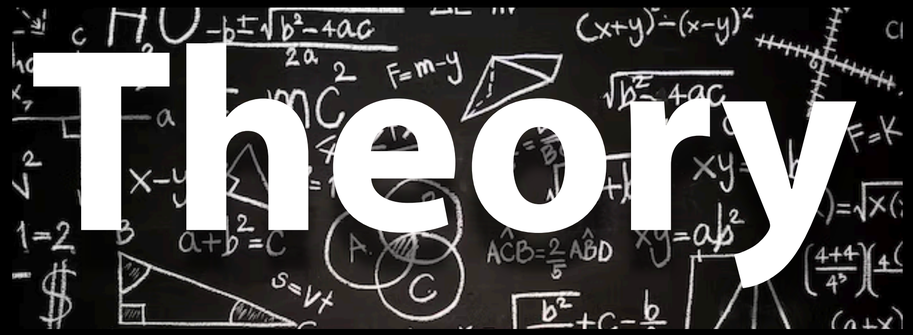
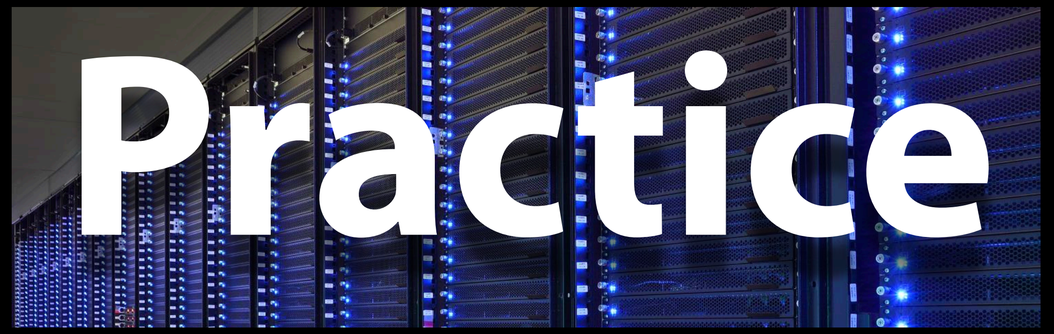
Nuclear Structure





Paolo Finelli

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ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

Overview - References

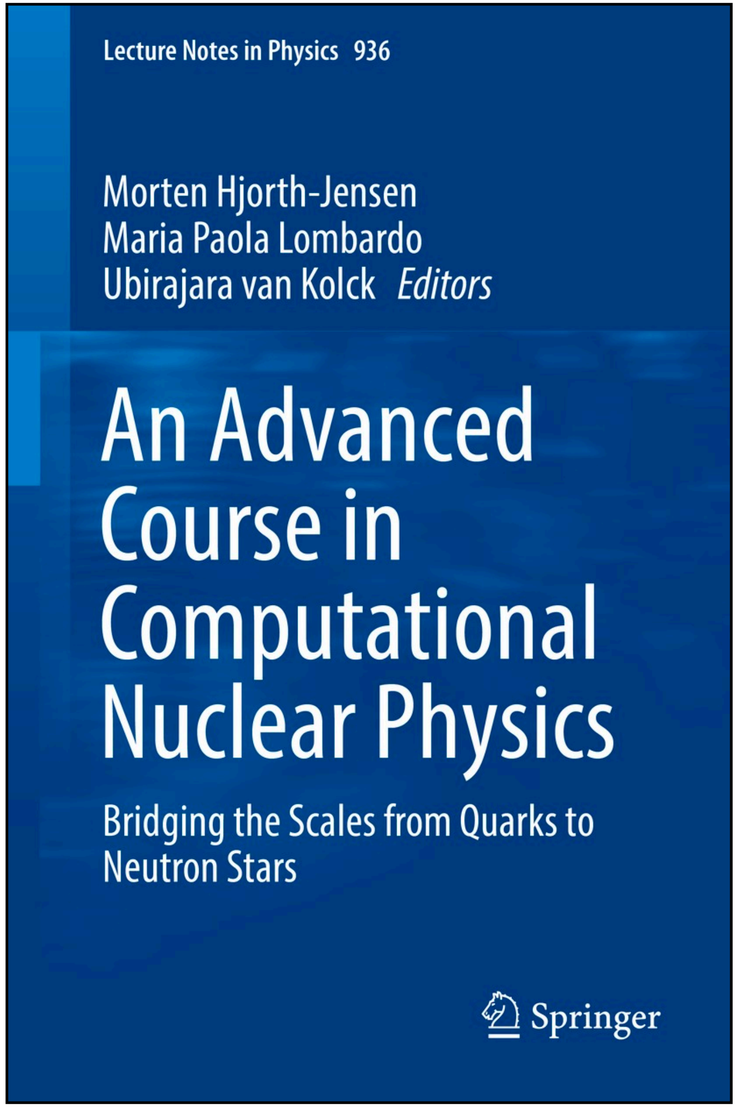
COURSE 2

ELEMENTARY FEATURES OF NUCLEAR STRUCTURE

B. Mottelson

NORDITA, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

Les Houches Summer School 1998



A Guided Tour of *ab initio* Nuclear Many-Body Theory

*Heiko Hergert**

Facility for Rare Isotope Beams and Department of Physics & Astronomy, Michigan State University, East Lansing, MI, United States

Over the last decade, new developments in Similarity Renormalization Group techniques and nuclear many-body methods have dramatically increased the capabilities of *ab initio* nuclear structure and reaction theory. Ground and excited-state properties can be computed up to the tin region, and from the proton to the presumptive neutron drip lines, providing unprecedented opportunities to confront two- plus three-nucleon interactions from chiral Effective Field Theory with experimental data. In this contribution, I will give a broad survey of the current status of nuclear many-body approaches, and I will use selected results to discuss both achievements and open issues that need to be addressed in the coming decade.

Eur. Phys. J. Plus (2018) **133**: 434
DOI 10.1140/epjp/i2018-12244-2

THE EUROPEAN PHYSICAL JOURNAL PLUS

Review

From the liquid drop model to lattice QCD*

A brief history of nuclear interactions

Vittorio Somà[a]

IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Received: 13 June 2018
Published online: 24 October 2018

Abstract. The present article aims to give a concise account of the main developments in nuclear structure theory, from its origin in the 1930s to date, taking the modelling of inter-nucleon interactions as guideline.

https://github.com/ManyBodyPhysics/LectureNotesPhysics
https://www.frontiersin.org/articles/10.3389/fphy.2020.00379/full
https://link.springer.com/article/10.1140/epjp/i2018-12244-2

Overview - References

- Short introduction

(Experimental evidences of *collective behaviour* and *single-particle motion)*

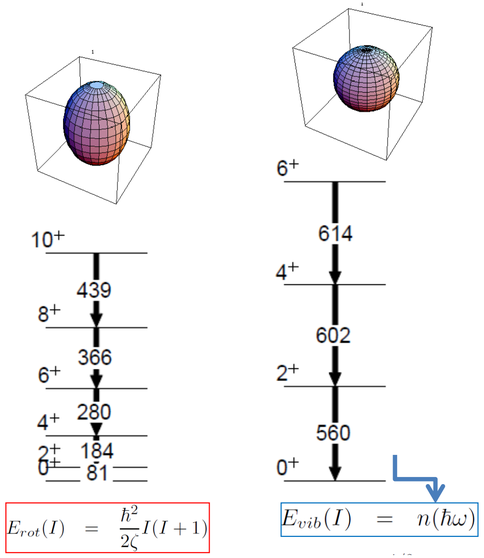
- How to treat the **nuclear many body problem**

1) Non-interacting shell model
2) Mean field approaches
3) Configuration interaction methods
4) Microscopic approaches (*ab-initio*)

- Numerical codes

Experimental data

Nuclear spectra - Collective motions



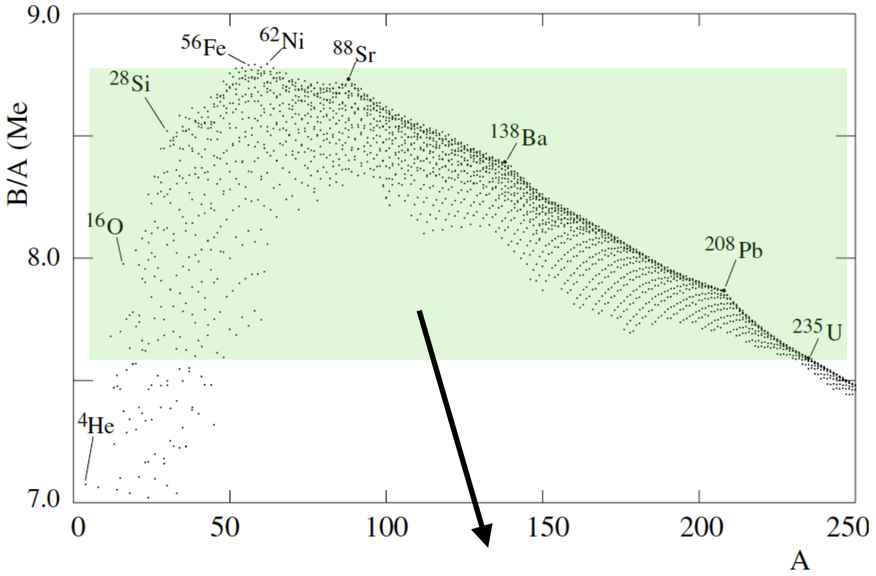
$E_{rot}(I) = \frac{\hbar^2}{2\zeta} I(I+1)$

$E_{vib}(I) = n(\hbar\omega)$

Rotations **Vibrations**

The nucleus looks like a collective ensemble of particles

Binding energy per nucleon



Because the number of pairs that can be taken from *A* particles is A(A-1), one might expect a term proportional to A. The strong force has a very limited range, therefore, the number of pairs of particles that actually interact is roughly proportional to *A*

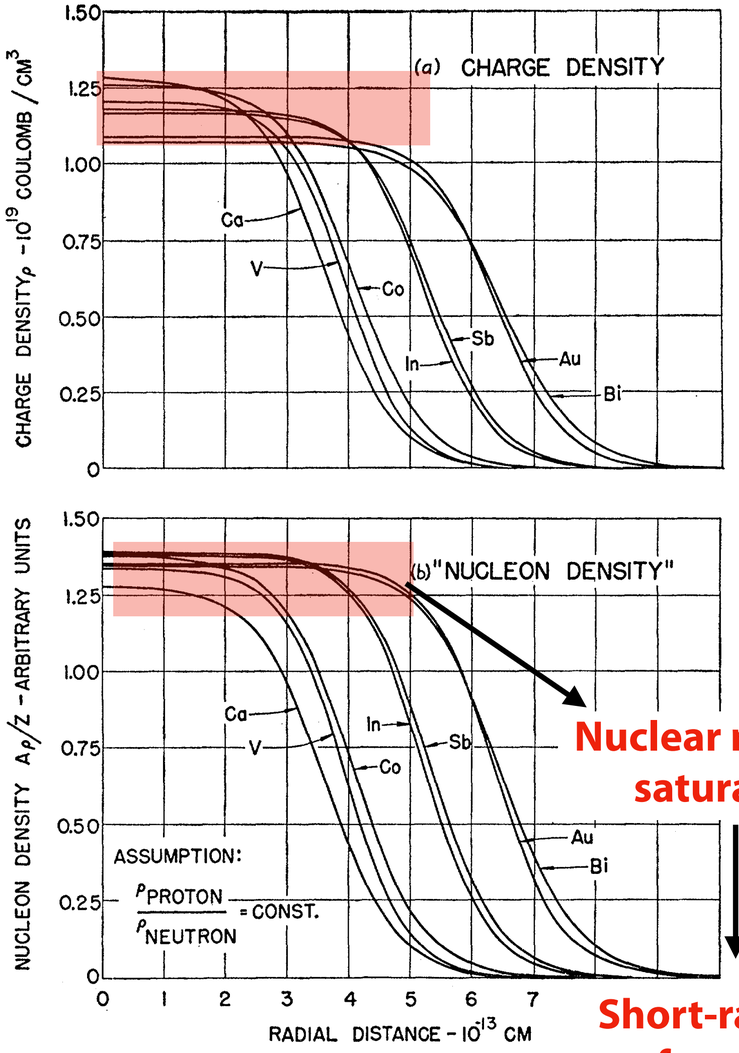
$R \sim A^{1/3} \rightarrow V \sim A$

$$E \simeq -\frac{1}{2} A(A-1)\langle U \rangle \frac{V_{nuc}}{V} \sim A$$

Binding energy goes like the volume (or A), at least at leading order..

© **Basdevant**, **Rich** and **Spiro**

Matter densities



Nuclear matter saturates

Short-range forces dominate

FIG. 14. (a) Charge distributions $\rho(r)$ for Ca, V, and Bi. They are Fermi smoothed uniform sha parameters given in Table III, and yield the cross in Figs. 3 and 8–12. (b) A plot of $(A/2Z)\rho(r)$ for the above nuclei. On the assumption that the distribution of matter in the nucleus is the same as the distribution of charge, this represents the "nucleon density."

© **Hofstadter**

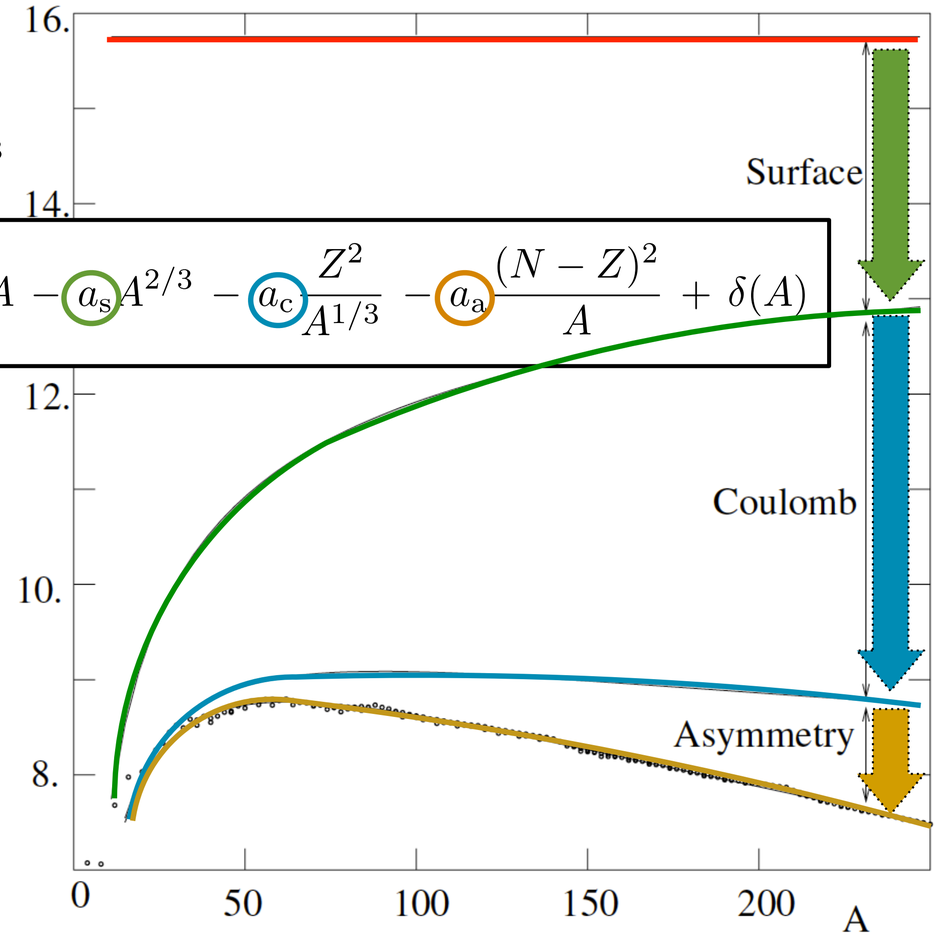
Liquid Drop Model (LDM) description

Think the nucleus as a drop of (incompressible) liquid with surface tension, where the competing processes produce a realistic binding energy ***B(A,Z)*** (Gamow, Bohr, Wheeler, Weizsäcker, Bethe,...)

$$R(\theta,\phi) = R_0\left(1+\sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\mu=\lambda}\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)\right)$$

$$R = R_0 A^{1/3}$$

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



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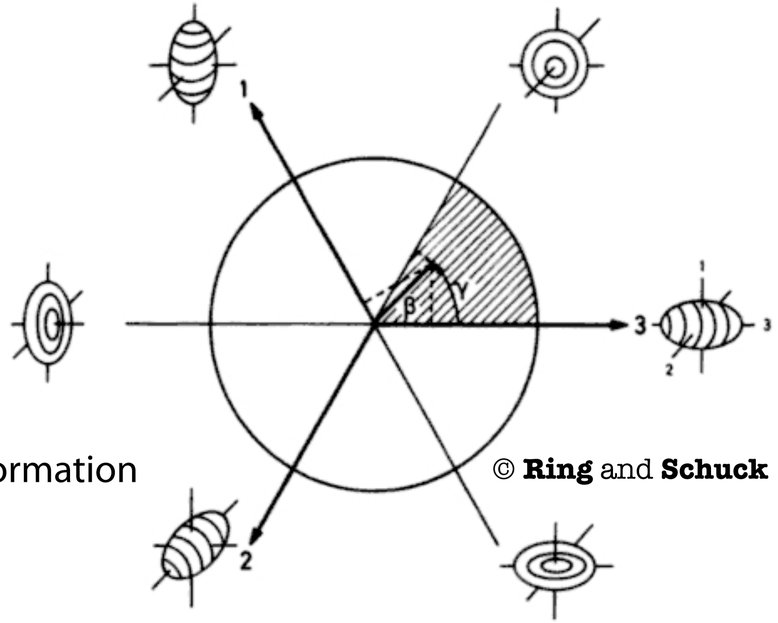
Volume

$\lambda = 0$ Compression

$\lambda = 1$ CoM translation

$\lambda = 2$ Quadrupole deformation



© **Ring** and **Schuck**

$$\alpha_{22} = \alpha_{2-2} = \beta \sin\gamma/\sqrt{2}$$

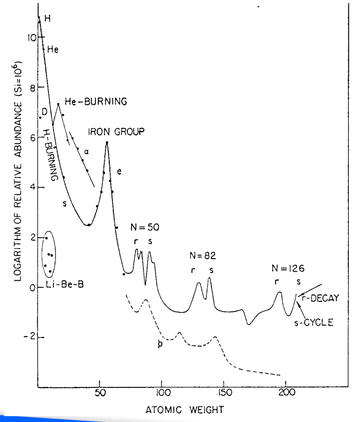
$$\alpha_{20} = \beta\cos\gamma$$

can be useful for collective motions, fission barriers,…

More experimental data - Evidences of single particle motion

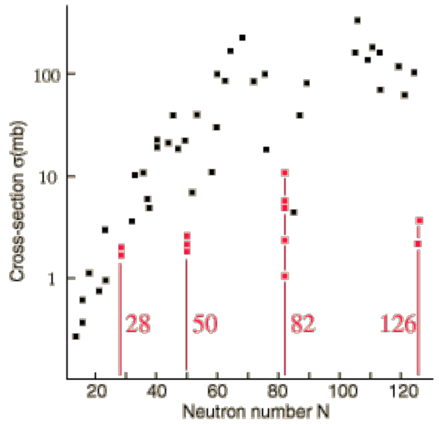
traces of magicity…

1. **Enhanced abundance** of elements for which Z or N is a magic number.
2. The **stable elements at the end** of the naturally occurring radioactive series have a "magic number" of neutrons or protons.
3. The **neutron absorption cross-sections** for isotopes where N = magic number are much **lower** than surrounding isotopes.
4. The **binding energy for the last neutron** is a **maximum** for a magic neutron number and drops sharply for the next neutron added.
5. The **excitation energy** from the ground nuclear state to the first excited state is **greater** for closed shells.
6. **Activation energy** for nuclear fission
7. **Deviations respect to LDM predictions**

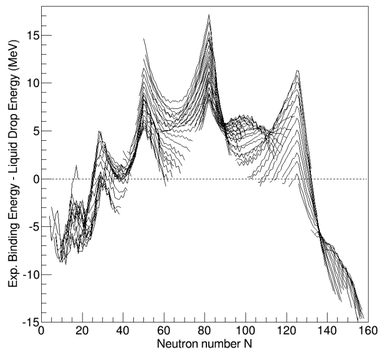


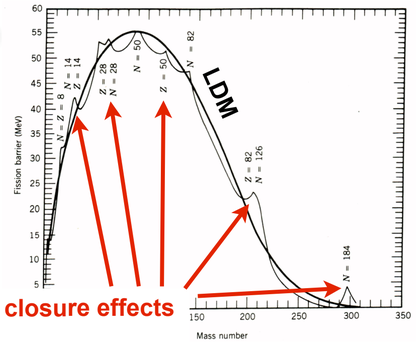
The Four Radioactive Series

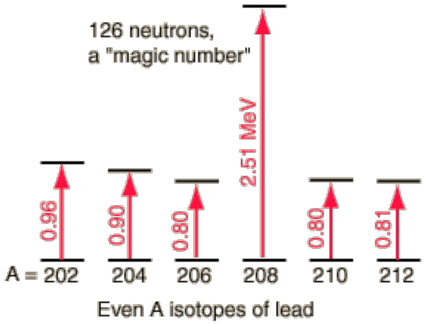
Series	Parent Lifetime	First Decay	End Product
Thorium	^{232}Th 1.40 x 10^{10}y	^{232}Th -> ^{228}Ra + a	^{208}Pb
Neptunium	^{237}Np 2.14 x 10^{6}y	^{237}Np -> ^{233}Pa + a	^{209}Bi
Uranium	^{238}U 4.17 x 10^{9}y	^{238}U -> ^{234}Th + a	^{206}Pb
Actinium	^{235}U 7.04 x 10^{8}y	^{235}U -> ^{231}Th + a	^{207}Pb

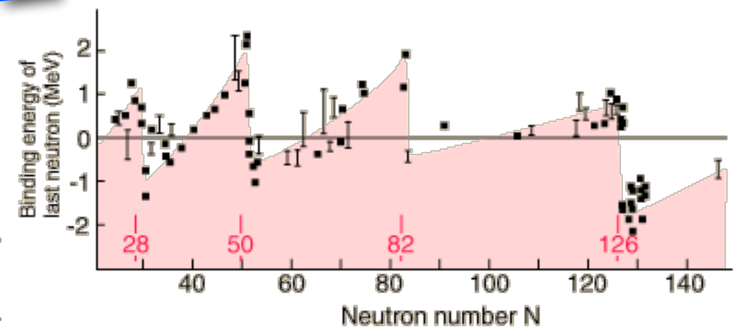


Nuclei with magic numbers of neutrons have neutron absorption cross-sections up to two orders of magnitude less than other nuclei with similar masses

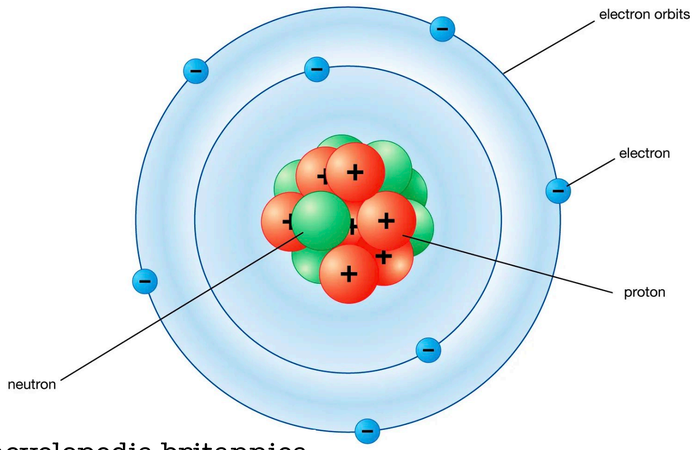








Independent particle motion



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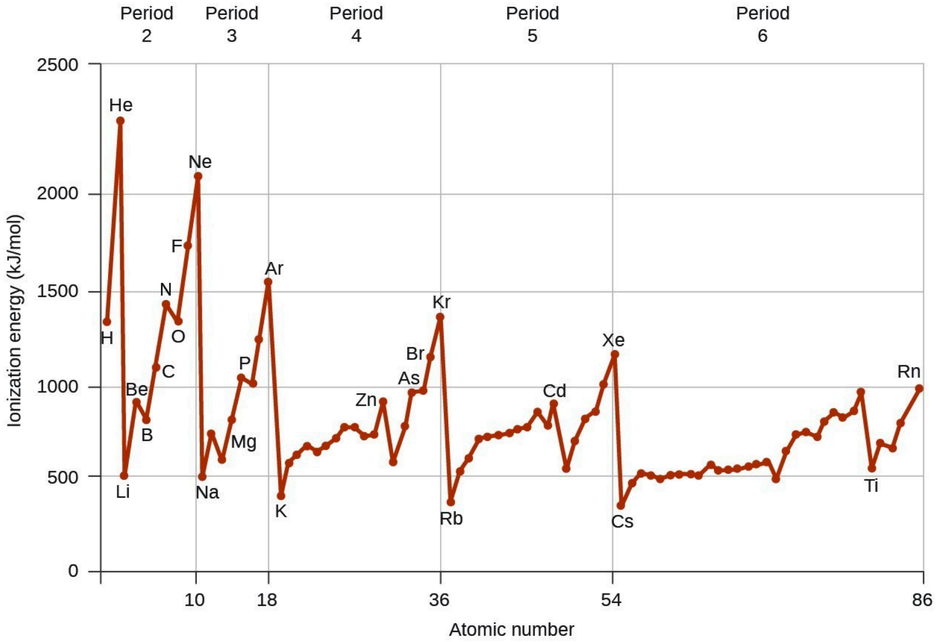
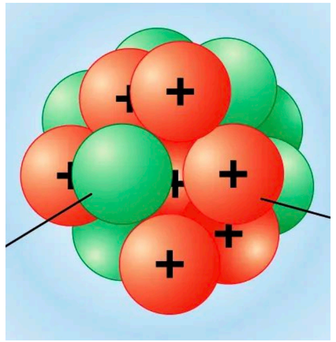
In atomic systems we clearly observe, i.e. for the ionisation energy, a clear pattern suggesting shell closures and single particle behaviours…



…but atoms are bound by the positive electric charge at its own center and *e-e* interaction can be treated perturbatively, since ***α=1/137***

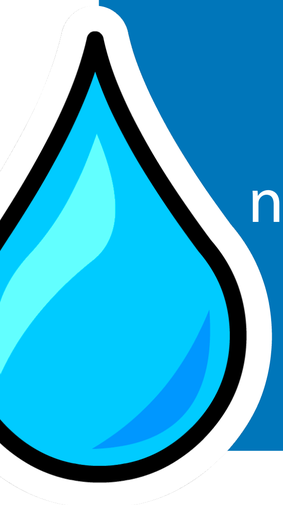
Nuclei are completely different!
Because they are **self-bound** and strong forces at low-energy can not be treated perturbatively



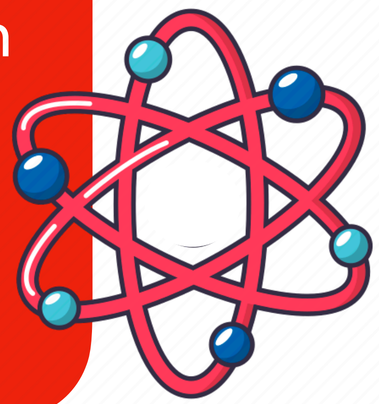
- Does it make sense talking about orbits?
- In particular with strong forces?
- Does it even make sense consider nucleons as point-particles?

LDM vs. Single Particle picture

The nucleus as a drop of incompressible liquid with no nucleonic degrees of freedom



Nucleons keep their own identities and moves in stationary orbits (nucleus ~ bunch of individual nucleons)



1. What is the **mean free path** when a nucleon moves through the nucleus?

2. How can the independent particle motion survive in the presence of the very strong, short-range, and complicated forces that act between each pair of nucleons?

A short digression on the nucleon mean free path

- Let's assume that an incoming neutron scatter towards a nucleus target. Depending on the energy it has a certain probability of colliding with one of the target nucleons.

TRANSMUTATIONS OF ATOMIC NUCLEI

By Professor NIELS BOHR

INSTITUTE OF THEORETICAL PHYSICS, UNIVERSITY OF COPENHAGEN

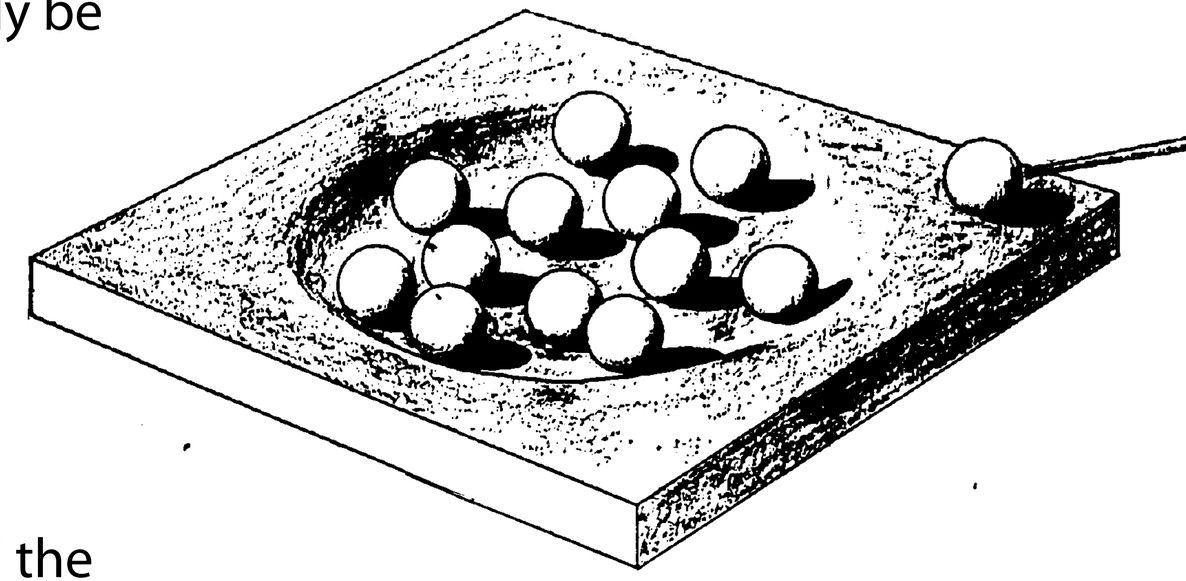
- Already the first collision implies a sharing of the energy of the incident neutron with the target nucleon so it will unlikely be able to escape from the nuclear binding field

($\mathbf{a}$: range of NN interaction)

$\boldsymbol{\rho} = 0.17$ nucleons/fm^3

$\mathbf{a} \sim 1$ fm $\rightarrow \boldsymbol{\sigma} = \mathbf{2\pi a^2} \sim 6$ fm^2

$$\lambda \sim 1/(\rho\sigma) \sim 1 \text{ fm} < R_{nuc}$$

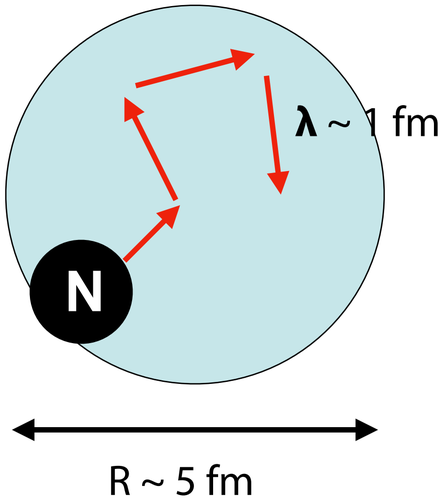


https://www.jstor.org/stable/1664129

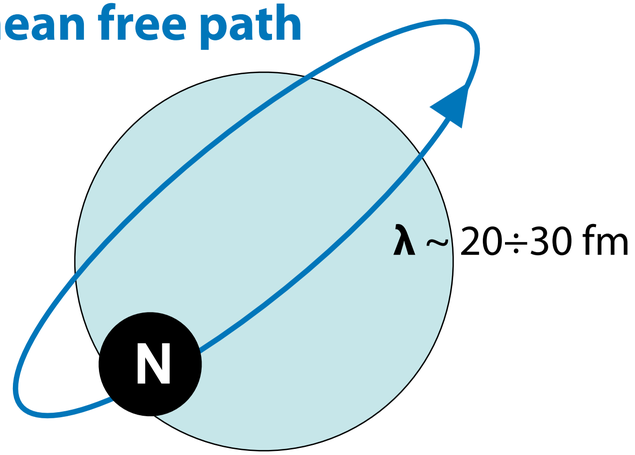
- Subsequent collisions between the incident neutron and the excited nucleons of the target will lead to a complicated state of motion which Bohr called the *compound nucleus* - a state in which the excitation energy is distributed statistically among all the available degrees of freedom of the composite system.

Nucleon mean free path

Short mean free path



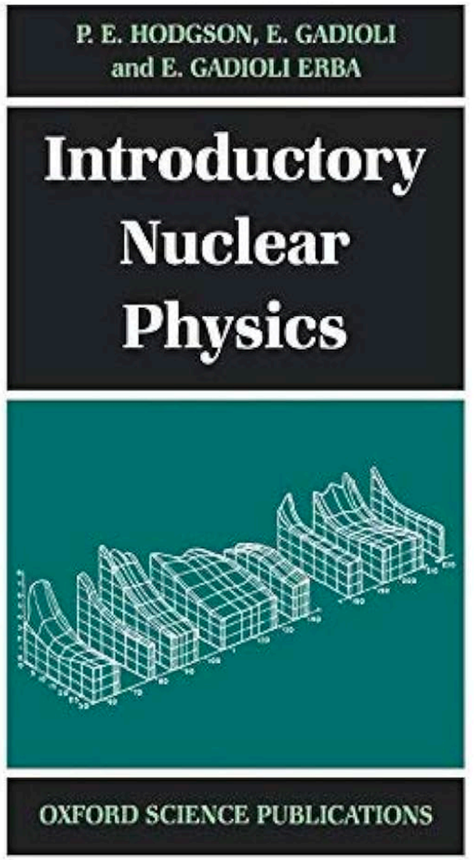
Long mean free path

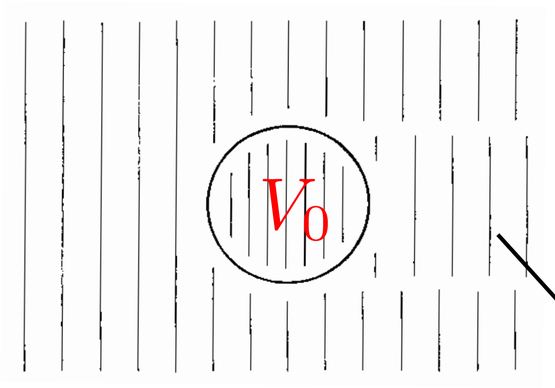


The successes of the collective model which assumes the nucleons to be strongly interacting and of the shell model which assumes that they move independently in an overall potential raise the question of the relationship between the two models.

What are the nucleons actually doing?

<u>It is not possible for them to be both strongly interacting and not interacting at all</u>. We know the cross-section for the interaction of two free nucleons, and this gives a mean free path that is far too short to be compatible with independent motion inside the nucleus. We can accept that different models should reflect different aspects of the nucleus, but they should be consistent with one another (Pag. 315)





The mean free path for a nucleon moving through a target nucleus can be directly measured in scattering experiments. An incident wave will be accelerated on entering the target, because of the nuclear attraction, and will then have a somewhat shorter wave length while inside the nucleus

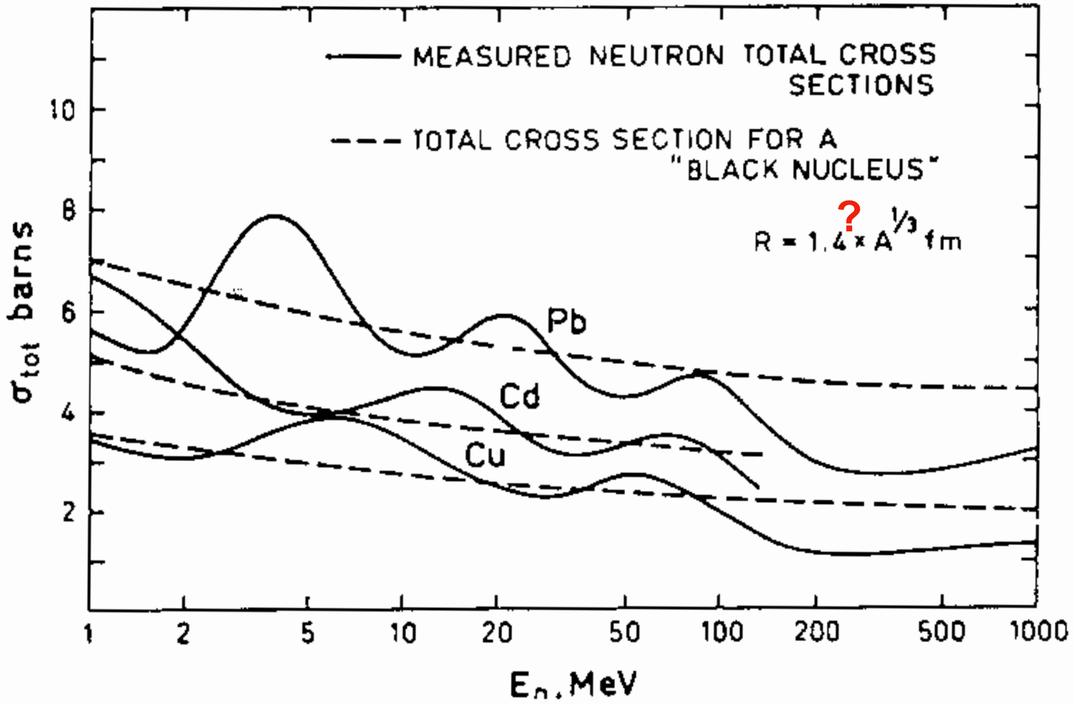
$$K_{in} = \sqrt{K_{out}^2 + \frac{2MV_0}{\hbar^2}}$$

Phase shift

$$\delta \sim (K_{in} - K_{out}) \times \ path$$

The interference between the transmitted and incident wave will give rise to oscillations in the cross section as a function of energy. The phase shift is a decreasing function of energy and an increasing function of the nuclear size (which determines the path length), and thus the maxima and minima in the cross sections shift to lower bombarding energies with increasing nuclear size.

$$K_{in} = \sqrt{K_{out}^2 + \frac{2MV_0}{\hbar^2}} + \frac{i}{2\lambda}$$



$V_0 = 50$ MeV

$\lambda = 30$ MeV $\gg R_{nuc}$

The mean free path is long compared to the nuclear size for a nucleon with energy close to the Fermi energy, in agreement with the evidence for shell structure in the nuclear spectra, but in striking disagreement with Bohr's assumption

© **Bohr** and **Mottelson**, Nuclear Structure: single-particle motion

Common wisdom

How can the independent particle motion survive in the presence of the very strong, short-range, and complicated forces that act between each pair of nucleons?

"The text books and literature agree with near total unanimity that the answer to this question is provided by the effects of the Pauli principle and the Fermi distribution. When two particles within the Fermi distribution interact, they cannot be scattered into states that are near-lying in energy and momentum because such final states are already occupied."

Ben Mottelson

$$P_{cl} d\boldsymbol{r}_1 d\boldsymbol{r}_2 = \rho(1)\rho(2) d\boldsymbol{r}_1 d\boldsymbol{r}_2 = \sum_m |\phi_m(1)|^2 d\boldsymbol{r}_1 \sum_n |\phi_n(2)|^2 d\boldsymbol{r}_2$$

$$P_F d\boldsymbol{r}_1 d\boldsymbol{r}_2 = \frac{1}{2} \sum_m \sum_n |\phi_m(1)\phi_n(2) - \phi_m(2)\phi_n(1)|^2 d\boldsymbol{r}_1 d\boldsymbol{r}_2$$

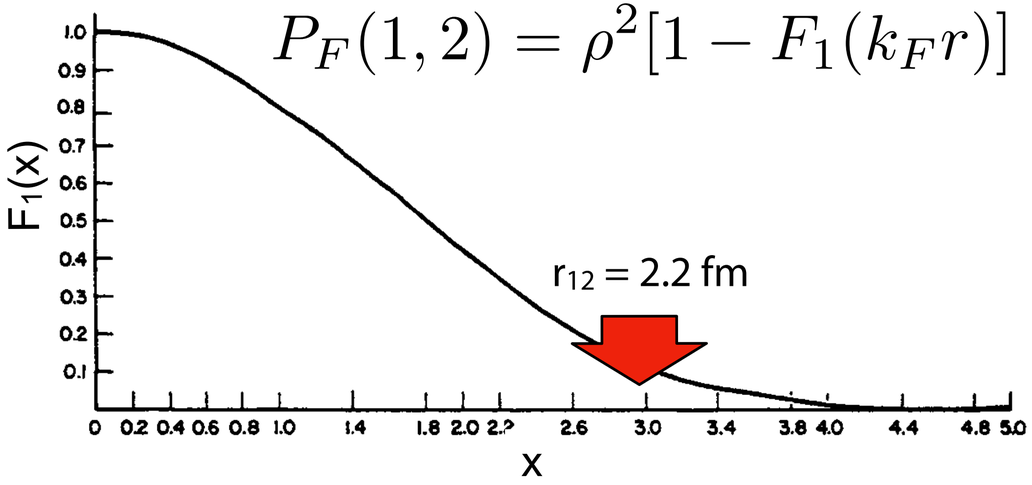
Pauli correlation

$$P_F - P_{cl} = -C^2(1,2) = -|\sum_m \phi_m(1)\phi_m^*(2)|^2$$

In nuclear matter, for uniform systems

$$\sum_m \phi_m(1)\phi_m^*(2) = \frac{4\pi}{(2\pi)^3} \int_0^{k_F} j_0(kr) k^2 dk = \frac{1}{2\pi^2} k_F^3 \frac{j_1(k_F r)}{k_F r}$$

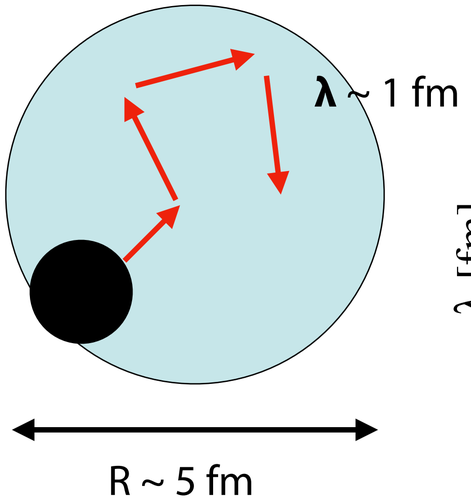
$$P_F(1,2) = \rho^2 [1 - F_1(k_F r)]$$



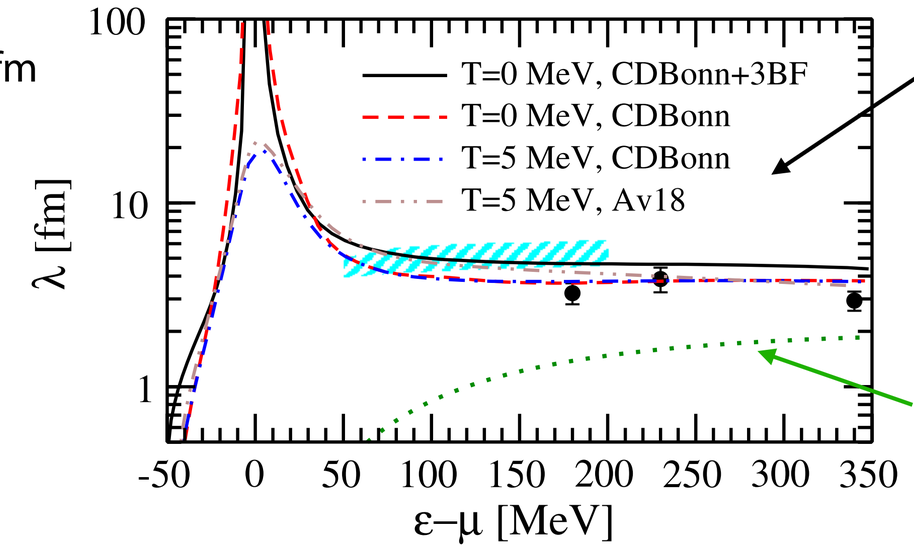
© **Praeston** and **Bhaduri**, Structure of the Nucleus

Nucleon mean free path again

Short mean free path



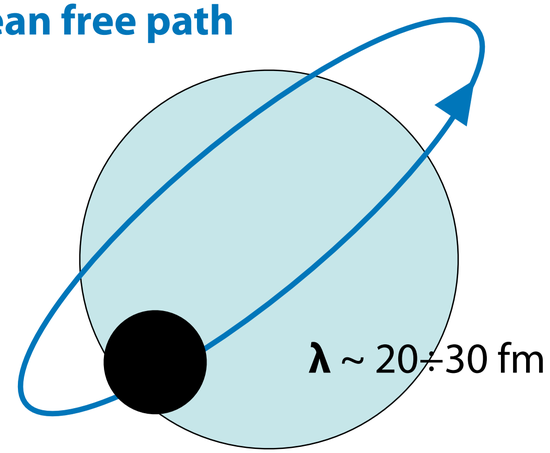
Mean free path of a nucleon in nuclear matter



It flattens at high energies, and remain constant, at a value of around 4–5 fm.

The kinetic theory prediction λ ~ 1/(ρσ) is well below all theoretical predictions

Long mean free path



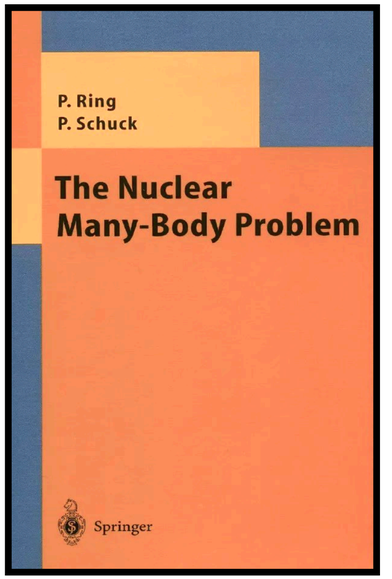
The mean free path is long compared to the nuclear size for a nucleon with energy close to the Fermi energy, in agreement with the evidence for shell structure in the nuclear spectra, but in striking disagreement with Bohr's assumption

the conclusion is inescapable… that nuclei are a nearly collisionless gas rather than a short-mean-free-path liquid drop

(S. Koonin)

Somà and **Rios**, Self-Consistent Green's Function Calculation of the Nucleon Mean Free Path

The nuclear many-body problem



For a system of $A = N + Z$ particles

$$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

Full Hamiltonian

(kinetic + many-body contributions)

Fully correlated state

for each state *n*

$\langle \boldsymbol{r} | \Psi_n \rangle$

Full A-body wave function

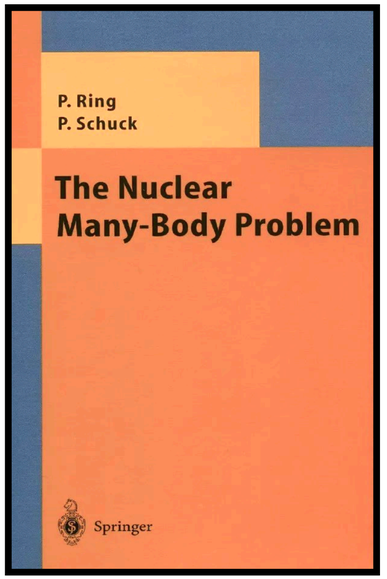
A-body energy spectrum

Ground (*n=0*) and excited states energy spectrum

The nuclear many-body problem (ii)

For a system of $A = N + Z$ particles

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$



Formal manipulation

$$\hat{H} = \hat{T} + \hat{V}_{2b} + \hat{V}_{3b} + \dots$$

Kinetic energy

Two- and three-body potential

$$\hat{T} = \sum_{i=1}^{A} \frac{\hat{\boldsymbol{p}}_i^2}{2m_i}$$

$$\sum_{i<j}^{A} \hat{V}_{2b}(\boldsymbol{r}_i, \boldsymbol{r}_j) + \sum_{i<j<k}^{A} \hat{V}_{3b}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k)$$

Nucleon-nucleon potential: phenomenology

Constraints due to **rotational invariance**, **invariance under parity**, **time reversal invariance**, **hermiticity** and **invariance with respect to nucleon labels**

$$\left\{\mathbf{1}_{\rm spin},\ \vec{\sigma}_1\cdot\vec{\sigma}_2,\ S_{12}(\vec{r}),\ S_{12}(\vec{p}),\ \vec{L}\cdot\vec{S},\ (\vec{L}\cdot\vec{S})^2\right\}\times\{\mathbf{1}_{\rm isospin},\ \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\}$$

or, in momentum space,

$$\left\{\mathbf{1}_{\rm spin},\ \vec{\sigma}_1\cdot\vec{\sigma}_2,\ S_{12}(\vec{q}),\ S_{12}(\vec{k}),\ i\vec{S}\cdot\vec{q}\times\vec{k},\ \vec{\sigma}_1\cdot\vec{q}\times\vec{k}\,\vec{\sigma}_2\cdot\vec{q}\times\vec{k}\right\}\times\{\mathbf{1}_{\rm isospin},\ \boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\}$$

NN potentials can be decomposed as follows

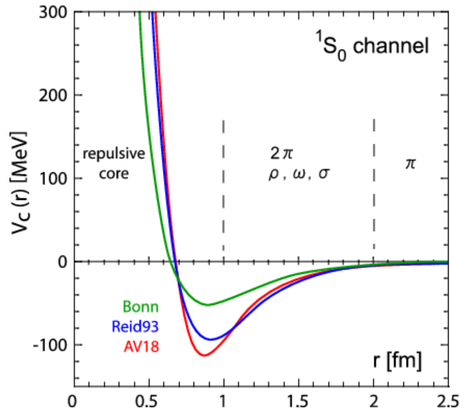
$$V_c(r)=V_0(r)+V_\sigma(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2+V_\tau(r)\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2+V_{\sigma\tau}(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2$$ central

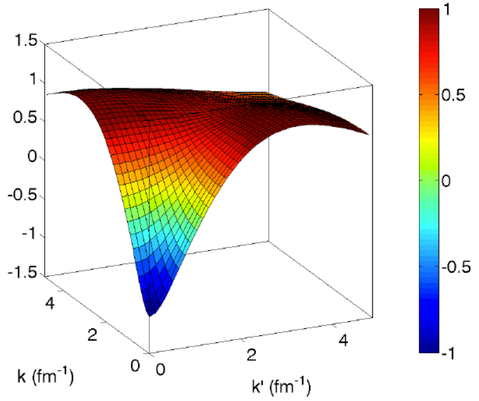
$$V_T(r)=[V_T(r)+V_{T\tau}(r)]S_{12}(\hat{r})$$ tensor

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

$$V_{LS}(r)=V_{LS0}\boldsymbol{L}\cdot\boldsymbol{S}$$ **spin-orbit**

Central potential





$$V_{L=0}(k,k')\propto\langle k|V_{L=0}|k'\rangle\propto\int d^3r\,j_0(kr)\,V(r)\,j_0(k'r)\implies V_{kk'}\ \text{matrix}$$

Tensor potential

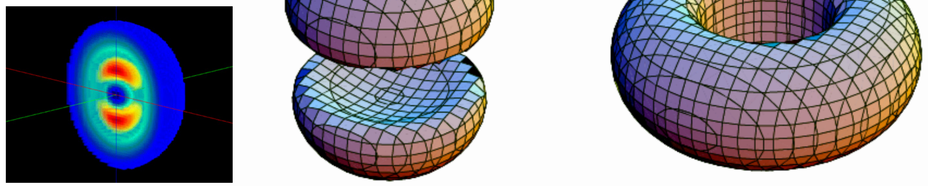
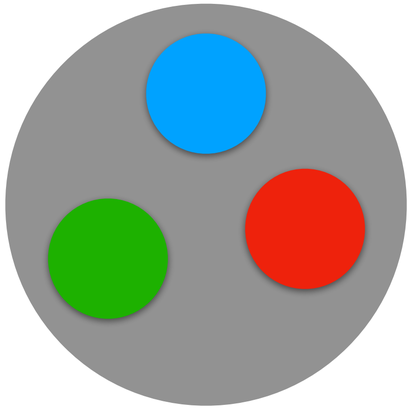
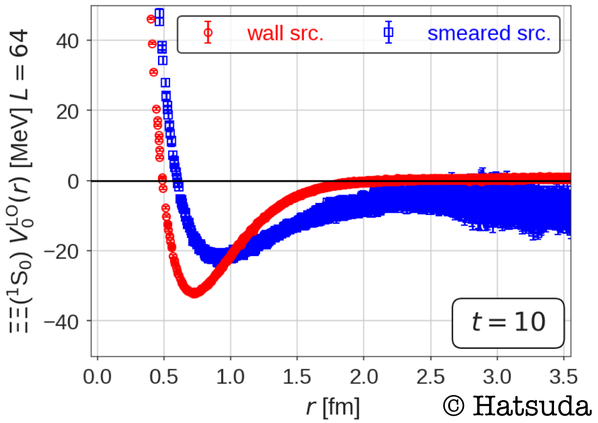


Figure 1.24: Surfaces of constant density in the deuteron ($\rho^{(2)}_{1M_S}=0.005\text{fm}^{-3}$) for $M_S=\pm1$ on the left and $M_S=0$ on the right. The plots are done for the Argonne V18 interaction.

Ring and **Schuck**, The Nuclear Many-Body Problem

Nucleon-nucleon potential: features





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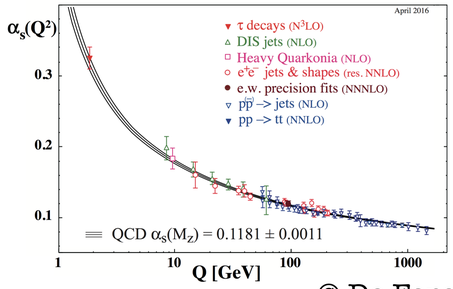

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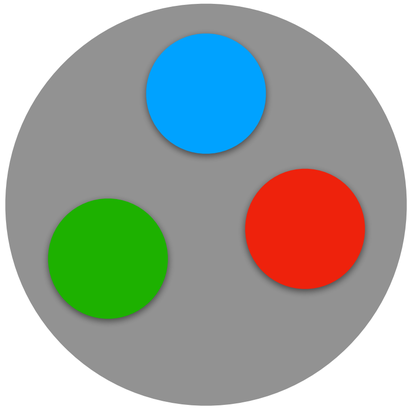
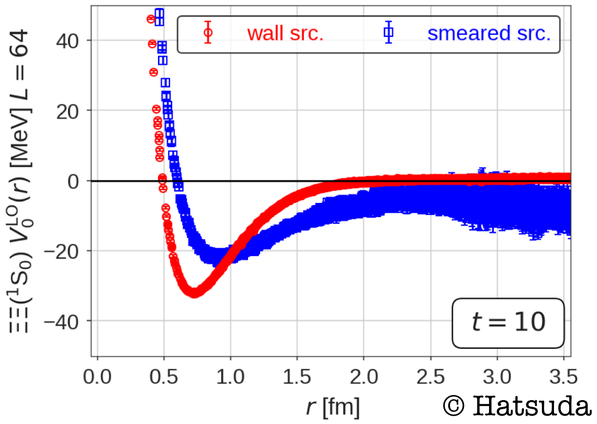
- In this energy regime, QCD is strictly **non-perturbative**

Nucleon-nucleon potential: features



$$F_p(Q^2) \approx \left(\frac{1}{1+(Q/800\,\mathrm{MeV})^2}\right)^2$$



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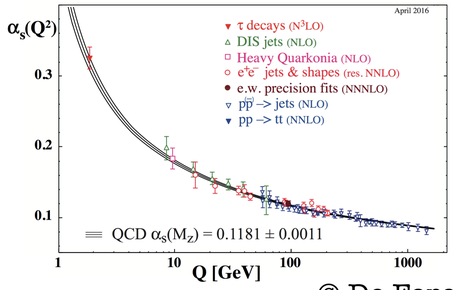

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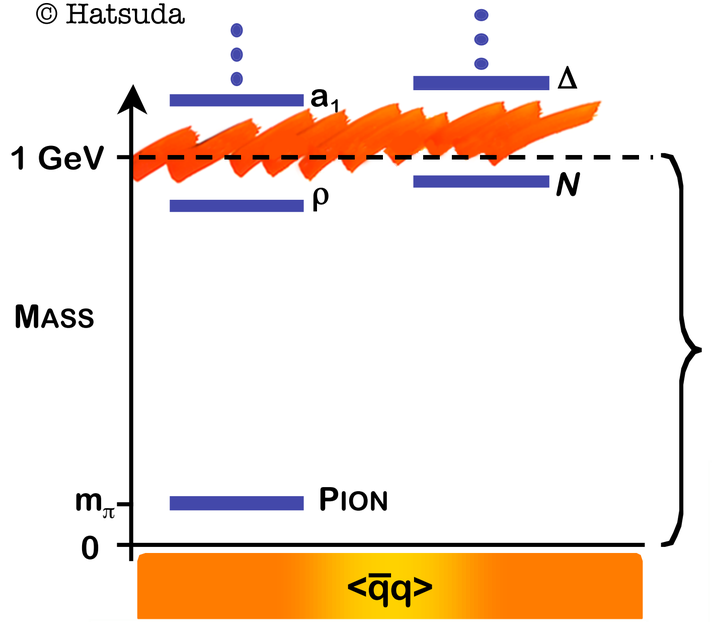
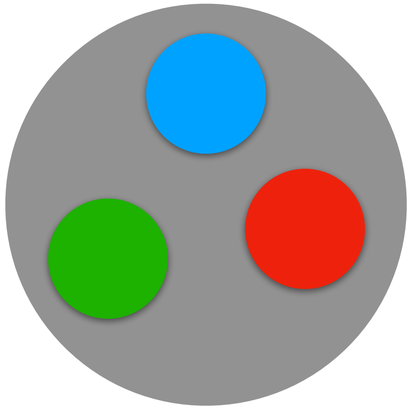


GAP

$\Delta = 4\,\pi\,f_\pi$

~ 1 GeV

Nucleon-nucleon potential: features



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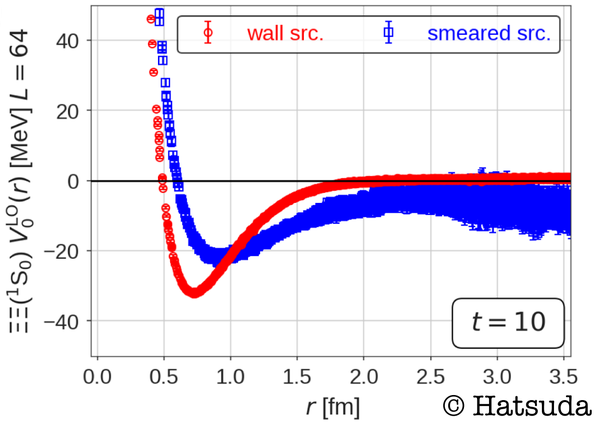

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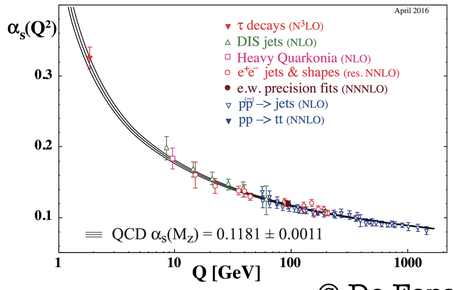

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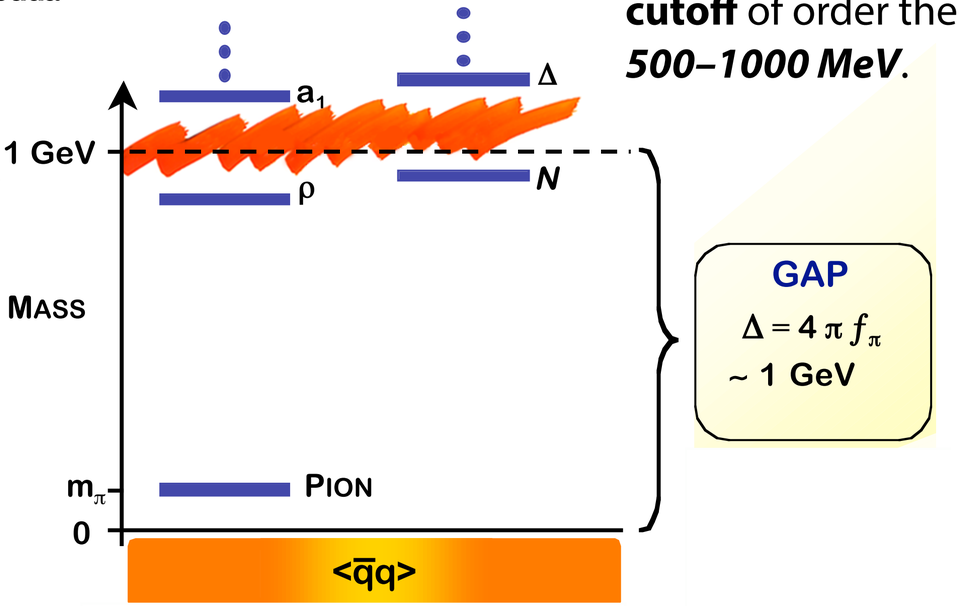
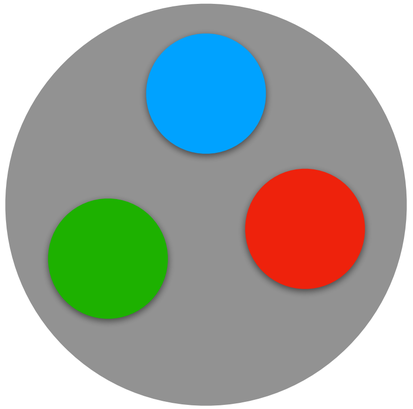
- It looks like an energy spectrum of a quantum systems exhibiting a **spontaneous symmetry breaking** pattern… **if pions would be massless**
- The broken symmetry is **chiral symmetry**
- $SU(2)_R$ X $SU(2)_L$ or $SU(2)_V$ X $SU(2)_R$ ➡ $SU(2)_V$
- Pions are massive since the symmetry is also explicitly broken by quark masses (GOR relation)



Nucleon-nucleon potential: features



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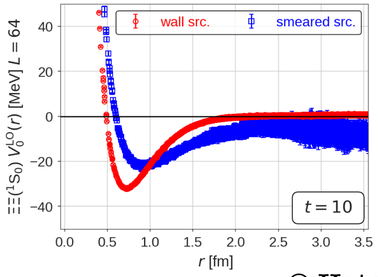

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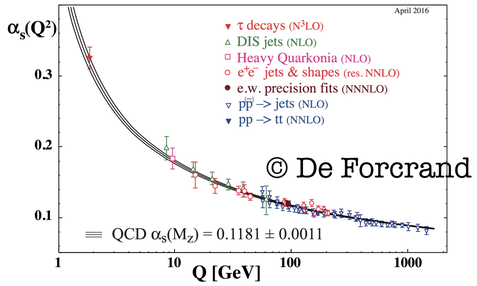

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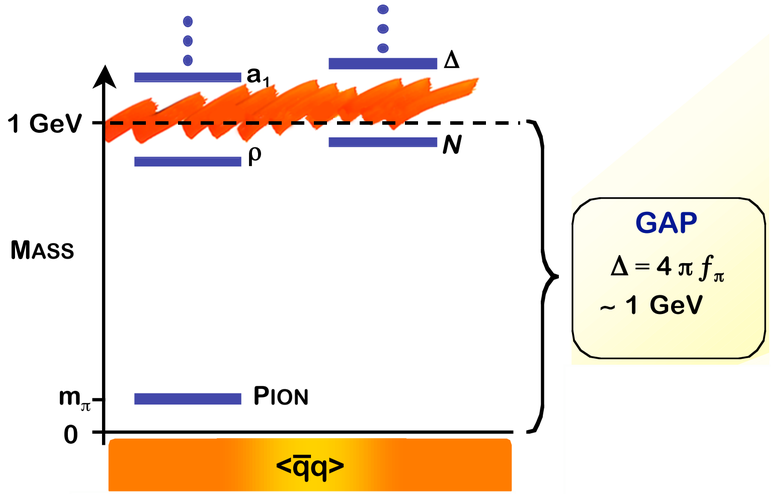

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- Our effective theory, therefore, should have a **cutoff** of order the color resolution scale, ***Λc ≈ 500–1000 MeV***.
- Heavy hadrons, like the proton, neutron, Δ, ρ, and so on, have masses of order the cutoff or larger and so cannot be relativistic. These are most efficiently treated as **pointlike nonrelativistic particles**

*For low energy processes it's enough to consider **explicit long-range** dynamics and **simplified (contact)** interactions for the **short range** part*

Weinberg, Phenomenological Lagrangians

(**don't forget symmetries!!**)

Nucleon-nucleon potential: modern point of view

1. Identify the soft and hard scales and the appropriate degrees of freedom: **pions** and **nucleons**
2. Identify the relevant **symmetries** of low-energy QCD and investigate if and how are broken
3. Construct the **most general Lagrangian** consistent with symmetry and symmetry breaking patterns
4. Design a computational scheme, i.e. a low-momentum expansion (**power counting**)

At first order

$$\mathcal{L}_{\pi N}^{(1)} = \bar{N}\left(i\gamma^\mu D_\mu - m + \frac{g_A}{2}\gamma^\mu\gamma_5 u_\mu\right) N$$

$$-\frac{1}{4f_\pi^2}(\bar{\Psi}\gamma_\mu\vec{\tau}\Psi)\cdot\left(\vec{\Phi}\times(\partial^\mu\vec{\Phi})\right) \qquad +\frac{1}{2f_\pi}(\bar{\Psi}\gamma_\mu\gamma_5\vec{\tau}\Psi)\partial^\mu\vec{\Phi}$$

Weinberg-Tomozawa coupling

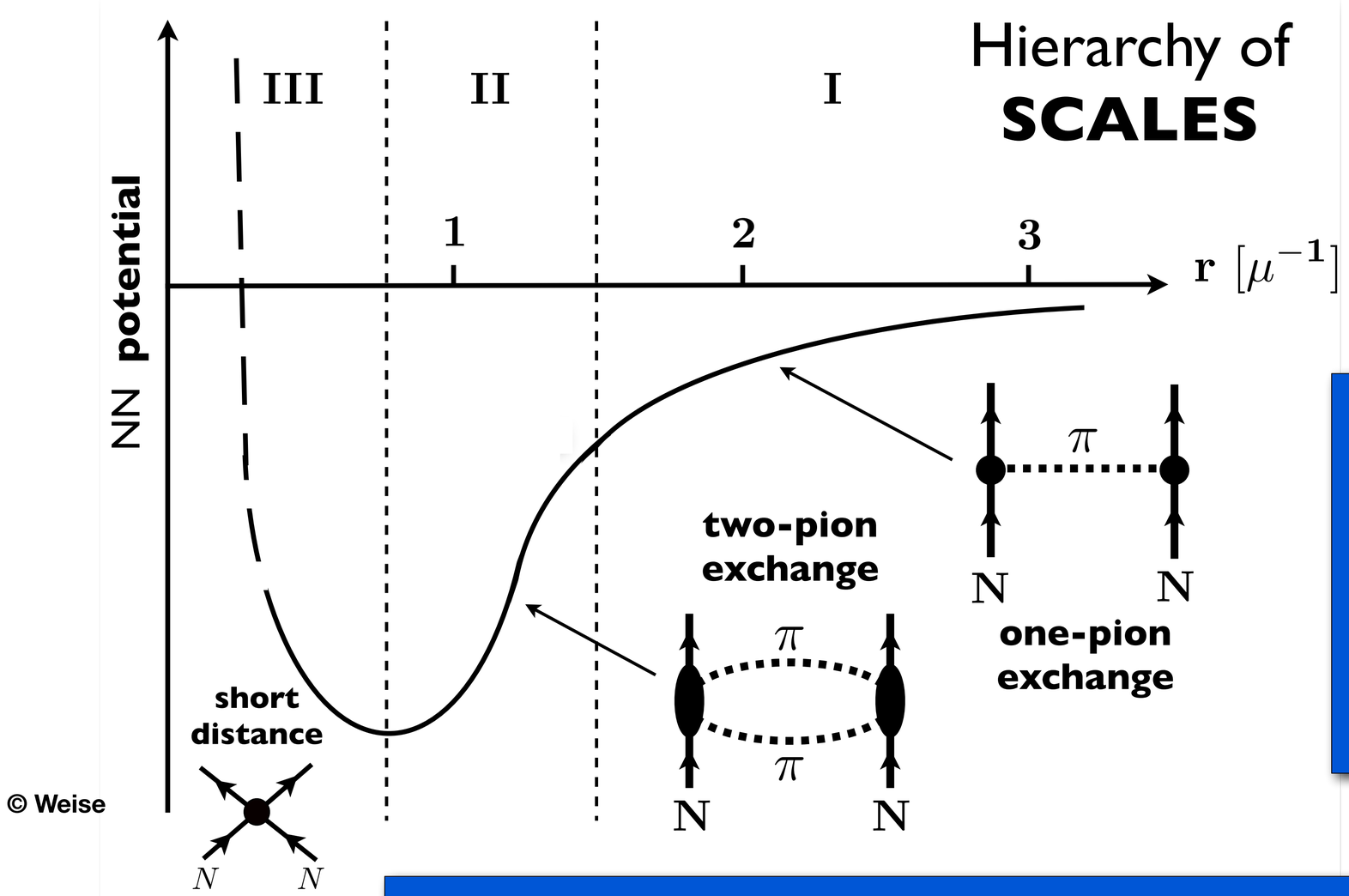
$$u_\mu \equiv iu^\dagger(\partial_\mu U)u^\dagger = -\frac{\boldsymbol{\tau}\cdot\partial_\mu\boldsymbol{\pi}}{F} + \mathcal{O}(\boldsymbol{\pi}^3)$$

$$D_\mu N \equiv (\partial_\mu + \Gamma_\mu)N\,, \quad \text{with} \quad \Gamma_\mu \equiv \frac{1}{2}\left(u^\dagger\partial_\mu u + u\partial_\mu u^\dagger\right) = \frac{i}{4F^2}\boldsymbol{\tau}\cdot\boldsymbol{\pi}\times\partial_\mu\boldsymbol{\pi} + \mathcal{O}(\boldsymbol{\pi}^4)$$

$$\frac{Q}{\Lambda_\chi} \quad \frac{\text{Soft scale } (p_\pi,\, m_\pi)}{\text{Hard scale } (\Lambda\sim 4\pi f_\pi,\, M_N)}$$

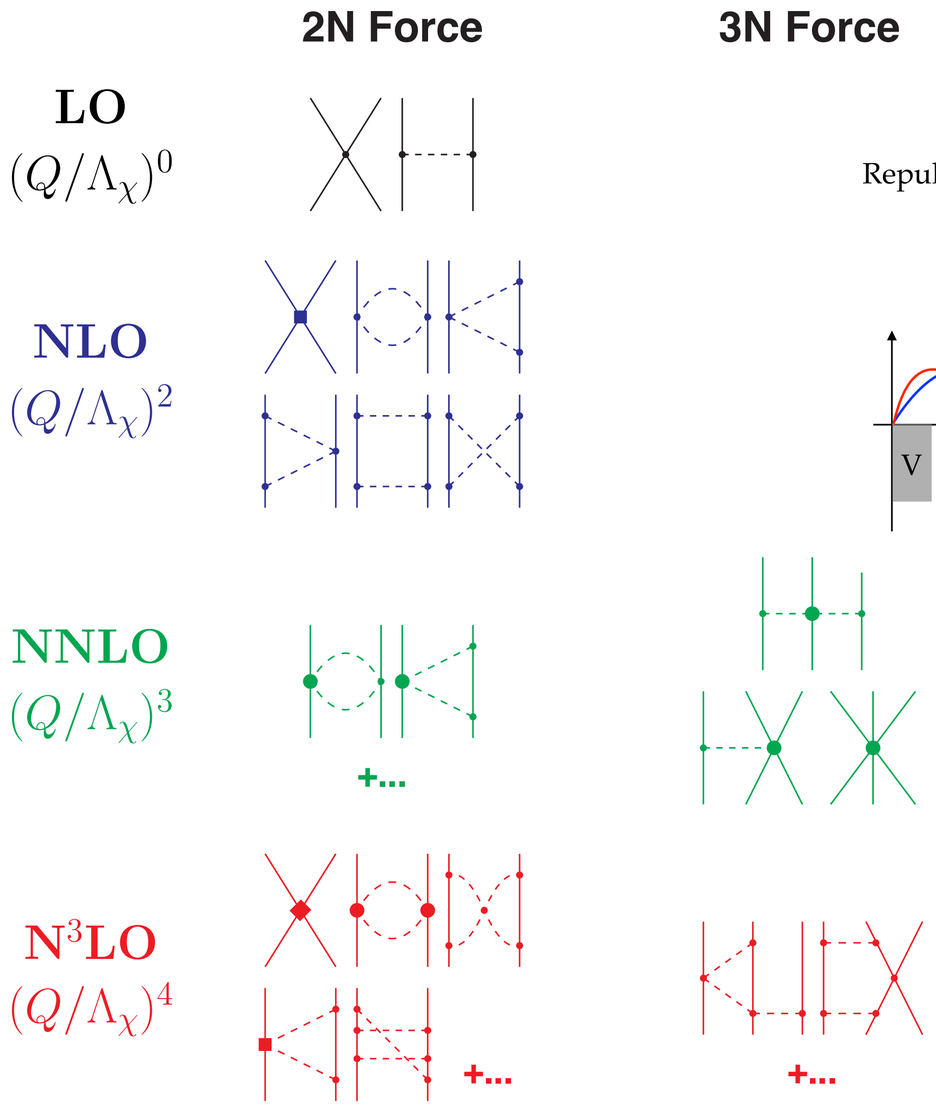
Contrary to the pion mass, the nucleon mass does not vanish in the chiral limit and introduces an **additional** hard **scale** in the problem

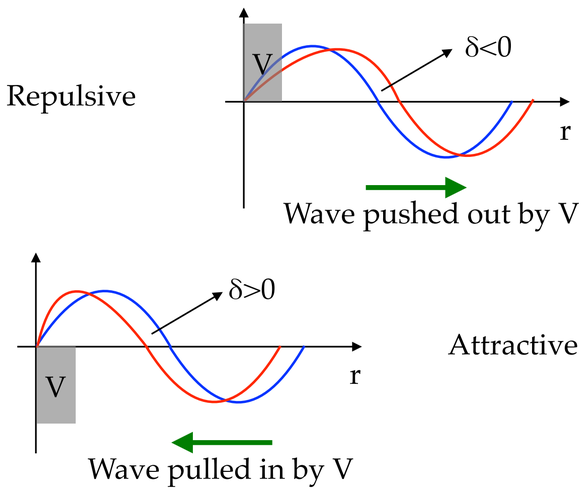
Nucleon-nucleon potential: modern point of view

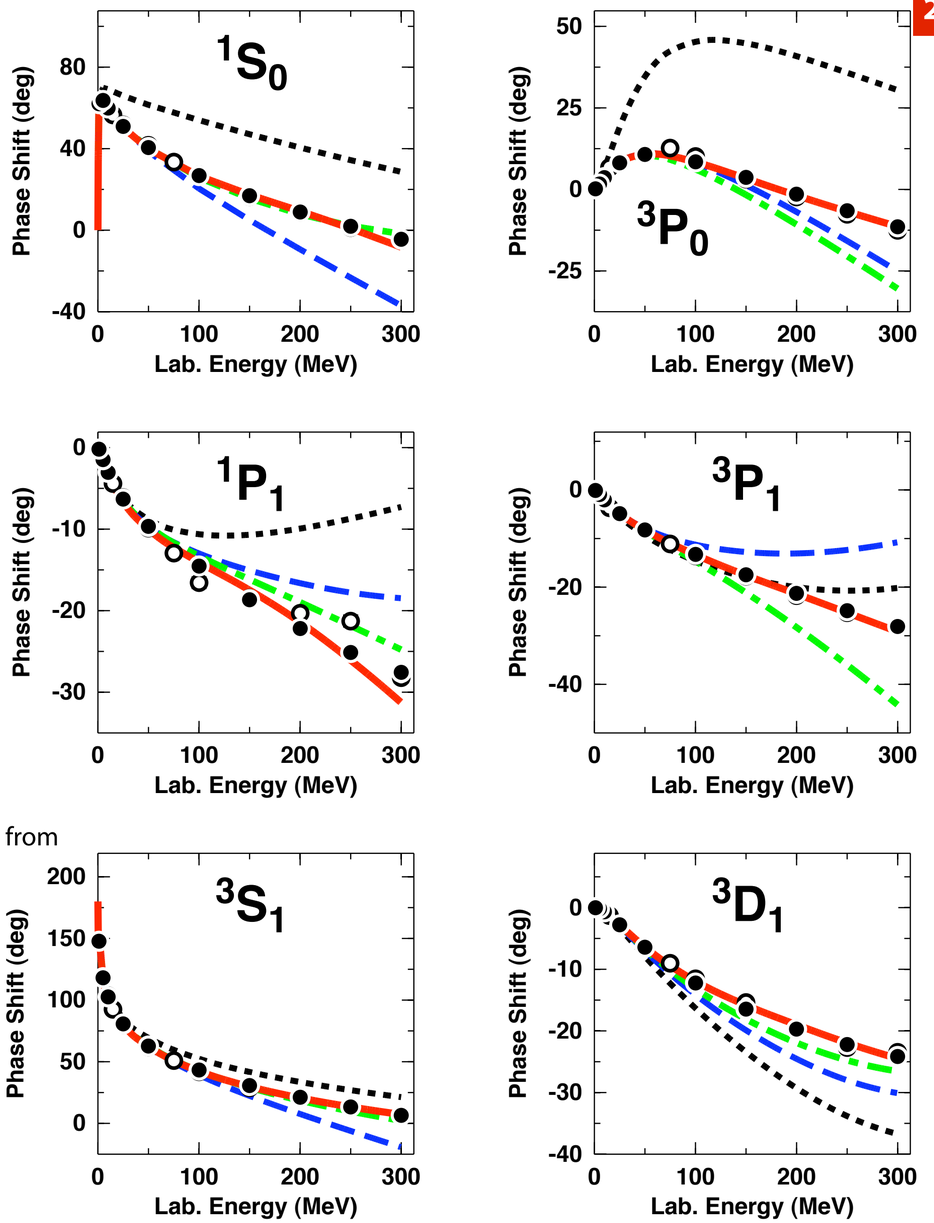


The nuclear force at large distances is governed by the exchange of one or multiple pions. This **long-range part** of the nuclear force is strongly constrained by the chiral symmetry of QCD

The **short-range** part of the nuclear force is driven by physics not resolved explicitly in reactions with typical nucleon momenta of the order of $M_\pi c$. It can be mimicked by zero-range contact interactions with an increasing number of derivatives.







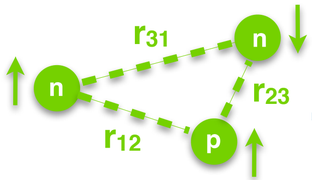
Phase shifts of np scattering as calculated from NN potentials at different orders of ChPT.

LO
NLO
NNLO
N3LO

Lectures and code on FRIB-TA Summer School
(https://github.com/fribtascattering/fribtascattering.github.io

R. **Machleidt** et al, Chiral effective field theory and nuclear forces, Phys. Rep. 503 (2011) 1-75
E. **Epelbaum** et al, Modern Theory of Nuclear Forces, Rev. Mod. Phys. 81 (2009) 1773-1825

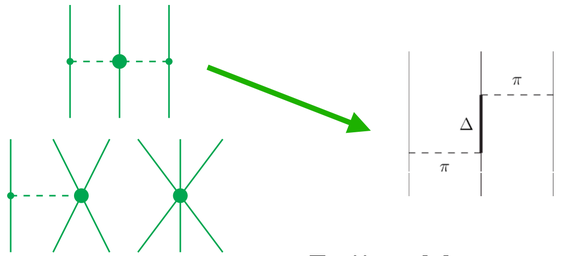
Do we really need three-body forces?



Theoretical argument

In the commonly accepted description of the NN interaction, **Chiral Perturbation Theory**, three nucleon forces (but also four-nucleon, five-nucleon,…) naturally arise.

NNLO
$(Q/\Lambda_\chi)^3$



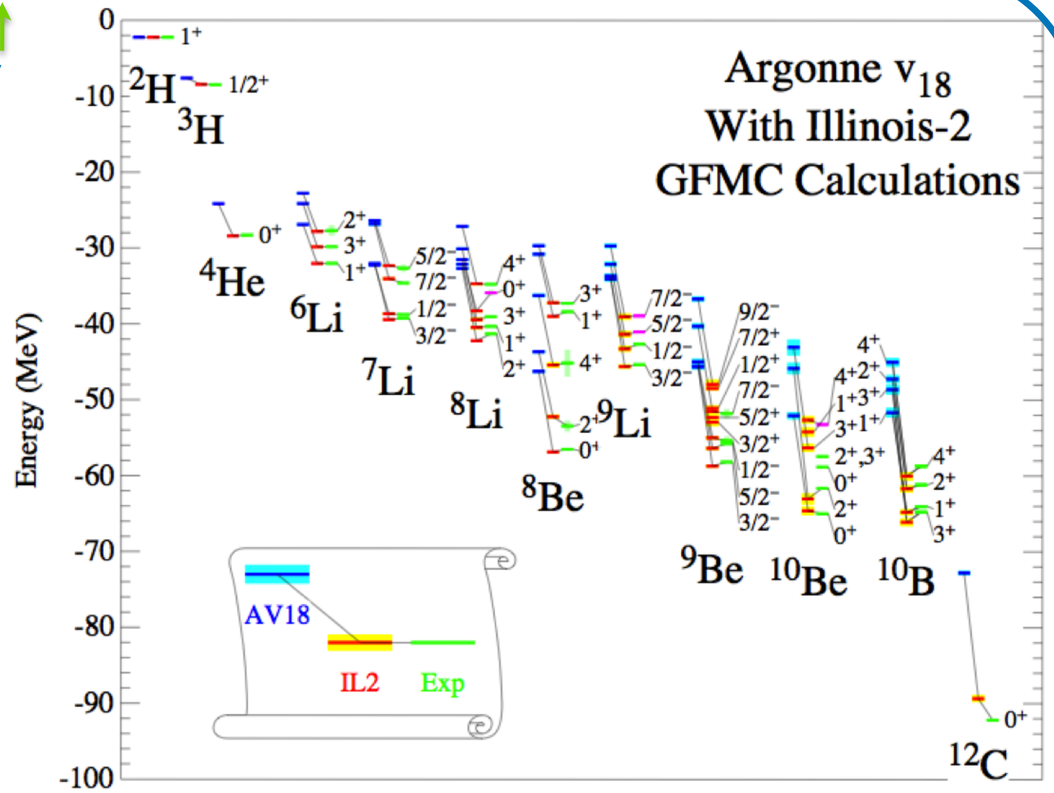
Fujita-Myazawa

N^{3}LO
$(Q/\Lambda_\chi)^4$

+…

+…

Computational argument

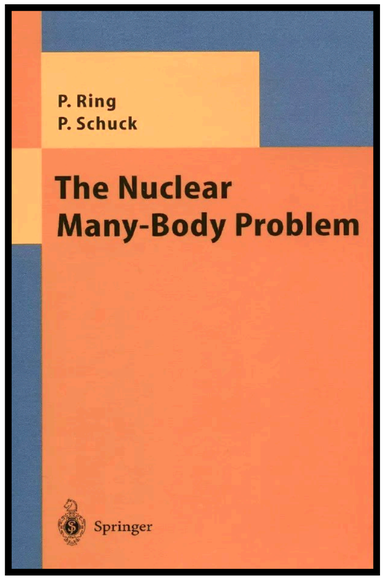


- NN potentials already reproduces 2-body with a χ2/datum ≃1
- Almost exhausted operator structure

But this is not the end of the story, strength can be shifted from 2-body matrix elements to 3-body…

The nuclear many-body problem (iii)

For a system of $A = N + Z$ particles $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$



Formal manipulation

$$\hat{H} = \hat{T} + \hat{V}_{2b} + \hat{V}_{3b} + \dots$$

Kinetic energy

$$\hat{T} = \sum_{i=1}^{A} \frac{\hat{\boldsymbol{p}}_i^2}{2m_i}$$

Two- and three-body potential

$$\sum_{i<j}^{A} \hat{V}_{2b}(\boldsymbol{r}_i, \boldsymbol{r}_j) + \sum_{i<j<k}^{A} \hat{V}_{3b}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k)$$

Add and subtract a 1-body potential U_{1b}

$$\hat{H} = \underbrace{\hat{T} + \hat{U}_{1b}}_{\hat{H}_0} + \underbrace{\left(\hat{V}_{2b} + \hat{V}_{3b} - \hat{U}_{1b}\right)}_{\hat{V}_{res}}$$

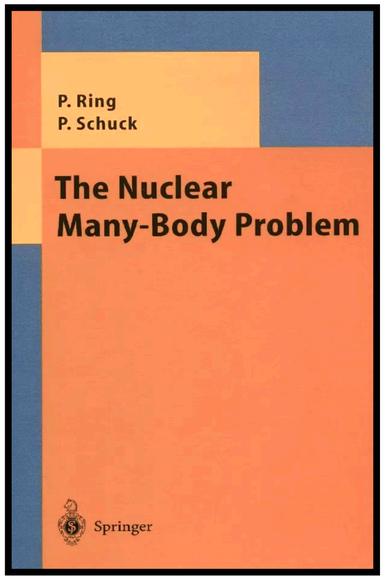
Mean-field Hamiltonian (or unperturbed)

- Sum of single-particle Hamiltonians -

Residual interaction (perturbation theory?)

The nuclear many-body problem (iv)

For a system of $A = N + Z$ particles $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$



Formal manipulation

$$\hat{H} = \hat{T} + \hat{V}_{2b} + \hat{V}_{3b} + \dots$$

$$\hat{H} = \underbrace{\hat{T} + \hat{U}_{1b}}_{\hat{H}_0} + \left(\underbrace{\hat{V}_{2b} + \hat{V}_{3b} - \hat{U}_{1b}}_{\hat{V}_{res}}\right)$$

$$\hat{H}_0 = \sum_{i=1}^{A} \frac{\boldsymbol{p}_i^2}{2m_i} + U_i(\boldsymbol{r}) = \sum_{i=1}^{A} \hat{h}_i$$

Extreme single-particle model

- No correlations
- Oversimplified
- Orthonormality - Matrix elements strongly simplified (factorised)

How to construct the basis: **one**-body basis

single particle nucleon basis $|\Phi_k\rangle = \left(|\phi_k^{space}\rangle \otimes |\chi_k^{spin}\rangle \right) \otimes |\xi_k^{isospin}\rangle$

$\{|\phi_k\rangle\}$

Set of eigenstates of a single nucleon **H**. We can assume something simple, i.e. harmonic oscillator

(special functions, i.e. Hermite, allow *nth*-order derivatives free of errors)

Be careful with asymptotic behaviours

$|nlm_l\rangle \qquad |sm_s\rangle = |\frac{1}{2}m_s\rangle \qquad |tm_t\rangle = |\frac{1}{2}m_t\rangle$

$$N \sum_{m_l, m_s} \left(\begin{array}{cc|c} l & \frac{1}{2} & j \\ m_l & m_s & m \end{array} \right) |nlm_l\rangle \otimes |\frac{1}{2}m_s\rangle \otimes |\frac{1}{2}m_t\rangle$$

$$\hat{h}_i|\Phi_k\rangle = \epsilon_k|\Phi_k\rangle \xrightarrow{\times\langle \boldsymbol{r}|} h_i\Phi_k(\boldsymbol{r}_i) = \epsilon_k\Phi_k(\boldsymbol{r}_i)$$

Postulate: The Hilbert space of state functions of a system of identical particles contains either *only symmetric* or *only antisymmetric* functions

(bosons) **(fermions)**

How to construct the basis: **many**-body basis

Nucleons are fermions → Pauli exclusion principle

$$\hat{P} = \frac{1}{A!}\sum_{\pi} \mathrm{sgn}(\pi) P_\pi$$

Permutation operator

$$P_{ij}|\ldots k_i \ldots k_j \ldots\rangle = |\ldots k_j \ldots k_i \ldots\rangle = -|\ldots k_i \ldots k_j \ldots\rangle$$

$$\Phi(r_1, r_2) = \frac{1}{\sqrt{2!}} \det \begin{vmatrix} \phi_{k1}(r_1) & \phi_{k1}(r_2) \\ \phi_{k2}(r_1) & \phi_{k2}(r_2) \end{vmatrix}$$

same place $r_1 = r_2$ → $\det = 0$

same state $k_1 = k_2$ → $\det = 0$

The many-body space is in general the product of many single particle Hilbert spaces

$$H^A = h_1 \otimes h_2 \otimes \cdots \otimes h_A$$

A-body uncorrelated state

Slater determinants

$$|\Phi\rangle = \hat{P}\underbrace{\{|\phi_{k_1}\rangle \otimes |\phi_{k_2}\rangle \otimes \ldots |\phi_{k_A}\rangle\}} \equiv |k_1 k_2 \ldots k_A\rangle$$

Antisymmetrized product of *A* 1-body state

Any antisymmetric state $|\Psi\rangle = \sum C_{k_i} |k_1 k_2 \ldots k_A\rangle \equiv \sum_i c_i |\Phi_i\rangle$

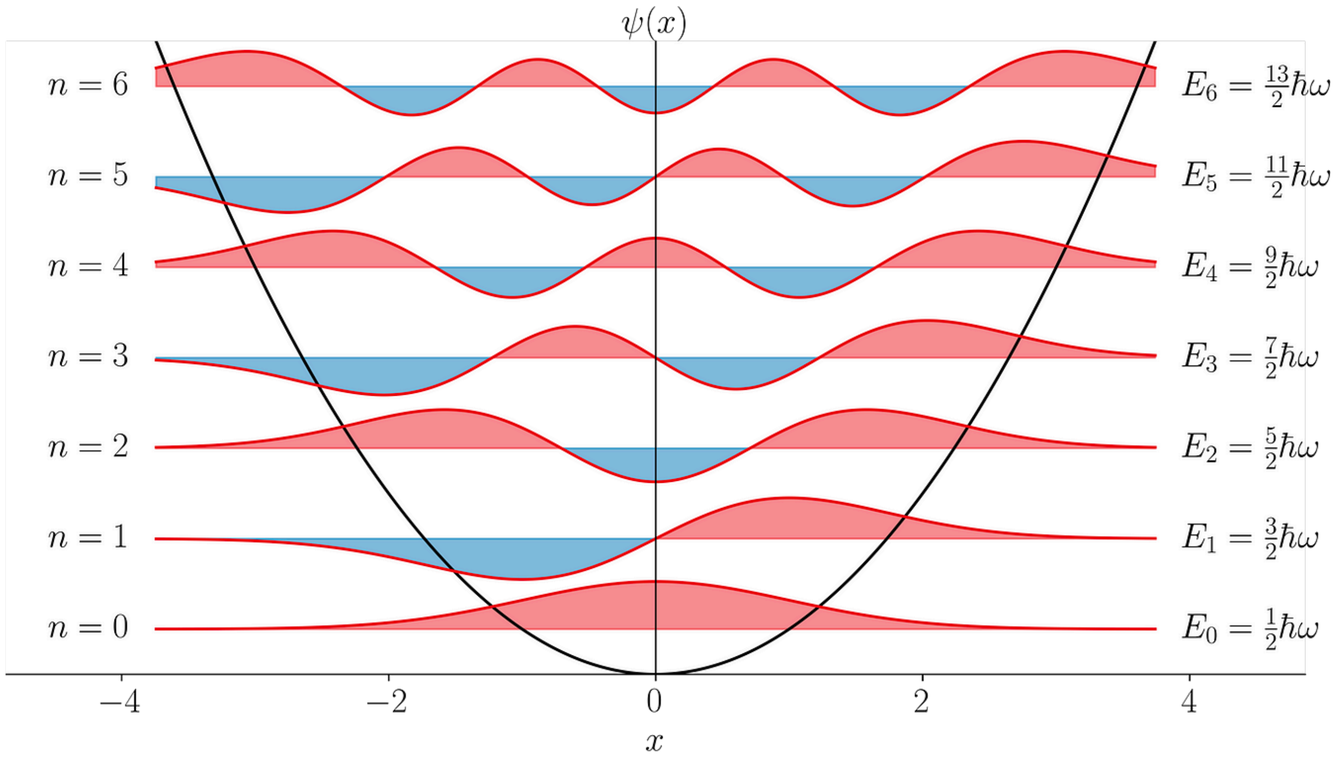
How to truncate the sum is a very complicated issue!!

Non-interacting shell model

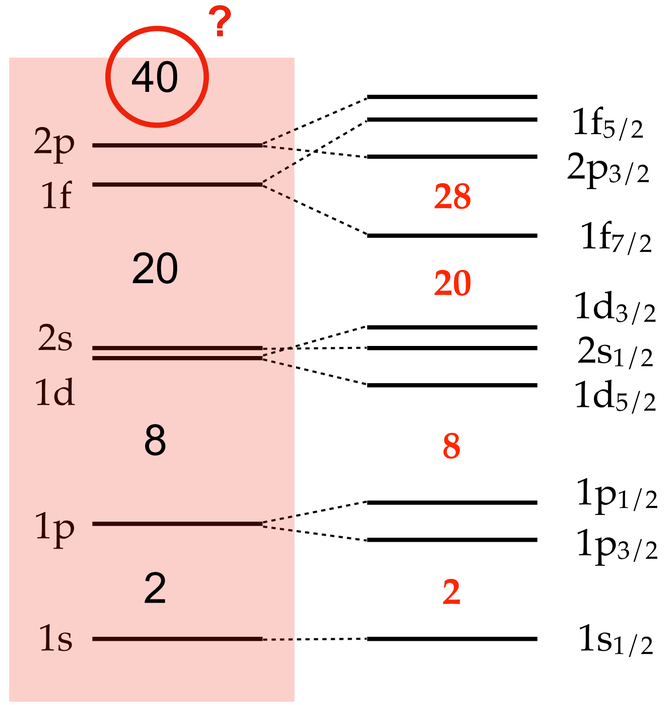
$$U_i = \frac{1}{2}m\omega^2 r_i^2 \rightarrow h_i = \frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 r_i^2$$

$$h_i \Phi_k(\boldsymbol{r}_i) = \epsilon_k \Phi_k(\boldsymbol{r}_i)$$

k={n,l,m,…}



$$\Phi_{nlm}(\boldsymbol{r}) = R_{nl}(r)Y_{lm}(\hat{r})$$



$$\epsilon_{nl}\left(N+\frac{3}{2}\right)\hbar\omega = \left(\underbrace{2(n-1)+l}_{N}+\frac{3}{2}\right)\hbar\omega$$

Non-interacting shell model

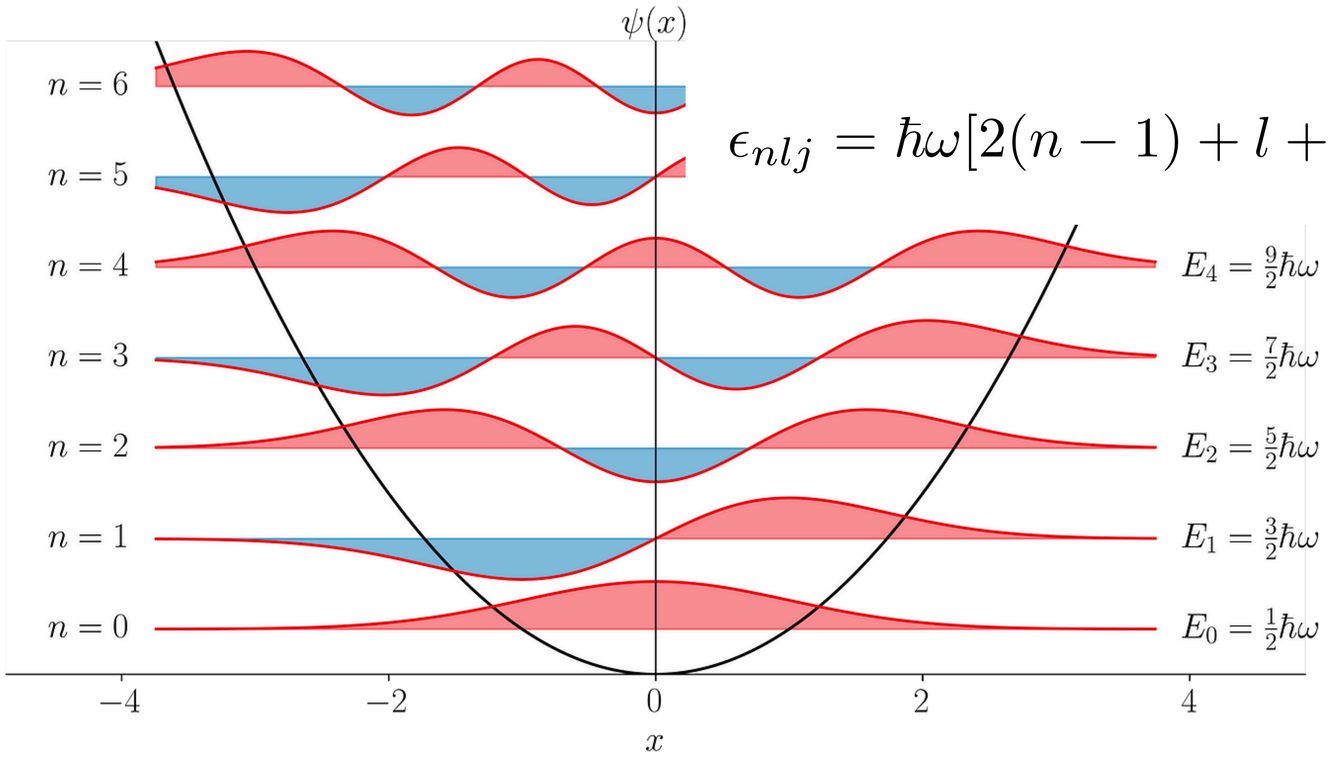
$$U_i = \frac{1}{2}m\omega^2 r_i^2 \rightarrow h_i = \frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 r_i^2$$

adding

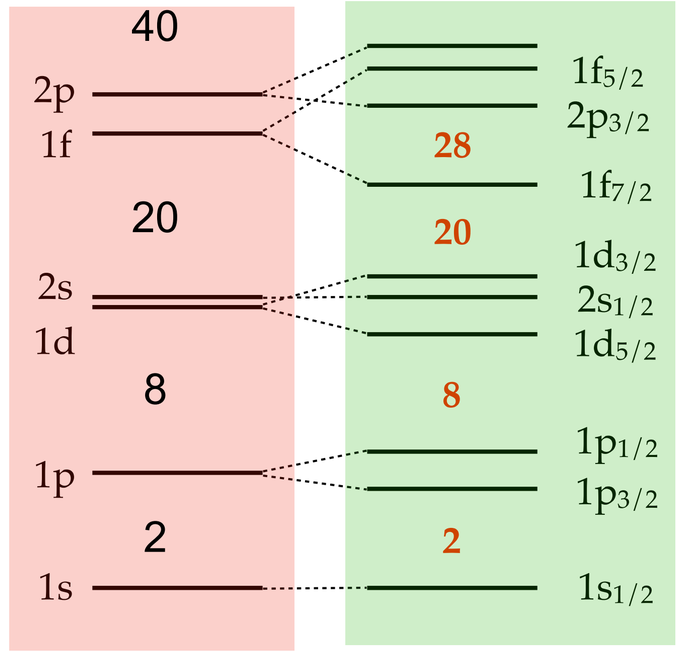
centrifugal + spin-orbit

$$U_{corr} = Dl^2 + C\boldsymbol{l}\cdot\boldsymbol{s}$$

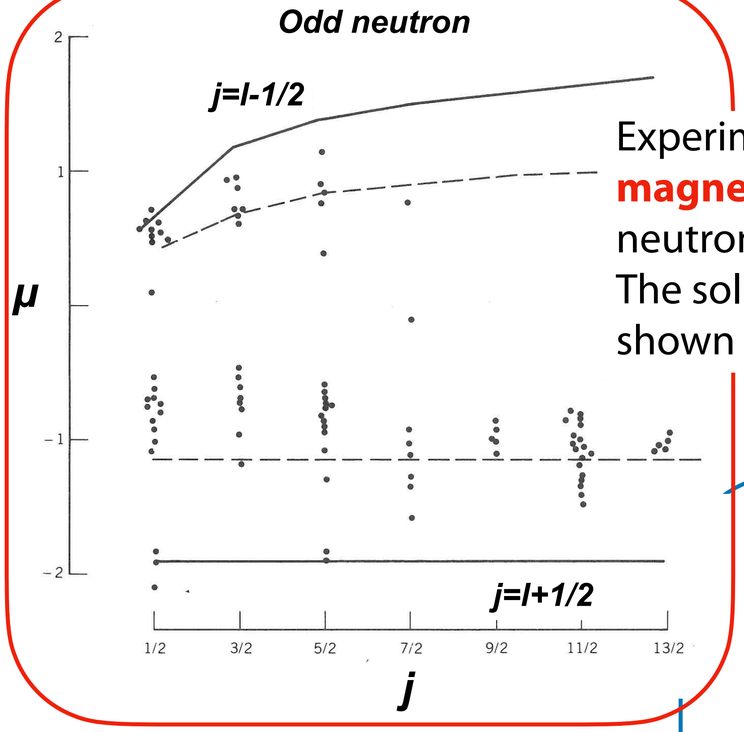
(Jensen, Goeppert Mayer,...)



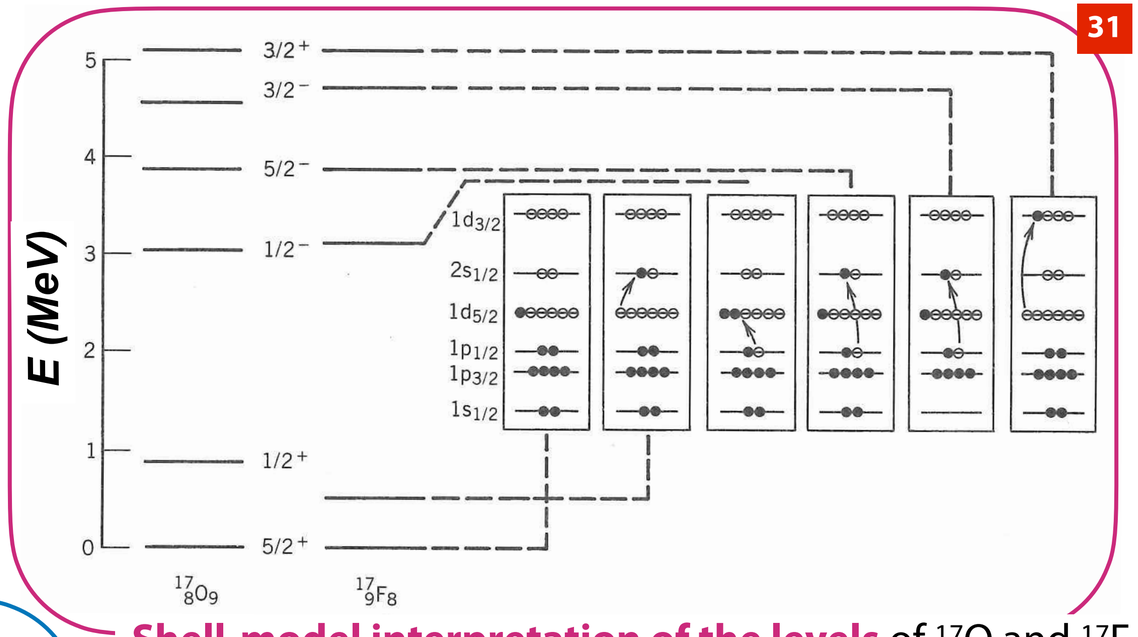
$$\epsilon_{nlj} = \hbar\omega[2(n-1)+l+3/2] + Dl(l+1) + C\begin{cases} l+1 & j=l-1/2 \\ -l & j=l+1/2 \end{cases}$$



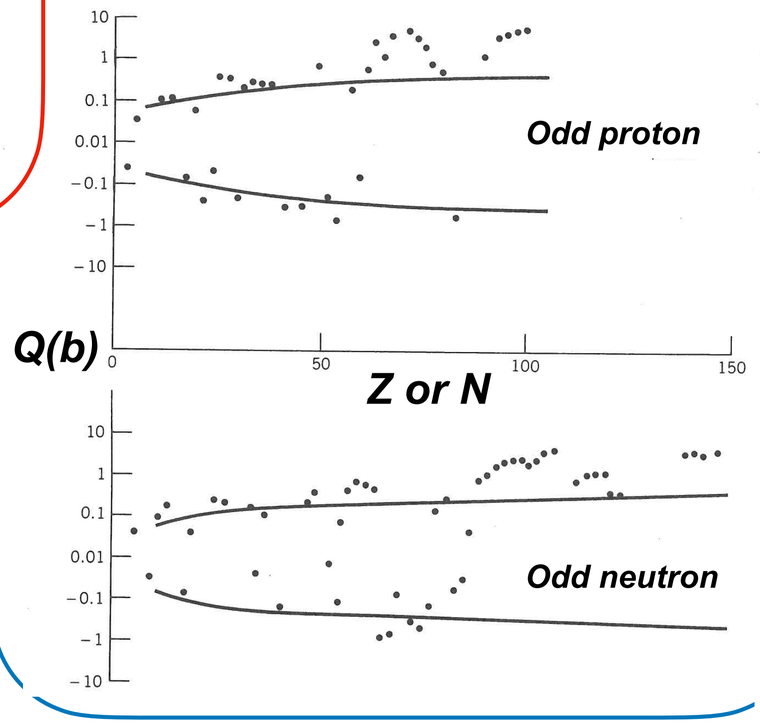
Non-interacting shell model - results



Experimental values for the **magnetic moments** of odd-neutron and odd-proton nuclei. The solid (**Schmidt**) lines are shown as shell-model predictions



Shell-model interpretation of the levels of ^{17}O and ^{17}F. All levels below about 5 MeV are shown, and the similarity between the levels of the two nuclei suggests they have common structures, determined by the valence nucleons.



Experimental values of **electric quadrupole moments** of odd-neutron and odd-proton nuclei. The solid lines are shown as shell-model predictions

K. **Krane**, Introductory Nuclear Physics

The nuclear many-body problem (v)

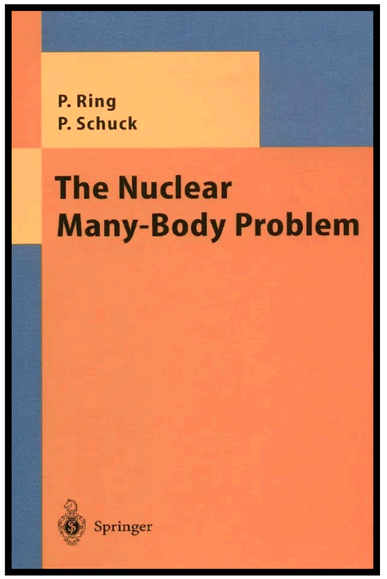
For a system of A = N + Z particles $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$

$$\hat{H} = \underbrace{\hat{T} + \hat{U}_{1b}}_{\hat{H}_0} + \underbrace{\left(\hat{V}_{2b} + \hat{V}_{3b} - \hat{U}_{1b}\right)}_{\hat{V}_{res}}$$

Mean-field Hamiltonian

(Sum of single-particle Hamiltonians)

Residual interaction



Derive a 1-body interaction in order to minimise V_{res}

Use an effective one-body Hamiltonian

$$\hat{H}_{eff}|\Phi\rangle = \bar{E}|\Phi\rangle$$

Mean field approach

H_{eff} determined by experimental data (*E/A*, *R*,…)

- Wavefunctions do not include explicit correlations
- Correlations encoded in the effective interaction (no control whatsoever)
- $|\Phi\rangle$ is not an eigenstate of H - check symmetries!!

need for symmetry restoration!

Mean field concept

Nucleons are non-relativistic point-particles

$v \ll c$

Energies involved are too low to explore the nucleon internal structure

Nucleons move independently in a mean field potential, i.e. *the average interaction contribution of the other A-1 nucleons*

Residual interaction is neglected

The mean field potential has in general a phenomenological nature (not always) and contains all the relevant contributions, central, spin-orbit, tensor,…including density- and isospin-dependence

What to include and when stop adding terms is basically a free choice

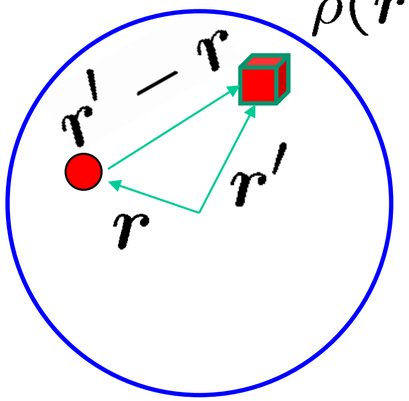
The mean field potential is determined by fitting exp. data

Different strategies lead to different use (finite nuclei, neutron stars, heavy-ion collisions,…)

Extrapolation into set of data not included into the fit procedure could be dangerous

Good for energies, radii, deformations, single particle dynamics (not always)

Hartree-Fock approach



$\rho(\boldsymbol{r}')d\boldsymbol{r}'$

$$\rho(\boldsymbol{r}) = \sum_i |\phi_i(\boldsymbol{r})|^2$$

Averaged potential over the nucleon distribution

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

Hartree equations

$$0 = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - \epsilon_i\right]\phi_i(\boldsymbol{r})$$

$$= \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r},\boldsymbol{r}')\left(\sum_j |\phi_j(\boldsymbol{r})'|^2\right)d\boldsymbol{r}' - \epsilon_i\right]\phi_i(\boldsymbol{r})$$

need to be antisymmetrized

Hartree-Fock equations

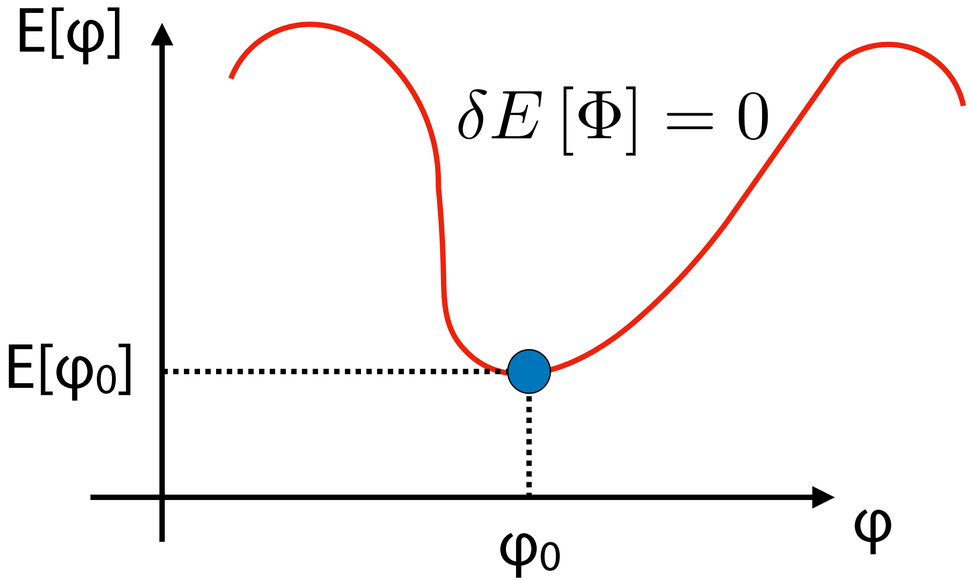
$$0 = \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r},\boldsymbol{r}')\left(\sum_j |\phi_j(\boldsymbol{r})'|^2\right)d\boldsymbol{r}' - \epsilon_i\right]\phi_i(\boldsymbol{r})$$

$$- \int v(\boldsymbol{r},\boldsymbol{r}')\left(\sum_j \phi_j^*(\boldsymbol{r}')\phi_i(\boldsymbol{r}')\right)d\boldsymbol{r}'\phi_j(\boldsymbol{r})$$

$$0 = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_l(\boldsymbol{r}) - \epsilon_i\right]\phi_i(\boldsymbol{r}) + \int d\boldsymbol{r}' V_{nl}(\boldsymbol{r},\boldsymbol{r}')\phi_i(\boldsymbol{r}')$$

local potential $V_l(\boldsymbol{r})$ — non-local potential $V_l(\boldsymbol{r},\boldsymbol{r}')$

Variational Problem - Ritz principle



Variational ansatz

$$E[\Phi] = \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle} \geq E_{\Psi_0}$$

true ground-state

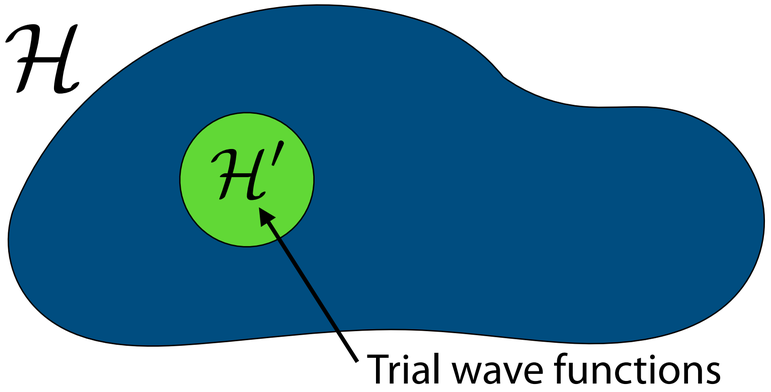
Theorem

Every state φ that produces a stationary state of E[φ] is an eigenstate of H and viceversa. The corresponding eigenvalue is the value of E[φ] corresponding to the stationary state.

(**Messiah**, Quantum mechanics)

$$\delta\langle \Psi | H | \Psi \rangle = 0$$
$$\langle \Psi | \Psi \rangle = 1$$
$$\langle \Psi | H | \Psi \rangle = E$$

$$H|\Psi\rangle = E|\Psi\rangle$$

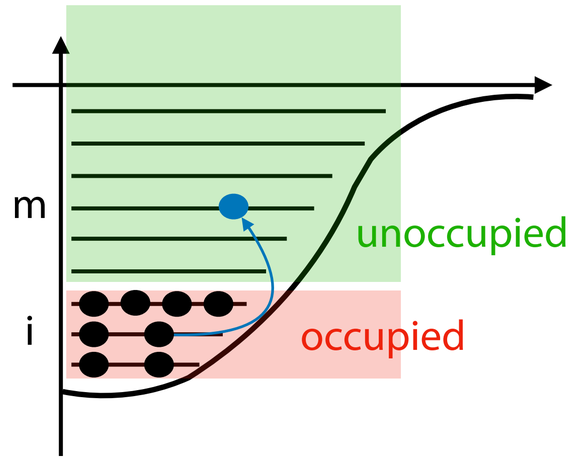


1p-1h state $|\Phi_i^a\rangle = \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle$

$$|\Phi_0\rangle = \left(\prod_{i \leq F} \hat{a}_i^\dagger \right) |0\rangle$$

$$|\Phi_0\rangle + |\delta\Phi_0\rangle = |\Phi_0\rangle + \eta a_m^\dagger a_i |\Phi_0\rangle \equiv |\Phi_0\rangle + \eta |\Phi_i^m\rangle$$

Minimization ⟶ $\langle \delta\Phi_0 | H | \Phi_0 \rangle = 0$



Brillouin theorem (about the residual interaction)

Stationary condition

$$\langle \delta\Phi_0 | H | \Phi_0 \rangle = \eta \langle \Phi_i^m | H | \Phi_0 \rangle = \eta \langle \Phi_0 | a_i^\dagger a_m H | \Phi_0 \rangle = 0$$

$$\hat{H} = \hat{T} + \hat{U}_{HF} + \left(\hat{V}_{2b} - \hat{U}_{HF} \right)$$

$\hat{V}_{res}$ Residual interaction

$$E_0 = \langle \Phi_0 | H | \Phi_0 \rangle$$

Choosing the Hartree-Fock solution it's equivalent to require that the residual interaction evaluated in the ground-state is zero.

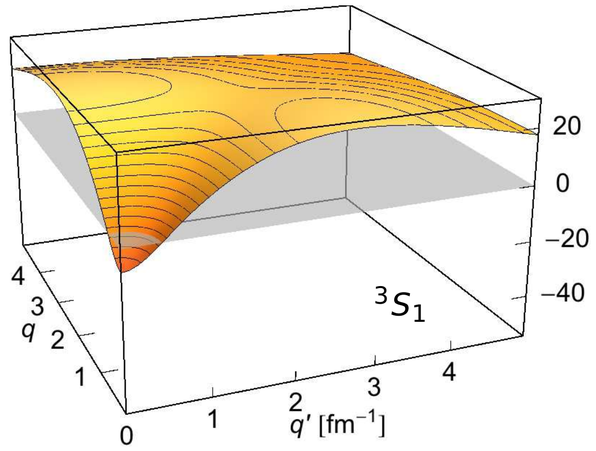
$$\langle \Phi_0 | V_{res} | \Phi_0 \rangle = 0$$

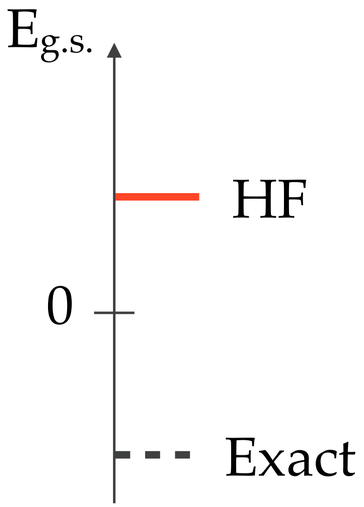
It is not enough to ensure that is valid solution

	$\lvert\Phi_0\rangle$	$\lvert\Phi_i^m\rangle$
$\lvert\Phi_0\rangle$	≠0	0
$\lvert\Phi_i^m\rangle$	0	≠0

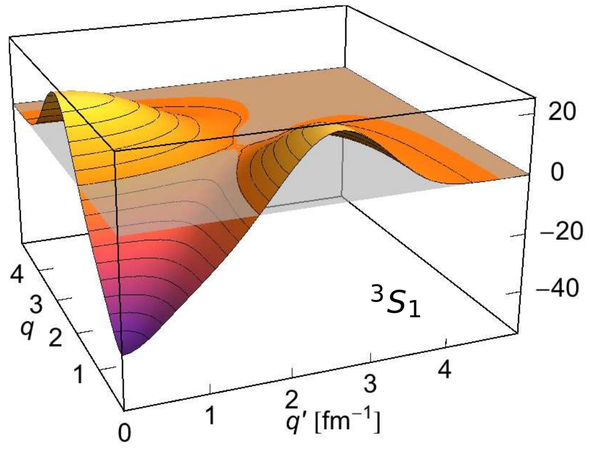
Hartree-Fock with ab initio interactions

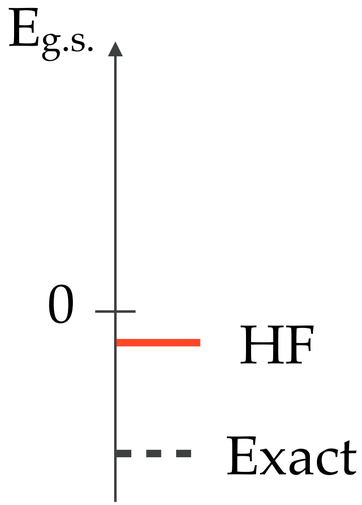
OBE potentials





Chiral potentials





Somà, Lecture @ Fiera di Primiero

Skyrme functionals

The Skyrme force was first introduced by **Skyrme** as an effective force for nuclear Hartree-Fock calculations and later by **Vautherin** and **Brink**

$$E\left(\rho_p,\rho_n\right)=\int \mathcal{H}_{Sk}d\vec{r}$$

$$\hat{h}_q=U_q-\nabla\cdot B_q\nabla-\frac{i}{2}\{\mathbb{W}_q,\nabla\sigma\}$$

$$\{\mathbb{W}_q,\nabla\sigma\}=\Sigma_{ij}\{W_{ij},\nabla_i\hat{\sigma}_j\}$$

$$U_q=\frac{\delta E}{\delta\rho_q}\qquad B_q=\frac{\delta E}{\delta\tau_q}$$

$$\mathcal{H}_{Sk}\left(\rho_{n,p},\tau_{n,p},\underset{n,p}{\vec{J}}\right)=\mathcal{H}_K\left(\tau_{n,p}\right)+\mathcal{H}_0+\mathcal{H}_3+\mathcal{H}_{eff}+\mathcal{H}_{fin}+\mathcal{H}_{so}+\mathcal{H}_{sg}+\mathcal{H}_C\left(\rho_p\right)$$

Kinetic

$$\mathcal{H}_K\left(\vec{r}\right)=\frac{\hbar^2}{2m}\left[\tau_p\left(\vec{r}\right)+\tau_n\left(\vec{r}\right)\right]$$

Two body

$$\mathcal{H}_0\left(\vec{r}\right)=\frac{t_0}{2}\left[\left(1+\frac{1}{2}x_0\right)\rho^2-\left(x_0+\frac{1}{2}\right)\left(\rho_p^2+\rho_n^2\right)\right]$$

$$\mathcal{H}_3\left(\vec{r}\right)=\frac{1}{12}t_3\rho^\sigma\left[\left(1+\frac{1}{2}x_3\right)\rho^2-\left(x_3+\frac{1}{2}\right)\left(\rho_p^2+\rho_n^2\right)\right]$$

Two body density dependent

(mimicking an effective 3-body force)

An alternative:
Berger, **Girod** and **Gogny**, Comp. Phys. Comm., 63 (1991) 365
Dechargé and **Gogny**, Phys. Rev. C 21., (1980) 1568

Skyrme, Phil. Mag. 1 (1956), 1043, Nucl. Phys. 9 (1959), 615
Vautherin and **Brink**, Phys. Lett. 32B (1970), 149, Phys. Rev. C5 (1972), 626
Bender, **Heenen**,, **Reinhard**, Rev.Mod.Phys. 75 (2003) 121-180

Skyrme functionals

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$$E\left(\rho_p,\rho_n\right)=\int \mathcal{H}_{Sk}d\vec{r}$$

$$\mathcal{H}_{sg}\left(\vec{r}\right)=\frac{1}{16}\left[\left(t_1-t_2\right)\sum_{i=p,n}\overrightarrow{J}_i^2-\left(t_1x_1+t_2x_2\right)\overrightarrow{J}^2\right]$$

Tensor term

$$\mathcal{H}_{so}\left(\vec{r}\right)=\frac{W_0}{2}\left(\vec{J}\cdot\vec{\nabla}\rho+\sum_{i=p,n}\vec{J}_i\cdot\vec{\nabla}\rho_i\right).$$

Spin-orbit

$$\mathcal{H}_{Sk}\left(\rho_{n,p},\tau_{n,p},\overrightarrow{J}_{n,p}\right)=\mathcal{H}_K\left(\tau_{n,p}\right)+\mathcal{H}_0+\mathcal{H}_3+\mathcal{H}_{eff}+\mathcal{H}_{fin}+\mathcal{H}_{so}+\mathcal{H}_{sg}+\mathcal{H}_C\left(\rho_p\right)$$

Effective mass

$$\mathcal{H}_{eff}\left(\vec{r}\right)=\frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right]\tau\rho+\frac{1}{4}\left[t_2\left(x_2+\frac{1}{2}\right)-t_1\left(x_1+\frac{1}{2}\right)\right]\left(\tau_p\rho_p+\tau_n\rho_n\right)$$

Finite-range

$$\mathcal{H}_{fin}\left(\vec{r}\right)=\frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\left(\nabla\rho\right)^2-\frac{1}{16}\left[3t_1\left(x_1+\frac{1}{2}\right)+t_2\left(x_2+\frac{1}{2}\right)\right]\left(\left(\nabla\rho_n\right)^2+\left(\nabla\rho_p\right)^2\right.$$

EV8
Sky3D
HFBRAD
HFODD
SKY3D

Skyrme, Phil. Mag. 1 (1956), 1043, Nucl. Phys. 9 (1959), 615
Vautherin and **Brink**, Phys. Lett. 32B (1970), 149, Phys. Rev. C5 (1972), 626
Bender, **Heenen**,, **Reinhard**, Rev.Mod.Phys. 75 (2003) 121-180

$U_i^{(n)}$

Single-particle potentials

Diagonalize the Hamiltonian

Solve the 1-body Schrödinger equation

$\phi^{(n+1)}$

Determine the resulting wave functions

END YES

Convergence criterion

$||\phi^{(n+1)} - \phi^{(n)}|| \ll \epsilon$

NO

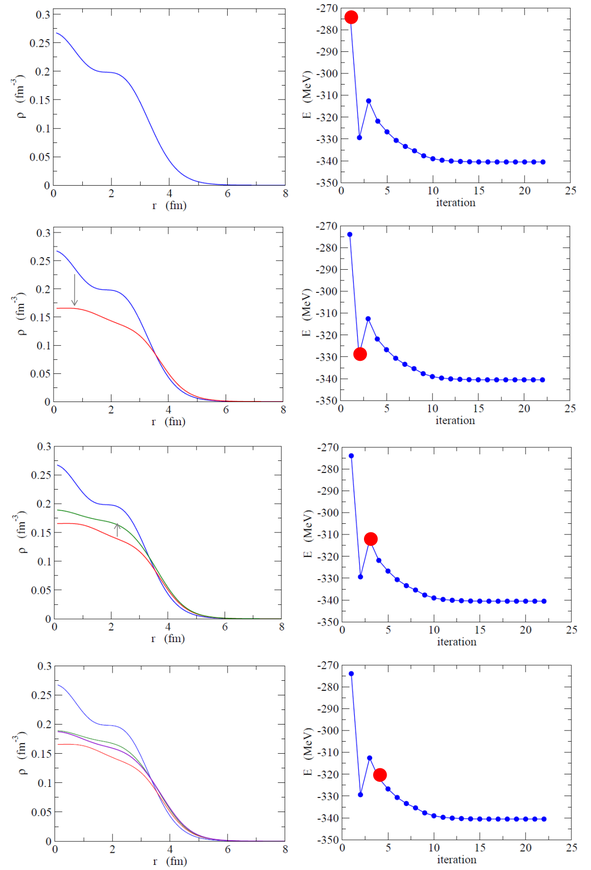
$\rho_i^{(n+1)}, J_i^{(n+1)}$

Calculation of new densities and currents

$U_i^{(n+1)}$

Calculation of new potentials

$U_i^{(n+1)}$



Covariant interactions (Walecka-Serot)

$$E = \int d^3r\, \mathcal{E}_{\mathrm{RMF}} + E_{\mathrm{Coul}} + E_{\mathrm{pair}} - E_{\mathrm{cm}},$$

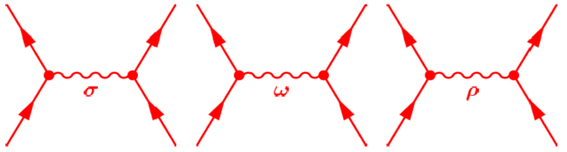
$$\mathcal{E}_{\mathrm{RMF}} = \mathcal{E}_{\mathrm{nucl}} + \mathcal{E}_{\mathrm{meson}} + \mathcal{E}_{\mathrm{coupl}} + \mathcal{E}_{\mathrm{nonl}},$$

$$\mathcal{E}_{\mathrm{nucl}} = \sum_{\alpha=1}^{\Omega} v_\alpha^2 \bar{\psi}_\alpha (-i\gamma\cdot\nabla + m_{\mathrm{B}})\, \psi_\alpha,$$

$$\mathcal{E}_{\mathrm{meson}} = \sum_{\mathcal{M}=\sigma,\omega,\rho} \frac{1}{2} \Phi_{\mathcal{M}} (-\Delta + m_{\mathcal{M}}) \Phi_{\mathcal{M}},$$

$$\mathcal{E}_{\mathrm{coupl}} = g_\sigma \Phi_\sigma \rho_{s0} + g_\omega \Phi_\omega^\mu \rho_{\mu 0} + g_\rho \Phi_\rho^\mu \rho_{\mu,1},$$

$$\mathcal{E}_{\mathrm{nonl}} = \frac{1}{3} b_2 \Phi_\sigma^3 + \frac{1}{4} b_3 \Phi_\sigma^4 + \frac{1}{4} c_3 (\Phi_{\omega,\mu} \Phi_\omega^\mu)^2$$



PRO

- Exploit the covariant formulation of the problem
- Free parameters: masses and couplings (mesons are effective degrees of freedom)
- Spin-orbit determined by the interplay between the scalar and the vector component
- Odd-terms determined by the even components (no free parameters)

CONS

- Antiparticle degrees of freedom (*no sea approximation)*
- Extension of the functional hard to identify (more non-linearities? More mesons?)

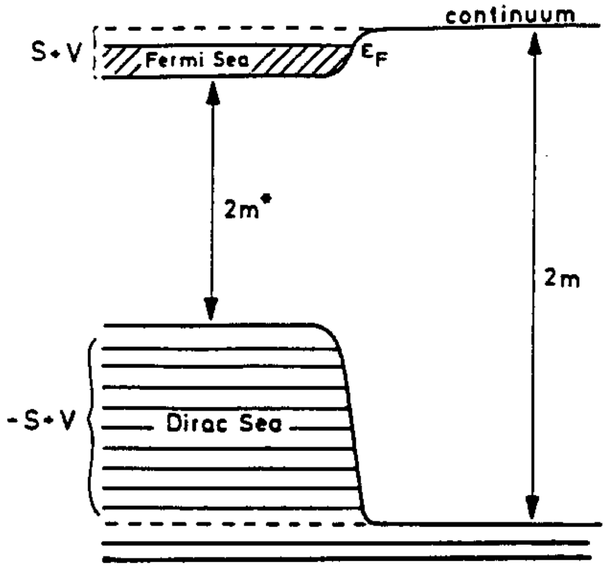
Ring, Relativistic mean field theory in finite nuclei, PPNP 37 (1996) 193

Covariant interactions (Walecka-Serot)

Dirac equation
(and Klein-Gordon for meson fields)

$$\{\gamma_\mu(i\partial^\mu + V^\mu) + m + S\}\psi_i = 0$$

$$\begin{aligned} S(x) &= g_\sigma \Phi_\sigma(x) \\ V^\mu(x) &= g_\omega \Phi^\mu_\omega(x) + g_\rho \vec{\tau} \Phi^\mu_\rho + \dots \end{aligned}$$



The qualitative structure of the scalar field S and the vector field V in a finite nucleus as a function of the distance from the origin. In realistic calculations these potentials are not completely flat in the nuclear interior, but show small quantum fluctuations.

$$\left[-\nabla \frac{1}{2m_{eff}} \nabla + V_c + \frac{1}{2m^2}(\nabla V_{ls})(\boldsymbol{p} \times \boldsymbol{s})\right] \phi = \epsilon \phi$$

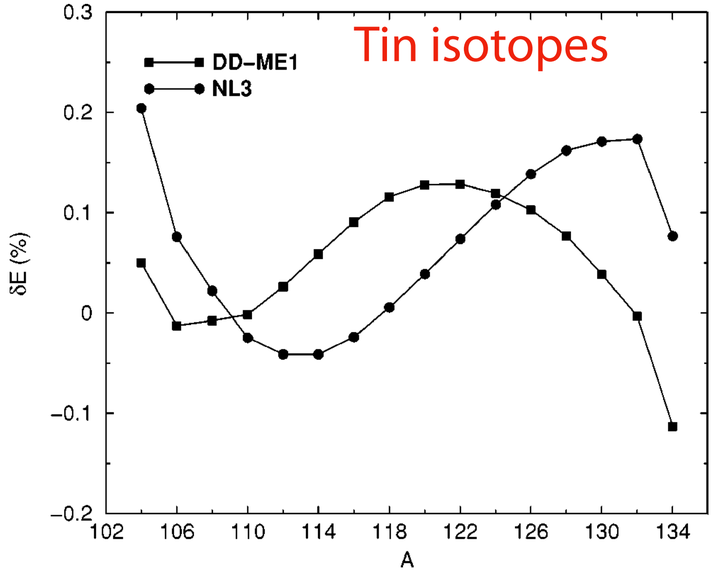
$$m_{eff} = m - \frac{1}{2}(V - S)$$

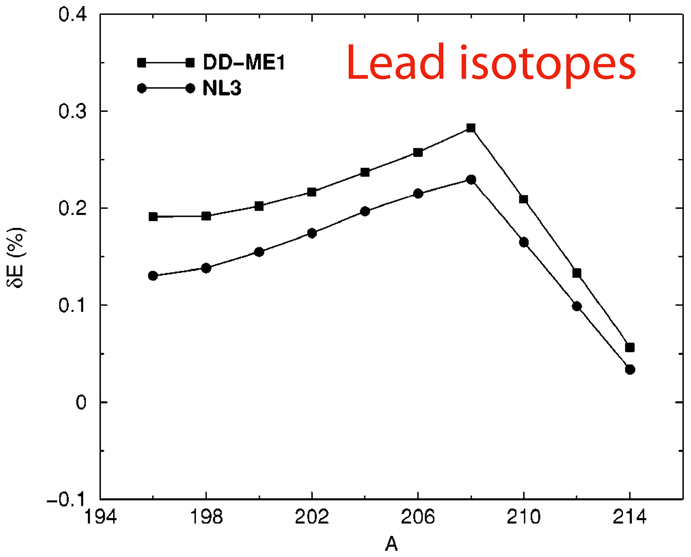
$$V_c = V + S$$

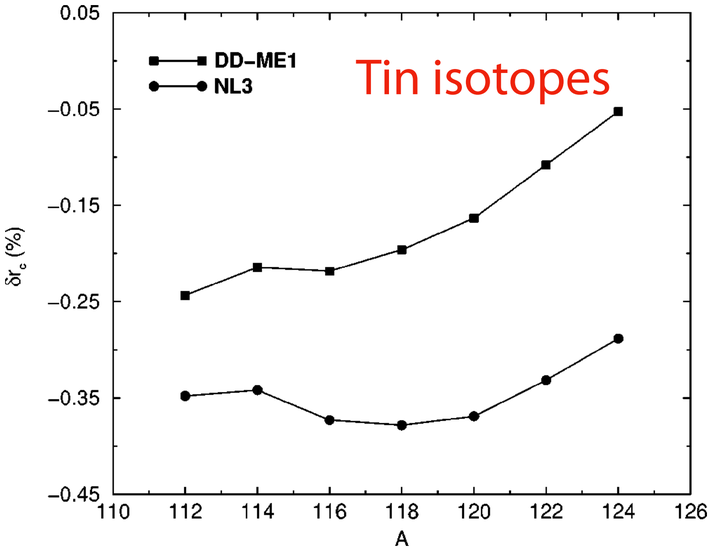
$$V_{ls} = \frac{m}{m_{eff}}(V - S)$$

Ring, Relativistic mean field theory in finite nuclei, PPNP 37 (1996) 193

Covariant interactions - some results







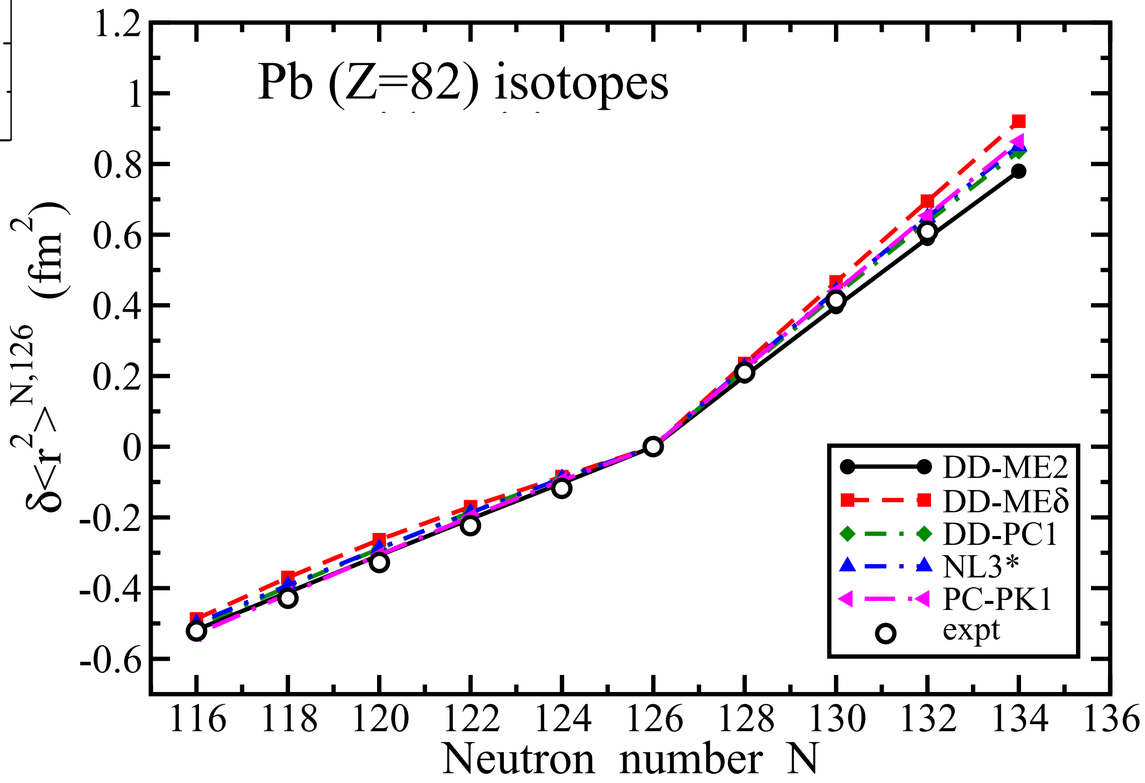
% deviations from experimental data

Niksic, **Vretenar**, **Finelli** , and **Ring**

Relativistic Hartree-Bogoliubov model with density-dependent meson-nucleon couplings

The differential mean-square charge radius of the Pb isotopes relatively to ^{208}Pb obtained with different parametrizations

$$\delta\langle r^2\rangle_p^{N,N'} = \langle r^2\rangle_p(N) - \langle r^2\rangle_p(N')$$
$$= r_{ch}^2(N) - r_{ch}^2(N'),$$

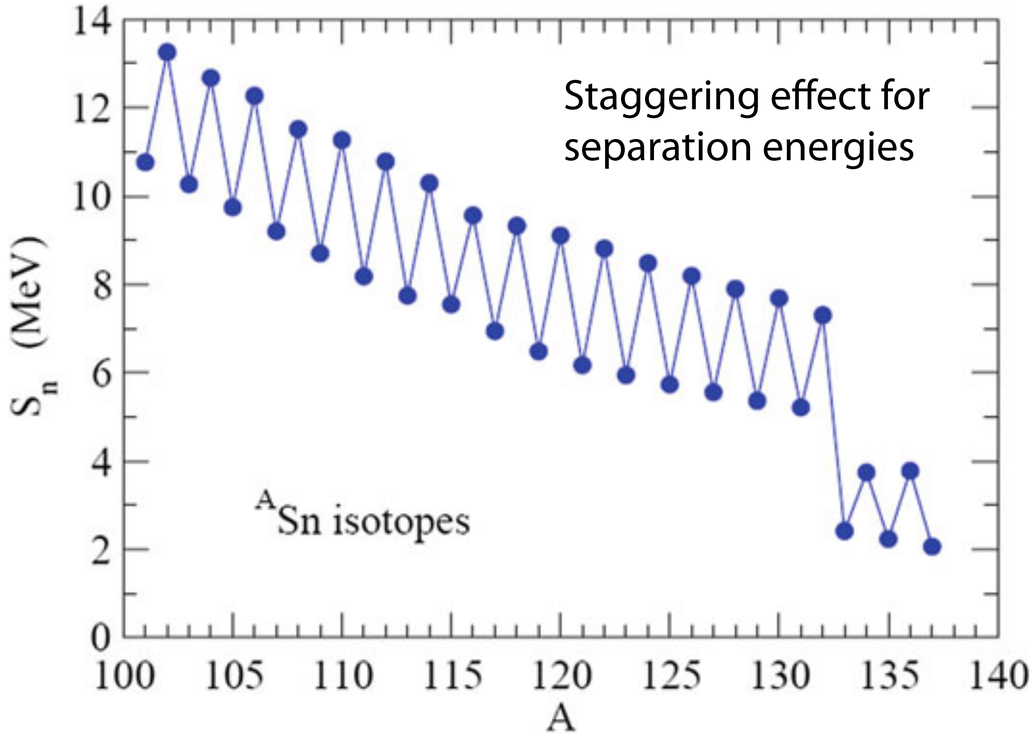


Perera, **Afanasjev**, and **Ring**

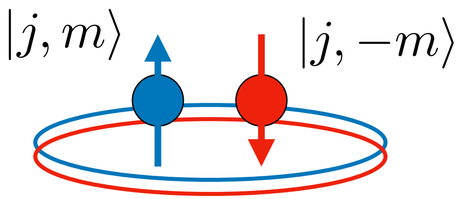
Charge radii in covariant density functional theory: A global view

Pairing - inclusion of pp correlations

1. The energy difference between the ground and the first excited states in even-even nuclei is significantly larger than that of even-odd nuclei. For example, a typical energy difference between the first excited and the ground states is more than 1 MeV in even Sn isotopes, while there are many states below a few hundreds keV in odd Sn isotopes.
2. The moment of inertia of deformed rare-earth nuclei is typically one half of the rigid rotor one because of the superfluidity.
3. The so-called pairing energy gap manifests itself in the mass staggering between even and odd mass nuclei over wide regions of the mass table.

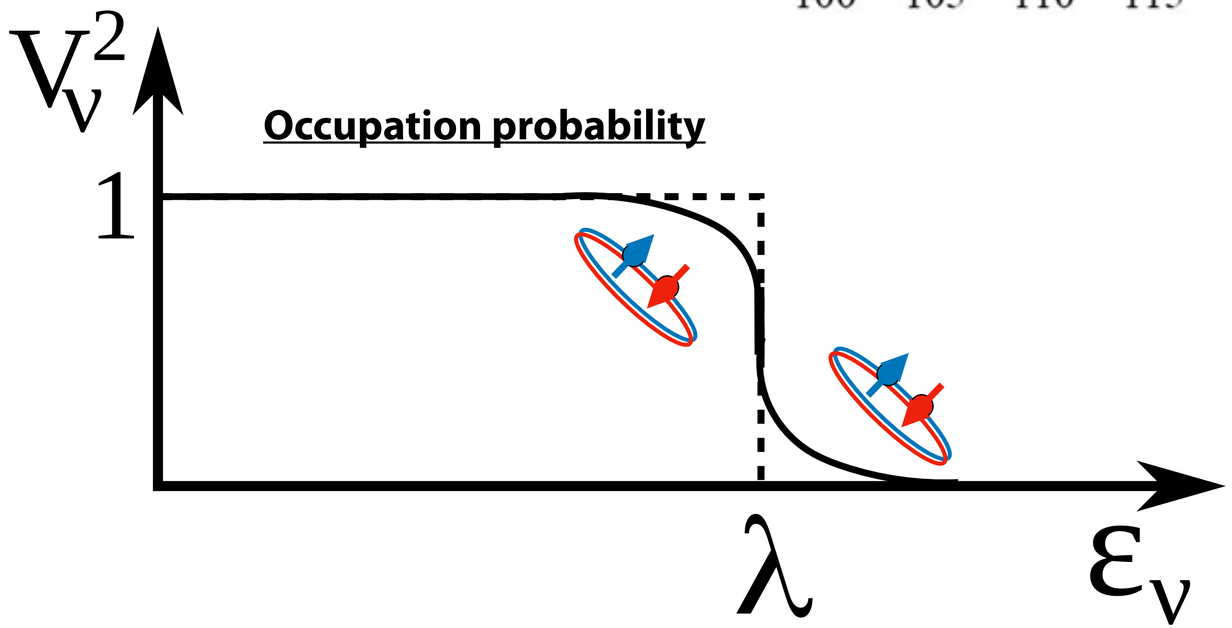


$^1S_0$ - isotriplet



Time-reversed orbits

$$|J = 0^+\rangle$$



Pairing - inclusion of pp correlations

- To take into account the pairing correlations on top of the mean field HF model, the BCS or HF+Bogolyubov model are often introduced.
- The basic novelty is to introduce a new type of fermions, the "quasi-particles". The simplicity of single-particle models is preserved.
- However, the ground state is no longer a single-Slater determinant, but will be defined as the so-called BCS vacuum (it does not have a definite number of physical particles)

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}}$$

$$\alpha_{\bar{k}} = v_k a_k^\dagger + u_k a_{\bar{k}}$$

Bogolyubov transformation

$$a_{\bar{k}}^\dagger \equiv a_{jm}^\dagger = (-1)^{j+m} a_{j-m}^\dagger$$

$$|HF\rangle \rightarrow |BCS\rangle$$

$$\alpha_k |\mathrm{BCS}\rangle = 0$$

$$|\mathrm{BCS}\rangle = \prod_k \alpha_k |0\rangle \Rightarrow |\mathrm{BCS}\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|0\rangle$$

$$|u_k|^2 + |v_k|^2 = 1$$

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \lambda}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta_k^2}}\right)$$

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_k - \lambda}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta_k^2}}\right)$$

What V_{pp} to use?

- Realistic forces
- Phenomenological ansatz

How to reconcile LDM and single-particle description?

The most important correlation effects in nuclear structure stem from large-amplitude collective motion. Low-lying excited states are mixed into the calculated mean-field ground state which can be treated by configuration mixing, i.e., superposition of several mean-field states.

This embraces nuclear surface vibrations related to low-lying excitation spectra and zero-energy modes (translation, rotation, etc.) related to the restoration of symmetries broken by the mean-field ground state.

Given a family of *N*-body wave functions depending on a **collective variable *q***

$$|\Psi_k\rangle = \int dq\,|\Phi(q)\rangle f_k(q)$$

$$E_k = \frac{\langle\Psi_k|\hat{H}|\Psi_k\rangle}{\langle\Psi_k|\Psi_k\rangle}$$

$$\int dq'\,[\mathcal{H}(q,q') - E_k\mathcal{I}(q,q')]f_k(q') = 0$$ Hill-Wheeler equation

$$\mathcal{H}(q,q') = \langle\Phi(q)|\hat{H}|\Phi(q')\rangle$$

$$\mathcal{I}(q,q') = \langle\Phi(q)|\Phi(q')\rangle.$$

Generator Coordinate Method

Restoration of symmetries

The main application of the generator coordinate method involves the restoration of broken symmetries. The family of the wave functions $|\varphi(q)\rangle$ is generated by the symmetry operations: rotation in coordinate space for angular momentum, rotation in gauge space for particle number, or parity transformation (in which case, the mixing is discrete). In these cases, the generating function $f_k(q)$ is determined *a priori* by the properties of the symmetry operator.

Particle number projection

BCS (or HFB) states are not eigenstates of the particle-number operator. They give the desired particle numbers *N* and *Z* only on average

$$\hat{P}_N = \frac{1}{2\pi}\int_0^{2\pi} d\phi_N e^{i\phi_N(\hat{N}-N)}$$

Angular momentum projection

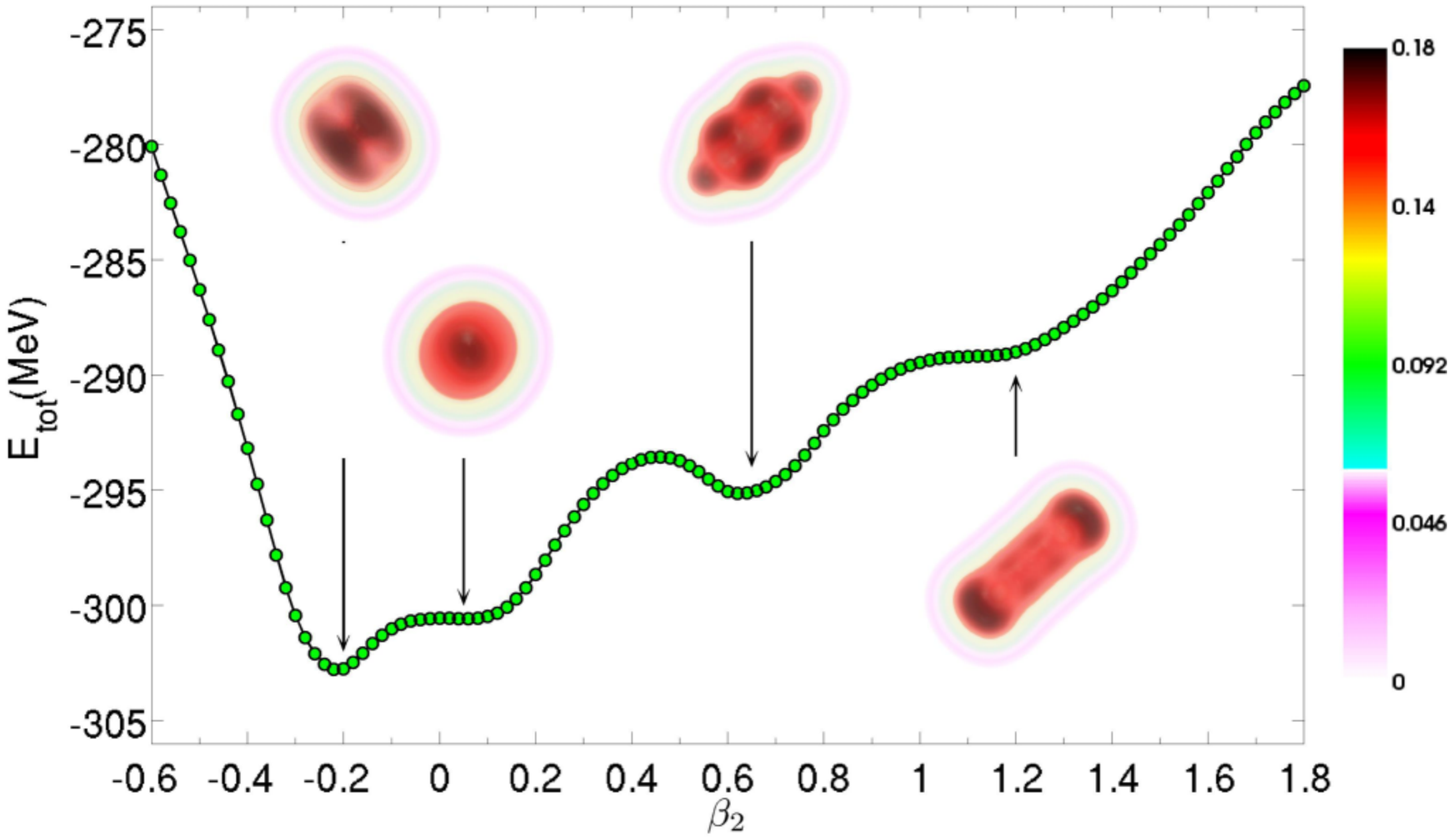
Deformed mean-field states are not eigenstates of the total angular momentum. An eigenstate with eigenvalue J is obtained by projecting the mean-field wave function

$$|\Phi, JM\rangle = \frac{\sum_K g_K \hat{P}^J_{MK}|\Psi\rangle}{\sqrt{\sum_K |g_K|^2 \langle\Psi|\hat{P}^J_{KK}|\Psi\rangle}}$$

$$\hat{P}^J_{MK} = \frac{2J+1}{8\pi^2}\int d\Omega D^{J*}_{MK}(\Omega)\hat{R}(\Omega)$$

Some recent theoretical results from DFT approaches

- Self-consistent binding energy curves of ^{36}Ar as functions of the quadrupole deformation parameter β_2, calculated with the functional DD- ME2.
- The insets display the corresponding intrinsic nucleon density distributions in the reference frame defined by the principal axes of the nucleus.



Ebran, **Khan**, **Niksic**, and **Vretenar**,
Density functional theory studies of cluster states in nuclei

The nuclear many-body problem (vi)

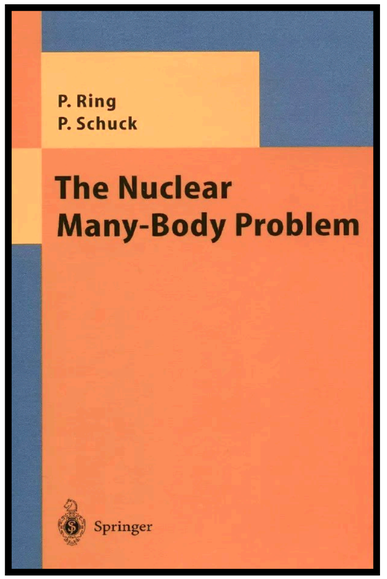
For a system of A = N + Z particles $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$

$$\hat{H} = \underbrace{\hat{T} + \hat{U}_{1b}}_{\hat{H}_0} + \underbrace{\left(\hat{V}_{2b} + \hat{V}_{3b} - \hat{U}_{1b}\right)}_{\hat{V}_{res}}$$

Mean-field Hamiltonian

(Sum of single-particle Hamiltonians)

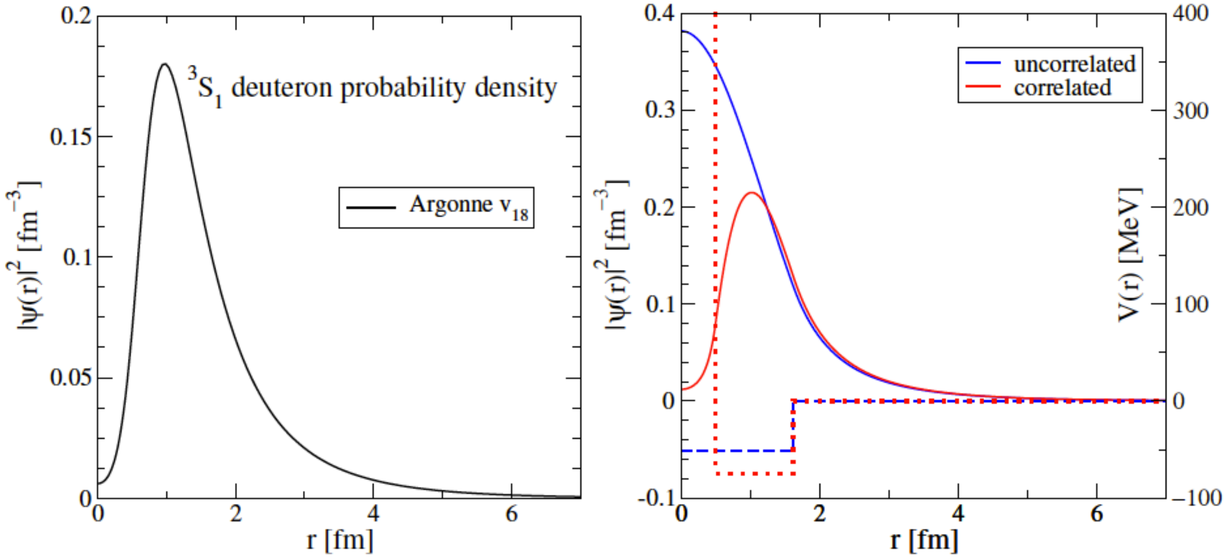
Residual interaction

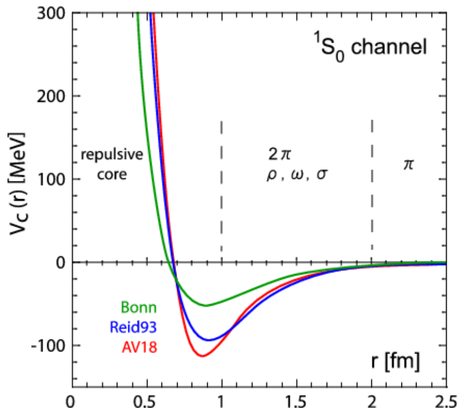


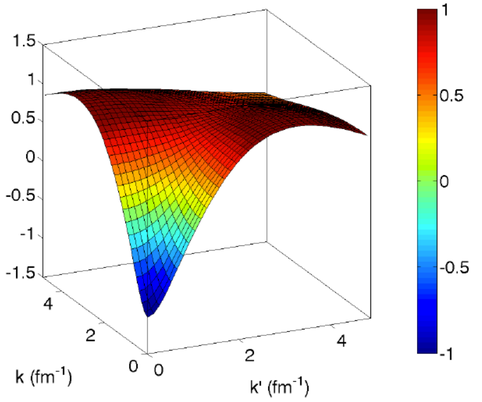
It's time to introduce back the NN interaction in our models…

Could it be simplified?

Nucleon-nucleon potential: how to soften V_{NN}?







$$V_{L=0}(k,k') \propto \langle k|V_{L=0}|k'\rangle \propto \int d^3r\, j_0(kr)\, V(r)\, j_0(k'r)$$?

- Probability at short distances suppressed, i.e. correlations
- Short-distance structure ~ high momentum components

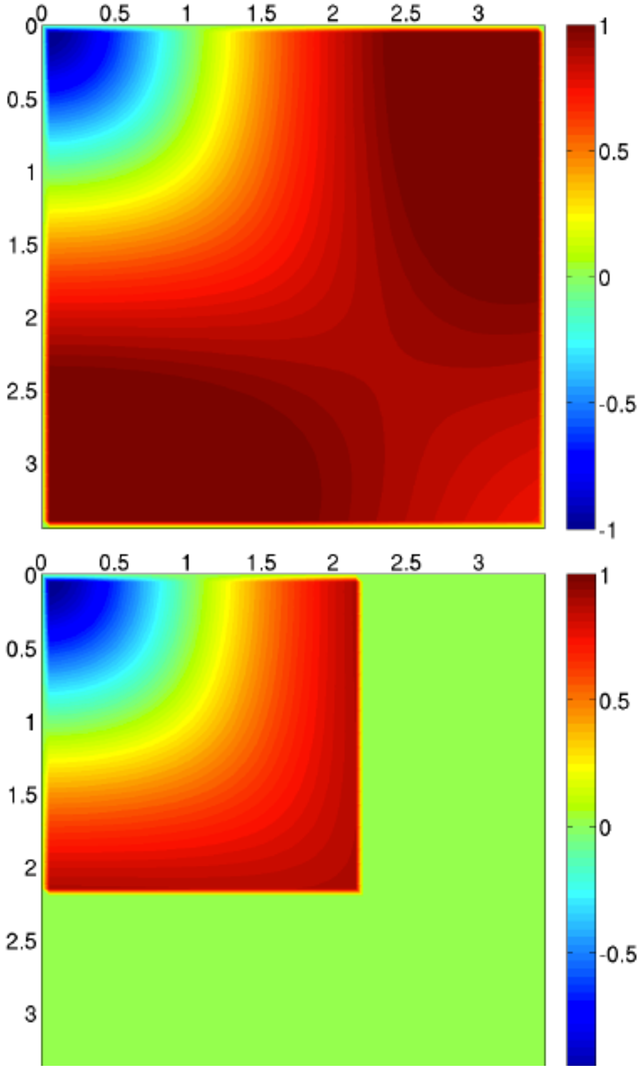
Sources of nonperturbative physics
- Strong short-range repulsion (“hard core”)
- Iterated tensor interaction
- Near zero-energy bound states

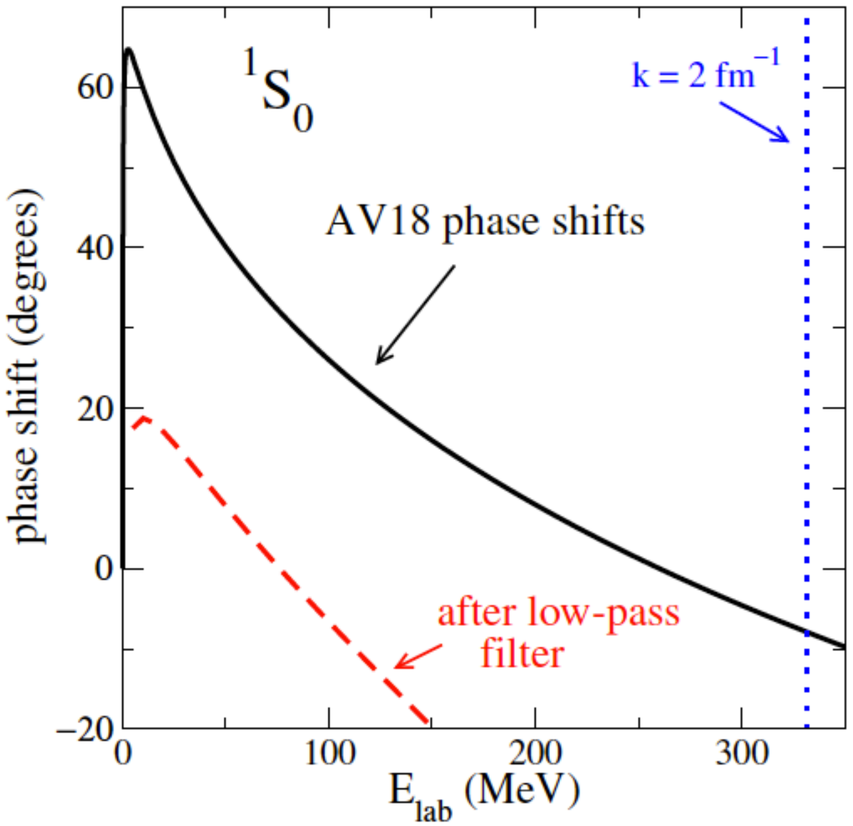
Consequences:
- Strong correlations are overwhelming.
- Diagrammatic analyses become hopelessly complicated.

Is it possible to tame the effect of correlations imposing a cutoff?

Nucleon-nucleon potential: how to soften V_{NN}?

Is it possible to tame the effect of correlations imposing a cutoff?





lower consistently the cutoff

Renormalization Group

Bogner, **Furnstahl** and **Perry**, Similarity Renormalization Group for Nucleon-Nucleon Interactions
Johnson, Tracing the evolution of nuclear forces under the similarity renormalization group

Nucleon-nucleon potential: how to soften V_{NN}? SRG

The flow equation

$$H_\alpha = U_\alpha \, H_0 \, U_\alpha^\dagger$$

α flow parameter ➡ energy cutoff

$$\frac{\mathrm{d}H_\alpha}{\mathrm{d}\alpha} = \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} U_\alpha^\dagger \, H_\alpha - H_\alpha \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} U_\alpha^\dagger$$

$$\eta_\alpha = \frac{\mathrm{d}U_\alpha}{\mathrm{d}\alpha} U_\alpha^\dagger = -\eta_\alpha^\dagger$$

anti-hermitian generator

$$\frac{\mathrm{d}H_\alpha}{\mathrm{d}\alpha} = [\eta_\alpha, H_\alpha], \qquad H_0 = H_{\alpha=0}$$

This flow equation generates a set of ***α***-dependent unitarily equivalent Hamiltonians H_α

Wenger-Wilson Ansatz

$$\eta_\alpha = [\mathrm{diag}(H_\alpha), H_\alpha]$$

basis $\{|i\rangle\}$

$$\mathrm{diag}(H_\alpha) = \sum_i |i\rangle\langle i|H_\alpha|i\rangle\langle i|$$

For more details and codes see https://github.com/pietropalladino/SRG-project

Nucleon-nucleon potential: how to soften V_{NN}? SRG

with the choice

$$\eta_\alpha = [\mathrm{diag}(H_\alpha), H_\alpha]$$

$$\begin{aligned}\frac{\mathrm{d}\,H_\alpha}{\mathrm{d}\alpha} &= [[\mathrm{diag}(H_\alpha), H_\alpha]\,,\, H_\alpha] \\ &= \mathrm{diag}(H_\alpha)\,H_\alpha\,H_\alpha - 2\,H_\alpha\,\mathrm{diag}(H_\alpha)\,H_\alpha + H_\alpha\,H_\alpha\,\mathrm{diag}(H_\alpha)\end{aligned}$$

separating the off-diagonal and the diagonal matrix elements $\eta_{ij} = H_{ij}\,(H_{ii} - H_{jj})$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha}H_{ij} &= \sum_k [H_{ii}\,(H_{ik}+H_{kk})(H_{kj}+H_{jj}) \\ &+ (H_{ii}+H_{ik})(H_{kj}+H_{kk})\,H_{jj} \\ &- 2\,(H_{ii}+H_{ik})\,H_{kk}\,(H_{kj}+H_{jj})] \\ &= (H_{ii}\,H_{jj} - H_{ii}\,H_{ii} + H_{ii}\,H_{jj} - H_{jj}\,H_{jj})\,H_{ij} \\ &+ \sum_k (H_{ii}+H_{jj}-2\,H_{kk})\;H_{ik}\,H_{kj} \\ &= \boxed{-(H_{ii}-H_{jj})^2\,H_{ij} + \sum_k (H_{ii}+H_{jj}-2\,H_{kk})\;H_{ik}\,H_{kj}.}\end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}H_{ii}}{\mathrm{d}\alpha} &= \sum_k (2\,H_{ii} - 2\,H_{kk})\;H_{ik}\,H_{ki} \\ &= 2\sum_k (H_{ii}-H_{kk})\;|H_{ik}|^2.\end{aligned}$$

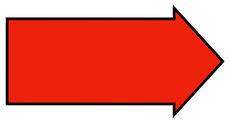
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\sum_i H_{ii}^2 = \sum_i \frac{\mathrm{d}}{\mathrm{d}\alpha}H_{ii}^2 = \sum_i 2H_{ii}\frac{\mathrm{d}}{\mathrm{d}\alpha}H_{ii}$$

For more details and codes see https://github.com/pietropalladino/SRG-project

Nucleon-nucleon potential: how to soften V_{NN}? SRG

H is hermitian, therefore its diagonal elements are real numbers whose squares are positive. The square of the absolute value of the off-diagonal elements and therefore the product of both parts is also positive. A summation of positive elements leads to an increasing result. Thus the derivative of the square of the matrix elements has to increase.

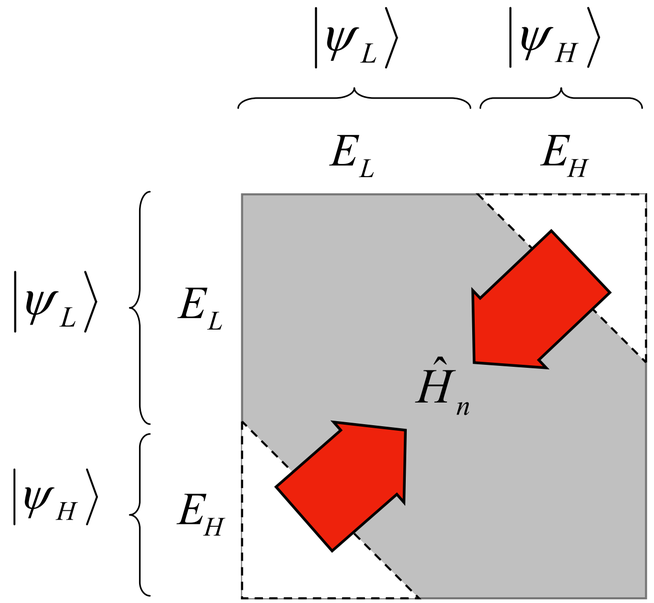
$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\alpha}\sum_i H_{ii}^2 &= 2\sum_{i,\,k} 2\,H_{ii}\,(H_{ii}-H_{kk})\;|H_{ik}|^2 \\
&= 2\sum_{i,\,k} (2\,H_{ii}\,H_{ii}-2\,H_{ii}\,H_{kk})\;|H_{ik}|^2 \\
&= 2\sum_{i,\,k} (H_{ii}-H_{kk})^2\;|H_{ik}|^2 \geq 0.
\end{aligned}$$



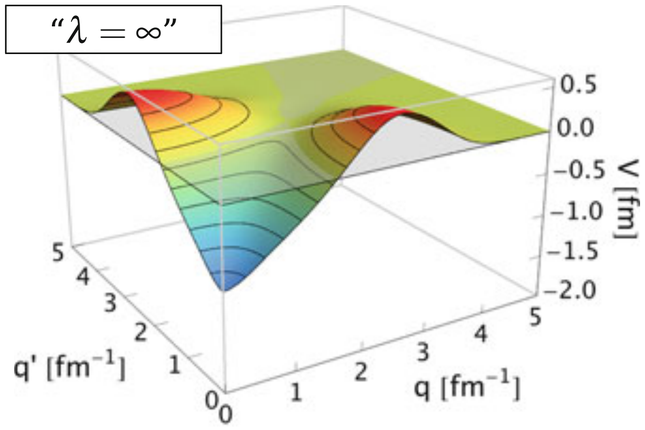
The off-diagonal elements must decrease

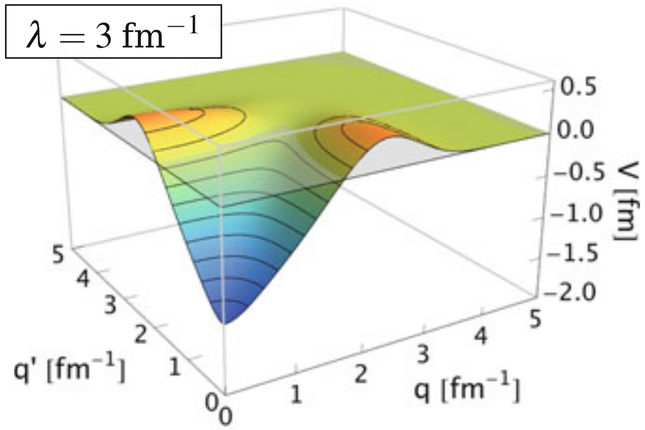
Since the sum of the squares of the diagonal matrix elements has to increase, the off-diagonal matrix elements must decrease monotonically to satisfy this equation. This shows, that the flow equation with the Wenger generator causes the desired diagonalization of the Hamiltonian.

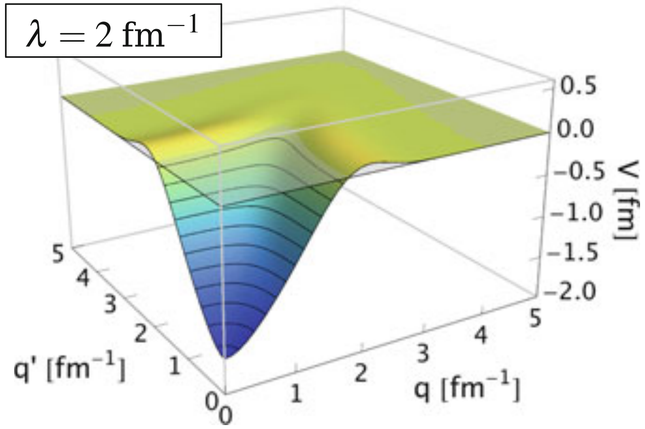
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\mathrm{Tr}\left(H^2\right) = \frac{\mathrm{d}}{\mathrm{d}\alpha}\sum_{i,j}\left(H_{ii}^2+|H_{ij}|^2\right) = 0$$

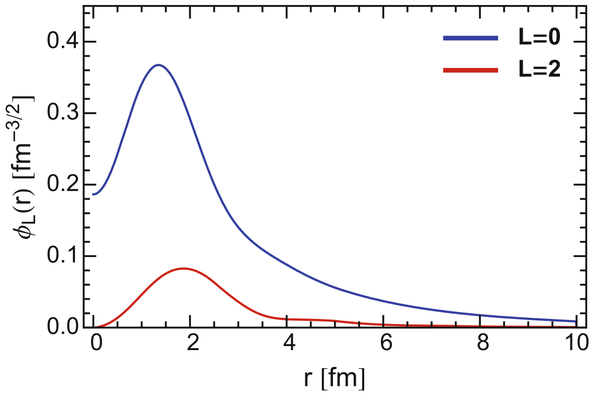


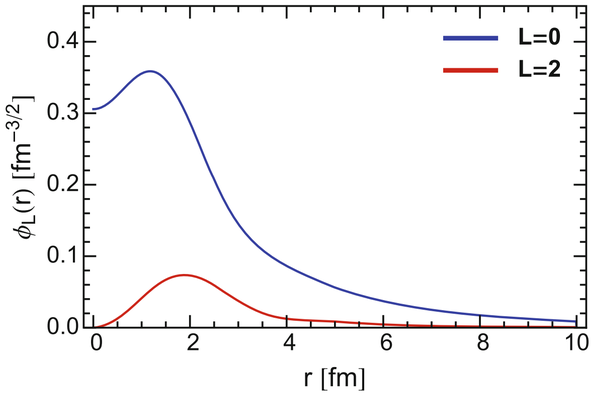
For more details and codes see https://github.com/pietropalladino/SRG-project

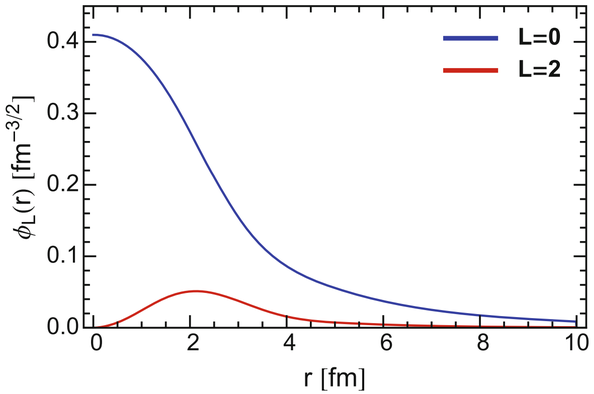






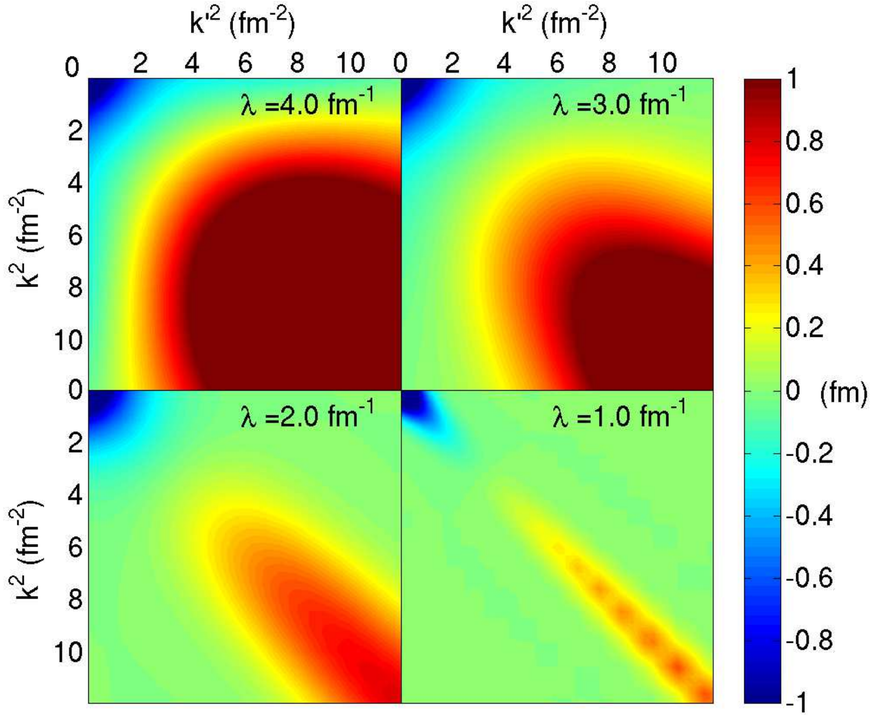


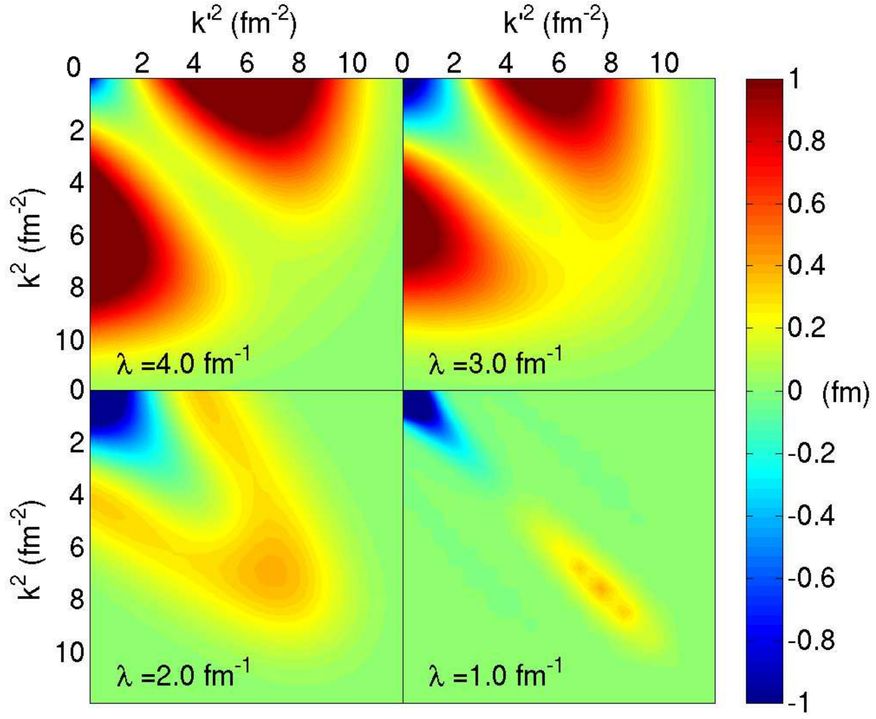


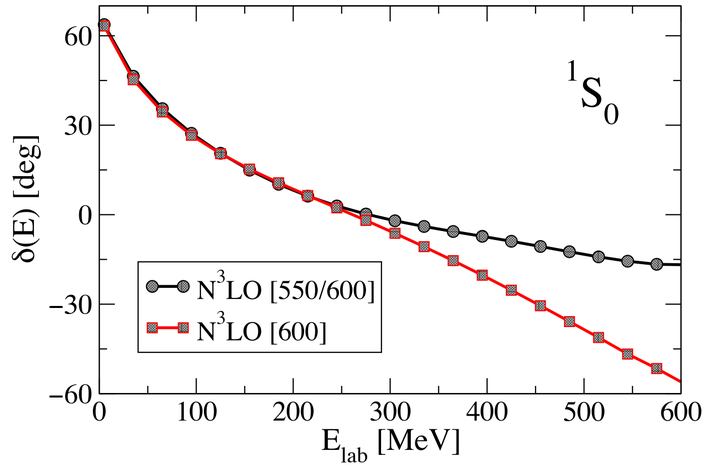


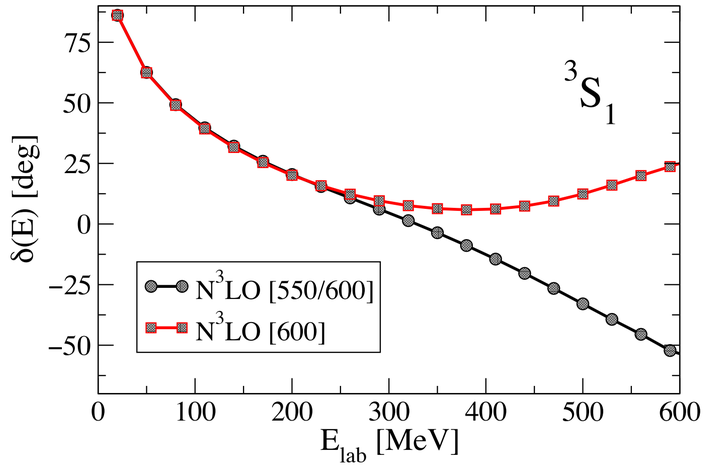
- SRG evolution of the chiral N3LO nucleon-nucleon interaction by Entem and Machleidt, with initial cutoff 500 MeV.
- In the *left column*, we show the momentum-space matrix elements of the interaction in the *S*1 partial wave for different values of the SRG resolution scale .
- In the *right column*, we show the *S*- and *D*-wave components of the deuteron wave function that is obtained by solving the Schrödinger equation with the corresponding SRG-evolved interaction

Nucleon-nucleon potential: how to soften V_{NN}? SRG









Advantages

1. Unitary transformation designed **to decouple** low- and high-energy states
2. All **observables preserved**
3. No relevant changes to low energy observables even when high momenta are removed
4. Natural hierarchy of many-body forces maintained

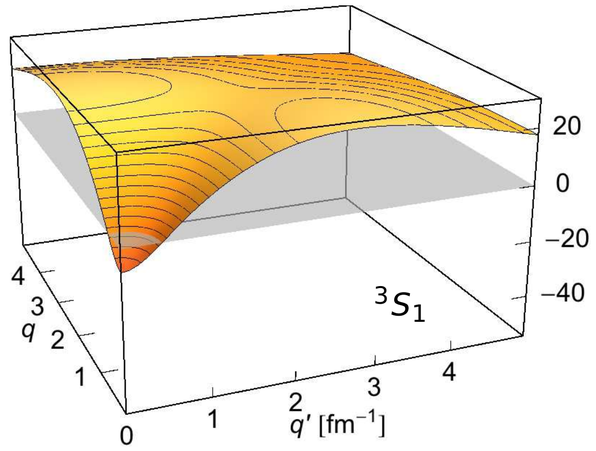
Disadvantages

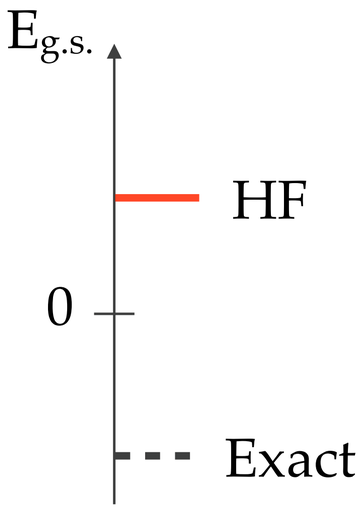
Induces many-body forces

© **Perry** and **Furnstahl** (Ohio) and **Bogner** (NSCL)

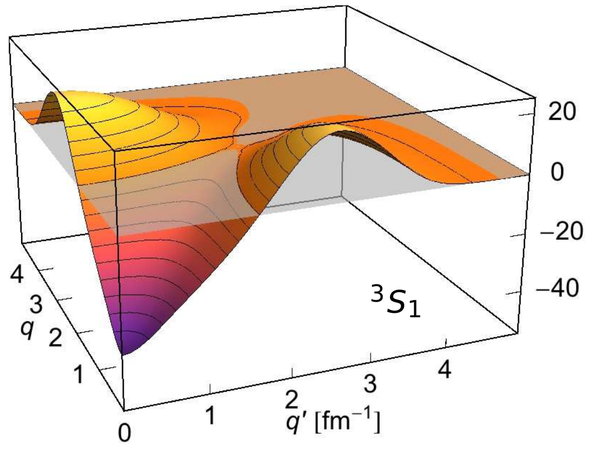
Hartree-Fock with ab initio interactions

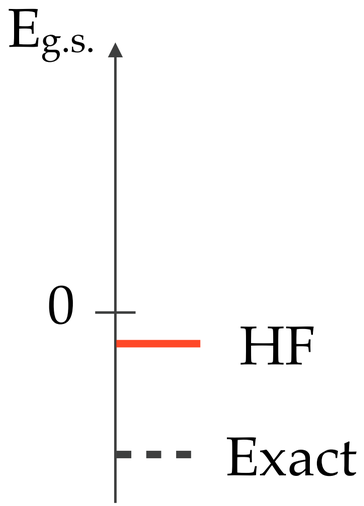
OBE potentials



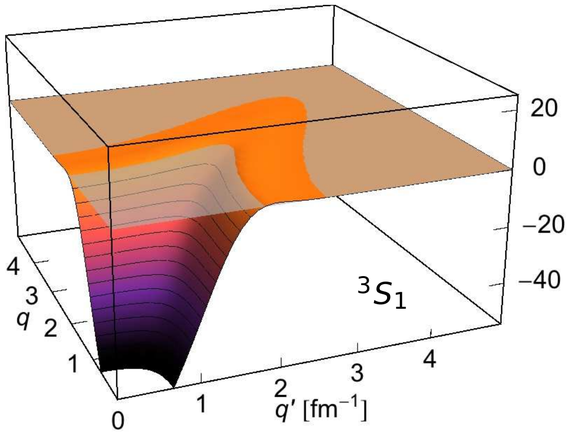


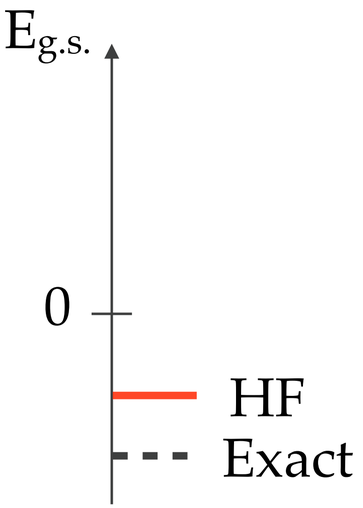
Chiral potentials





SRG potentials





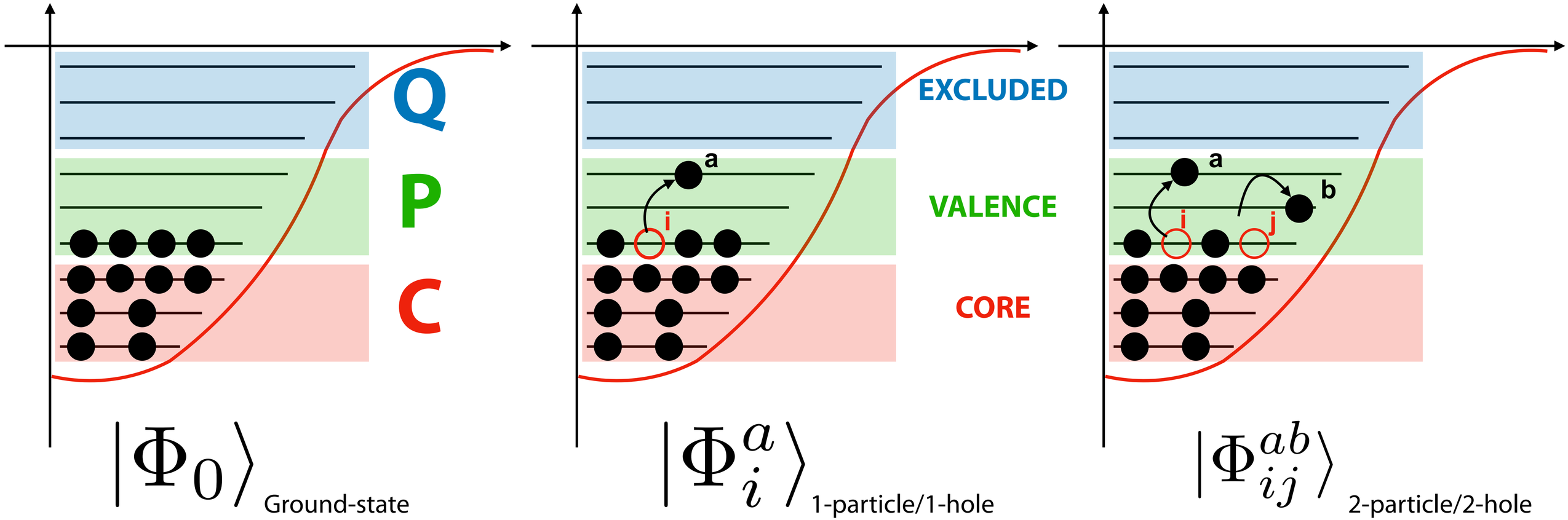
Somà, Lecture @ Fiera di Primiero

What about the residual interaction? Interacting shell model

In the previous slides we have seen that it's always possible to write

$$|\Psi\rangle = \sum C_{k_i} |k_1 k_2 \dots k_A\rangle \equiv \sum_i c_i |\Phi_i\rangle$$

Slater determinants



$|\Phi_0\rangle$ Ground-state

$|\Phi_i^a\rangle$ 1-particle/1-hole

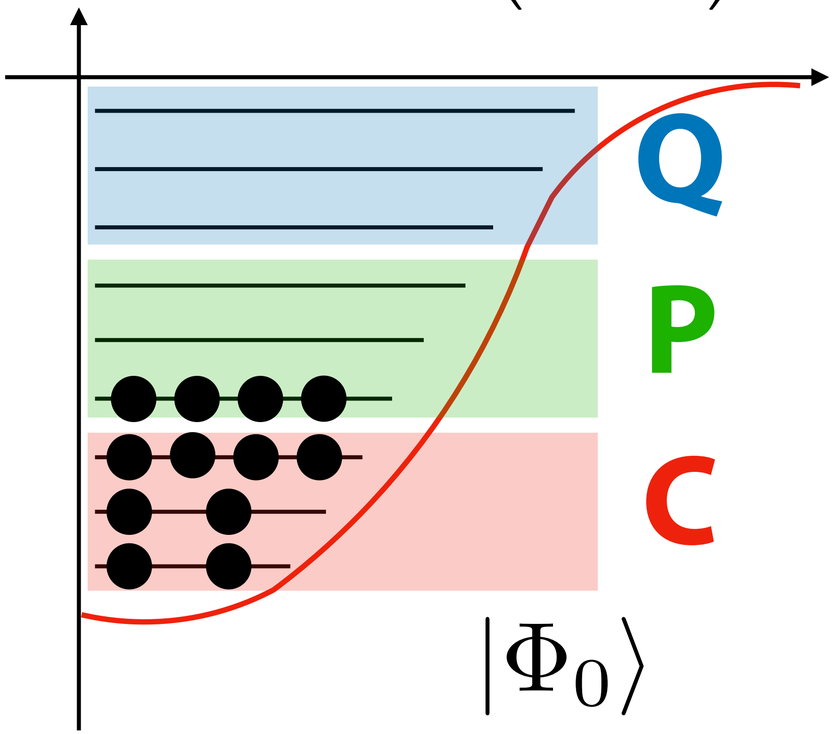
$|\Phi_{ij}^{ab}\rangle$ 2-particle/2-hole

Interacting shell model - Ansatz for the ground state (2nd quant.)

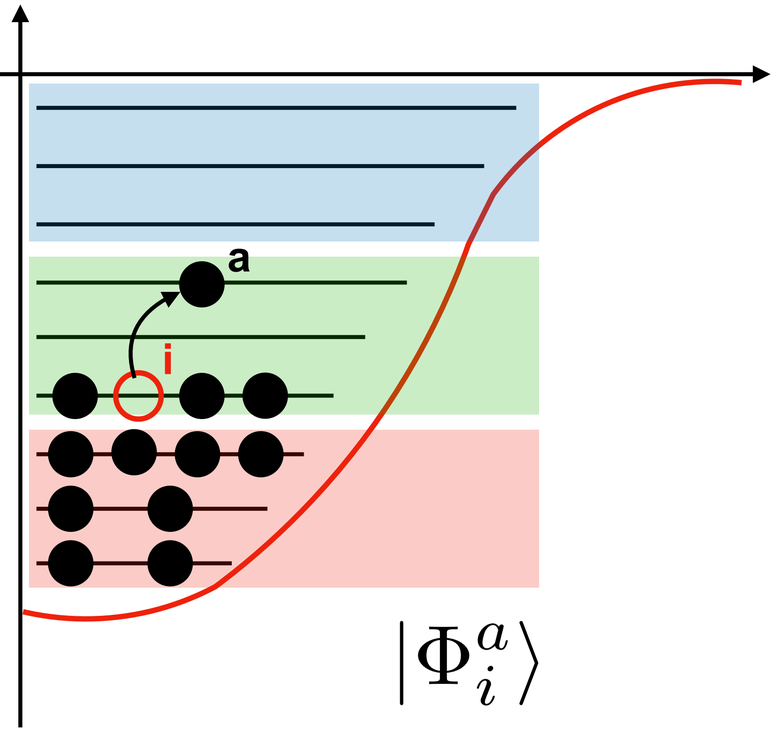
$$|\Phi_0\rangle = \left(\prod_{i\leq F} \hat{a}_i^\dagger\right)|0\rangle$$

1p-1h state $|\Phi_i^a\rangle = \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle$

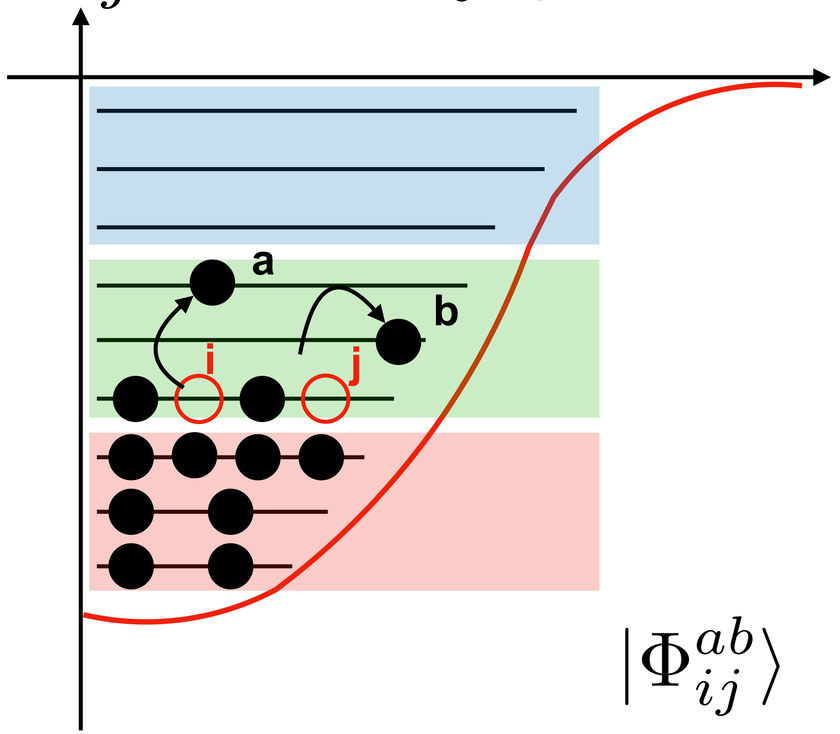
2p-2h state $|\Phi_{ij}^{ab}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle$



$|\Phi_0\rangle$



$|\Phi_i^a\rangle$



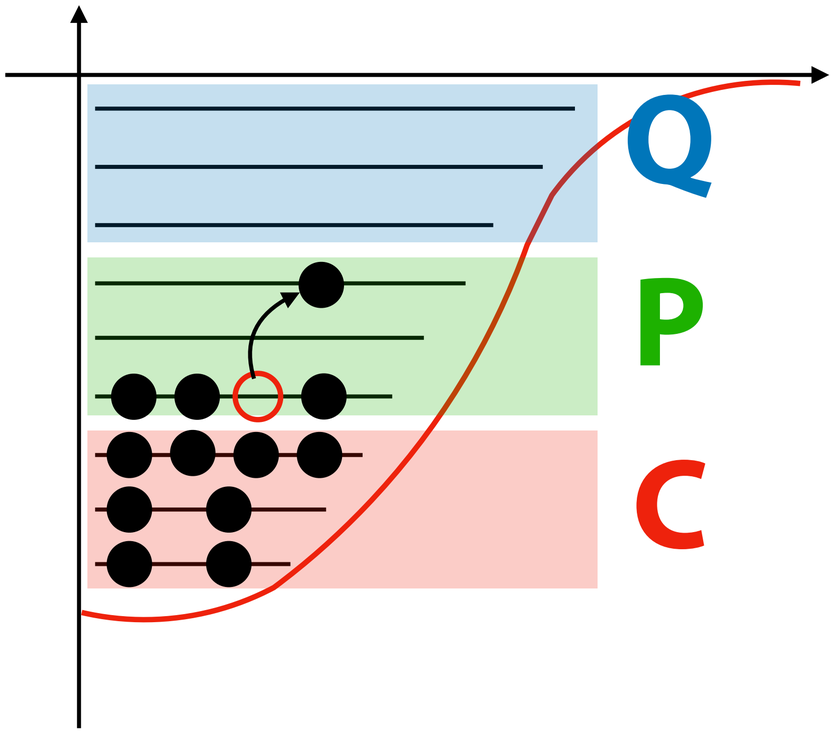
$|\Phi_{ij}^{ab}\rangle$

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{a,i} C_i^a|\Phi_i^a\rangle + \sum_{ab,ij} C_{ij}^{ab}|\Phi_{ij}^{ab}\rangle + \cdots = (C_0 + \hat{C})|\Phi_0\rangle$$

Correlation operator

Interacting shell model - A simple recipe

1) Construct orbitals from H_0, i.e. harmonic oscillator
2) Orbitals could be divided in
   - Inert core (orbitals always full) **C**
   - Valence space (*p-h* excitations) **P**
   - Excluded space (orbitals always empty) **Q**
3) Starting from V_{res} build V_{eff} (renormalised interaction for the active space **P**)
4) Solve the Schrödinger equation by diagonalising $H = H_0 + V_{eff}$



- The residual two-body interaction V_{res} has to be "effective", i.e. V_{res} has to take implicitly into account of the degrees of freedom that are explicitly considered frozen.
- This means that V_{res} should contain core-polarization and particle-particle excitations , so that the eigenvalues of the shell-model hamiltonian should be the same (or at least very close) to those of the nuclear many-body hamiltonian diagonalized in the full Hilbert space

Interacting shell model - A simple treatment

$$H|\psi\rangle = E|\Psi\rangle$$

approximation

$$|\Psi\rangle = \sum_{i}^{N_{cut}} c_i |\Phi_i\rangle$$

$\langle\Phi_j|\times$

$$\sum_{i}^{N_{cut}} c_i \langle\Phi_j|H|\Phi_i\rangle = E \sum_{i}^{N_{cut}} c_i \langle\Phi_j|\Phi_i\rangle$$

$$H_{ij} \qquad \delta_{ij}$$

Eigenvalue problem for ***H***

$$\boldsymbol{Hc} = \boldsymbol{Ec}$$

$$(H = H^{\dagger})$$

Hermitian

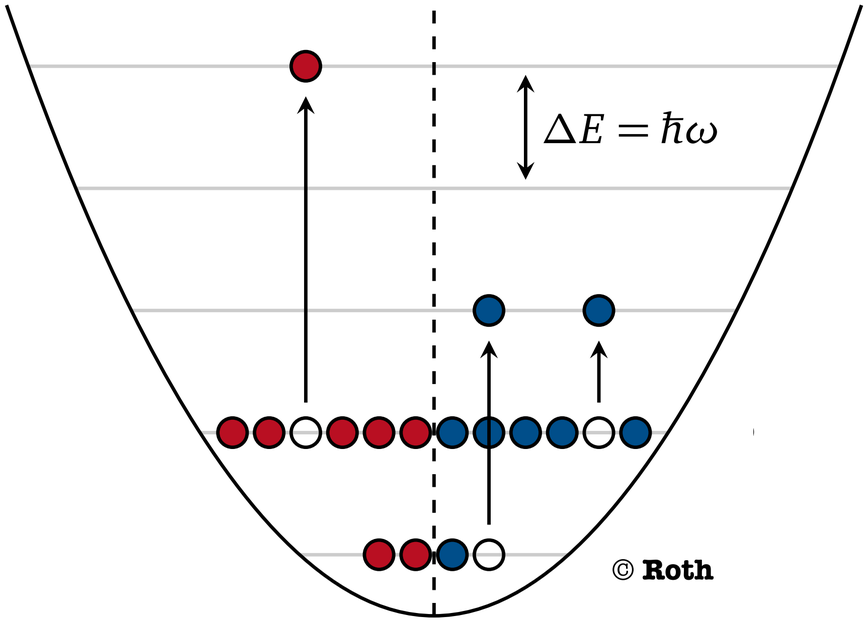
$$\begin{bmatrix} \vdots \\ \dots \; H_{ji} \; \dots \\ \vdots \end{bmatrix} \begin{bmatrix} \vdots \\ C_i^{(k)} \\ \vdots \end{bmatrix} = E_k \begin{bmatrix} \vdots \\ C_j^{(k)} \\ \vdots \end{bmatrix}$$

Model space truncations

FCI

Full configuration interaction

truncate the 1-body basis (at some maximum single-particle energy e_{max})



NO-CORE

No-core shell model basis

Cut the many-body basis (total number of HO excitation quanta N_{max})

Example: $N_{max} = 6$

KSHELL

BIGSTICK

ANTOINE

NUSHELLX

CoSMo

Eigenvalue problem for ***H***

$$\boldsymbol{Hc} = \boldsymbol{Ec}$$

$$(H = H^{\dagger})$$

Hermitian

$$\begin{bmatrix} \vdots \\ \dots \; H_{ji} \; \dots \\ \vdots \end{bmatrix} \begin{bmatrix} \vdots \\ C_i^{(k)} \\ \vdots \end{bmatrix} = E_k \begin{bmatrix} \vdots \\ C_j^{(k)} \\ \vdots \end{bmatrix}$$

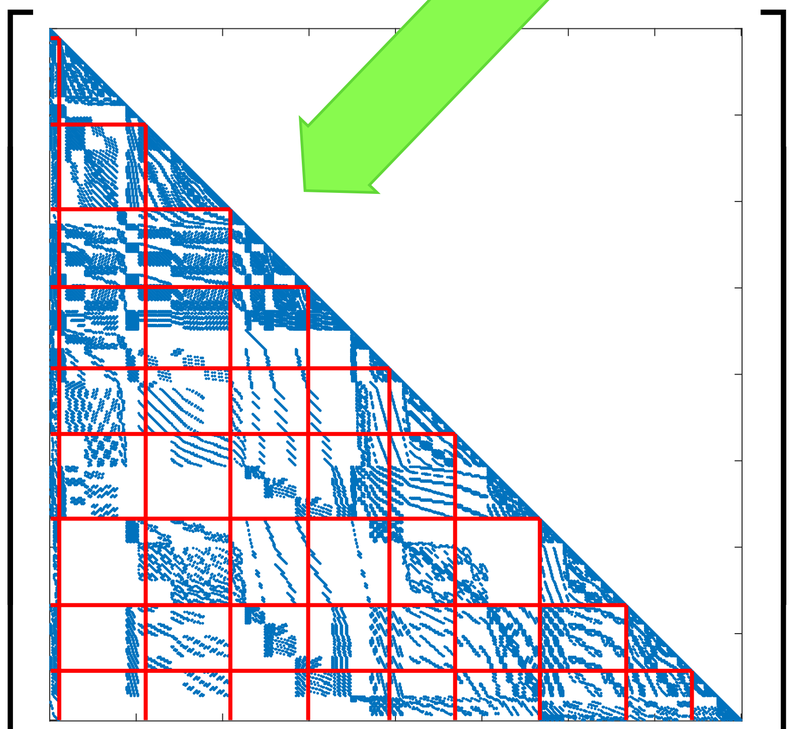
Sparse matrix

↓

Only the lowest energy eigenvalues are interesting

↓

Lanczos algorithm



$$\begin{bmatrix} \\ \\ \\ \end{bmatrix} \begin{bmatrix} \vdots \\ C_i^{(k)} \\ \vdots \end{bmatrix} = E_k \begin{bmatrix} \vdots \\ C_j^{(k)} \\ \vdots \end{bmatrix}$$

How to treat the NN potential

The possible ways to derive a shell-model residual interaction V_{res} can be grouped

Empirical V_{res} fitted on experimental data

The V_{res} two-body matrix elements are treated as free parameters

They are derived by a best-fit procedure to a selected set of experimental data

Pros: these shell-model interactions are a very refined tool, very successful, and still the most widely employed ones

Cons: the predictions of the physics that characterize unexplored features of the spectroscopy of the nuclei could be biased by the choice of the experimental databases

Empirical V_{res} with a simple analytical expression

They have a simple analytical expression, i.e.

- pairing or pairing plus quadrupole interactions
- surface delta interaction

Pros: they are very useful in order to understand what is the relevant physics underlying the spectroscopic structure of the nucleus

Cons: out-of-date

Realistic effective V_{res} derived microscopically from the free nucleon-nucleon potential V_{NN}

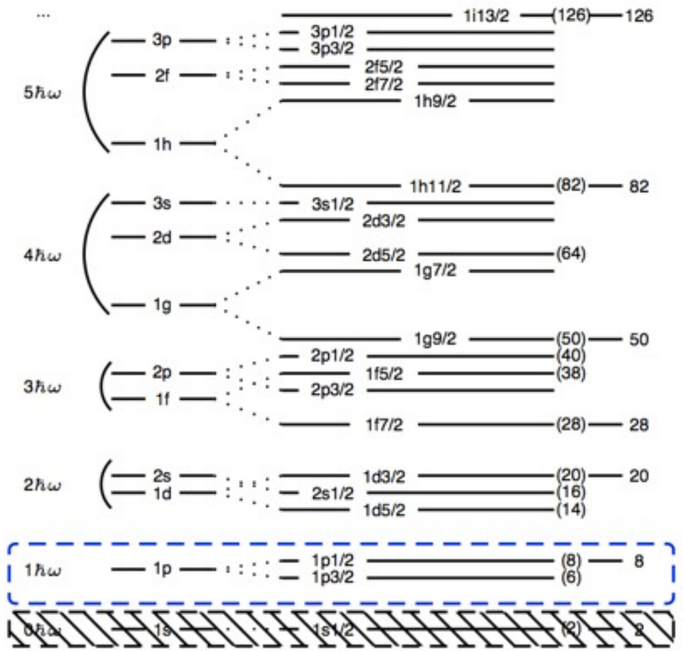
The shell-model V_{res} is derived directly from the free nucleon-nucleon potential

Pros: no parameters are involved in the shell-model calculation, apart the single-particle energies

Cons: the theory to derive these interactions is very complicated and still under investigation

Coraggio, Lecture @Nuclear Physics School "Raimondo Anni", 5th course

Interacting shell model - Phenomenological way



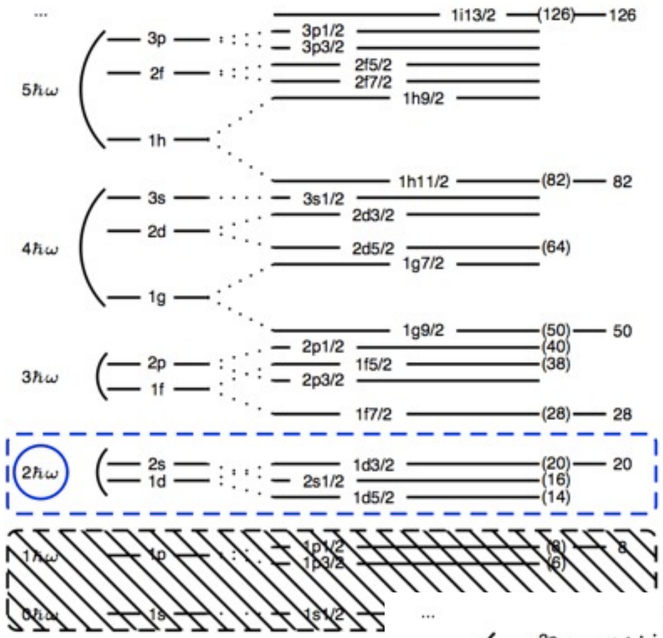
p-shell nuclei

$4 \leq A \leq 16$

Cohen-Kurath

VALENCE SPACE

CORE



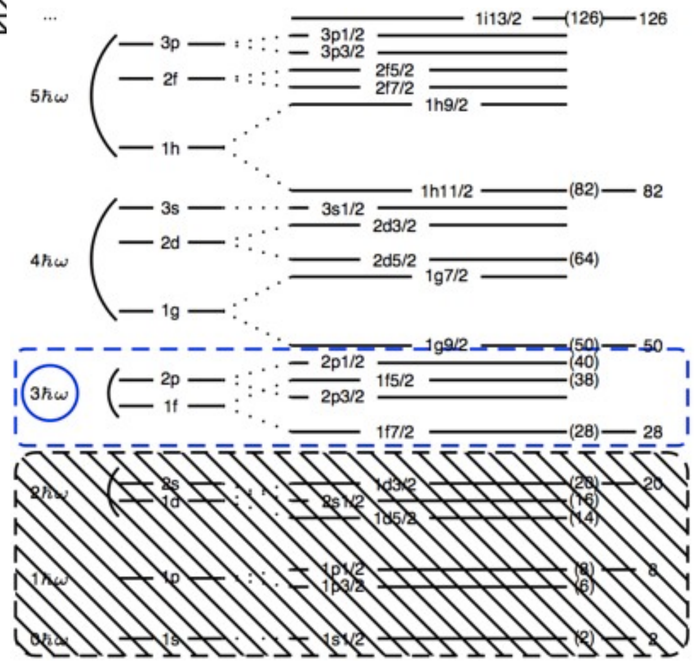
sd-shell nuclei

$16 \leq A \leq 40$

USD interaction

VALENCE SPACE

CORE



pf-shell nuclei

$40 \leq A \leq 80$

GXPF1 interactions

VALENCE SPACE

CORE

...

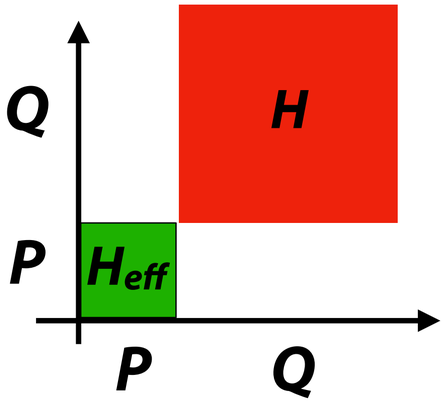
The effective interaction is a set of two-body matrix elements tuned to reproduce experimental data

Example: for nuclei ranging from ^{16}O to ^{40}Ca, we consider the 0*s* and the 0*p* shells filled by 8 protons and 8 neutrons (^{16}O core), and the valence nucleons interact in the 6 1*s* 0*d* proton and neutron orbitals

Bacca, Lecture @EXOTIC 2015: Re-writing Nuclear Physics textbooks

Effective interactions in the valence space

Define a valence space ***P***



$$P = \sum_{i=1}^{d} |\Phi_i\rangle\langle\Phi_i| \qquad Q = 1 - P,$$

$$P^2 = P, \quad Q^2 = Q, \quad PQ = QP = 0$$

$$H|\Psi_\nu\rangle = E_\nu|\Psi_\nu\rangle \Rightarrow PH_{\text{eff}}P|\Psi_\alpha\rangle = (E_\alpha - E_C)P|\Psi_\alpha\rangle$$

E_C energy of the core

Currently there are several ways to derive an effective SM Hamiltonian starting from the bare interactions between nucleons.

1. Many-body perturbation theory
2. Lee-Suzuki transformation
3. Valence-space in-medium similarity renormalization group (VS-IMSRG)
4. Shell-model coupled cluster (SMCC)
5. No-core shell model (NCSM) with a core based on the Lee-Suzuki similarity transformation

$$H_{\text{eff}} = e^{\mathcal{G}} H e^{-\mathcal{G}}$$

$$QH_{\text{eff}}P = 0$$

@ **Coraggio and Itaco,** Perturbative Approach to Effective Shell-Model Hamiltonians and Operators

Effective interactions in the valence space

This means that we are looking for a new Hamiltonian ***H*** whose eigenvalues are the same as those of the Hamiltonian ***H*** for the *A*-nucleon system but which satisfies the decoupling equation between the model space ***P*** and its complement ***Q***

$$H_{\text{eff}} = P\mathcal{H}P \qquad Q\mathcal{H}P = 0$$

$$\mathcal{H} = X^{-1}HX \longrightarrow X = e^{\omega} \longrightarrow \omega = Q\omega P$$

$$H_{\text{eff}} = P\mathcal{H}P = PHP + PHQ\omega \longrightarrow QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0$$

The matrix equation is non-linear

Recursive relation

$$H_1^{\text{eff}}(\omega) = \hat{Q}(\epsilon_0) - PH_1Q\frac{1}{\epsilon_0 - QHQ}\omega H_1^{\text{eff}}(\omega)$$

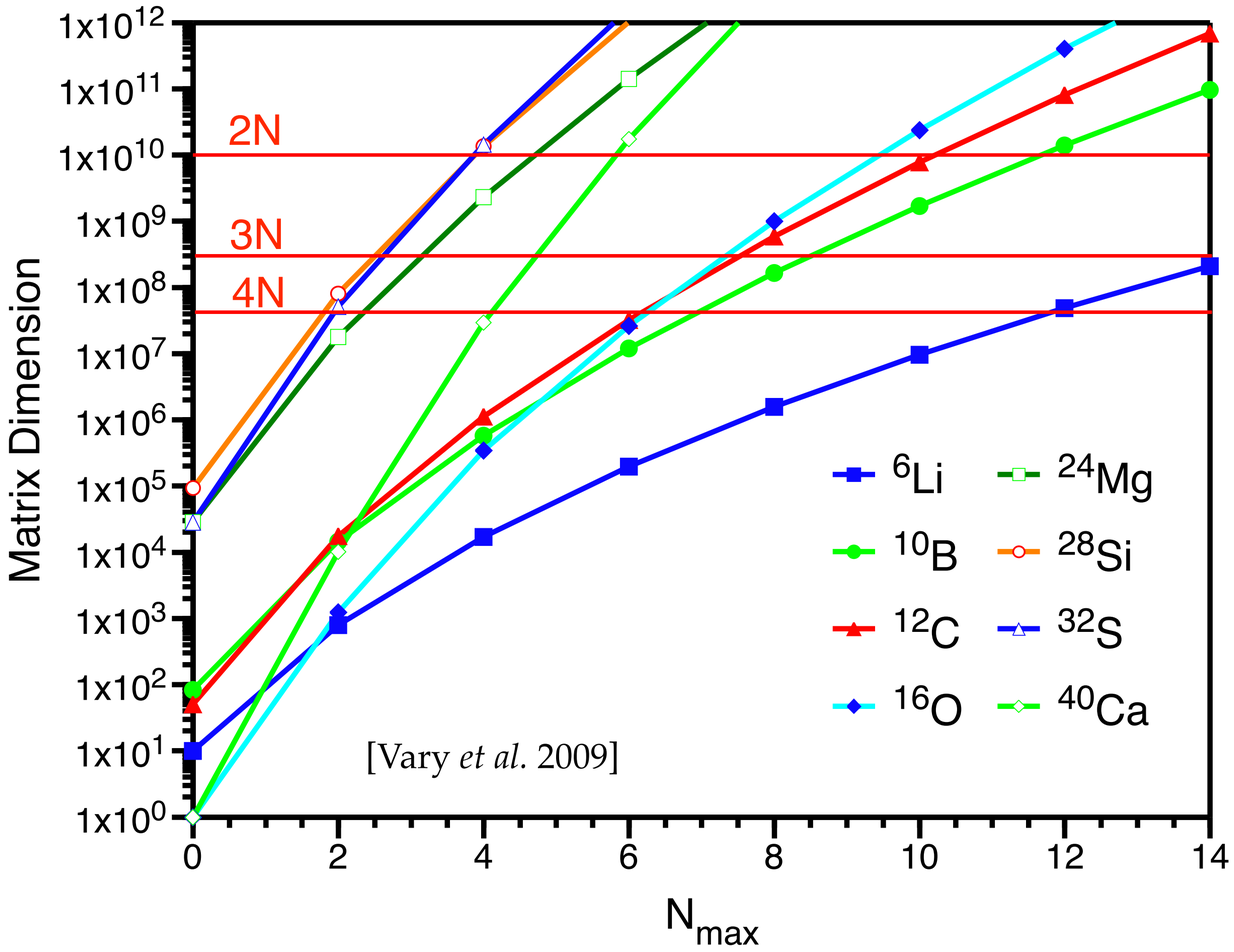
$$H_0 = \sum_{i=1}^{A}\left(\frac{p_i^2}{2m} + U_i\right)$$

$$H_1 = \sum_{i<j=1}^{A} V_{ij}^{NN} - \sum_{i=1}^{A} U_i$$

$$\hat{Q}(\epsilon) = PH_1P + PH_1Q\frac{1}{\epsilon - QHQ}QH_1P$$

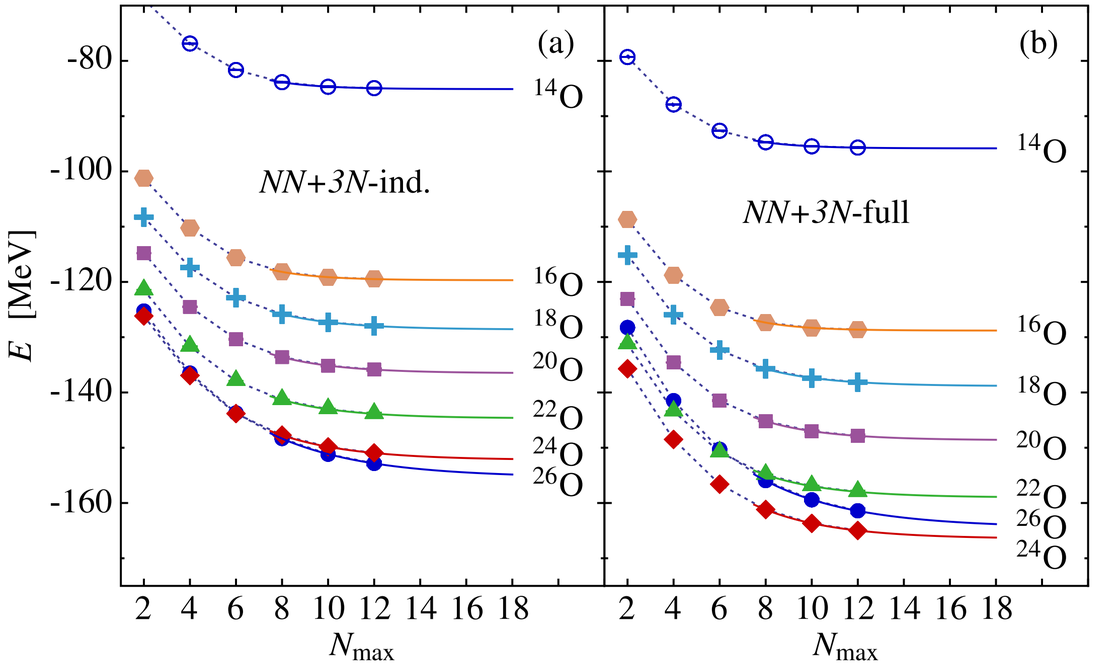
@ **Coraggio and Itaco,** Perturbative Approach to Effective Shell-Model Hamiltonians and Operators

Dimensionality



Importance truncation: prior to diagonalisation

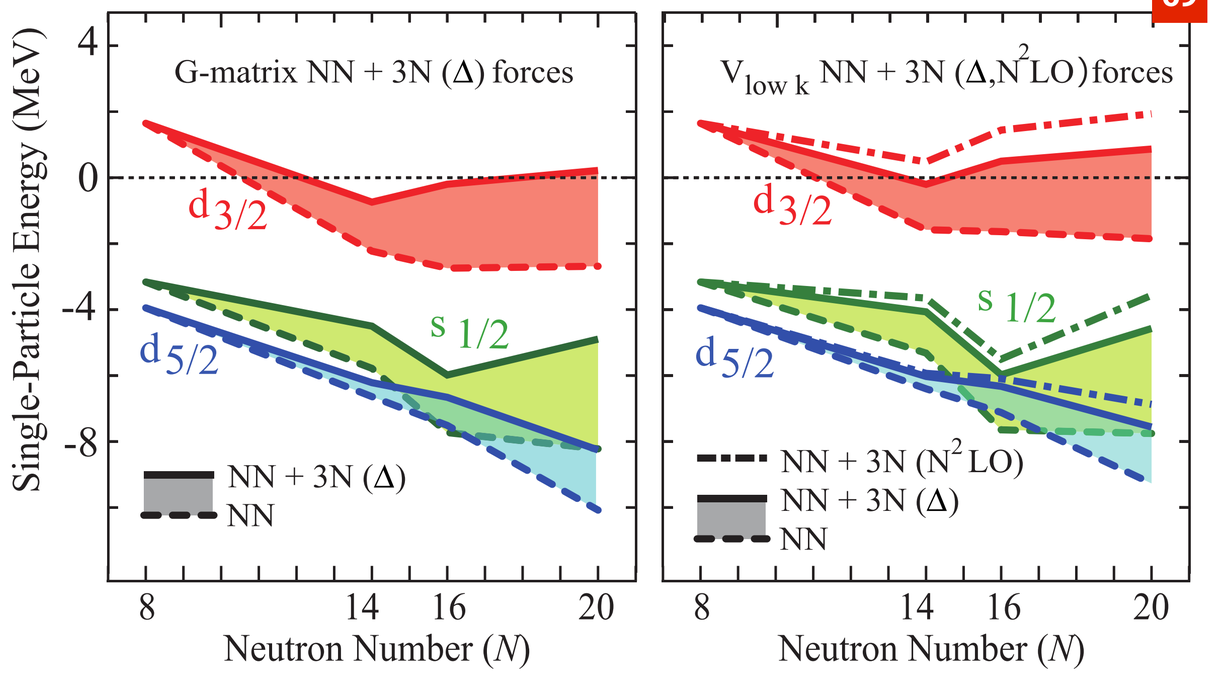
- Estimate the size of each entry upon a given criterion
- Discard irrelevant elements
- Construct importance-truncated space

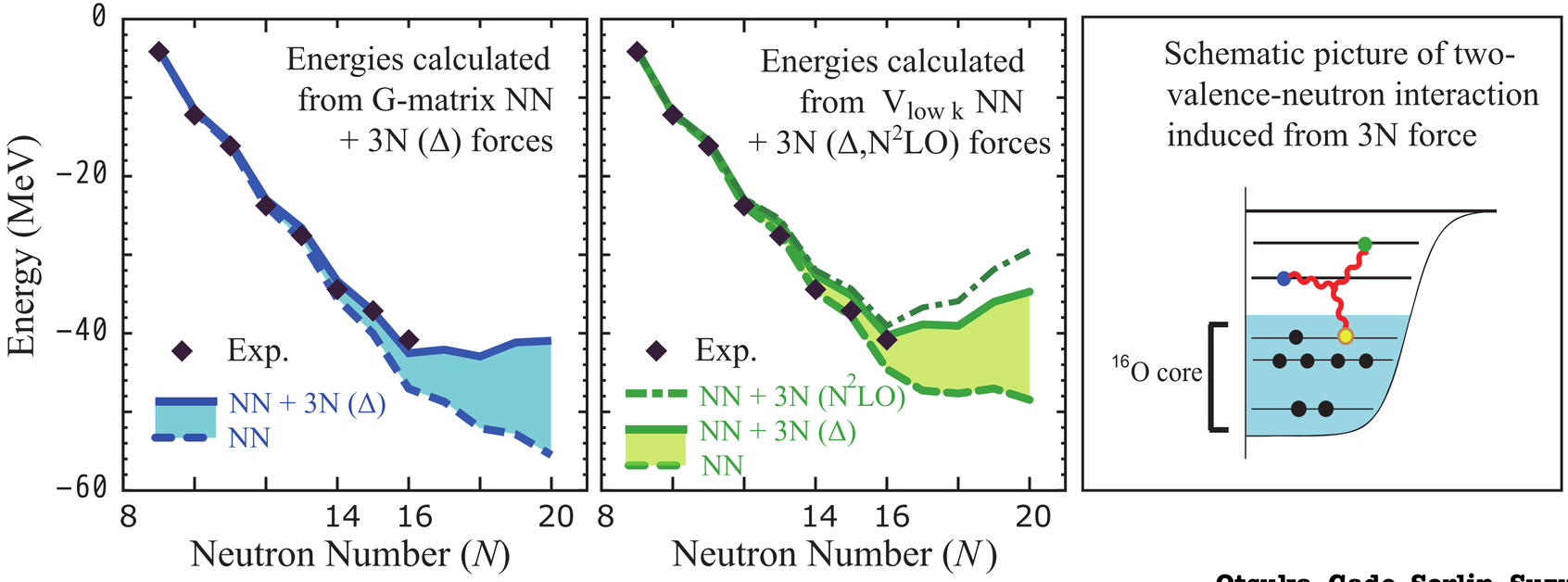


Hergert, Binder, **Calci**, **Langhammer**, and **Roth**, Ab Initio Calculations of Even Oxygen Isotopes with Chiral Two-Plus-Three-Nucleon Interactions

Shell model: Predictions

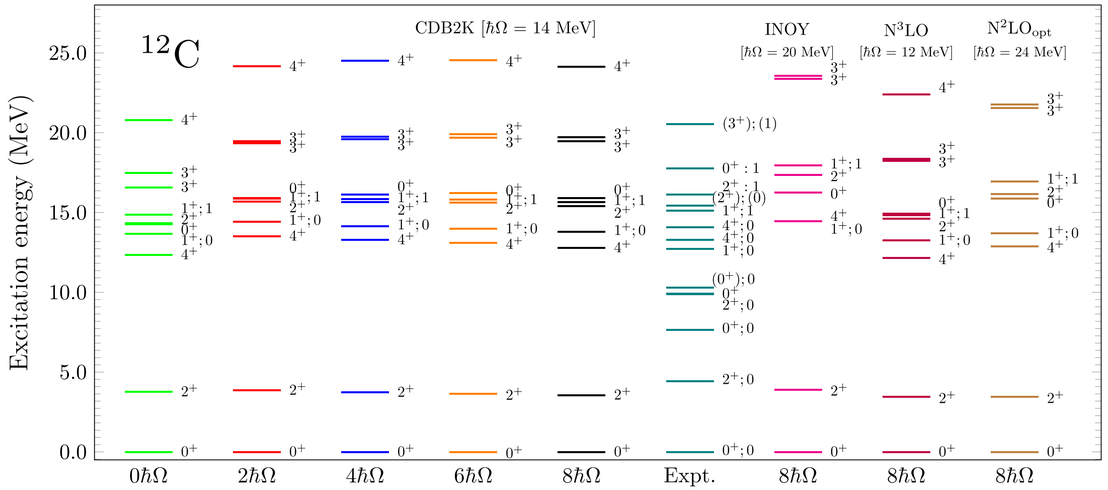
- Neutron Single Particle Energies (SPE) of the oxygen isotopes starting from the stable O to heavier ones with more neutrons. The SPEs calculated with NN interactions in the G-matrix formalism put the neutron dripline incorrectly beyond ^{28}O.
- The repulsive 3N contributions become significant with increasing N.
- The general trend seems to suggest that a good fraction of the effects of the 3NF, and perhaps other 3NFs in general, is included empirically in shell-model interactions.
- The 3NF changes them to be very close to experimental values and places the dripline correctly.

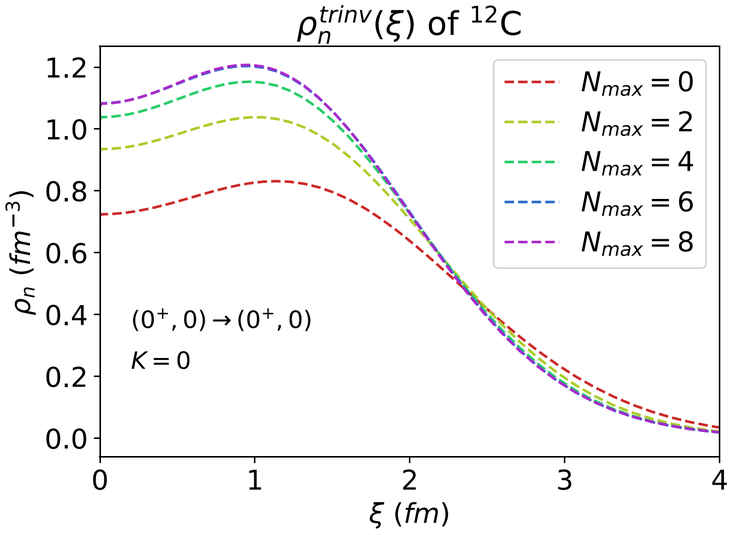


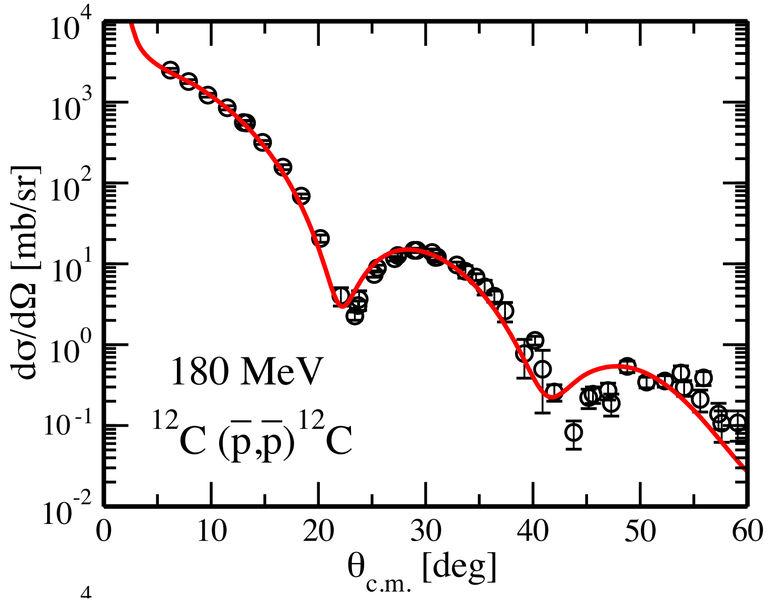


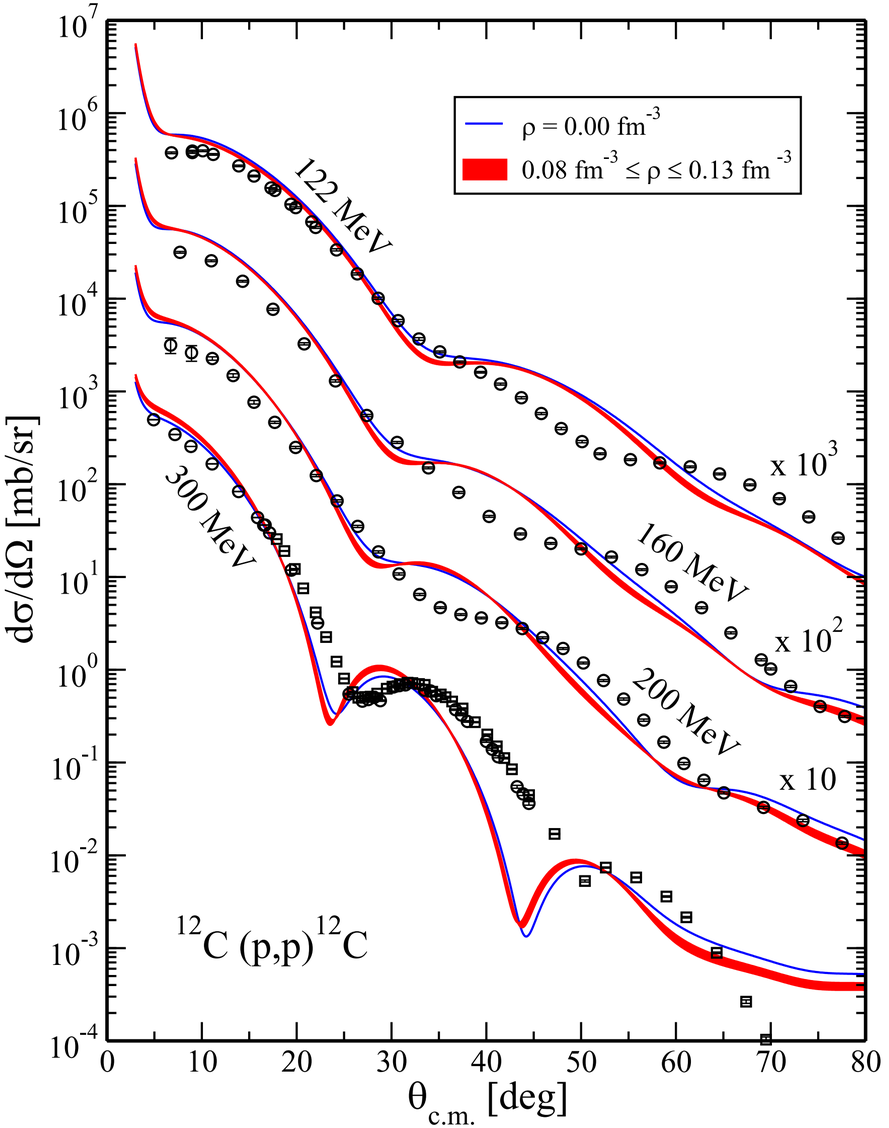
Otsuka, Gade, **Sorlin**, **Suzuki**, and **Utsuno**, Evolution of shell structure in exotic nuclei

No-core shell model









Choudhary, **Srivastava** ,**Gennari**, and **Navrátil**, Ab initio no-core shell-model description of 10−14C isotopes

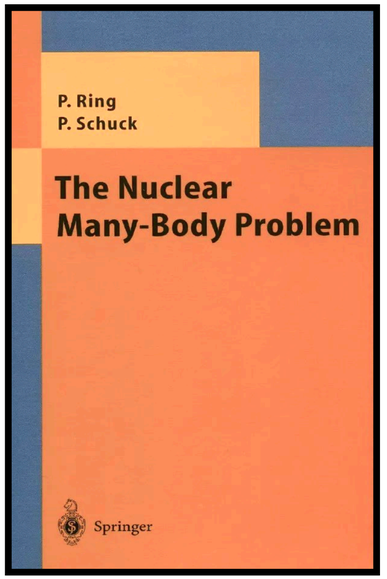
Vorabbi, **Gennari**, **Finelli** ,**Giusti**, **Navrátil**, and **Machleidt**, Impact of three-body forces on elastic nucleon-nucleus scattering observables

Vorabbi, **Gennari**, **Finelli** ,**Giusti** ,and **Navrátil**, Elastic Antiproton-Nucleus Scattering from Chiral Forces

The nuclear many-body problem (vii)

For a system of $A = N + Z$ particles

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$



Formal manipulation

$$\hat{H} = \hat{T} + \hat{V}_{2b} + \hat{V}_{3b} + \dots$$

Kinetic energy

Two- and three-body potential

$$\hat{T} = \sum_{i=1}^{A} \frac{\hat{\boldsymbol{p}}_i^2}{2m_i}$$

$$\sum_{i<j}^{A} \hat{V}_{2b}(\boldsymbol{r}_i, \boldsymbol{r}_j) + \sum_{i<j<k}^{A} \hat{V}_{3b}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k)$$

Try to solve the nuclear Schrödinger problem from a ***ab-initio*** approach

"exact" or, at least, formally exact

"realistic interaction"

Alternative approaches: Self-consistent Green Functions

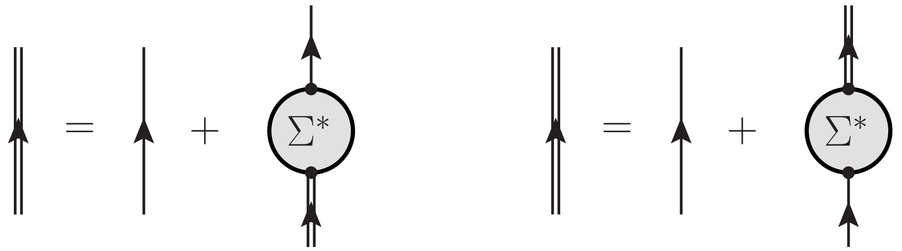
Dyson equation

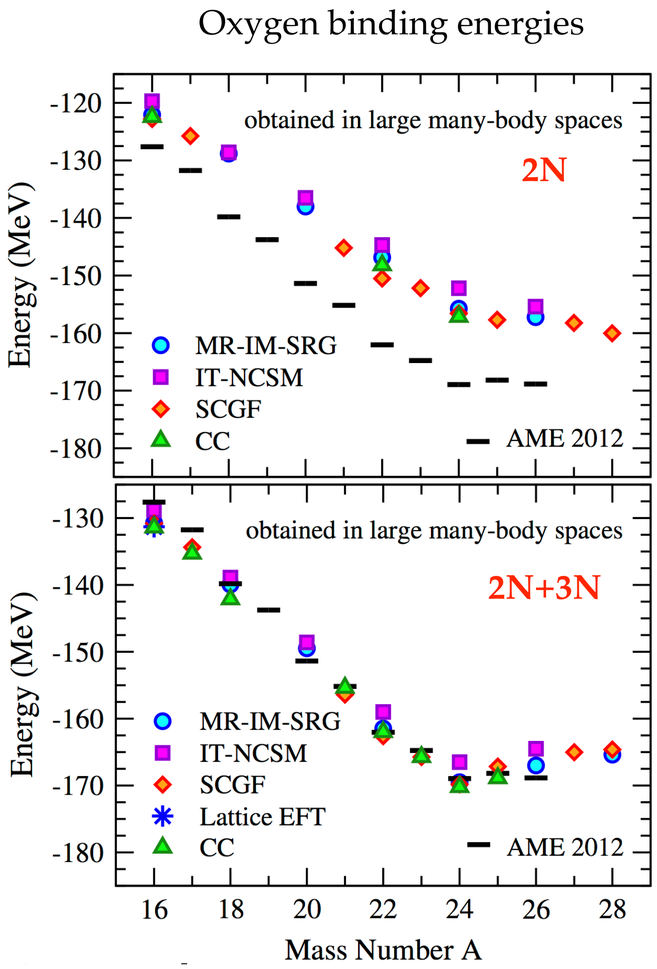
$$G = G^{(0)} + G^{(0)} \Sigma G$$

The problem is simplified by truncating the expansion of G in terms of 1-particle, 2-particle objects

unperturbed Green's function

many-body effects contained in the **self-energy** Σ





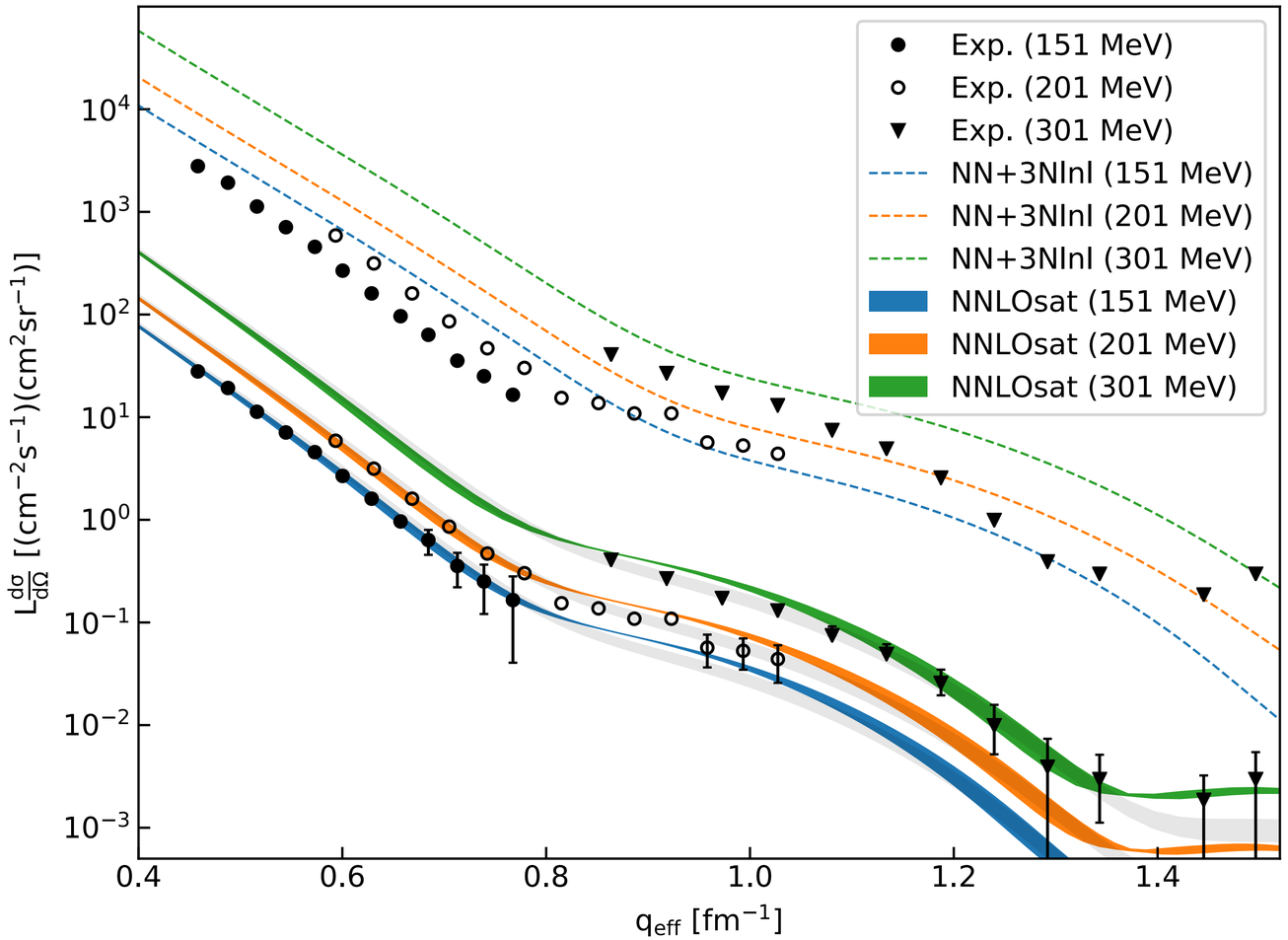
Through the one-body Green's function:

- Ground-state energy
- One-body observables (radii, densities…)
- Spectroscopy of the $A \pm 1$-body systems
- Elastic nucleon-nucleus scattering

Barbieri and **Carbone**, Self-consistent Green's function approaches

Alternative approaches: Self-consistent Green Functions

Dyson equation $$G = G^{(0)} + G^{(0)} \Sigma G$$



Hamiltonian

- Chiral EFT
  Bare NNLOsat
  Bare NN+3NInl
- Effective 3NF

Basis parameters

- $\hbar\Omega = 10$ to 14 MeV
- $N_{max} = 11 - 13$
- $E_{3max} = 16$

Arthuis, **Barbieri Vorabbi,** and **Finelli**, Ab Initio Computation of Charge Densities for Sn and Xe Isotopes

Alternative approaches: Coupled Cluster

Coester and Kümmel developed the ideas that led to coupled cluster theory in the late 1950s. The correlated wave function of a many-body system $|\Psi\rangle$ can be formulated as an exponential of correlation operators T acting on a reference state

$$|\Psi\rangle = \exp\left(\hat{T}\right)|\Phi\rangle$$

ground-state

$$|\Psi_0\rangle = |\Psi_{CC}\rangle = e^{\hat{T}}|\Phi_0\rangle = \left(\sum_{n=1}^{A}\frac{1}{n!}\hat{T}^n\right)|\Phi_0\rangle$$

A represents the maximum number of particle-hole excitations

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$$

$$\hat{T}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i_1,i_2,\ldots i_n \\ a_1,a_2,\ldots a_n}} t_{i_1 i_2 \ldots i_n}^{a_1 a_2 \ldots a_n} a_{a_1}^\dagger a_{a_2}^\dagger \ldots a_{a_n}^\dagger a_{i_n} \ldots a_{i_2} a_{i_1}$$

$$E_{\mathrm{CC}} = \langle\Phi_0|\overline{H}|\Phi_0\rangle$$

$$\overline{H} = e^{-\hat{T}}\hat{H}_N e^{\hat{T}}$$

$$\hat{H}_N = \hat{H} - \langle\Phi_0|\hat{H}|\Phi_0\rangle$$

Lietz, Novario, Jansen, Hagen, and **Hjorth-Jensen**, Computational Nuclear Physics and Post Hartree-Fock Methods

Alternative approaches: IMSRG

Choosing a single Slater determinant as the reference state, we can rewrite the Hamiltonian *exactly* in terms of normal-ordered operators

$$\hat{H} = E + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

Wick theorem

IMSRG2

$$\hat{\eta}(s) \approx \hat{\eta}^{(1)}(s) + \hat{\eta}^{(2)}(s)\,,$$

$$\hat{H}(s) \approx E(s) + f(s) + \Gamma(s)\,,$$

$$\frac{d}{ds}\hat{H}(s) \approx \frac{d}{ds}E(s) + \frac{d}{ds}f(s) + \frac{d}{ds}\Gamma(s)\,.$$

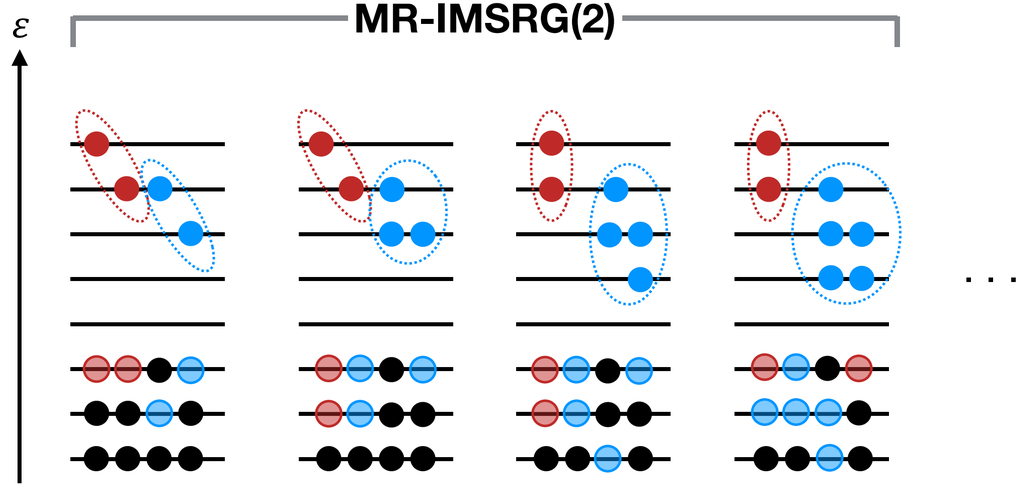
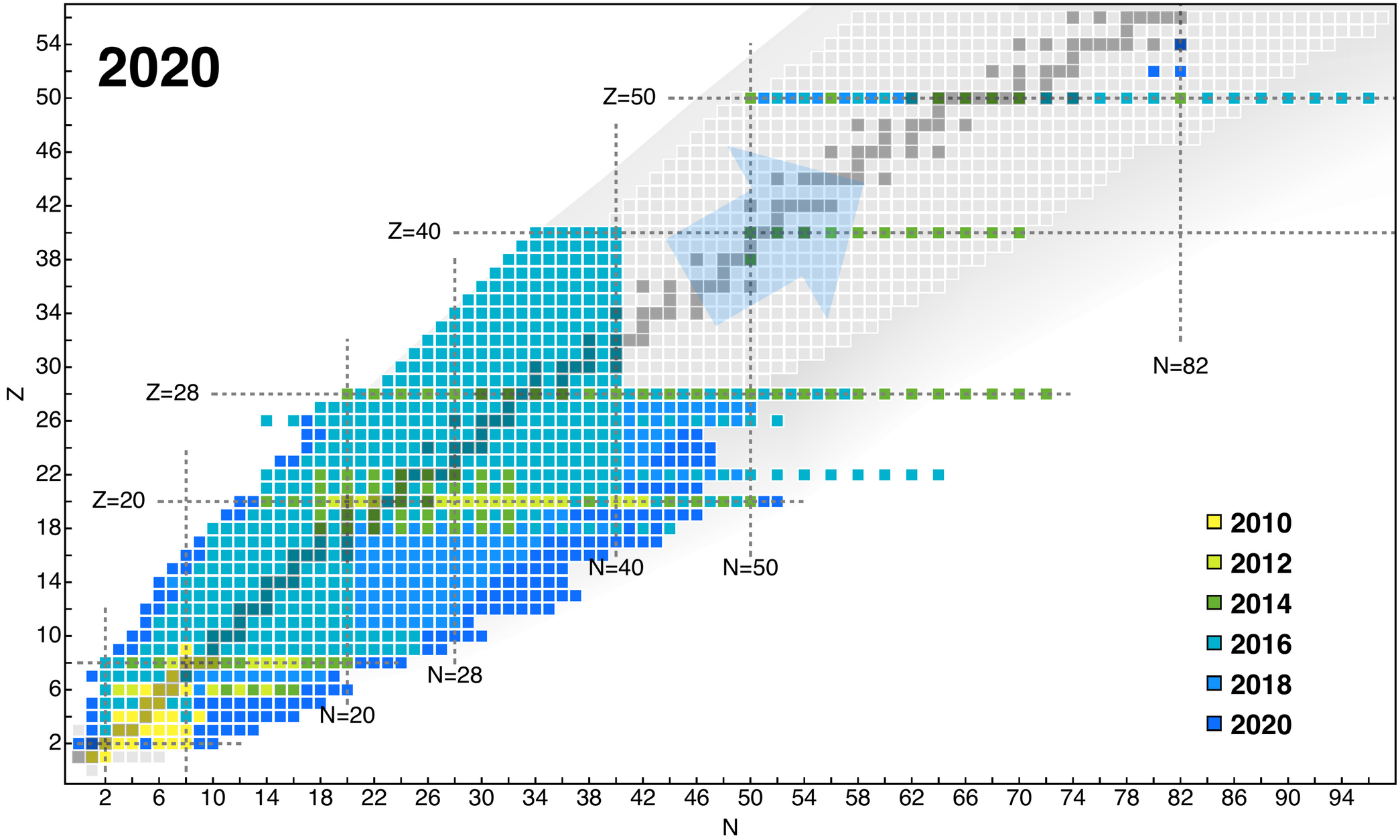


FIGURE 4 | Schematic view of correlations in nuclei. Solid circles indicate nucleons, transparent circles hole states, and dashed ellipses indicate correlations between nucleons. Certain 2p2h, 3p3h and higher correlations (indicated in blue) are built into a correlated wave function that then serves as the reference state for an MR-IMSRG(2) calculation (capturing correlations indicated in red), while up to an IMSRG(A) calculation would be needed for an equivalent description in the conventional framework.


2020
Z=50
Z=40
Z=28
Z=20
N=82
N=40
N=50
N=28
N=20
2010
2012
2014
2016
2018
2020
Z
N
2
6
10
14
18
22
26
30
34
38
42
46
50
54
58
62
66
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74
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82
86
90
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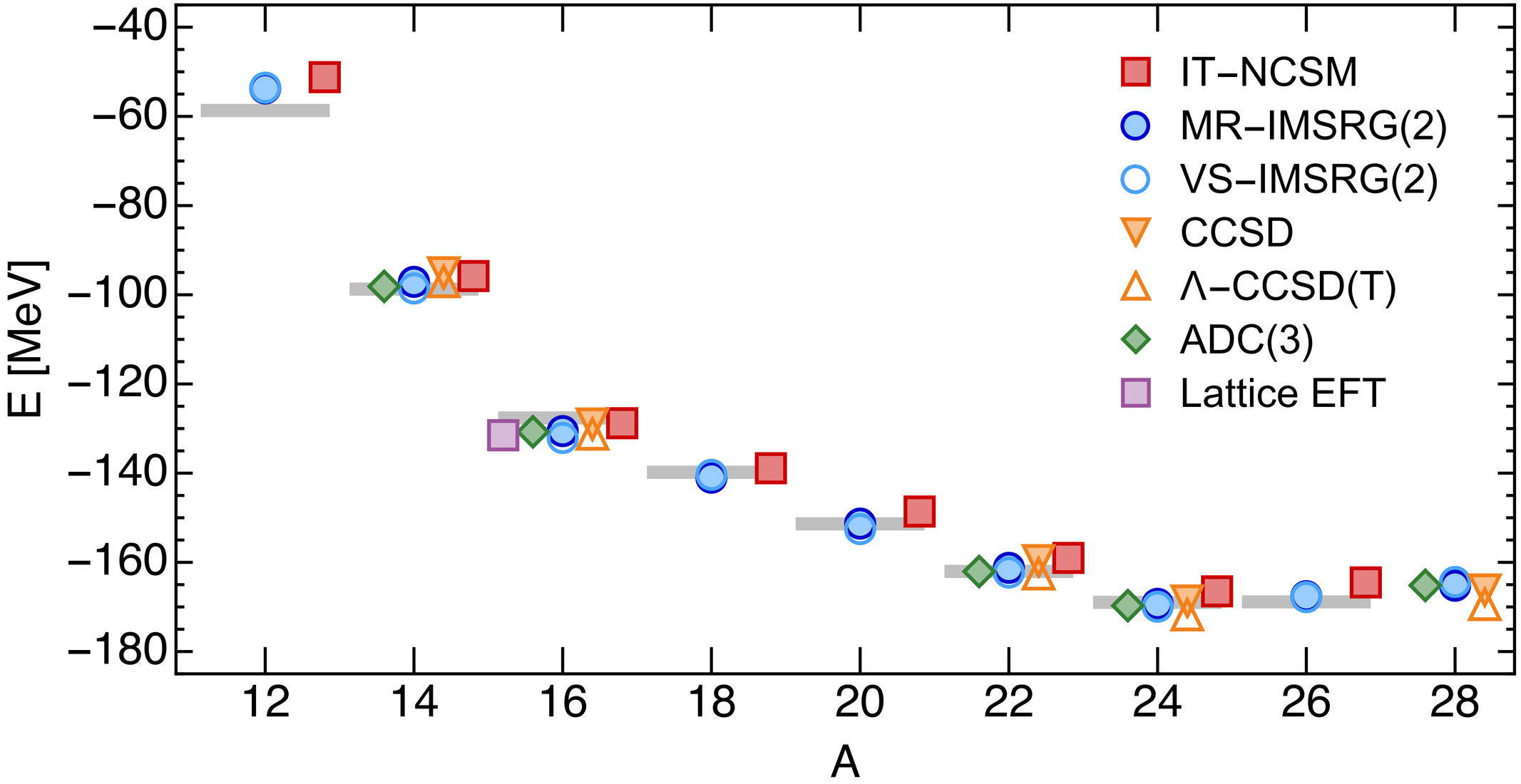
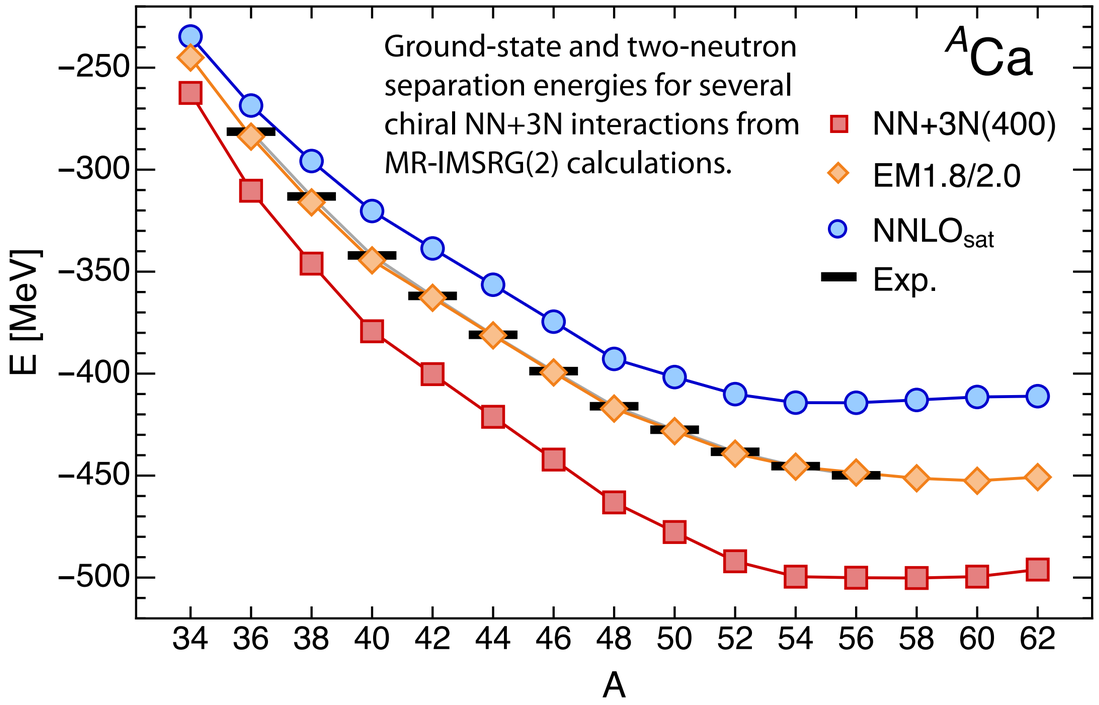
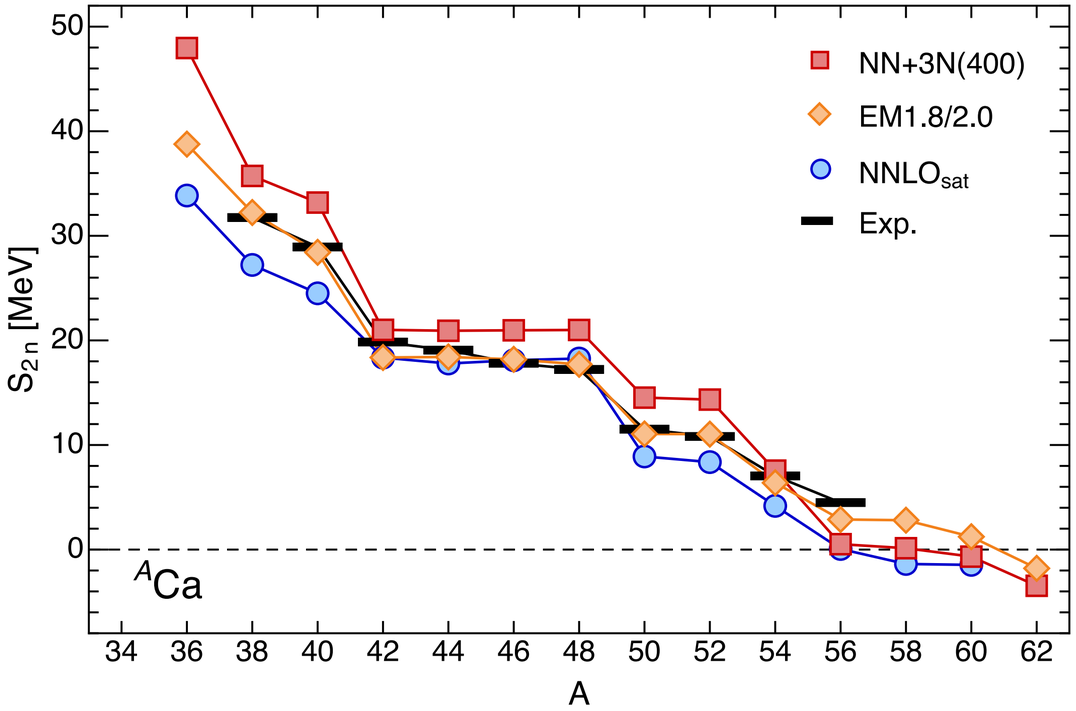
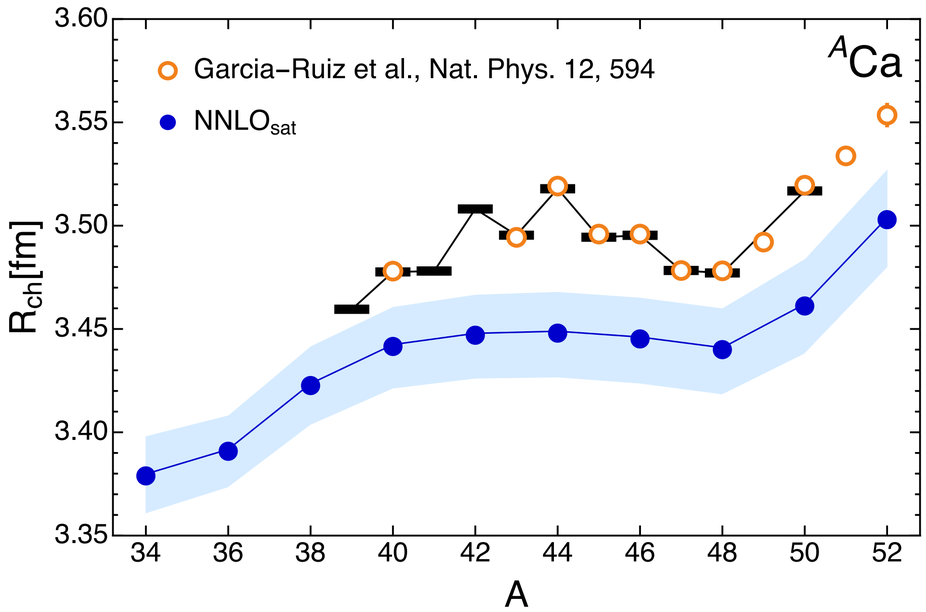


Ground-state energies of the oxygen isotopes for various many-body approaches, using the chiral NN+3N(400) interaction at $\lambda = 1.88$ fm^{-1}

Hergert, A Guided Tour of ab initio Nuclear Many-Body Theory







Calcium charge radii from MR-IMSRG(2) calculations with NNLOsat
The shaded area indicates uncertainties from basis convergence. Black bars and orange circles indicate experimental data

Numerical Codes

Computer Physics Communications
Volume 187, February 2015, Pages 175-194

Go to Computer Physics Communications

Solution of the Skyrme–HF+BCS equation on a 3D mesh, II: A new version of the Ev8 code

W. Ryssens [a], V. Hellemans [a], M. Bender [b c], P.-H. Heenen [a]

EV8

The main characteristic of **Ev8** is that it solves the Hartree–Fock plus BCS equations for Skyrme type functionals.

This allows flexibility since the same mesh can be used to describe the oblate deformed, spherical, prolate deformed, superdeformed and fission configurations of a given nucleus.

Code https://data.mendeley.com/datasets/pbv7bz59rj/1
Paper http://dx.doi.org/10.1016/j.cpc.2014.10.001

Programming language: FORTRAN-90.

Solution method: The program expands the single particle wavefunctions on a 3D Cartesian mesh. The nonlinear mean-field equations are solved by the imaginary time step method. A quadratic constraint is used to obtain states corresponding to given values of the monopole and quadrupole operators.

Restrictions: Ev8 assumes time-reversal invariance and nuclear shapes exhibiting three plane-reflection symmetries. Pairing correlations are treated at the BCS level of approximation.

Running time: Few minutes

Computer Physics Communications
Volume 185, Issue 7, July 2014, Pages 2195-2216

The code **Sky3D** solves the static or dynamic equations on a three-dimensional Cartesian mesh with isolated or periodic boundary conditions and no further symmetry assumptions.

Pairing can be included in the BCS approximation

The TDHF code Sky3D ☆

J.A. Maruhn [a], P.-G. Reinhard [b], P.D. Stevenson [c], A.S. Umar [d]

Code https://data.mendeley.com/datasets/pv8p3r69cb/1
Code(1.1) https://data.mendeley.com/datasets/vzbrzvyrn4/1
Paper https://doi.org/10.1016/j.cpc.2014.04.008

Sky3D

Programming language: FORTRAN-90, OpenMP and MPI for parallelization. LAPACK, FFTW3 as external libraries.

Solution method: The wavefunction are represented on a three-dimensional Cartesian mesh with no further symmetry restrictions. All spatial derivatives are evaluated using the finite Fourier transform method. The code solves the static Hartree–Fock equations with a damped gradient iteration method and the time-dependent Hartree–Fock equations with an expansion of the time-development operator. Any number of initial nuclei can be placed into the mesh in with arbitrary positions and initial velocities.

Restrictions: The reliability of the mean-field approximation limits the scope of applications to collision energies about a few MeV per nucleon above the Coulomb barrier and to relatively short interaction times. Similarly, some of the missing time-odd terms may restrict the applications to even–even nuclei.

Running time: The running time depends strongly on the size of the grid, the number of nucleons, and the duration of the collision. For a single-processor PC-type computer it can vary between a few minutes and weeks.

Computer Physics Communications
Volume 168, Issue 2, 1 June 2005, Pages 96-122

Coordinate-space solution of the Skyrme–Hartree–Fock– Bogolyubov equations within spherical symmetry. The program HFBRAD (v1.00) ☆

K. Bennaceur [a], J. Dobaczewski [b c d]

The code **HFBRAD** solves the Skyrme–Hartree–Fock or Skyrme–Hartree–Fock– Bogolyubov equations in the coordinate representation with spherical symmetry.

A realistic representation of the quasiparticle wave functions on the space lattice allows calculations to be performed up to the particle drip lines.

Zero-range density- dependent interactions are used in the pairing channel.

HFBRAD

Code https://data.mendeley.com/datasets/4vzsg8tbr6/1
Paper https://doi.org/10.1016/j.cpc.2005.02.002

Programming language: FORTRAN-95

Solution method: The program determines the two-component Hartree–Fock–Bogolyubov quasiparticle wave functions on the lattice of equidistant points in the radial coordinate. This is done by solving the eigensystem of two second-order differential equations using the Numerov method. A standard iterative procedure is then used to find self-consistent solutions for the nuclear product wavefunctions and densities.

Restrictions: The main restriction is related to the assumed spherical symmetry.

Running time: Less than a minute for a heavy nucleus

Computer Physics Communications
Volume 216, July 2017, Pages 145-174

Solution of the Skyrme-Hartree–Fock–Bogolyubovequations in the Cartesian deformed harmonic-oscillator basis. (VIII) HFODD (v2.73y): A new version of the program ☆

N. Schunck [a], J. Dobaczewski [b c d e], W. Satuła [d e], P. Bączyk [d], J. Dudek [f g], Y. Gao [c], M. Konieczka [d], K. Sato [h], Y. Shi [c i j], X.B. Wang [c k], T.R. Werner [d]

The code **HFODD** solves the nuclear Skyrme Hartree–Fock or Skyrme Hartree–Fock–Bogolyubov problem by using the Cartesian deformed harmonic-oscillator basis.

It allows (i) full proton–neutron mixing, (ii) the Gogny force in both ph and pp channels, (iii) parallel capabilities, (iv) the Lipkin translational energy correction method with pairing, (v) higher-order Lipkin particle-number corrections, (vi) isospin-symmetry-breaking terms, and (vii) the Augmented Lagrangian Method for calculations with 3D constraints on angular momentum and isospin.

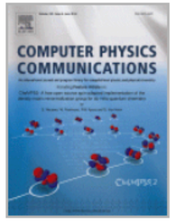
HFODD

Code https://data.mendeley.com/datasets/3b28fs62wc/1
Paper https://doi.org/10.1016/j.cpc.2017.03.007

Programming language: FORTRAN-90. The user must have access to the LAPACK, LINPACK and BLAS libraries

Solution method: The program uses the Cartesian harmonic oscillator basis to expand single-particle or single-quasiparticle wavefunctions of neutrons and protons interacting by means of the Skyrme or Gogny effective interactions and zero-range or finite-range pairing interactions. The expansion coefficients are determined by the iterative diagonalization of the mean-field Hamiltonians or Routhians which depend non-linearly on the local or nonlocal neutron, proton, or mixed proton–neutron densities. Suitable constraints are used to obtain states corresponding to a given configuration, deformation or angular momentum.

Computer Physics Communications
Volume 185, Issue 6, June 2014, Pages 1808-1821



DIRHB—A relativistic self-consistent mean-field framework for atomic nuclei ☆

T. Nikšić [a], N. Paar [a], D. Vretenar [a], P. Ring [b]

DIRHB

The DIRHB package consists of three Fortran computer codes for the calculation of the ground-state properties of even–even atomic nuclei using the framework of relativistic self-consistent mean-field models.

Each code corresponds to a particular choice of spatial symmetry: the DIRHBS, DIRHBZ and DIRHBT codes are used to calculate nuclei with spherical symmetry, axially symmetric quadrupole deformation, and triaxial quadrupole shapes, respectively. Reflection symmetry is assumed in all three cases.

Code https://elsevier.digitalcommonsdata.com/datasets/cx55fkbjy6/1
Paper https://doi.org/10.1016/j.cpc.2014.02.027

Programming language: FORTRAN-77

Solution method: The codes solve the stationary relativistic Hartree–Bogoliubov equations in a self-consistent iteration scheme. At each iteration the matrix elements of the equations are updated using the modified Broyden method or the linear mixing method. The single-nucleon wave functions are expanded in a basis of spherical, axially symmetric or triaxial harmonic oscillator, depending on the assumed symmetry of the nuclear shape. For calculations that constrain the shape to specific values of the deformation parameters, the augmented Lagrangian method is used.

Restrictions: Time-reversal and reflection symmetries are assumed. Open-shell even–even spherical and quadrupole deformed nuclei can be considered.

Running time: from few seconds (spherical) up to few hours (triaxial)

Computer Physics Communications
Volume 184, Issue 1, January 2013, Pages 142-161

Random Phase Approximation (RPA) is used to study nuclear giant resonances and low-lying collective excitations, in terms of a nuclear effective interaction (the Skyrme forces).

Self-consistent RPA calculations with Skyrme-type interactions: The skyrme_rpa program ☆

RPA

Gianluca Colò [a], Ligang Cao [b c a], Nguyen Van Giai [d], Luigi Capelli [a 1]

Code https://data.mendeley.com/datasets/9hdvznfzvs/1
Paper https://doi.org/10.1016/j.cpc.2012.07.016

Programming language: FORTRAN-90/95; easily downgradable to FORTRAN-77

Solution method: The Hartree–Fock (HF) equations are solved in a radial mesh, using a Numerov algorithm. The solutions are iterated until self-consistency is achieved. In the obtained mean field, unoccupied states necessary for the RPA calculations are found. For all single-particle states, box boundary conditions are assumed. To solve the RPA problem for a given value of total angular momentum and parity J is constructed and the RPA matrix is diagonalized. The transition amplitudes and transition strengths associated to given external operators are calculated. The HF densities and RPA transition densities are also evaluated.

Restrictions: The main restrictions are related to the assumed spherical symmetry and absence of pairing correlations.

Running time: The typical running time depends strongly on the nucleus, on the multipolarity, on the choice of the model space and of course on the computer. It can vary from a few minutes to several hours.

ANTOINE

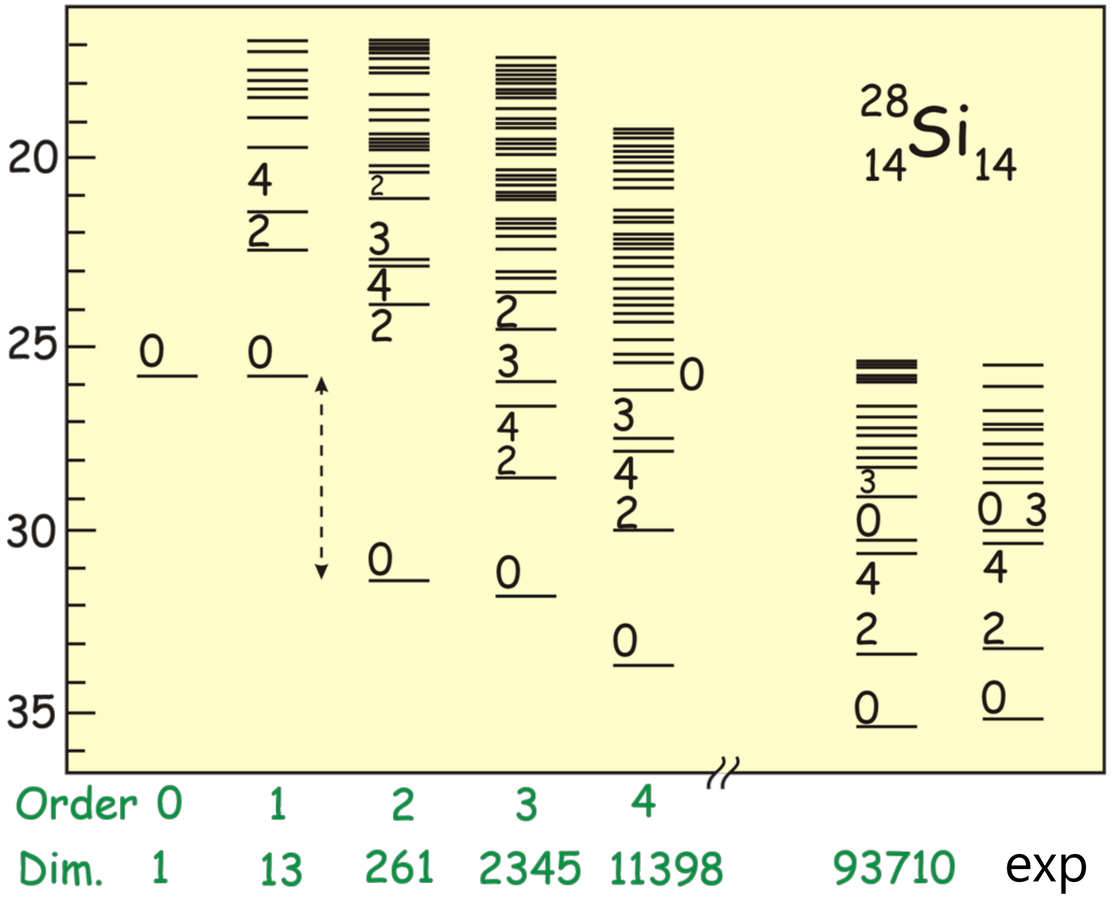
Programming language: FORTRAN-77

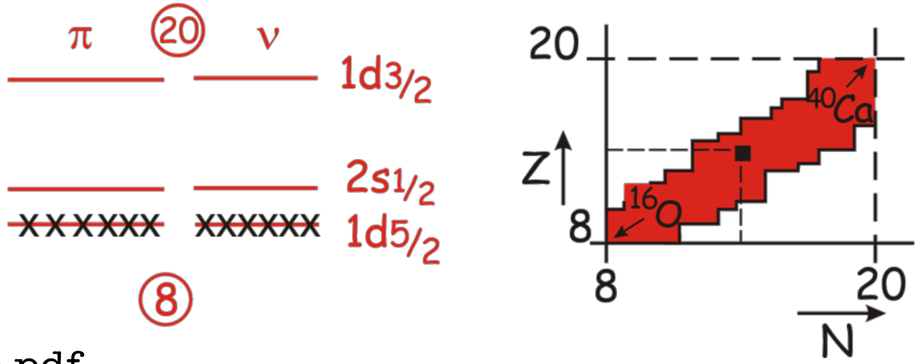
Solution method: This code works with shell model wavefunctions written in a M-scheme: each Slater Determinant is represented by an integer word and each bit of the word associated to a given individual state $|nljmt>$. Each bit has the value 1 or 0 depending on whether the state is occupied or empty. Only J_z and T_z are good quantum numbers, therefore all the possible *(J,T)* states are in the basis.

The diagonalization of the matrices are done with the Lanczos method.

It includes No Core Shell Model (NCSM)

Restrictions: Dimension of the matrix in the Lanczos procedure (yrast band of ^{52}Fe, for example)





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Code Send an email to E. Courier and F. Nowacki (Strasbourg)
Manual https://wiki.portal.chalmers.se/ff/uploads/Antoine/antoine.pdf
Paper https://www.actaphys.uj.edu.pl/index_n.php?I=R&V=30&N=3#705

Code https://github.com/cwjsdsu/BigstickPublick
Paper https://arxiv.org/abs/1801.08432

Programming language: FORTRAN-90 with some 95 extensions

Distribution: MIT Open Source License

- **BIGSTICK** is a flexible configuration-interaction open-source shell-model code for the many-fermion problem.
- It looks for low-lying eigenvalues of the Hamiltonian of a many fermion system; it does this by creating a basis of many-body states of Slater determinants. The Slater determinants are antisymmetrized products of single-particle states with good angular momentum, typically derived from some shell-model-like potential; hence we call this a shell-model basis.
- The Hamiltonian is assumed to be rotationally invariant and to conserve parity, and is limited to two- and, optionally, three-body forces. Otherwise no assumptions are made about the form of the single-particle states or of the Hamiltonian.
- It utilizes a factorized on-the-fly algorithm for computing many-body matrix elements, and has both MPI (distributed memory) and OpenMP (shared memory) parallelization.
- It allows both phenomenological (major valence shell space) and ab initio (the so-called no-core shell model) calculations.
- It can generate energy spectra, static and transition one-body densities, and expectation values of scalar operators. Using the built-in Lanczos algorithm one can compute transition probability distributions and decompose wave functions into components defined by group theory.

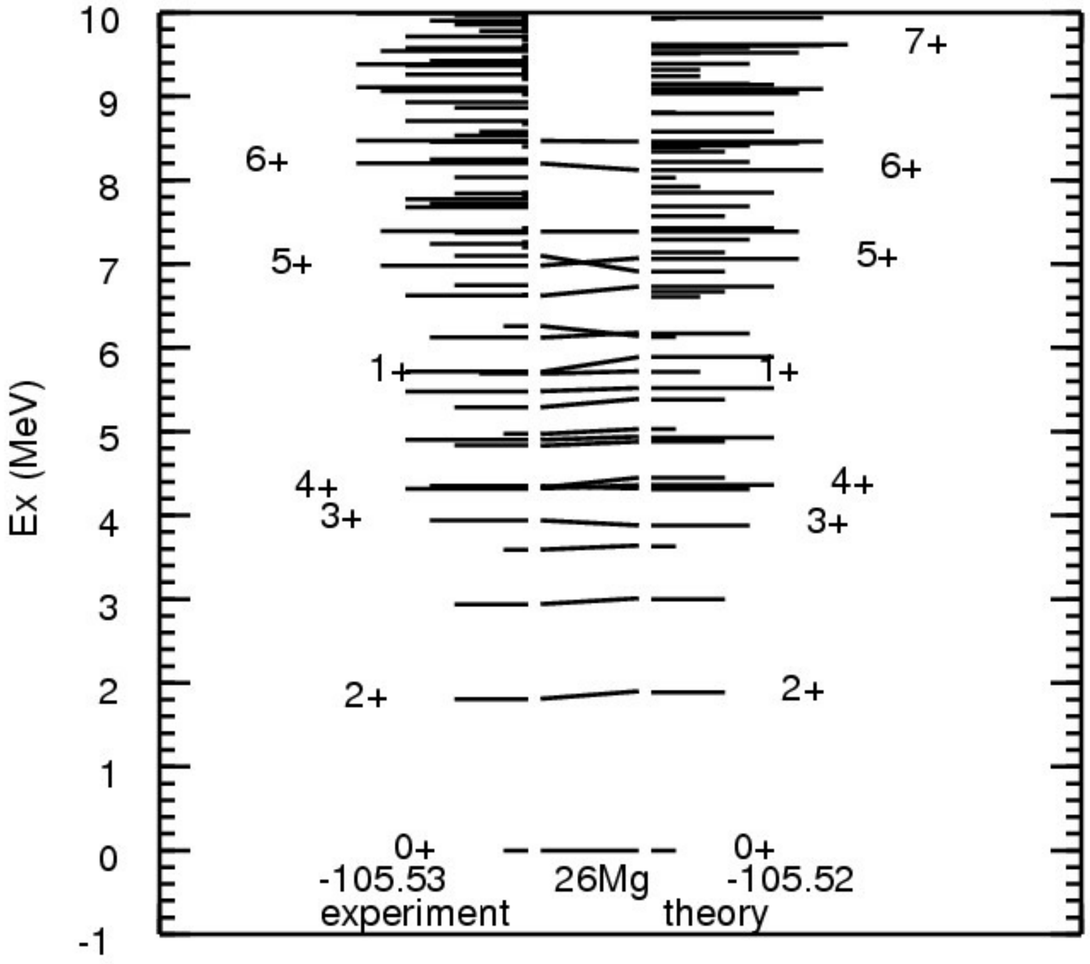
NUSHELLX

NuShell

- Replaces old shell model code OXBASH
- JT-projected M-scheme
- Stores complete matrix, which limits the size of calculations

NuShellX

- Calculates Hamiltonian "on the fly"
- Utilizes NuShell modules for protons and neutrons J-scheme built on coupling between protons and neutrons
- Most time-consuming step in CI calculation is diagonalization
- OpenMP and MPI
- LAPACK
- Lanczos procedure



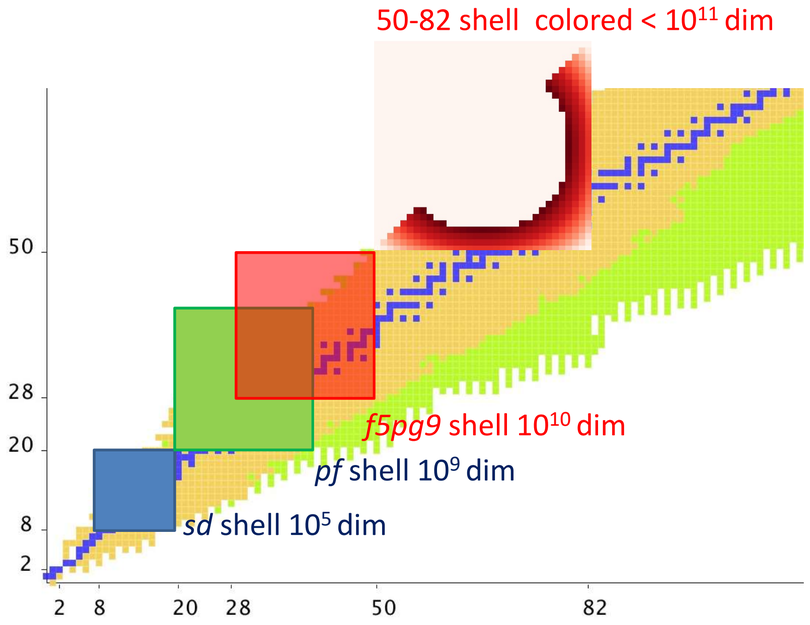
Code http://www.garsington.eclipse.co.uk/

Paper 1 https://github.com/NuclearStructure/PHY981/blob/master/doc/LectureNotes/nushellxtutorial.pdf

Paper 2 https://www.sciencedirect.com/science/article/pii/S0090375214004748?via%3Dihub

KSHELL

- The "KSHELL" code performs nuclear shell-model calculations with M- scheme representation
- MPI+OpenMP parallel implementation



Energy relative to ^{16}O core

Excitation energy

Energy levels

	N	2J	prty	N_Jp	2T	E(MeV)	Ex(MeV)
0^+_1	1	0	+	1	0	-135.938	0.000
2^+_1	2	4	+	1	0	-133.950	1.987
4^+_1	3	8	+	1	0	-131.279	4.659
0^+_2	4	0	+	2	0	-130.927	5.011
3^+_1	5	6	+	1	0	-129.771	6.167
4^+_2	6	8	+	2	0	-128.901	7.037
0^+_3	7	0	+	3	0	-128.699	7.239
2^+_2	8	4	+	2	0	-128.415	7.522
2^+_3	9	4	+	3	0	-128.032	7.906
1^+_1	10	2	+	1	0	-127.998	7.940

B(E2) larger than 1.0 e^2 fm^4

2Ji	Ei	2Jf	Ef	Ex
0+(1)	-135.938	4+(1)	-133.950	1.987
0+(1)	-135.938	4+(3)	-128.032	7.906
8+(2)	-128.901	4+(2)	-128.415	0.485
8+(2)	-128.901	4+(3)	-128.032	0.869

Experiment (Nudat2)

E_{level} (keV)	Jπ
0.0	0+
1779.030 11	2+
4617.86 4	4+
4979.92 8	0+
6276.20 7	3+
6690.74 15	0+
6878.79 8	3-
6887.65 10	4+
7380.59 9	2+
7416.26 9	2+
7799.01 9	3+

Programming language: FORTRAN; BLAS, LAPACK library

Distribution: GNU General Public License

Website https://sites.google.com/alumni.tsukuba.ac.jp/kshell-

Code https://github.com/jorgenem/kshell_public

Paper 1 https://arxiv.org/abs/1310.5431

Paper 2 https://www.sciencedirect.com/science/article/pii/S0010465519301985?via%3Dihub

CoSMo

Continuum Shell Model

- CoSMo is a comprehensive shell model code suite designed for nuclear shell model and configuration interaction calculations.
- The highly structural and templated nature of the CoSMo code allows for flexibility and ease in applications, including those to open quantum systems with non-Hermitian Hamiltonians, clustering, and time-dependent dynamics.

$$|\alpha; E\rangle = \sum_1 \alpha_1(E)|1\rangle + \sum_c \int dE'\, \alpha_c(E'; E)|c; E'\rangle$$

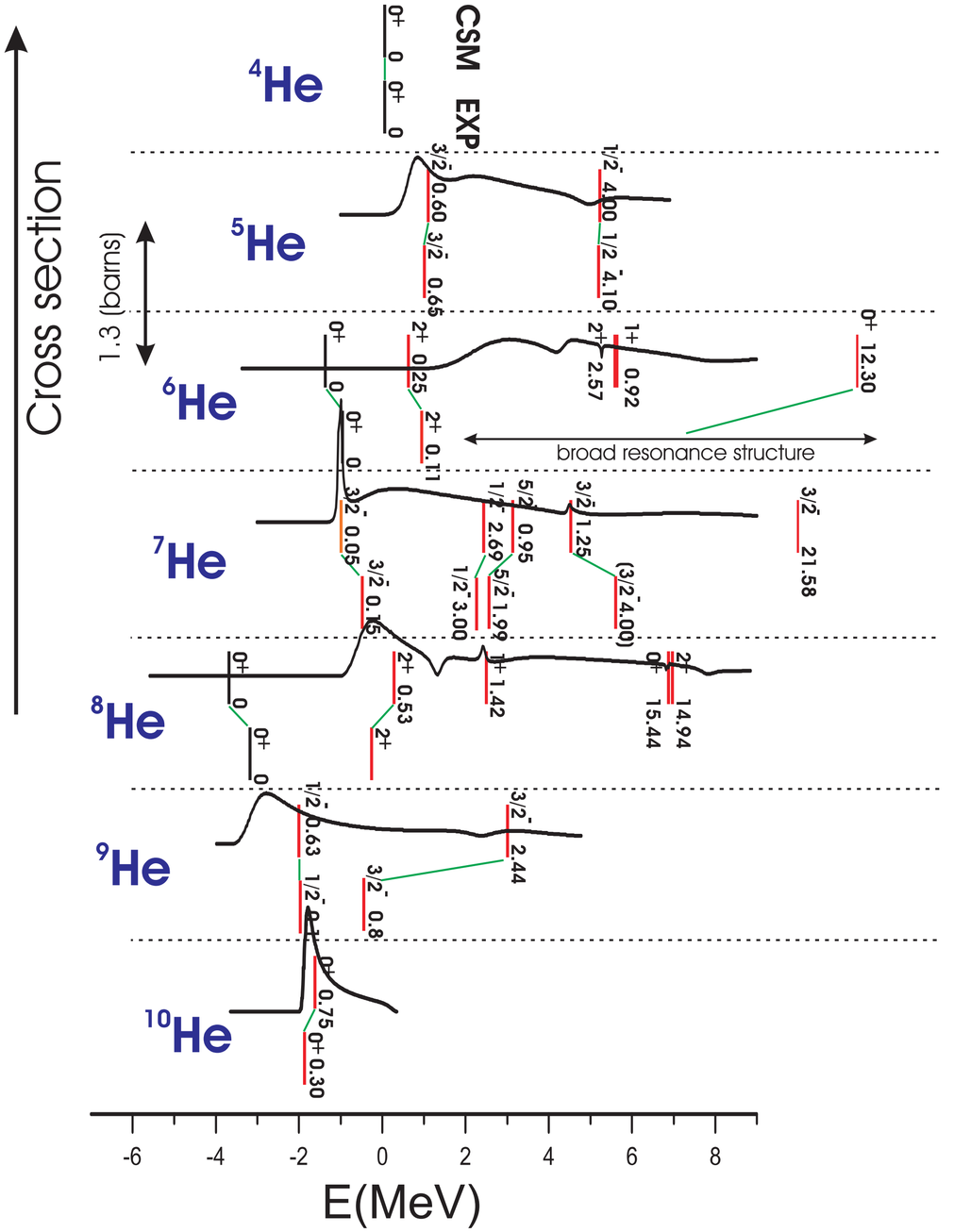
continuum

$$\sum_2 \left[\langle 1|H|2\rangle + \sum_c \int dE' \frac{A_1^c(E', E) A_2^c(E', E)^*}{E - E' + i0} - \delta_{12} E \right] \alpha_2 = 0$$

Programming language: C++

Distribution: GNU General Public License

Website https://www.volya.net/index.php?id=cosmo
Code https://github.com/alvolya/cosmo
Paper https://iopscience.iop.org/article/10.1088/1742-6596/49/1/016



CENS is a graphical user interface (GUI) written in Python which coordinates:

- Many programs in Fortran 90/95 for computing effective two-body interactions starting with free nucleon-nucleon interactions (proton-neutron formalism).
- A shell-model code and a transition code. Source code in C/C++ (portable to all systems) which allows you to address systems up to 10^9 basic states. Parallel codes for larger systems available upon demand.

NN potentials

- Charge symmetry breaking (CSB): available for N3LO and CD-Bonn interactions. The Argonne V18 model includes CSB.
- Isospin symmetry breaking (ISB): available for N3LO and CD-Bonn interaractions. The Argonne V18 model includes CSB.
- Coulomb: Argonne includes Coulomb by default. All other interaction models can or cannot include the Coulomb interaction as an option.

Nuclear structure applications

- Shell model code
- Hartree-Fock (HF) and TDHF
- Neutron stars equation of state
- IMSRG

Dealing with the NN potentials, can compute a renormalized two-body interaction using

- a no-core shell-model prescription
- a G-matrix prescription
- a V_{lowk} prescription
- a renormalization group prescription in momentum space or in oscillator space (not ideal for shell-model calculations)

Programming language: Python, C/C++ and Fortran 95

Website, Code, Refs https://github.com/ManyBodyPhysics/CENS

NuHamil

The numerical code **NuHamil** generates the nucleon-nucleon (NN) and three-nucleon (3N) matrix elements expressed in a spherical harmonic-oscillator basis, inputs of many-body calculations.

$$V^{\mathrm{NN},J}_{p'q'pq} = \sum_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} J^{\mathrm{NN}}_{\mathrm{rel}} S} \sum_{n'l'nl} T^{p'q'J}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} n'l'SJ^{\mathrm{NN}}_{\mathrm{rel}}} \times V^{SJ^{\mathrm{NN}}_{\mathrm{rel}}}_{n'l'nl} \; T^{pqJ}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} nlSJ^{\mathrm{NN}}_{\mathrm{rel}}} .$$

$$T^{pqJ}_{N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} nlSJ^{\mathrm{NN}}_{\mathrm{rel}}} = (-1)^{L^{\mathrm{NN}}_{\mathrm{cm}}+l+S+J} \sqrt{[j_p][j_q][S][J^{\mathrm{NN}}_{\mathrm{rel}}]} \times \sum_{\Lambda} [\Lambda] \begin{Bmatrix} l_p & 1/2 & j_p \\ l_q & 1/2 & j_q \\ \Lambda & S & J \end{Bmatrix} \begin{Bmatrix} L^{\mathrm{NN}}_{\mathrm{cm}} & l & \Lambda \\ S & J & J^{\mathrm{NN}}_{\mathrm{rel}} \end{Bmatrix} \times \langle N^{\mathrm{NN}}_{\mathrm{cm}} L^{\mathrm{NN}}_{\mathrm{cm}} nl : \Lambda | n_p l_p n_q l_q : \Lambda \rangle_1 .$$

Programming language: Modern Fortran; OpenMP, MPI, BLAS, LAPACK, GSL

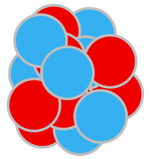
Distribution: GPLv3

Code https://github.com/Takayuki-Miyagi/NuHamil-public
Paper https://link.springer.com/article/10.1140/epja/s10050-023-01039-y

NuclearToolkit.jl provides self-contained codes for nuclear physics covering from nuclear forces to various nuclear many-body methods. Users can generate nucleon-nucleon (NN) potentials based on chiral effective field theory and use them in many-body methods such as Hartree-Fock many-body perturbation theory (Møller–Plesset method), in-medium similarity renormalization group (IM-SRG), and valence shell model (configuration interaction method)

Nuclear Toolkit

NuclearToolkit.jl provides an interface that combines these various methods into one and works on a variety of environments, including Linux, Mac, and Windows. This is achieved thanks to the high readability and portability of the Julia programming language (Bezanson et al., 2012).



ShellModel.jl

Pros

- Easy to run
- Portability (no need to specify "magical" compiler options specific to each environment)
- Fast (e.g., 10 lowest eigenpairs of 28Si (in full sd shell) can be calculated in ~3 sec.)
- One can easily extend the code

Cons

- poorly parallerized (for # of threads >= 12)
- greedy (compared to the "on-the-fly" generation of matrix element)

Programming language: Julia programming language (Bezanson et al., 2012)

Code https://github.com/SotaYoshida/NuclearToolkit.jl
Paper https://joss.theoj.org/papers/10.21105/joss.04694

BoccaDorata

- The BcDor code is built upon a C++ class library that is meant for the computation of many-body Green's functions (propagators) in finite systems. This is written in *J*-coupled formalism and it is therefore mostly suitable for the ab-initio computation of finite nuclei in the medium mass range.
- The public version of BcDor contains all the basic components of this library and allow for calculation of closed-shell nuclei up to second order in the self-energy expansion and up to the coupled cluster with doubles approximation. This will allow for simple computations of binding energies, of the nuclear self-energy (which provides an optical potential) and of the spectral function.

Programming language: C++; LAPACK, BLAS

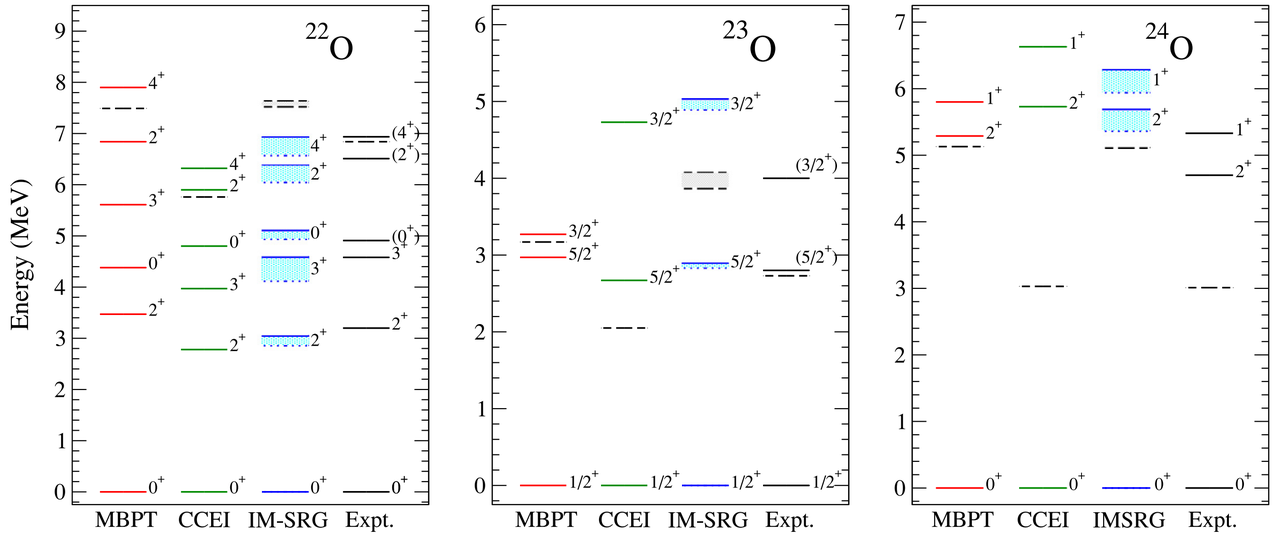
Distribution: Free

Code https://gitlab.com/cbarbieri/BoccaDorata

Papers Prog. Part. Nucl. Phys. 52, p. 377 (2004), Phys. Rev. A76, 052503 (2007), Phys. Rev. C79, 064313 (2009), Phys. Rev. C89, 024323 (2014).

IMSRG

- In-Medium Similarity Renormalization Group software for nuclear structure calculations. It is capable of performing Hartree-Fock, single-reference IM-SRG, and valence-space IM-SRG calculations.



Programming language: C++ Python; BOOST, ARMADILLO libraries

Distribution: GNU Public License

Code https://github.com/ragnarstroberg/imsrg

Paper http://link.aps.org/doi/10.1103/PhysRevLett.106.222502
http://www.sciencedirect.com/science/article/pii/S0370157315005414