei as large as ^{12}C) are currently carried out on leadership-class computers



Spectral function & Quantum Monte Carlo

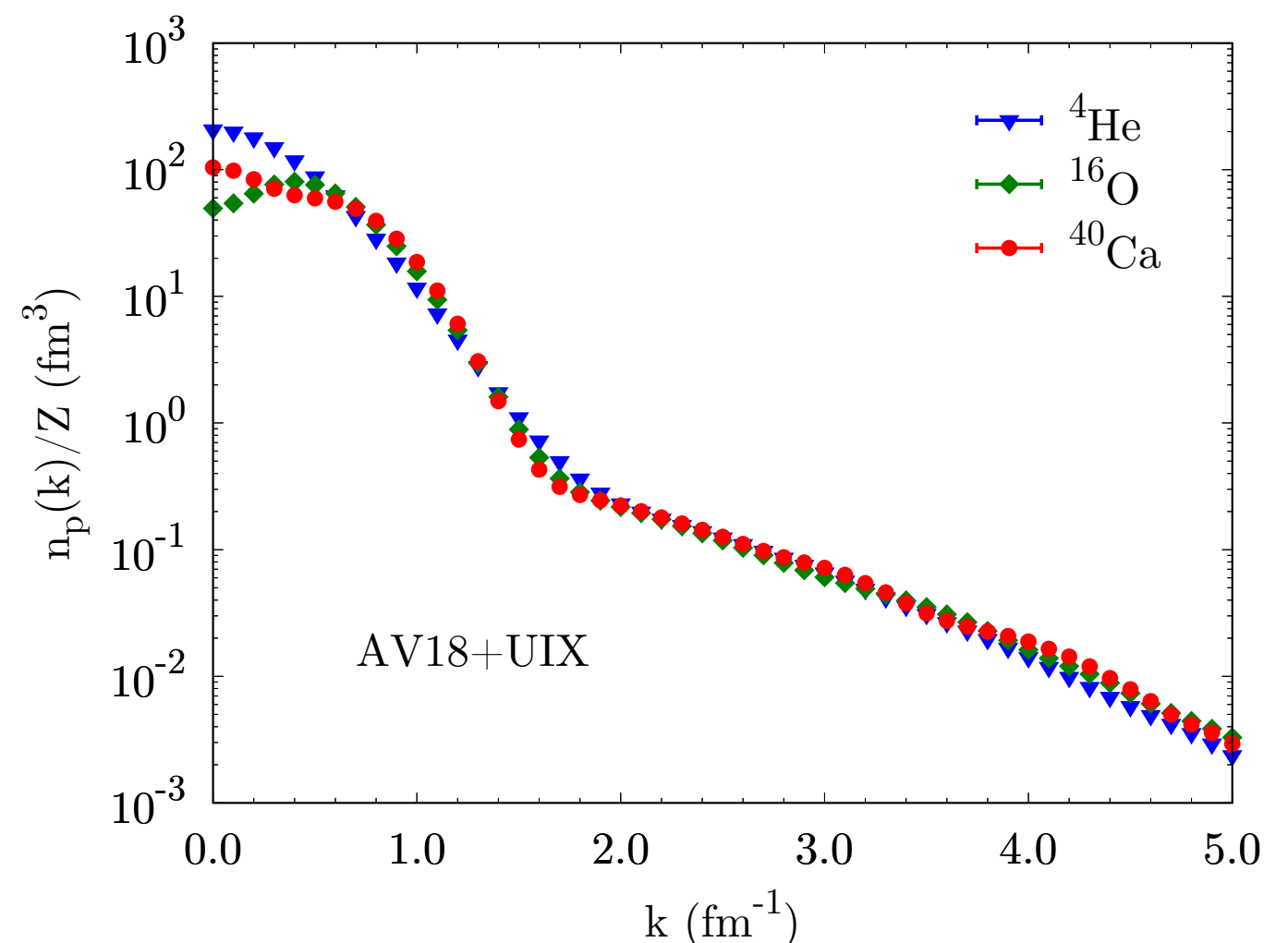
In the relativistic regime, the final state includes at least one particle carrying large momentum, whereas the initial nuclear state is still an eigenstate of the nuclear Hamiltonian.

The spectral function formalism allow one to circumvent the difficulties associated with the relativistic treatment of the nuclear final state and current operator, while at the same time preserving essential features (such as correlations) inherent to the realistic description of nuclear dynamics

The sum rule of the spectral function corresponds to the momentum distribution

$$\int dE P(\mathbf{k}, E) = n(\mathbf{k})$$

The momentum distribution of nuclei as large as ^{16}O and ^{40}Ca has been computed using QMC fully accounting for the correlations of the nuclear ground state



Chapter 2

The nuclear many-body problem

Many-body methods

Non relativistic many body theory is aimed at solving the Schrödinger equation

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

$$H\Psi_n(x_1, \dots, x_A) = E_n\Psi_n(x_1, \dots, x_A)$$



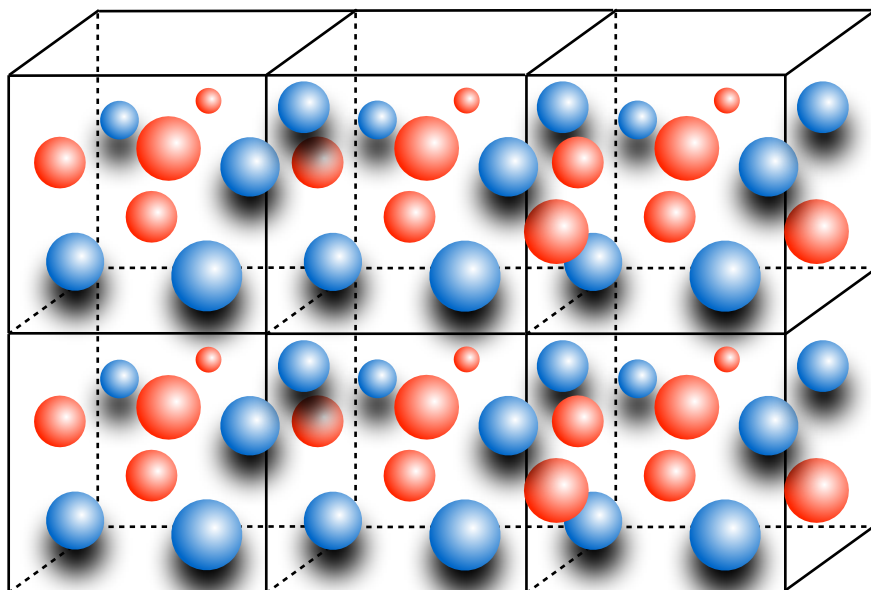
Many-body wave function

Within mean field approaches, the ground-state wave function is a Slater determinant of single particle wave functions

$$\Phi_0(x_1, \dots, x_A) = \mathcal{A}[\phi_{n_1}(x_1) \dots \phi_{n_A}(x_A)]$$

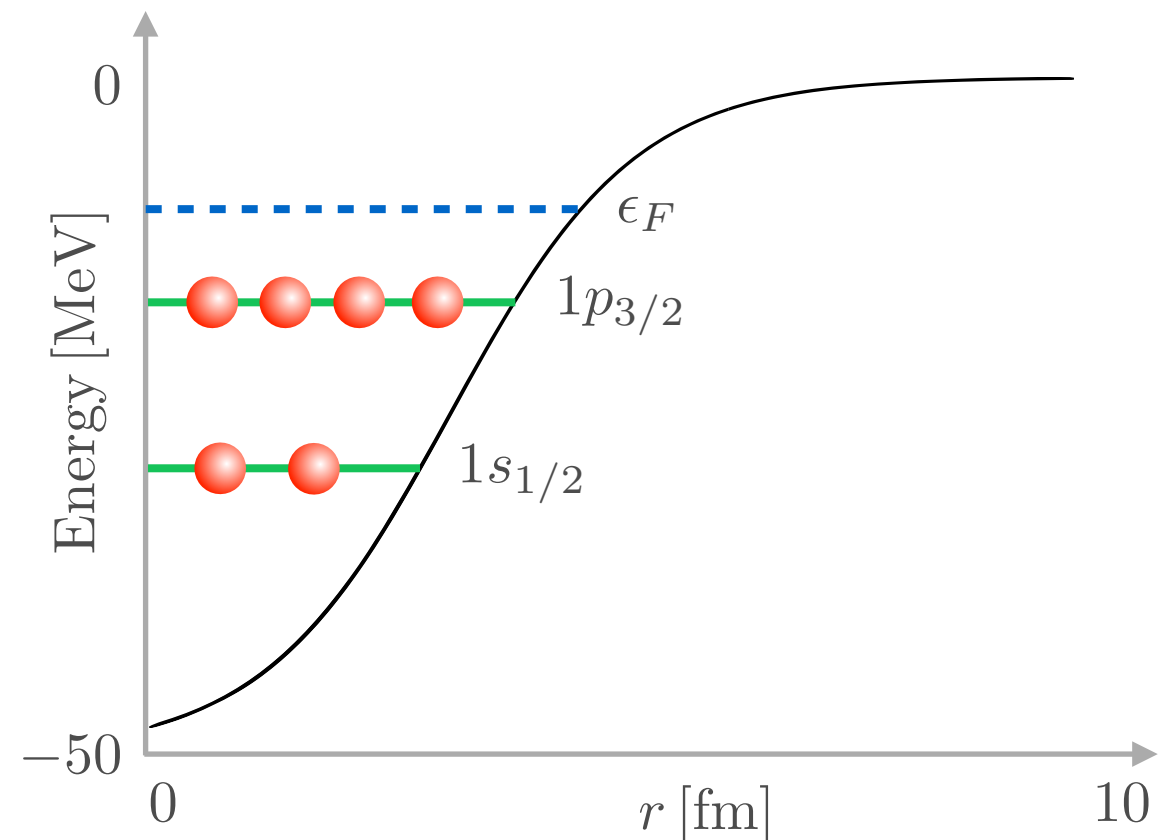
Infinite nuclear matter

- Single-particle wave functions are plane waves
- Box with periodic boundary conditions



Finite nuclei

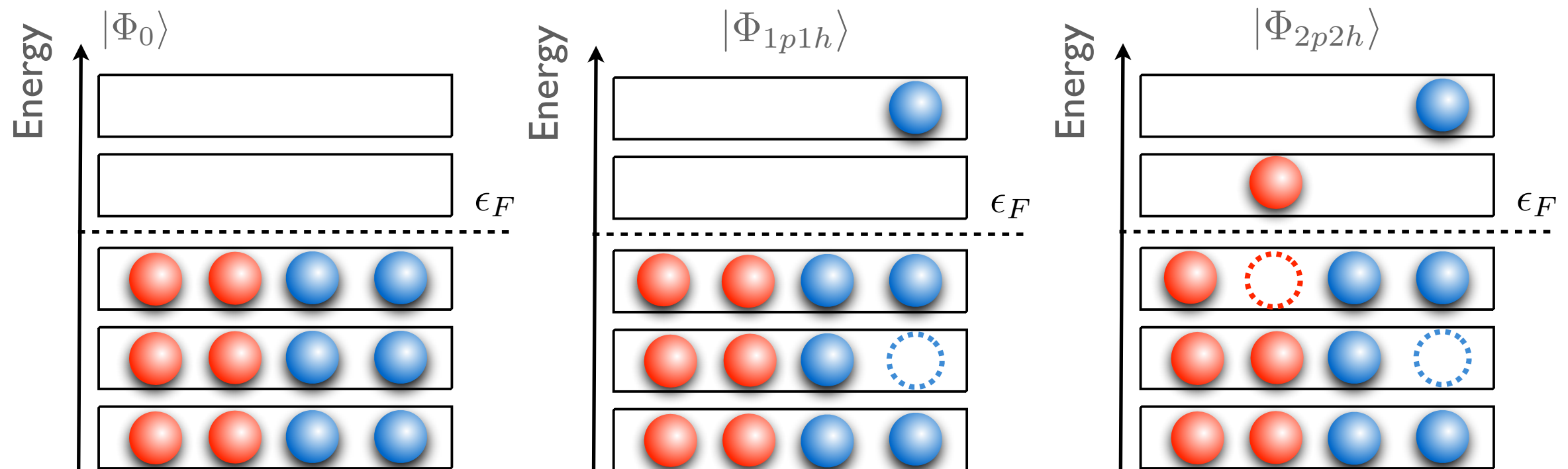
- Hartree-Fock solution



Many-body wave function

Excited states are constructed removing n occupied states from the Slater determinant and replacing them with n virtual (unoccupied) states

$$\Phi_{p_i, h_i}(x_1 \dots x_A) = \mathcal{A}[\phi_{n_1}(x_1) \dots \phi_{p_i}(x_i) \dots \phi_{n_A}(x_A)]$$



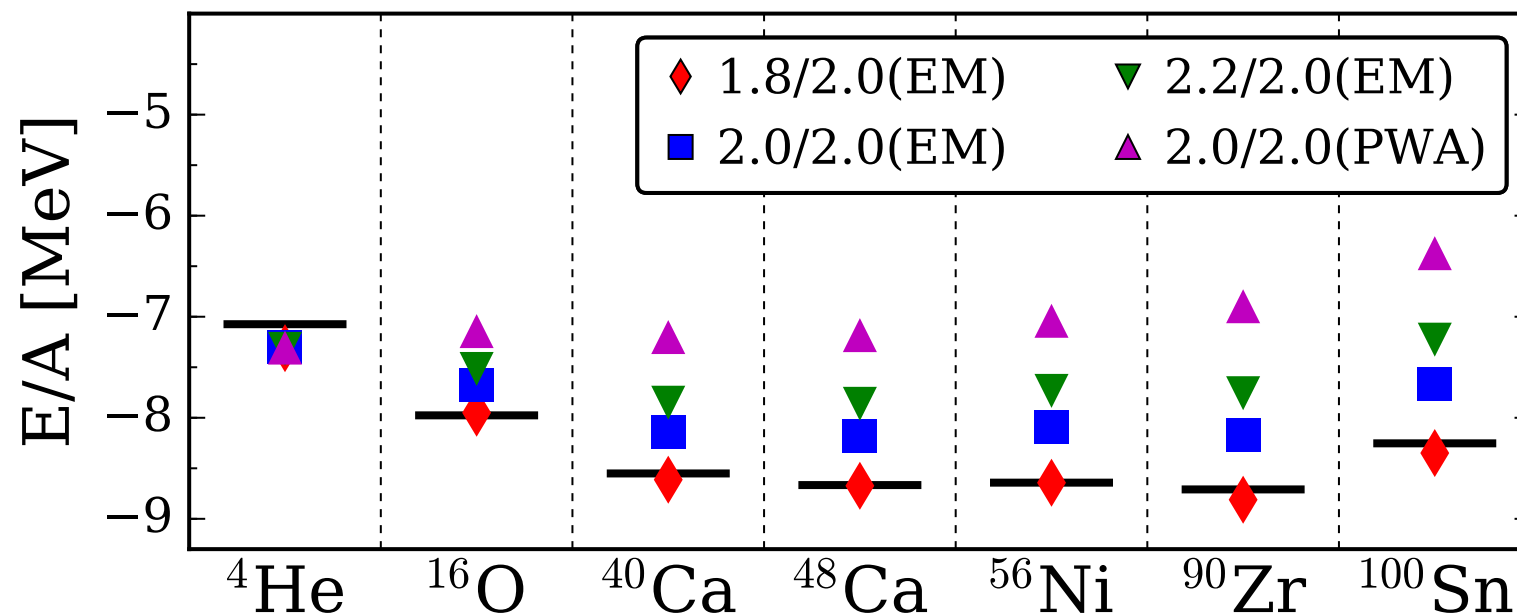
The eigenstate of the Hamiltonian is a linear combination of n-particles n-holes states

$$|\Psi_n\rangle = \sum c_{p_i, h_i}^n |\Phi_{p_i, h_i}\rangle \quad H|\Psi_n\rangle = E_n |\Psi_n\rangle$$

Many-body wave function

One class of many-body methods includes those relying on single-particle basis expansions, such as the no-core shell model (NCSM), the coupled-cluster (CC) method, the in-medium similarity renormalization group, and self-consistent Green's function methods

Medium-mass and heavy nuclei, up to ^{101}Sn , the heaviest doubly magic nucleus with equal number of neutrons and protons, can be described in terms of individual interactions between their constituents



Despite their remarkable achievements, these many-body methods have difficulties in dealing with the high-momentum components of the nuclear wave function

Correlated wave functions

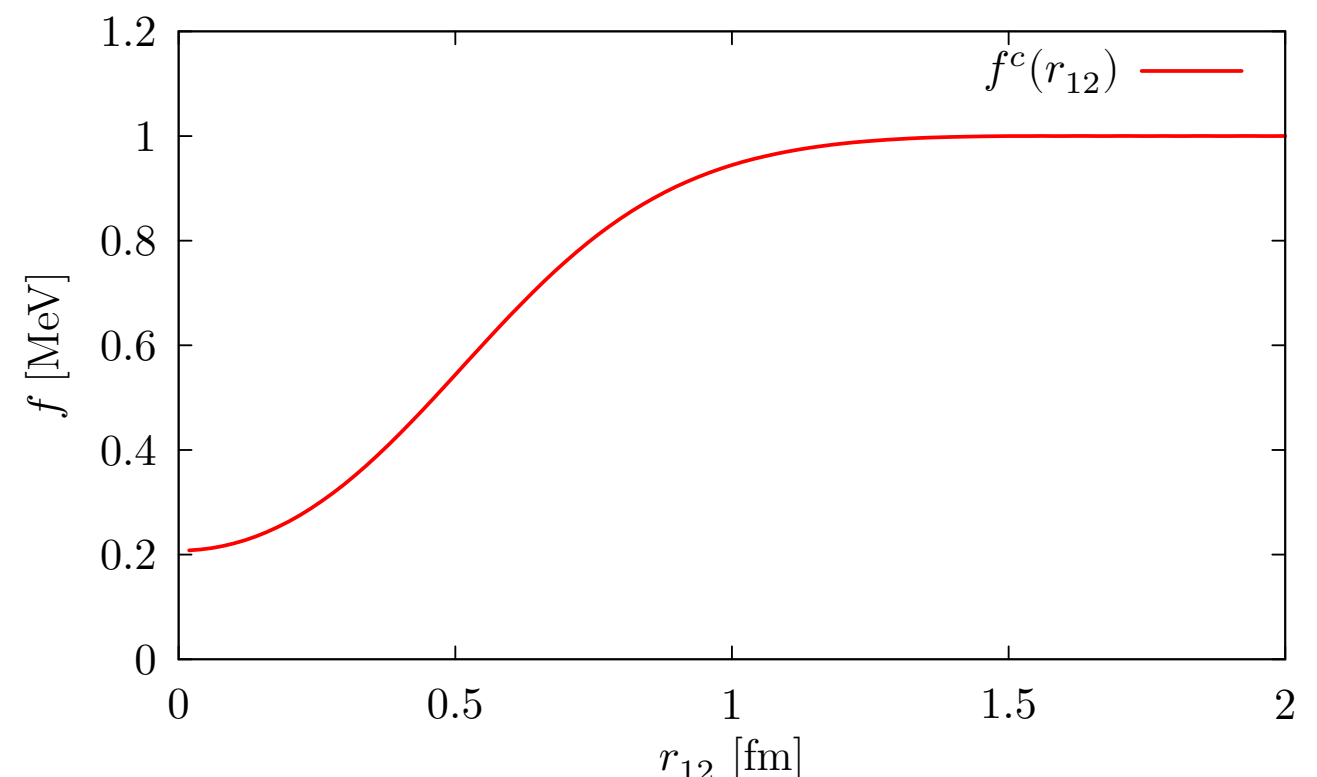
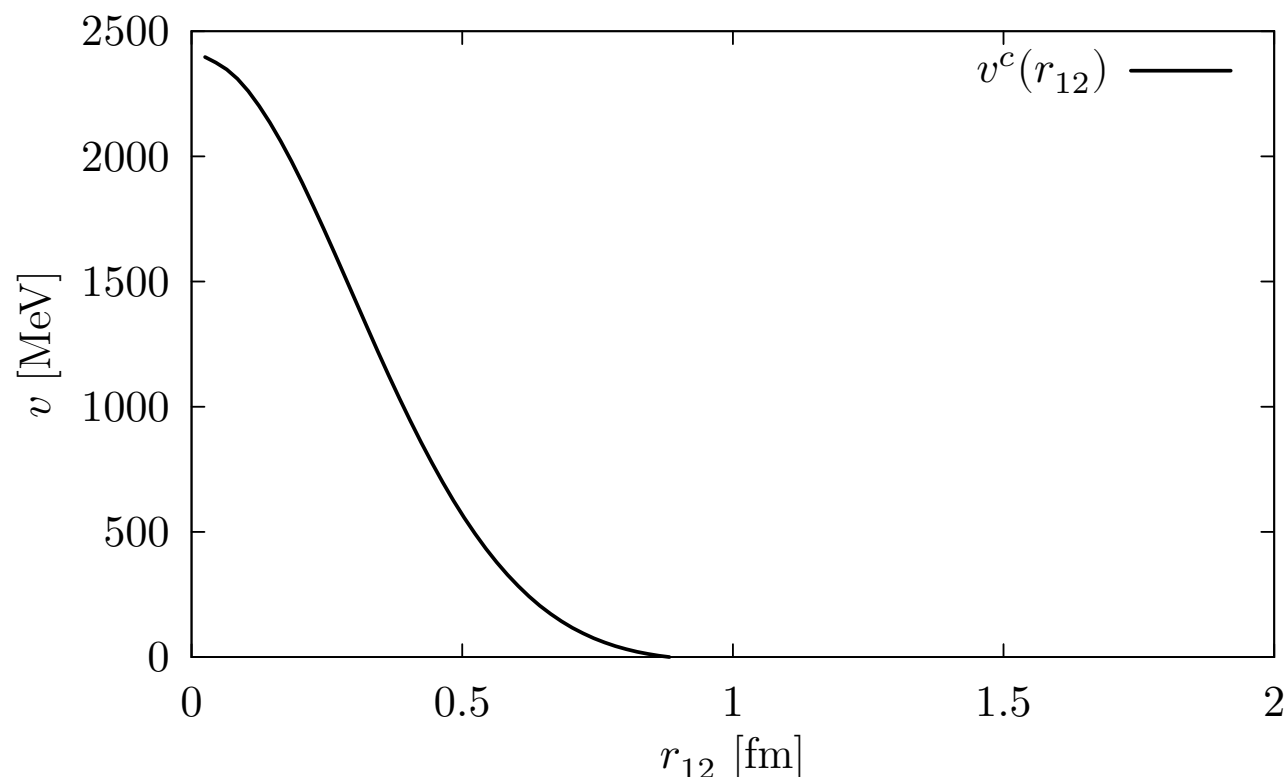
Quantum Monte Carlo methods explicitly account for the correlations induced by the nuclear interactions

$$\Phi_n(x_1 \dots x_A) \longrightarrow \mathcal{F} \Phi_n(x_1 \dots x_A)$$

The correlation operator reflects the spin-isospin dependence of the nuclear interaction

$$\mathcal{F} \equiv \left(\mathcal{S} \prod_{i < j} F_{ij} \right) \qquad F_{ij} \equiv \sum_p f_{ij}^p O_{ij}^p$$

The shape of f_{ij}^p is determined by minimizing the variational energy $E_V \simeq \langle \Phi_0 | \mathcal{F}^\dagger H \mathcal{F} | \Phi_0 \rangle$



Chapter 3

Quantum Monte Carlo

Quantum Monte Carlo methods

Let us assume that

- The temperature of the system is much smaller than the Fermi energy
- We are interested in the ground-state properties of the system

Quantum Monte Carlo methods give us two options for solving the many-body Schrödinger equation

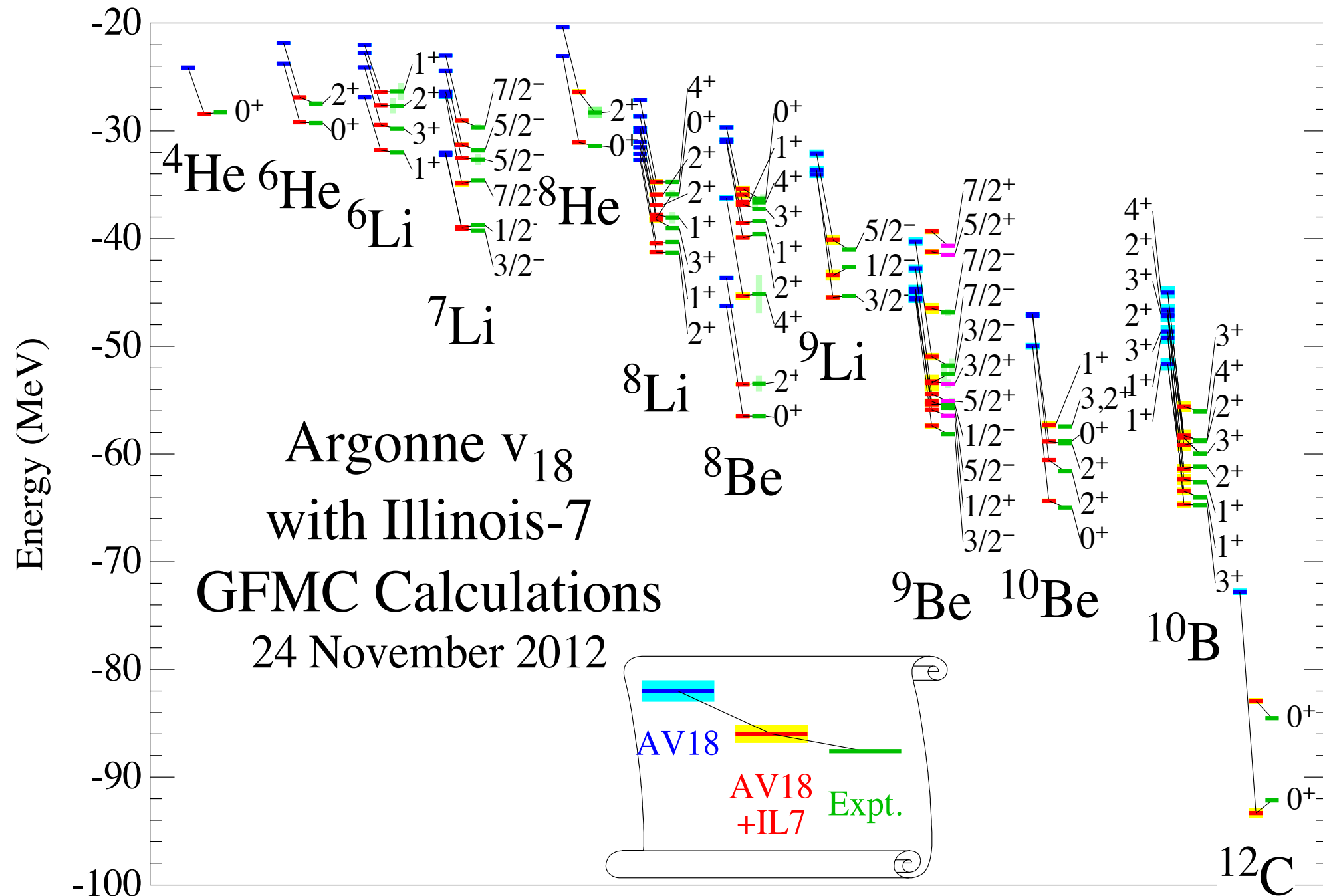
Variational Monte Carlo (VMC)

In VMC, one assumes a form for the trial wave function and optimizes its variational parameters, typically by minimizing the energy and/or the variance of the energy. The expectation of the Hamiltonian is evaluated by means of Monte Carlo method.

Diffusion Monte Carlo (DMC)

“Exactly” solve the problem by projecting the ground state from an arbitrary initial guess of the wave function by means of a propagation in imaginary time.

Quantum Monte Carlo methods



Variational Monte Carlo

Variational Monte Carlo uses the stochastic integration method to evaluate the expectation value of the Hamiltonian for a chosen trial wave function, which depends on a set of variational parameters.

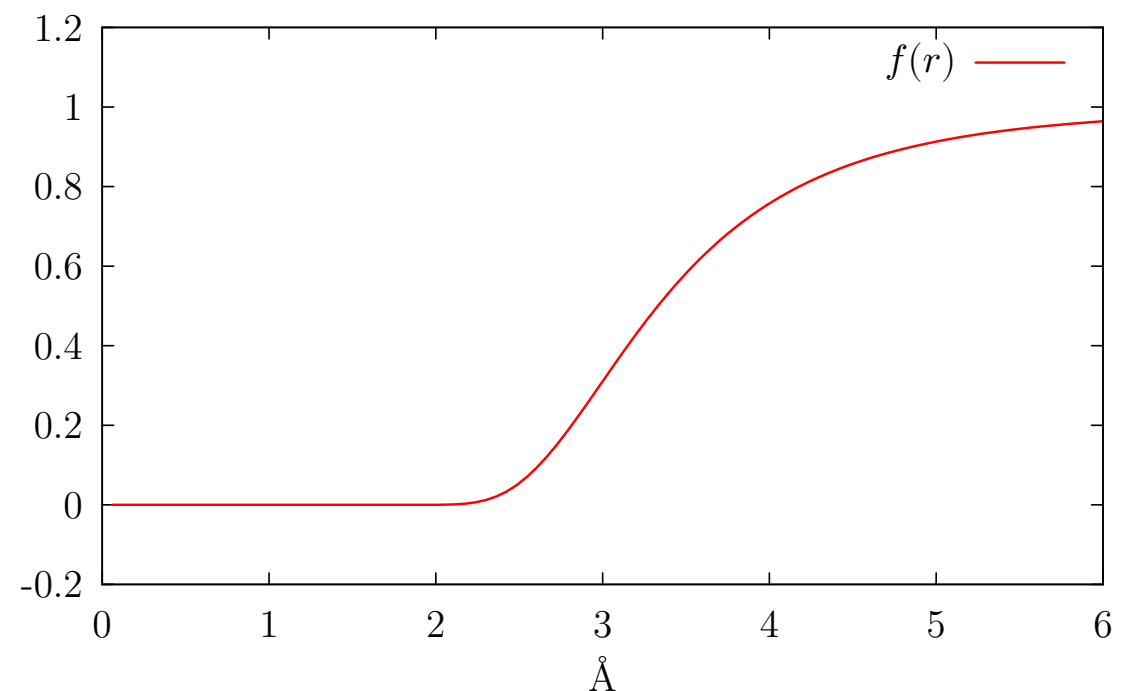
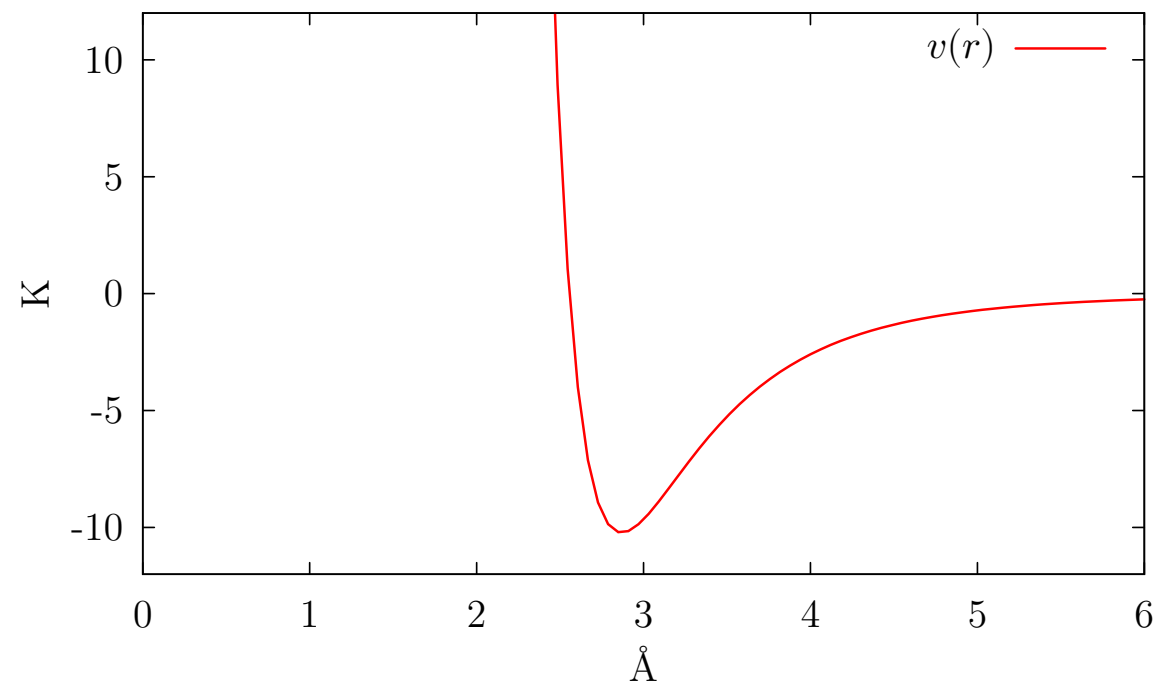
The interaction between ^4He atoms forming an homogeneous liquid can be parametrized by means of the two-body Lennard-Jones potential

$$v(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

A reasonable trial wave function is small where the potential is repulsive and large where the potential is attractive

$$\Psi_T(R) = \prod_{i < j} f(r_{ij})$$

$$f(r) = \exp \left[-\frac{1}{2} \left(\frac{b}{r} \right)^5 \right]$$



Variational Monte Carlo

The variational principle guarantees that the energy of the trial wave function is greater than or equal to the ground-state energy with the same quantum numbers as

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

The variational parameters are determined by minimizing the trial energy. In the atomic liquid ^4He atoms case this amounts to

$$\frac{\partial E_T}{\partial b} = 0$$

Note that, in order to compute the trial energy for a given set of variational parameters, the following multi-dimensional integral in the degrees of freedom of the system (coordinates, spin and isospin) has to be evaluated

$$E_T = \frac{\int dR \Psi_T^*(R) H \Psi_T(R)}{\int dR \Psi_T^*(R) \Psi_T(R)}$$

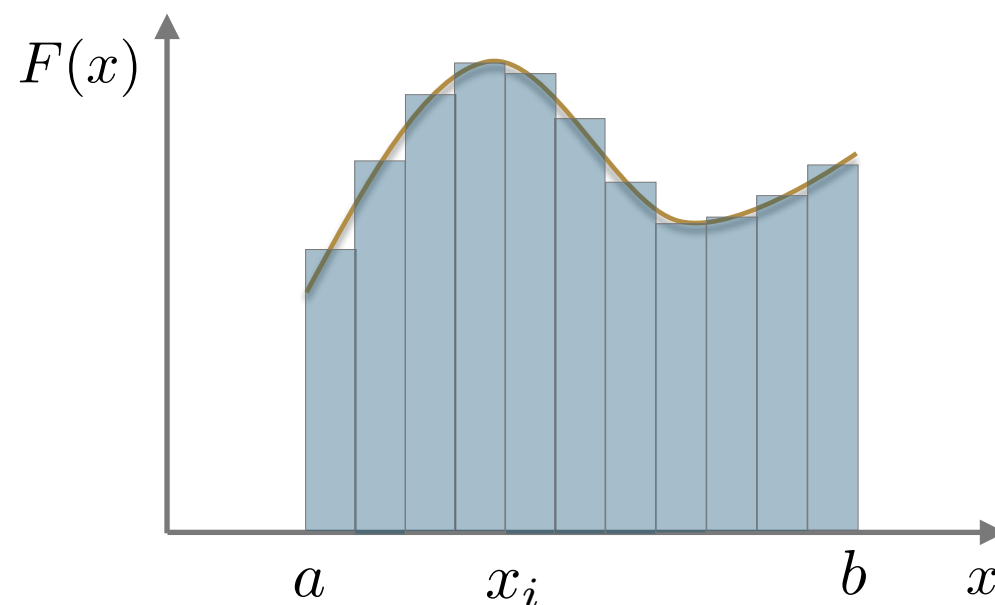
$$R \equiv \mathbf{r}_1, \dots, \mathbf{r}_A$$

Multi dimensional integrals

Our goal consists in computing the following D-dimensional integral

$$I(D) = \int_{a_1}^{b_1} dx_1 \dots \int_{a_D}^{b_D} dx_D F(x_1, \dots, x_D)$$

In the one-dimensional case, we can divide the area below to the curve into rectangles



$$\left\{ \begin{array}{l} I(1) \simeq h \sum_i F(x_i) \\ \Delta(1) = h^2 |F'(x_i)| + O(h^3) \\ h \propto \frac{1}{N} \end{array} \right.$$

How many points do we need to achieve a given precision ?

$$\frac{\Delta(1)}{I(1)} = \epsilon \quad \Rightarrow \quad N \propto \frac{1}{\epsilon}$$

Multi dimensional integrals

A generalization of the As for the D-dimensional case, it is easy to find

$$\left\{ \begin{array}{l} I(D) \simeq h^D \sum_i F(x_i) \\ \Delta(D) = h^{D+1} |\nabla F(x_i)| + O(h^{D+2}) \\ h \propto \frac{1}{N^D} \end{array} \right. \quad \Rightarrow \quad N \propto \frac{1}{\epsilon^D}$$

Note that more clever methods can be used, but the error is always proportional to h^α .

Suppose we want to compute the expectation value of the Hamiltonian for a system containing 12 particles interacting with a central potential with a precision $\epsilon = 0.1$

Because the potential is central, we will be dealing with a 36-dimensional integral

$$D = 36 \quad \Rightarrow \quad N \propto 10^{36} \quad \Rightarrow \quad 10^{17} \text{ hours on Mira!!!}$$

Nobody is going to award us that many hours of computing time!

The central limit theorem

Suppose that the N continuum random variables x_1, \dots, x_N are drawn from the probability distribution $P(x)$ and consider the function $f(x)$. We may define a new random variable

$$S_N = \frac{1}{N} \sum_{i=1}^N f(x_i)$$

If the samples are statistically independent, the **central limit theorem** states that the probability distribution of S_N is gaussian

$$P(S_N) = \frac{1}{\sqrt{2\pi\sigma_N^2}} e^{-\frac{(S_N - \bar{S}_N)^2}{2\sigma_N^2}}$$

where the average and the variance of S_N are given by

$$\bar{S}_N = \int dx P(x) f(x) \quad \sigma_N = \sqrt{\frac{1}{N} \left[\int dx P(x) f^2(x) - \bar{S}_N^2 \right]}$$

These results hold true for any dimensionality of the space in which the variable x is defined

The central limit theorem

Therefore, the central limit theorem provides a recipe to numerically evaluate multi-dimensional integrals of the form

$$I = \int dx f(x)$$

- Since the probability density has to be positive definite, rewrite the integral as:

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

- Sample N (with N “large”) points from the probability density $P(x)$
- Average the N values of $f(x_i)$ and $f^2(x_i)$

$$I = \frac{1}{N} \sum_{i=1}^N f(x_i) \pm \sqrt{\frac{1}{(N-1)} \left[\frac{1}{N} \sum_{i=1}^N f^2(x_i) - \left(\frac{1}{N} \sum_{i=1}^N f(x_i) \right)^2 \right]}$$

Variational Monte Carlo

Remember that the numerator of the expectation value of the Hamiltonian for a system of A particles interacting with a spin-independent potential reads

$$E_T = \int dR \Psi_T^*(R) H \Psi_T(R) \quad R \equiv \mathbf{r}_1, \dots, \mathbf{r}_A$$

In order to use the central limit theorem, the former integral has to be rewritten as

$$E_T = \int dR |\Psi_T(R)|^2 E_L(R)$$

where we have defined the **local energy**

$$E_L(R) \equiv \frac{H \Psi_T(R)}{\Psi_T(R)}$$

Since it is positive and integrable, $|\Psi_T(R)|^2$ can be regarded as a probability density.

In order to compute the trial energy one has to find a way to sample $|\Psi_T(R)|^2$

M(RT)² algorithm

The algorithm was first described in a paper by Metropolis, Rosenbluth, Rosenbluth, Teller and Teller M(RT)². It shares common features to the rejection techniques because:

- It involves explicitly proposing a tentative value of the variable we want to sample, which may be rejected.
- The normalization of the sampled function is irrelevant.

M(RT)² algorithm has its own advantages and disadvantages:

Pros

- It can be used to sample essentially any density function regardless of analytic complexity in any number of dimensions
- It is of very great simplicity.

Cons

- Sampling is correct only asymptotically
- Consecutive variables produced are often very strongly correlated
- Not well suited to sample distributions with parameters that change frequently.


M(RT)² algorithm

To begin with, consider a 1-D harmonic oscillator. We want to sample the probability distribution described by the modulus squared of our trial wave function

$$P(x) \equiv |\Psi_T(x)|^2 \qquad \Psi_T(x) = \exp\left(-\alpha \frac{x^2}{2}\right)$$

M(RT)² algorithm is based on the idea of random walk in the space of the random variable x . The game consists of generating a random variable applying a transformation to another. This “moving” point is called walker.

$$P_{i+1}(x_{i+1}) = \int dx_i P_i(x_i) T(x_i \rightarrow x_{i+1})$$

 **Transition probability**

By recursively applying the same transformation we get

$$P_n(x_n) = \int dx_1 \dots dx_{n-1} P_1(x_1) T(x_1 \rightarrow x_2) \dots T(x_{n-1} \rightarrow x_n)$$

Under some very general conditions it can be proven that

$\lim_{n \rightarrow \infty} P_n(x_n) = P(x) \Rightarrow$ where $P(x)$ only depends on T

M(RT)² algorithm

Let us impose a further condition, i.e. that the asymptotic distribution is an “equilibrium” state:

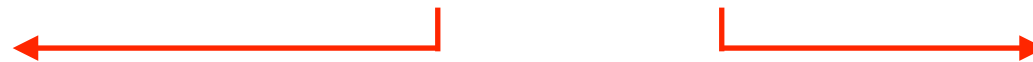
$$P(x)T(x \rightarrow y) = P(y)T(y \rightarrow x)$$

The latter is called detailed balance condition, because it does not hold only on average, but it tells that point by point there is no net flux of probability!

We can arbitrarily split the transition probability in two terms

$$T(x \rightarrow y) = G(x \rightarrow y)A(x \rightarrow y)$$

It describes the probability of moving the walker from $x \rightarrow y$.



It tells whether the proposed move is accepted or rejected.

The detailed balance then reads

$$\frac{A(y \rightarrow x)}{A(x \rightarrow y)} = \frac{P(x)G(x \rightarrow y)}{P(y)G(y \rightarrow x)}$$

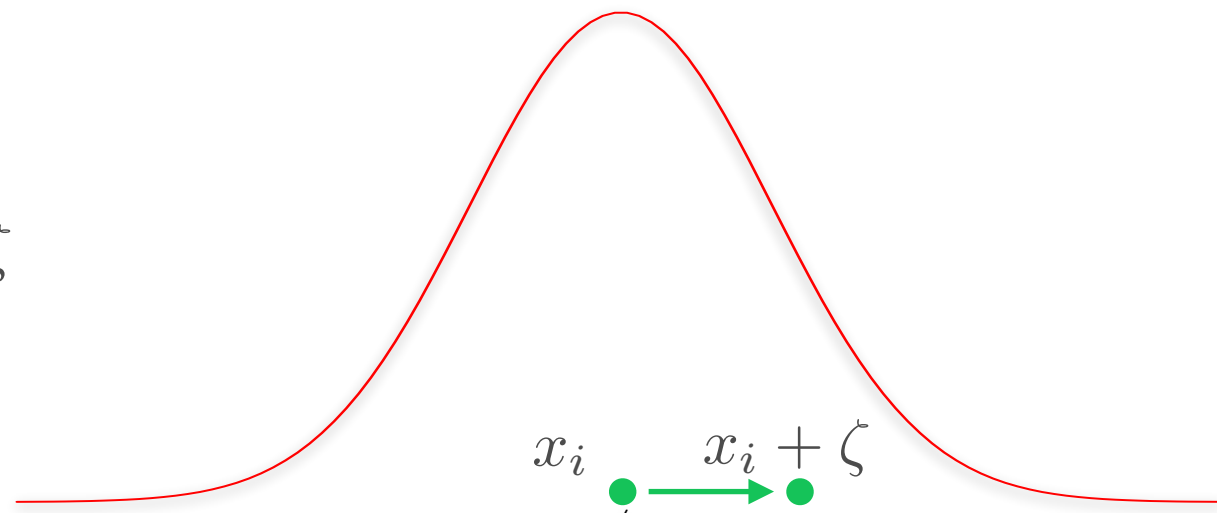
It can be easily checked that the following acceptance probability satisfies the above requirement

$$A(y \rightarrow x) = \min \left(1, \frac{P(x)G(x \rightarrow y)}{P(y)G(y \rightarrow x)} \right)$$

M(RT)² algorithm

In QMC we use a very simple prescription for $G(x \rightarrow y)$, which in 1-D corresponds to shifting a point by a value distributed according to a gaussian distribution

$$x_{i+1} = x_i + \zeta$$



In the many-particle case, the one dimensional gaussian is replaced by a three-dimensional one for each of the particles.

Since the probability of going from x to y is the same as the one for going from y to x , it turns out that

$$G(x \rightarrow y) = G(y \rightarrow x) \quad \longleftrightarrow \quad A(y \rightarrow x) = \min \left(1, \frac{P(x)}{P(y)} \right)$$

M(RT)² applied to VMC

At this point, we can describe the Metropolis algorithm for a VMC calculation in the 1-D case

Step 0 - Start from a “flat” distribution of walkers on the coordinate x

Step 1 - Move the walkers according to $G(x_i \rightarrow y_{i+1})$, i.e. $y_{i+1} = x_i + \zeta$

Step 2 - Compute the acceptance probability $A(x_i \rightarrow y_{i+1}) = \min \left(1, \frac{|\Psi_T(y_{i+1})|^2}{|\Psi_T(x_i)|^2} \right)$

Step 3 - Accept or reject the proposed move

$$\frac{|\Psi_T(y_{i+1})|^2}{|\Psi_T(x_i)|^2} > \xi \Rightarrow x_{i+1} = y_{i+1}$$

$$\frac{|\Psi_T(y_{i+1})|^2}{|\Psi_T(x_i)|^2} \leq \xi \Rightarrow x_{i+1} = x_i$$

Nuclear VMC wave function

A good trial wave function to describe a nucleus has to reflect the complexity of the nuclear potential

It contains 3-body correlations arising from the three-body potential

$$\Psi_T = \left[1 + \sum_{i < j < k} \tilde{U}_{ijk}^{\text{TNI}} \right] \Psi_P \longleftrightarrow \tilde{U}_{ijk} \equiv \tilde{\epsilon}_A V_{ijk}^A + \tilde{\epsilon}_R V_{ijk}^R$$

The pair correlated wave function is written in terms of operator correlations arising from the 2-body potential

$$\Psi_P = \left[\mathcal{S} \prod_{i < j} (1 + U_{ij}) \right] \Psi_J \longleftrightarrow U_{ij} = \sum_{p=2,6} u^p(r_{ij}) O_{ij}^p$$

The total antisymmetric Jastrow wave function depends on the quantum numbers of the given nucleus

$$\Psi_J = \left[\prod_{i < j < k} f_{ijk}^c \right] \left[\prod_{i < j} f_{ij}^c \right] \Phi_A(J, M, T, T_3)$$

Spin-isospin degrees of freedom

- A walker associated with wave function of the nucleus, do not only describes the positions of the protons and neutrons, but also their spin and isospin!
- The GFMC wave function is written as a complex vector, the coordinates of which represent a spin-isospin state of the system
- The ${}^3\text{H}$ case fits in the slide: the number of states grows exponentially with the number of nucleons

$$|\Psi_{3H}\rangle = \begin{pmatrix} a_{\uparrow\uparrow\uparrow} \\ a_{\uparrow\uparrow\downarrow} \\ a_{\uparrow\downarrow\uparrow} \\ a_{\uparrow\downarrow\downarrow} \\ a_{\downarrow\uparrow\uparrow} \\ a_{\downarrow\uparrow\downarrow} \\ a_{\downarrow\downarrow\uparrow} \\ a_{\downarrow\downarrow\downarrow} \end{pmatrix} \otimes \begin{pmatrix} a_{pnn} \\ a_{npn} \\ a_{nnp} \end{pmatrix}$$

