Quantum many-body problem in nuclear physics

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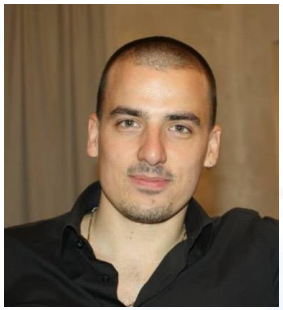

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Quantum many-body problem

Quantum many-body (QMB) problem:

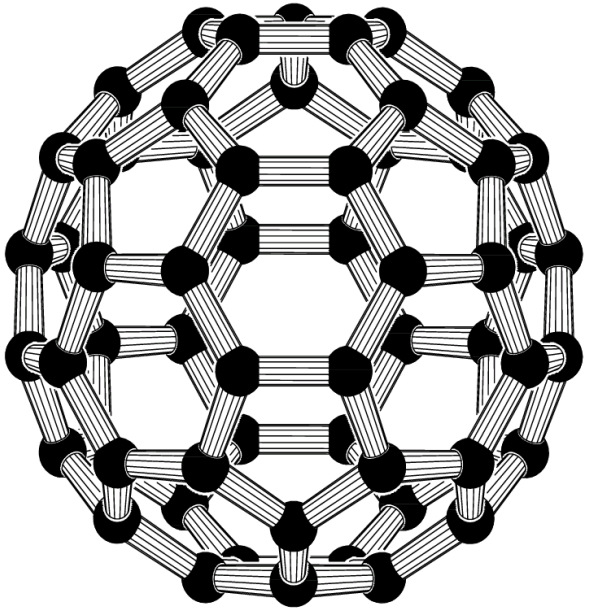
It is demanding to describe physical properties of **microscopic system** of **many** mutualy interacting **particles**.

- **microscopic system** = described within **quantum mechanics** approach
- **many particles** = whatever from 3 to any large (finite) number
- in some cases for 3 or 4 particles **exact solution** is possible (**Fadeev** or **Fadeev-Yakubovski** eqs.) … then we speak about **few-body problem**
- **infinite systems** can be often described within **statistical** approaches

Where solution of QMB is useful:

- **nuclear** physics
- **atomic** physics
- **molecular** physics
- **solid state** physics
- **nanoscopic systems**

(fullerens, quantum dots, nanowires...)

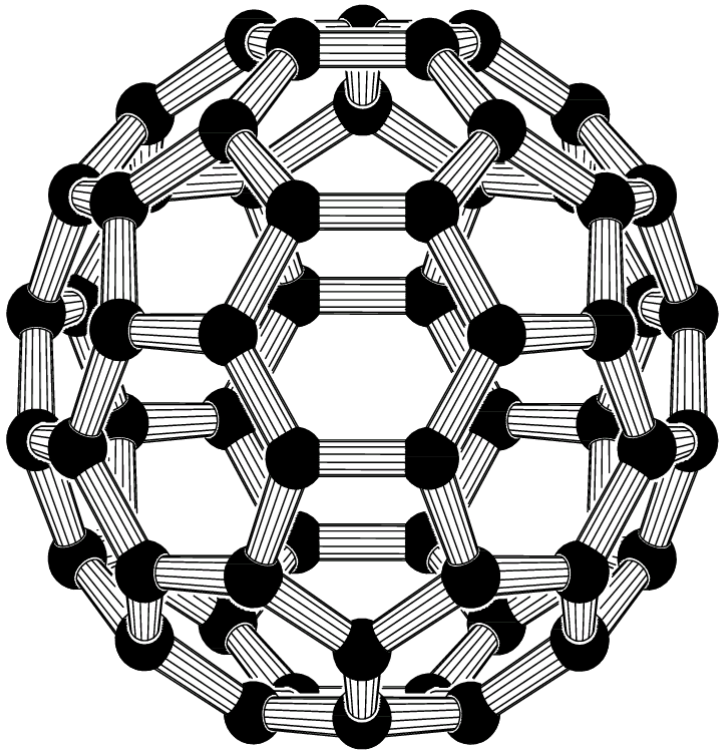


Quantum many-body problem

Main approaches to solve QMB problem:

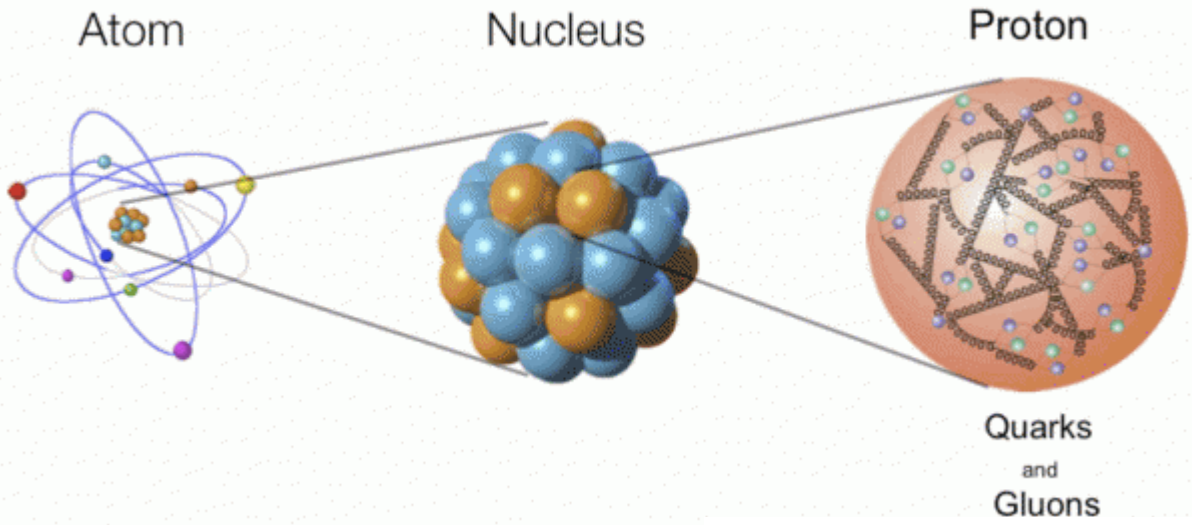
This is definitely not “complete list“ of theoretical approaches, only “well known“ examples:

- **Density functional theory** (DFT)
- **Mean-field methods** (Hartree-Fock, TDA, RPA)
- **Beyond mean-field** or “**post-Hartree-Fock**“ approaches
  - Coupled cluster
  - Configuration Interaction
  - **Equation of Motion Phonon Method** (EMPM)
- **Monte Carlo** approaches
  - Green‘s function Monte Carlo
  - Auxiliary field diffusion Monte Carlo method (AFDMC)
- **Self-consistent Green‘s function** (SCGF)



Atomic nucleus – playground for studying quantum many-body problem

Physics of atomic nucleus – what do we study (only QMB problem)?



Atomic nucleus as a bound system of nucleons

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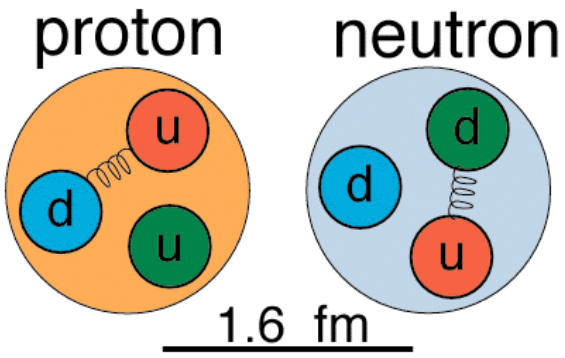
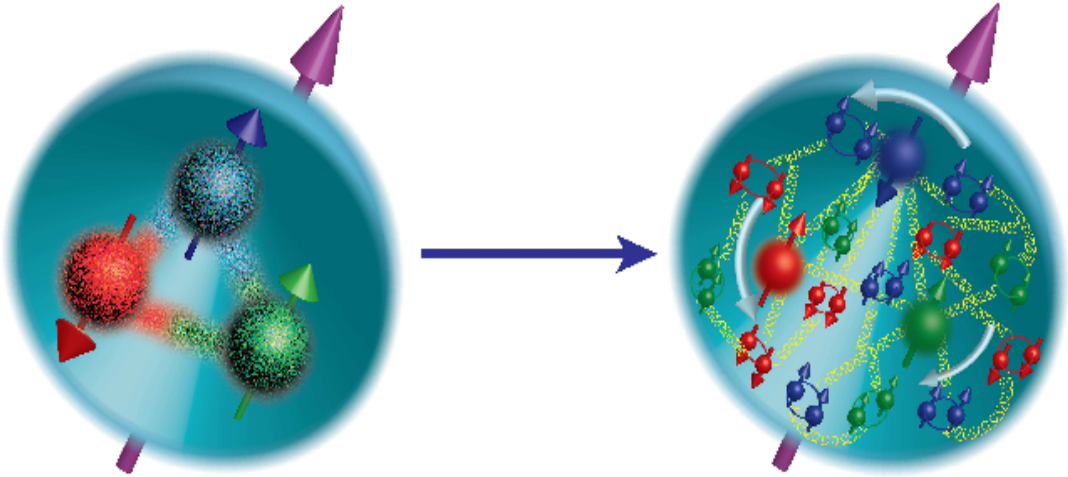
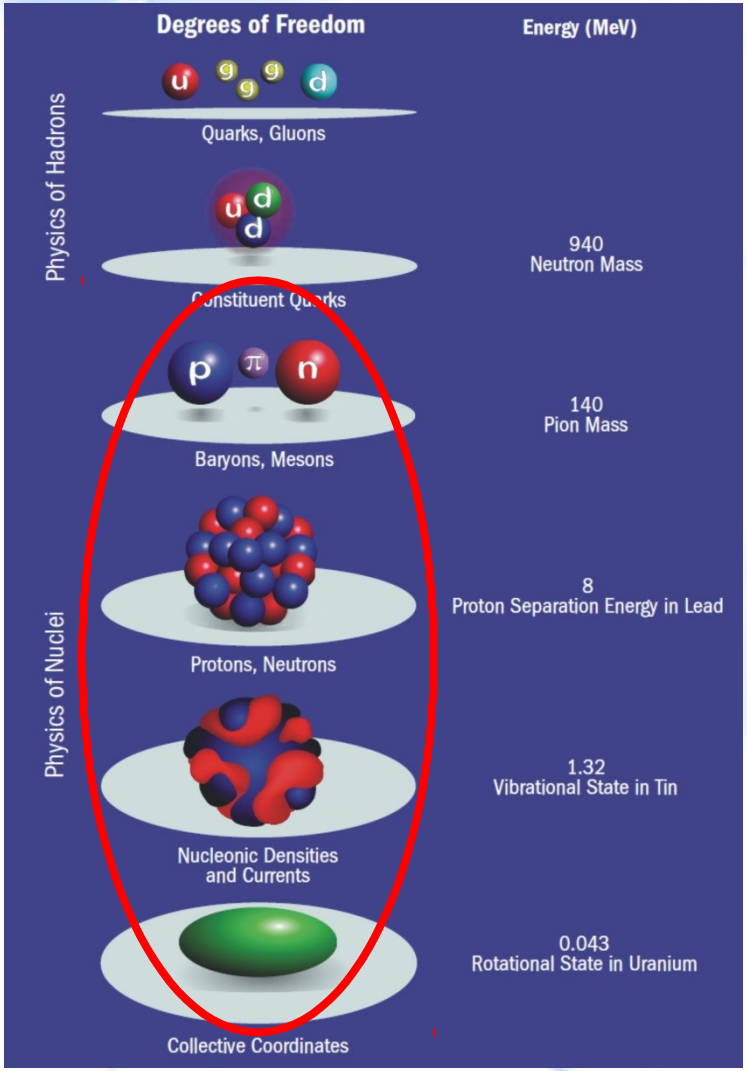
nucleons as a bound system of quarks





Atomic nucleus – playground for studying quantum many-body problem



What we see depends on resolution:

- **< 0.0001 fm: quarks**
- **0.1-1 fm : baryons, mesons**
- **1 fm: nucleons**
- **10 fm : collective modes**

Atomic nucleus – playground for studying quantum many-body problem

Implicit paradigm of theoretical nuclear physics:

Nucleus is **bound state of nucleons**. We describe nucleus by methods of **quantum mechanics** (QM) from **interactions** among **nucleons**.

This paradigm itself is not most **fundamental approach** – we should describe nuclei from **QCD.** Except of first pioneering attempts [**Phys. Rev. Lett.** 113, 252001 (2014)] **impossible**!!

Instead we employ the strategy: build **potential** among **nucleons** (**NN**, **NNN**, etc.) → solve **QMB** problem with given nucleon potential (i.e. **Hamiltonian**)

Building potentials itself is complicated task – **nucleons** as particles with the **inner structure**. Even the potentials cannot be build directly from **QCD**.

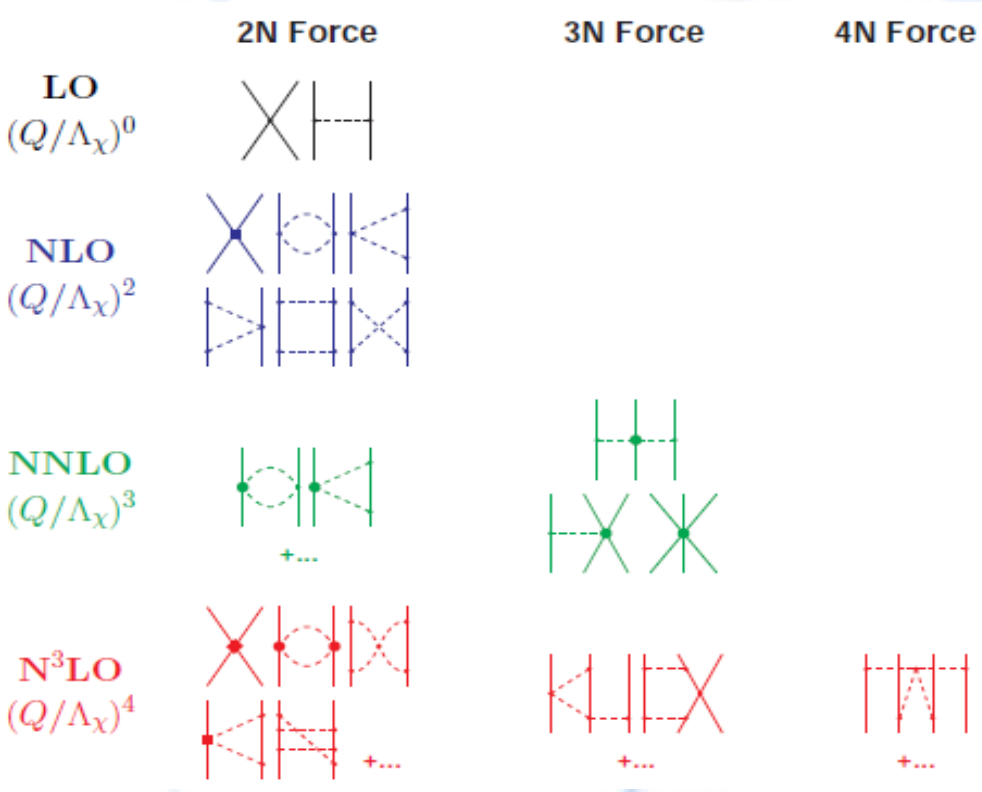
Models to describe **nucleon potentials**. For potentials suitable for nuclear calculations we need to solve **many-body nuclear problem**.

Solution of the nuclear **many-body problem** strongly depend on the employed **nucleon potential**.

Atomic nucleus – playground for studying quantum many-body problem

$$\mathcal{L}_{\pi N} = \mathcal{L}^{(1)}_{\pi N} + \mathcal{L}^{(2)}_{\pi N} + \mathcal{L}^{(3)}_{\pi N} + \ldots$$

$$\mathcal{L}^{(1)}_{\pi N} = \bar{N}\left[i\partial_0 - \frac{1}{4F_\pi^2}\vec{\tau}\cdot(\vec{\pi}\times\partial_0\vec{\pi}) - \frac{g_A}{2F_\pi}\vec{\tau}\cdot(\vec{\sigma}\cdot\vec{\nabla})\vec{\pi}\right] N + \ldots$$



Realistic nucleon potentials:

Effective field theory – instead of QCD field theory with elem. degrees of freedom (quarks, gluons) we build field theory with nucleons and pions. Must obey the same symmetries as QCD –> Chiral Perturbation Theory (ChPT)

Only mesons here are pions. But pion exchanges 2π, 3π, … till any order. Multi-pion exchanges replace presence of other types of mesons.

Diagrams of NN scatering can be divided to orders – perturbative theory (?)

Density functional theory

Hohenberg-Kohn theorem:

“The (non-degenerated) ground state wave function of a many-body fermionic system is a unique functional of the single-particle density.“

Basic words: **density functional**

$$\mathcal{H}(\vec{r}) = \mathcal{H}\left[\Psi(\vec{r})\right] = \mathcal{H}\left[\rho(\vec{r})\right]$$

single-particle density

$$\rho(\vec{r}) = \sum_{i=1}^{A} \phi_i^*(\vec{r})\phi_i(\vec{r})$$

$$\frac{\delta\mathcal{H}}{\delta\Psi} = \frac{\delta\mathcal{H}}{\delta\rho}\frac{\delta\rho}{\delta\Psi} = 0 \quad \Leftrightarrow \quad \frac{\delta\mathcal{H}}{\delta\rho} = 0 \quad \text{if} \quad \frac{\delta\rho}{\delta\Psi} \neq 0$$

Density functional theory

Skyrme functional – most usual form of DFT in nuclear physics:

$$\mathcal{H}_{Skyrme} = \frac{\hbar^2}{2m}\tau + \frac{b_0}{2}\rho^2 - \frac{b_0'}{2}\sum_q \rho_q^2 + \frac{b_3}{3}\rho^{\alpha+2} - \frac{b_3'}{3}\rho^\alpha \sum_q \rho_q^2$$

$$+b_1(\rho\tau - \vec{j}^2) - b_1'\sum_q(\rho_q\tau_q - \vec{j}_q^2) - \frac{b_2}{2}\rho\Delta\rho + \frac{b_2'}{2}\sum_q \rho_q\Delta\rho_q$$

$$+\tilde{b}_4(\vec{s}.\vec{T} - \vec{J}^2) + \tilde{b}_4'\sum_q(\vec{s}_q.\vec{T}_q - \vec{J}_q^2) - b_4(\rho\vec{\nabla}.\vec{J} + (\vec{\nabla}\times\vec{j}).\vec{s})$$

$$- b_4'\sum_q(\rho_q\vec{\nabla}.\vec{J}_q + (\vec{\nabla}\times\vec{j}_q).\vec{s}_q)$$

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r})$$

$$\tau(\vec{r}) = \sum_i \nabla\phi_i^*(\vec{r}).\nabla\phi_i(\vec{r})$$

$$J_k(\vec{r}) = \sum_i \varepsilon_{klm}((\nabla_l\phi_i^*(\vec{r}))\sigma_m\phi_i(\vec{r})$$

$$- \phi_i^*(\vec{r})\sigma_m(\nabla_l\phi_i(\vec{r})))$$

$$\vec{s}(\vec{r}) = \sum_i \phi_i^*(\vec{r})\vec{\sigma}\phi_i(\vec{r})$$

$$\vec{j}(\vec{r}) = \sum_i(\phi_i^*(\vec{r})\nabla\phi_i(\vec{r}) - (\nabla\phi_i^*(\vec{r}))\phi_i(\vec{r}))$$

$$\vec{T}(\vec{r}) = \sum_i \nabla\phi_i^*(\vec{r}).\vec{\sigma}\nabla\phi_i(\vec{r})$$

Time-even densities

Time-odd densities

Density functional theory

Advantage of **DFT**:

- Its applicability to basically whole **nuclear chart** (including superheavies)

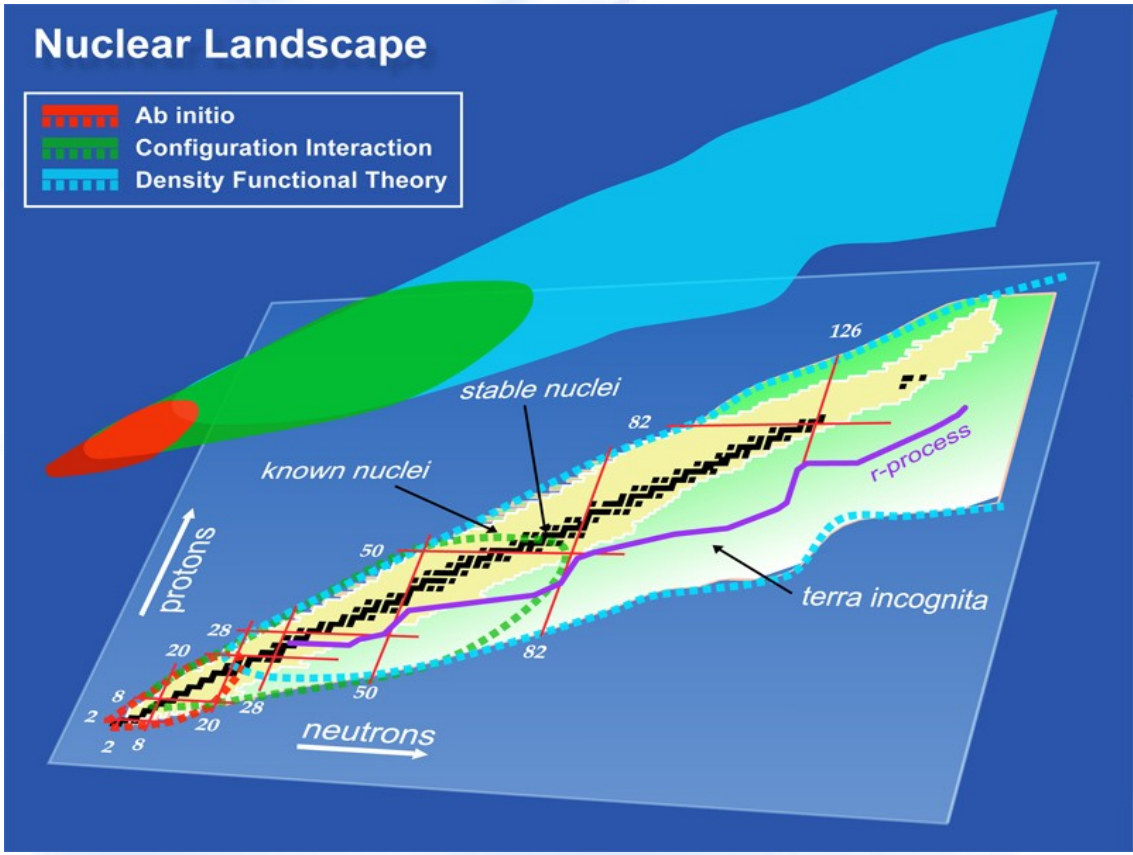
- Computational **simplicity**

Problem of **DFT**:

- No clear link **functional** ↔ **interaction**

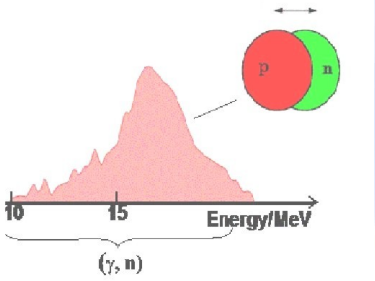
(**J. Dobaczewski**, J. Phys. G: Nucl. Part. Phys. 43 (2016) 04LT01)

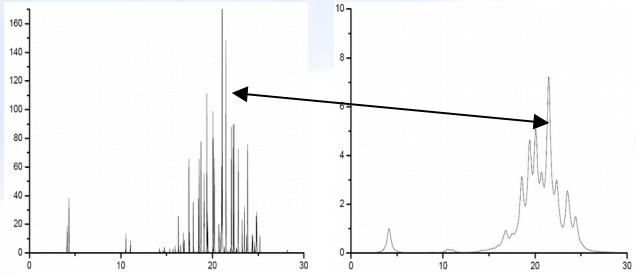
- DFT primarily for **ground states**, calculations of nuclear excited states in approaches based on DFT – mostly **collective excitations**



Photoabsorption total **cross section**:

$$\sigma(E\lambda\mu) = 8\pi^3 \frac{\lambda+1}{\lambda[(2\lambda+1)!!]^2} \sum_\nu \left(\frac{\omega_\nu}{\hbar c}\right)^{2\lambda-1} |<\nu|\hat{M}(\lambda\mu)|gs>|^2$$





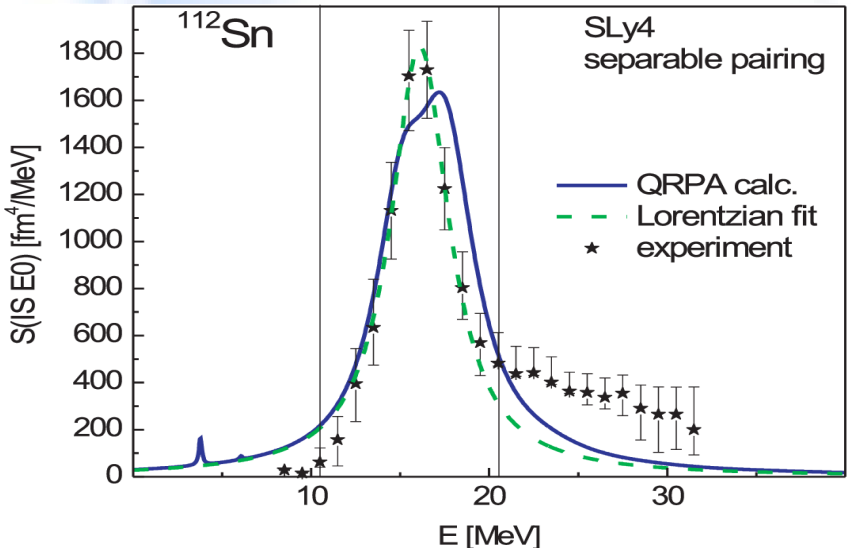
Density functional theory

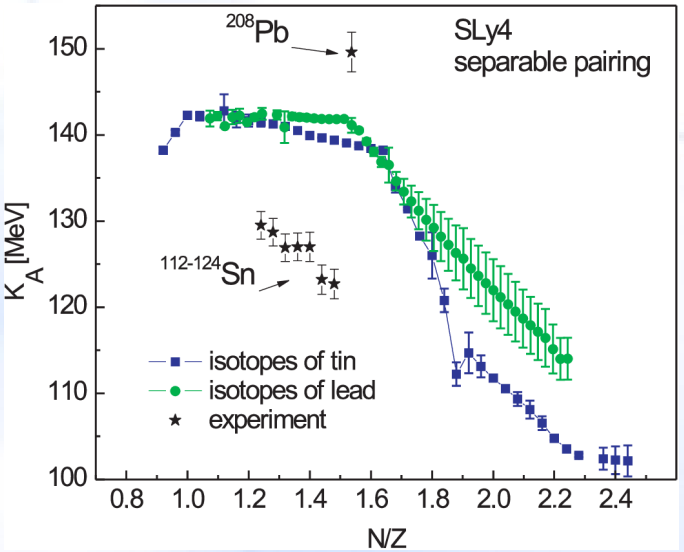
Giant monopole resonance – its **centroid** connected with the **incompressibility** of nucleus $\mathbf{K_A}$

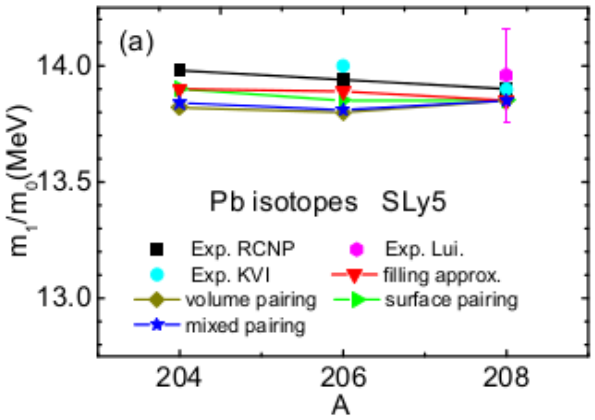
$$E_{GMR} = \frac{m_1}{m_0}$$

$$E_{GMR} = \sqrt{\frac{\hbar^2 K_A}{m\langle r^2\rangle}}$$

P.V. et al., **Phys. Rev. C 86**, 024303 (2012)





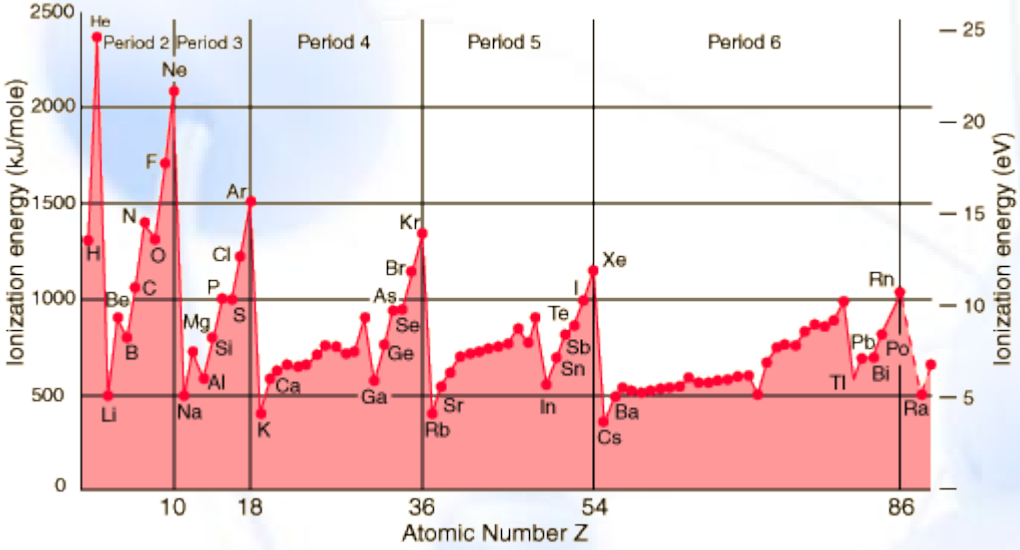


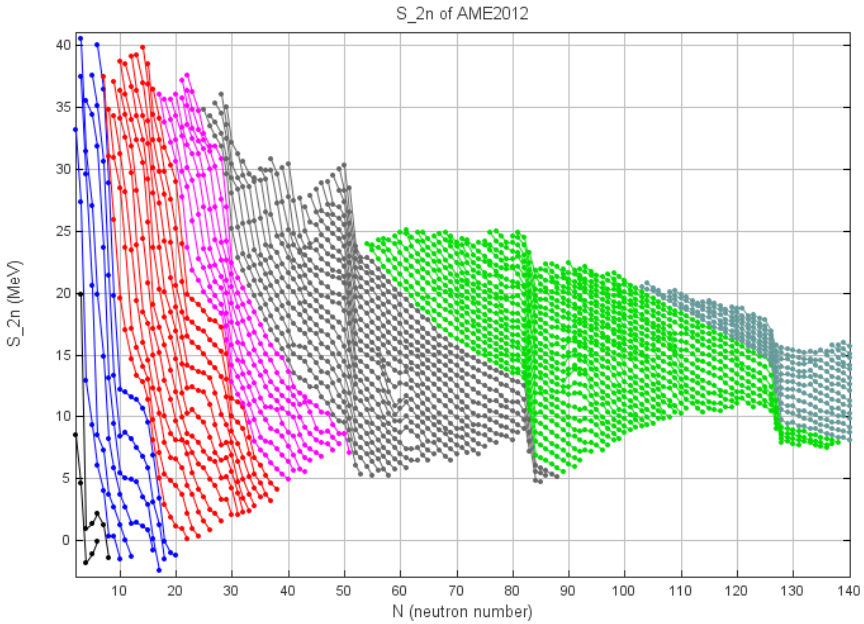
Tin isotopes much **“softer“** than ^{208}Pb

limitations of theory – theory (DFT) completely fails to describe incompressibility in **tin** and **lead simultaneously**

it cannot be caused by double close shell in ^{208}Pb

Nuclear mean field





Existence of “magic” numbers in atomic physic:

Consequence of movement of electrons in *Coulomb field* of atomic nucleus

Atomic nuclei

2n separation energies
S_2n = B(A,Z) – B(A-2,Z)

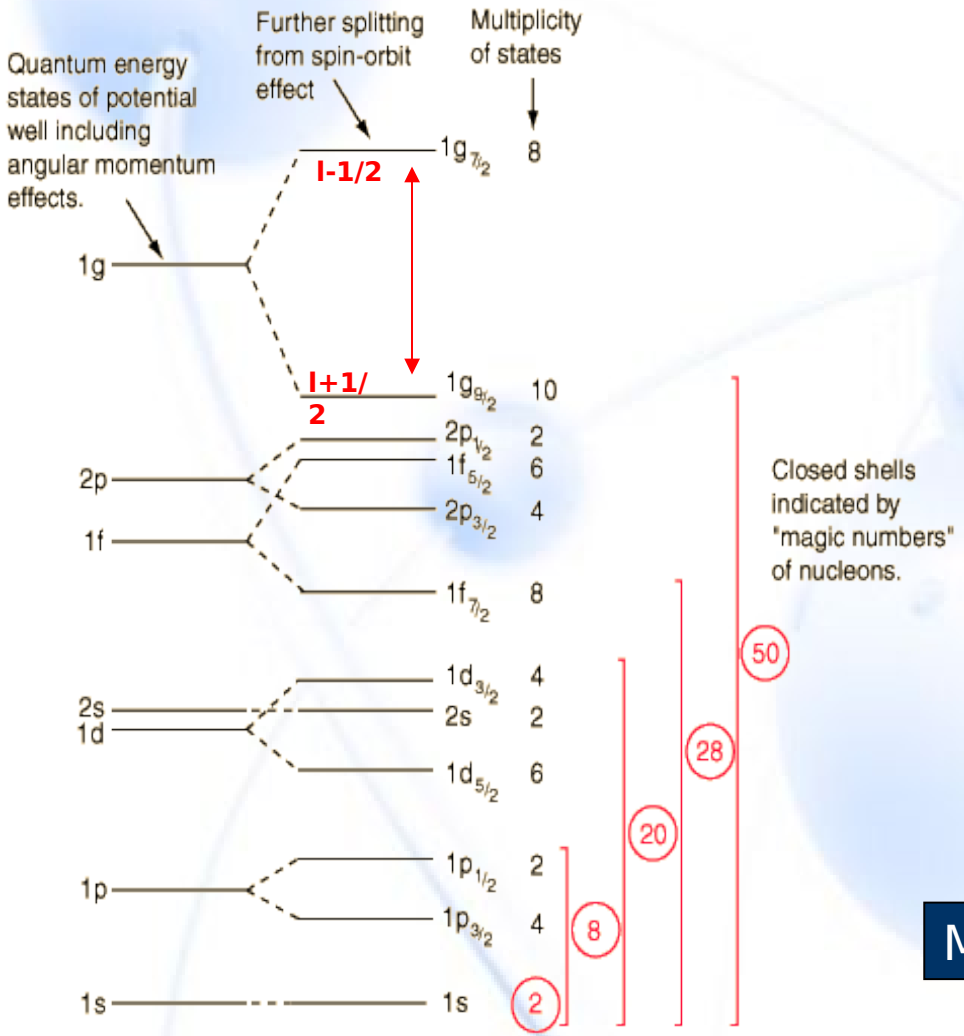
Shell corrections
-> magic numbers

Magic numbers 2,8,20,28,50,82,126

How shell structure occurs in nucleus?

Nuclear mean field

“original“ shell-model



M.Goepert-Mayer, J. H. D. Jensen
1963 Nobel prize for physics

“shell structure in nuclei and correct magic numbers“

Magic numbers 2,8,20,28,50,82,126

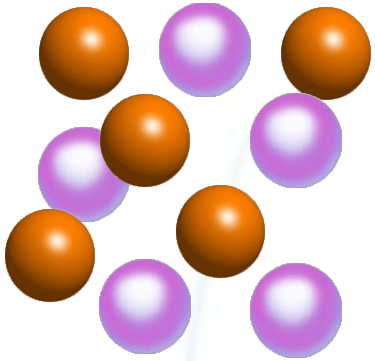
Nuclear mean field

How mean field occurs in nucleus? → change our perspective

nucleons as non-interacting particles in potential well → **mutual interaction of nucleons creates "mean field" → nucleons move in this field**

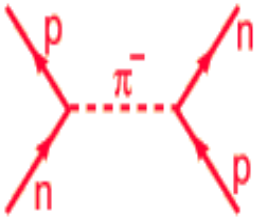
Hartree-Fock method – mean-field is generated "by itself" = self-consistence

$$\sum_{ij} t_{ij} a_i^\dagger a_j + \frac{1}{4}\sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k = \sum_{ij}\left\{ t_{ij} + \sum_{kl} V_{kilj} \langle\, |a_k^\dagger a_l| \,\rangle \right\} a_i^\dagger a_j + \frac{1}{4}\sum_{ijkl} V_{ijkl} : a_i^\dagger a_j^\dagger a_l a_k :$$



free nucleons

+



interaction

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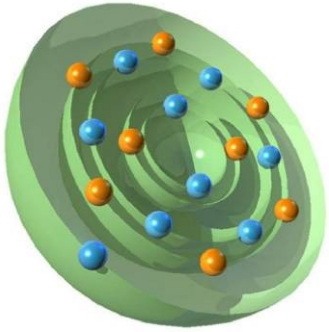
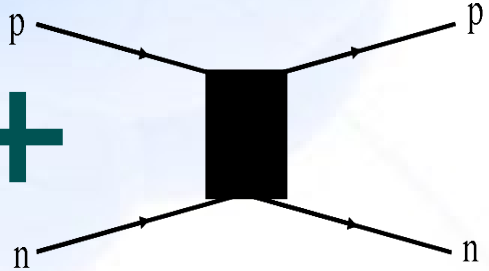


mean field

+



residual interaction

Nuclear mean field

Hartree-Fock method

H. Hergert, *PhD. thesis* (2008)

Phys. Rev. C 95, 024306, (2017)

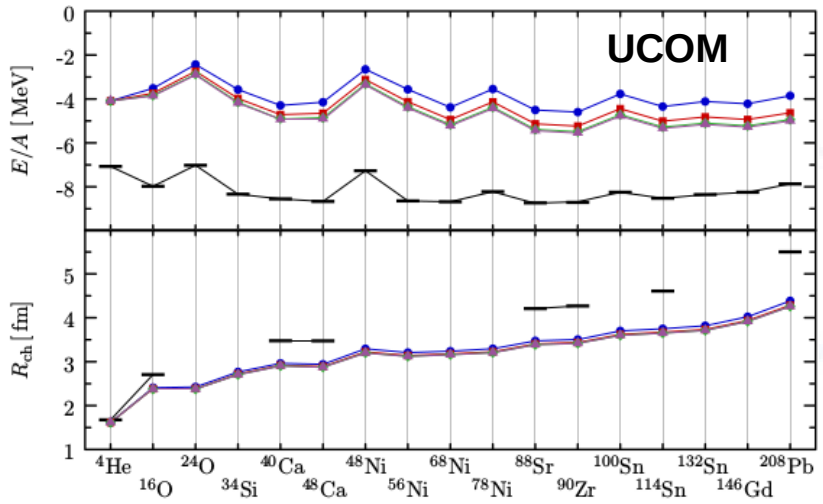


Figure 2.2: Ground-state energies and charge radii of closed-shell nuclei for $e_{max} = 12$. Shown V_{UCOM} with $I_\vartheta^{(1,0)} = 0.09\,\mathrm{fm}^3$ and $I_\vartheta^{(1,1)} = 0\,\mathrm{fm}^3$ (—●—), $0.02\,\mathrm{fm}^3$ (—■—), $0.05\,\mathrm{fm}^3$ (—◆—), and $0.07\,\mathrm{fm}^3$ (—▲—), compared to experimental data (——).

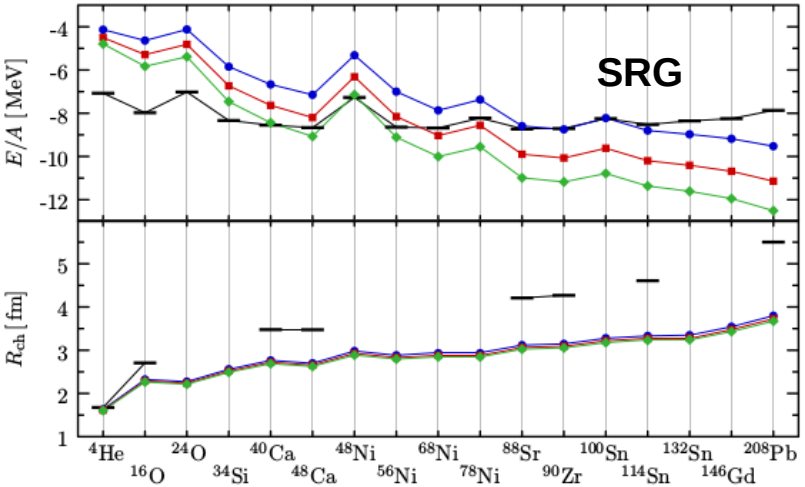
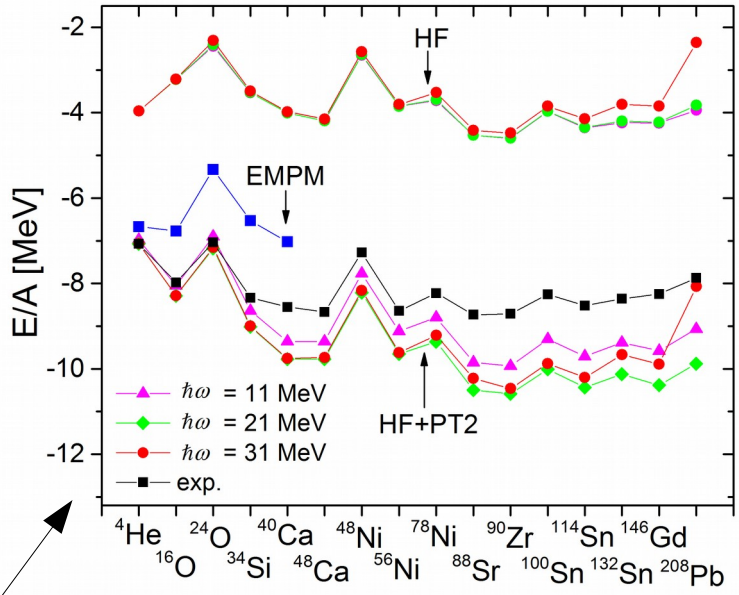


Figure 2.3: Ground-state energies and charge radii of closed-shell nuclei ($e_{max} = 12$) for V_α with $\bar{\alpha} = 0.025\,\mathrm{fm}^4$ (—●—), $0.030\,\mathrm{fm}^4$ (—■—), and $0.035\,\mathrm{fm}^4$ (—◆—), compared to experimental data (——).

E/A = binding energy per nucleon

R_{ch} = charged proton radius

NN interaction - chiral **$NNLO_{opt}$**



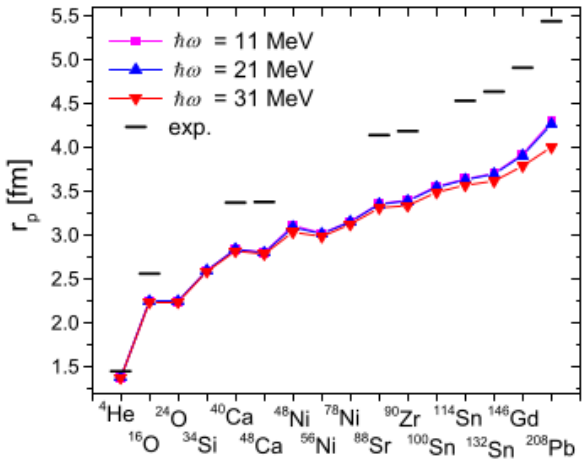
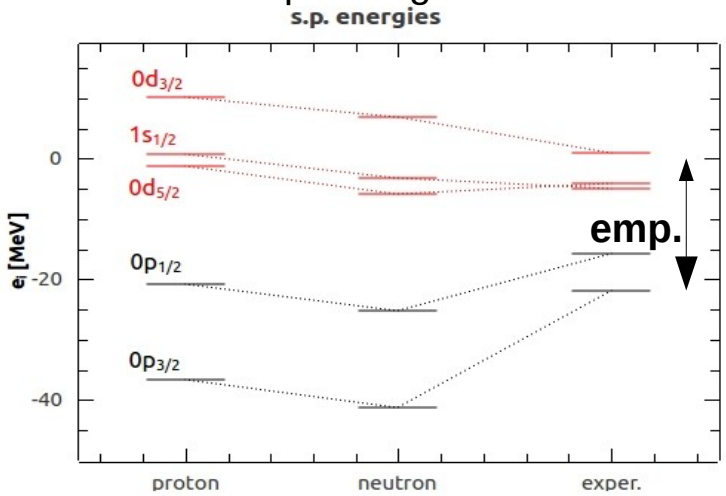


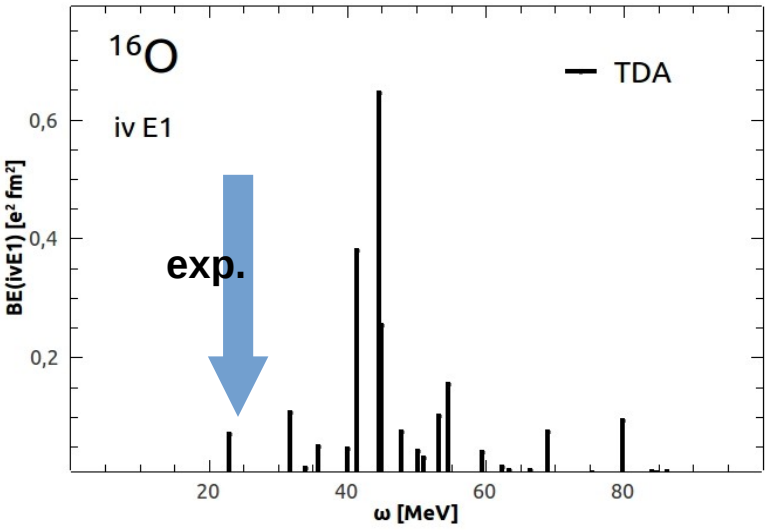
FIG. 6. Systematic of root-mean-square point proton radii computed in HF. The calculations are performed for $N_{max} = 14$ and different HO frequencies ω. The experimental data are from Ref. [49].

Nuclear mean field

nuclear **radius** → gaps **single-particle energies** → photoabsorption **excitation spectra**

unrealistic s.p. energies with realistic **NN interactions**





inclusion of 3-body NNN force

NN+NNN interaction
- χ **NNLO$_{sat}$**

bare and/or induced **NNN** improves **s.p. energies** but is worse for reproducing total **binding energy E/A** at the mean field (Hartree-Fock)

Phys. Scr. 94, 014006, (2019)

Table 1: The charge radii $r_{ch} = \sqrt{< r_{ch}^2 >}$ [fm] of ^{16}O and ^{40}Ca calculated with NN and $NN+NNN$ forces are compared with the experimental data (exp) [23].

$^A X$	NN	$NN+NNN$	exp
^{16}O	2.19	2.77	2.70
^{40}Ca	2.58	3.54	3.48

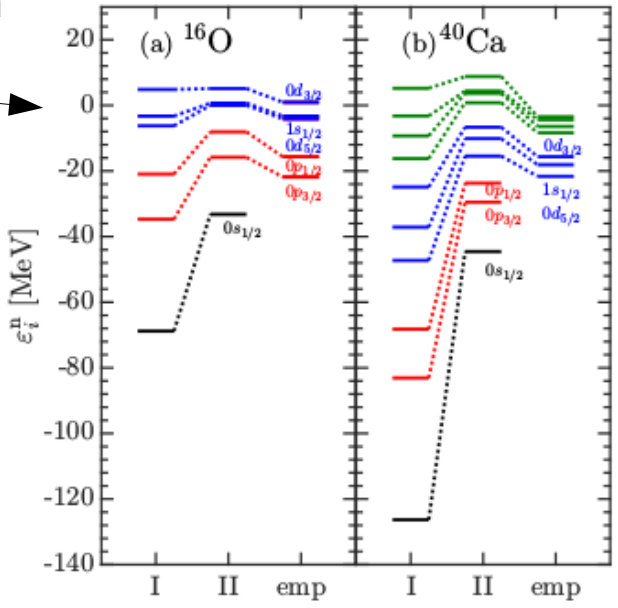


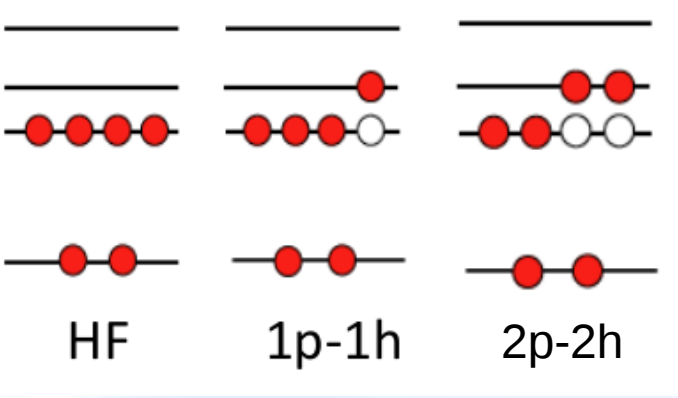
Fig. 3: The neutron single-particle energies ε_i^n of ^{16}O (a) and ^{40}Ca (b) calculated with NN (I) and $NN+NNN$ (II) interactions. The empirical data (emp) [24] are shown for comparison.

EMPM

Hilbert space – divided into subspaces

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus ... \oplus \mathcal{H}_n$$

HF – Hartree-Fock state (nucleons occupy lowest single-particle levels)
1p-1h = 1**particle** – 1**hole** excitation of HF
2p-2h = 2**particle** – 2**hole** excitation of HF
.
.
np-nh = n**particle** – n**hole** excitation of HF



Instead of multiple **particle-hole** excitations we can excite multiple **TDA phonons**

Tamm-Dancoff (TDA) phonons

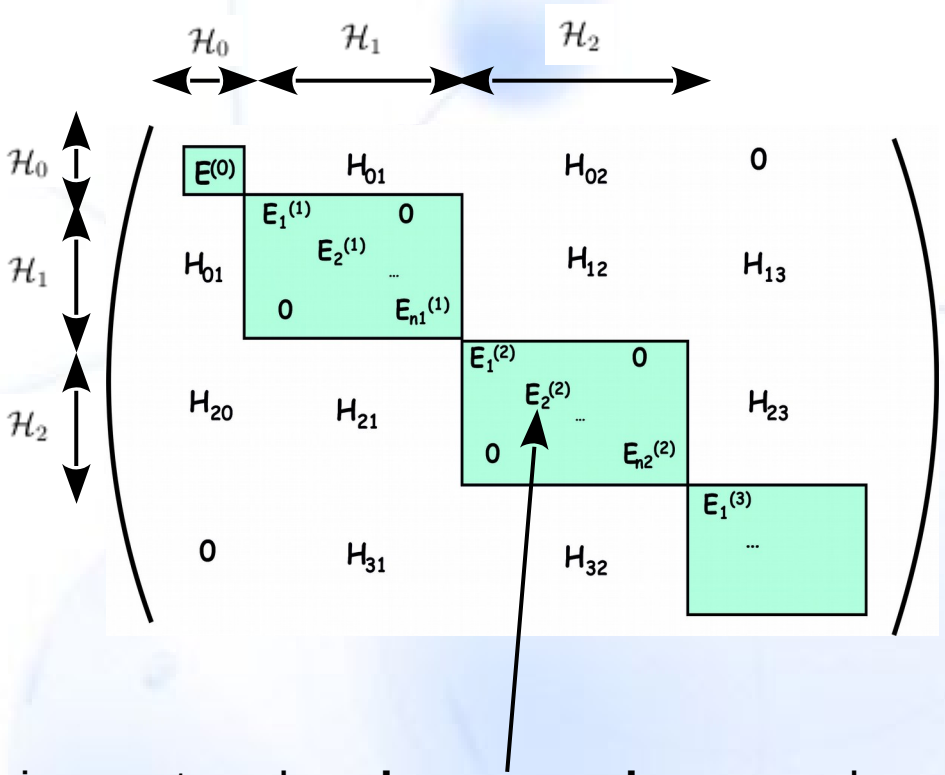
$$O^\dagger_\nu = \sum_{ph} c^\nu_{ph} a^\dagger_p a_{\hat{h}}$$

Phonons = linear combination of 1p-1h excitations
can represent **collective modes**

$$\begin{aligned}
\mathcal{H}_0 &= \{|HF>\} \\
\mathcal{H}_1 &= \{O^\dagger_{\nu_1}|HF>\} \\
\mathcal{H}_2 &= \{O^\dagger_{\nu_1} O^\dagger_{\nu_2}|HF>\} \\
&\cdot \\
&\cdot \\
\mathcal{H}_n &= \{O^\dagger_{\nu_1} O^\dagger_{\nu_2} ... O^\dagger_{\nu_n}|HF>\}
\end{aligned}$$

EMPM

$$
\begin{aligned}
\mathcal{H}_0 &= \{|HF>\} \\
\mathcal{H}_1 &= \{O^\dagger_{\nu_1}|HF>\} \\
\mathcal{H}_2 &= \{O^\dagger_{\nu_1}O^\dagger_{\nu_2}|HF>\} \\
&\cdot \\
&\cdot \\
\mathcal{H}_n &= \{O^\dagger_{\nu_1}O^\dagger_{\nu_2}...O^\dagger_{\nu_n}|HF>\}
\end{aligned}
$$



the total **Hamiltonian** mixes configurations from different **Hilbert subspaces**

Equation of Motion (EoM) – recursive eq. to solve **eigen-energies** on each **i**-phonon subspace while knowing the (**i-1**)-phonon solution

$$< i,\beta_i|[\hat{H},O^\dagger_\nu]|i-1,\alpha_{i-1}>=(E^i_{\beta_i}-E^{i-1}_{\alpha_{i-1}})<i,\beta_i|O^\dagger_\nu|i-1,\alpha_{i-1}>$$

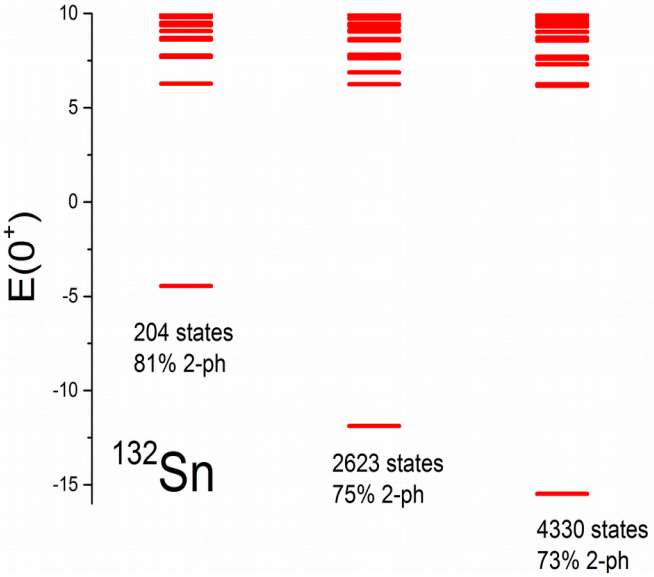
non-diagonal blocks of **Hamiltonian** calculated from amplitudes $<i,\beta_i|O^\dagger_\nu|i-1,\alpha_{i-1}>$

we diagonalize the total **Hamiltonian**

EMPM

Correlations and their effect on the nuclear **ground state**:

Phys. Rev. C 90, 014310, (2014)



NN interaction - χ **NNLO$_{opt}$**

A. Ekström et al., **PRL 110**, 192502 (2013)

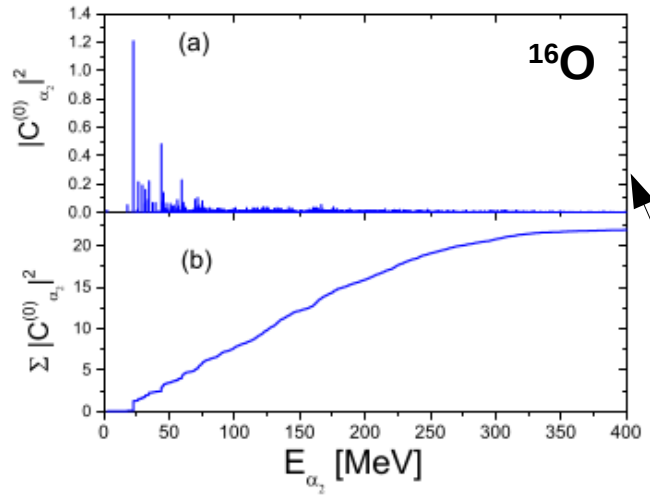
2-phonon correlations in the **g.s.**

$$|\Psi_{g.s.}> \approx C^{g.s.}_{HF}|HF> + \sum_{\mu_2} C^{g.s.}_{\mu_2}|i=2,\mu_2>$$

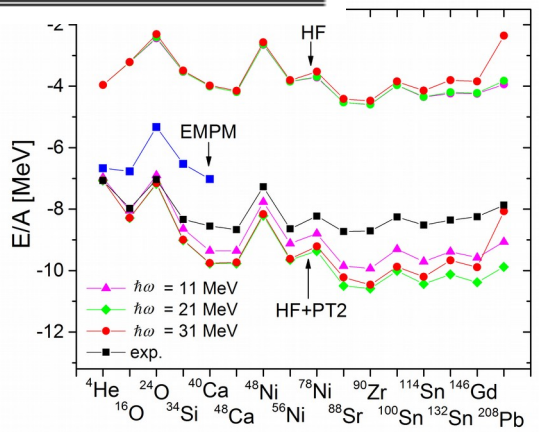
Phys. Rev. C 95, 024306 (2017)

TABLE I. Binding energies per nucleon. The EMPM value for ^{40}Ca was obtained for $N_{max} = 8$, which is not an extremal point.

	BE/A (MeV)			
$^A X$	HF	PT	EMPM	Exp.
^{4}He	3.96	7.07	6.67	7.07
^{16}O	3.22	8.29	6.77	7.98
^{40}Ca	4.00	9.77	7.02	8.55



running sum of contributions of the **2-phonon configurations** into the **correlated ground state**



EMPM

Correlations and their effect on the nuclear **radii**:

NN interaction - χ **NNLO$_{opt}$**

A. Ekström et al., **PRL 110**, 192502 (2013)

$$|\Psi_{g.s.}> \approx C^{g.s.}_{HF}|HF> + \sum_{\mu_2} C^{g.s.}_{\mu_2}|i=2,\mu_2>$$

proton **point radii**

$$< r_p^2 > = < \Psi_{g.s.}|r_p^2|\Psi_{g.s.} > = < r_p^2 >_{HF} + < r_p^2 >_{corr.}$$

small effect of correlations on **r$_p$**

satisfactory description of **radius** with **HF**

NNN forces play important role here!

diploma thesis of **J. Pokorný**

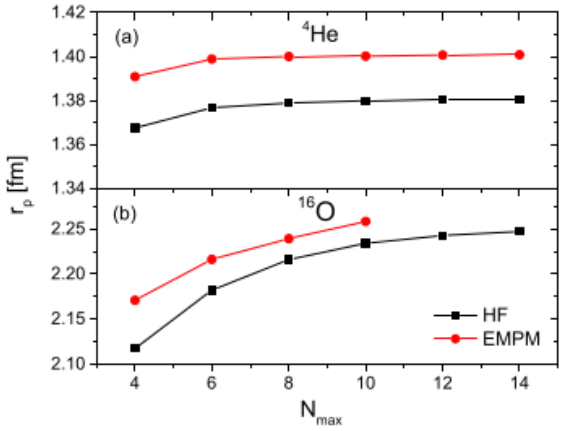
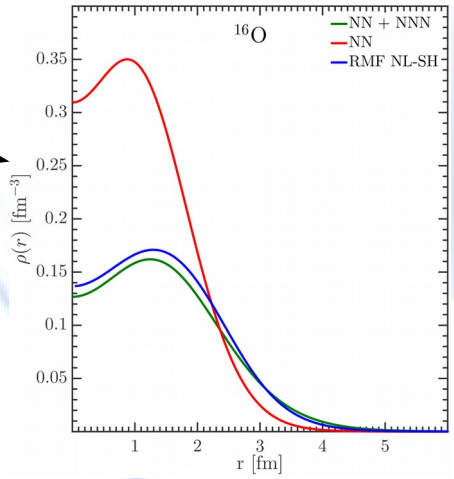


FIG. 7. HF and EMPM point proton radii of ^{4}He (a) and ^{16}O (b) versus N_{max} for fixed frequency ($\hbar\omega = 26$ MeV).



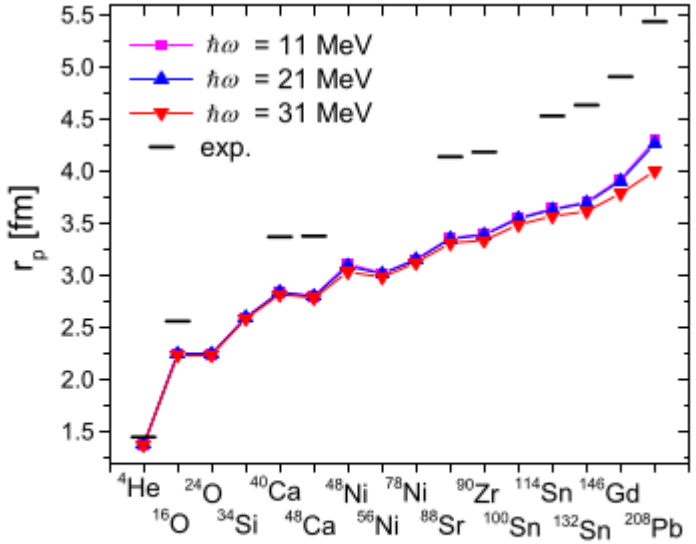


FIG. 6. Systematic of root-mean-square point proton radii computed in HF. The calculations are performed for $N_{max} = 14$ and different HO frequencies ω. The experimental data are from Ref. [49].

$^A X$	r_p (fm) HF	EMPM	Exp.
^{4}He	1.38	1.40	1.46
^{16}O	2.25	2.26	2.57

EMPM

Correlations and their effect on the nuclear **photoabsorption spectra**:

NN interaction - χ **NNLO**$_{opt}$

A. Ekström et al., **PRL 110**, 192502 (2013)

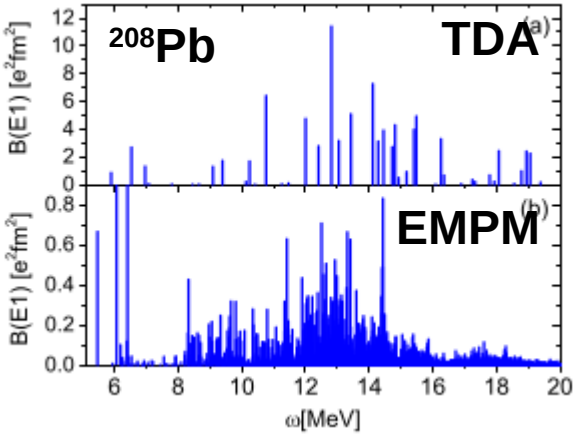
study of the dipole **photoabsorption spectrum**

B(E1, $0^+_{g.s.} \rightarrow 1^-_{exc.}$)

calculation of ^{208}**Pb** – see in **Phys. Rev. C 92**, 054315 (2015)

2-phonon configurations very important to describe richness of spectrum → **multifragmentation** of dipole resonance... we describe **width** of resonance

most of **1**$^-$ states have configurations beyond 1**phon**



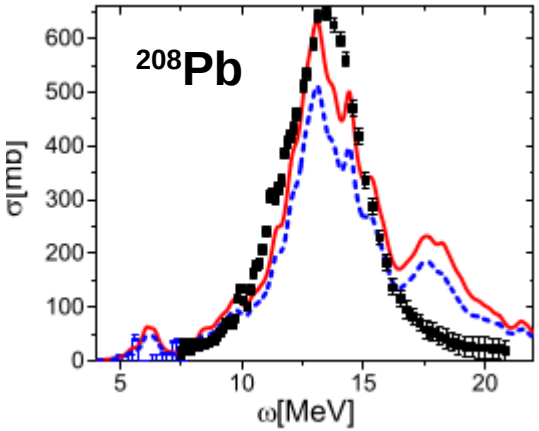


TABLE I. Phonon composition of the lowest twenty 1^- states.

J^π_ν	ω_ν (MeV)	$\lvert C_1^{(\nu)}\rvert^2$	$\lvert C_2^{(\nu)}\rvert^2$
1^-_1	4.42780	0.00017	0.99983
1^-_2	4.67271	0.00083	0.99917
1^-_3	4.96609	0.00014	0.99986
1^-_4	5.46012	0.95558	0.04442
1^-_5	5.93408	0.03132	0.96868
1^-_6	6.05979	0.90712	0.09288
1^-_7	6.18594	0.05422	0.94578
1^-_8	6.25179	0.04936	0.95064
1^-_9	6.26285	0.05409	0.94591
1^-_{10}	6.27701	0.00310	0.99690
1^-_{11}	6.38869	0.15931	0.84069
1^-_{12}	6.40474	0.69907	0.30093
1^-_{13}	6.42531	0.03371	0.96629
1^-_{14}	6.43502	0.03215	0.96785
1^-_{15}	6.48971	0.86985	0.13015
1^-_{16}	6.53002	0.00956	0.99044
1^-_{17}	6.55127	0.00485	0.99515
1^-_{18}	6.64103	0.00346	0.99654
1^-_{19}	6.71925	0.01301	0.98699
1^-_{20}	6.73778	0.00058	0.99942

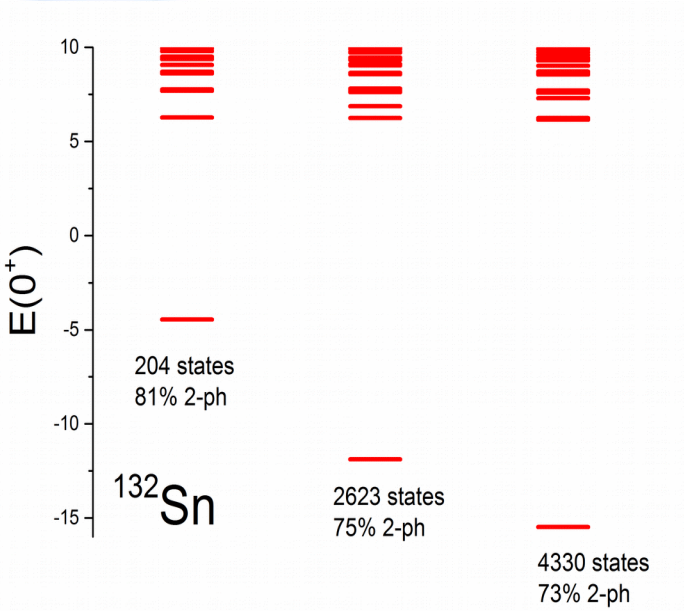
EMPM

Open problems:

- large scale **converged** (with respect to config. space) results up to **2-phonon**, but at least **3-** and **4- phonon** calcs. needed

- all **complex configurations** seem to **contribute** to the **correlated g.s.** wave function → not possible of drastic cut-offs

- **unconverged 3-phonon** calculations

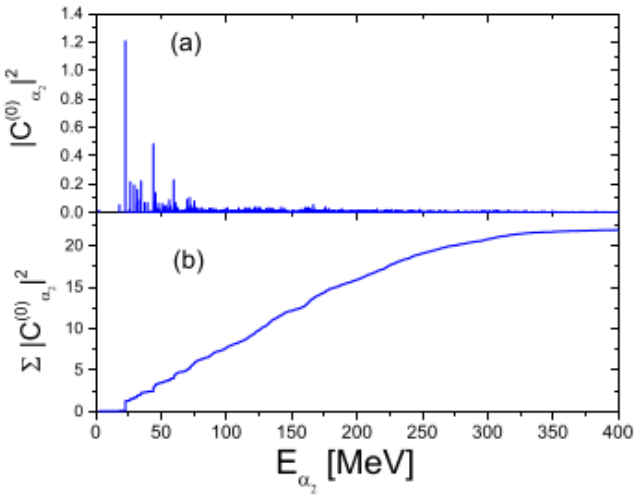


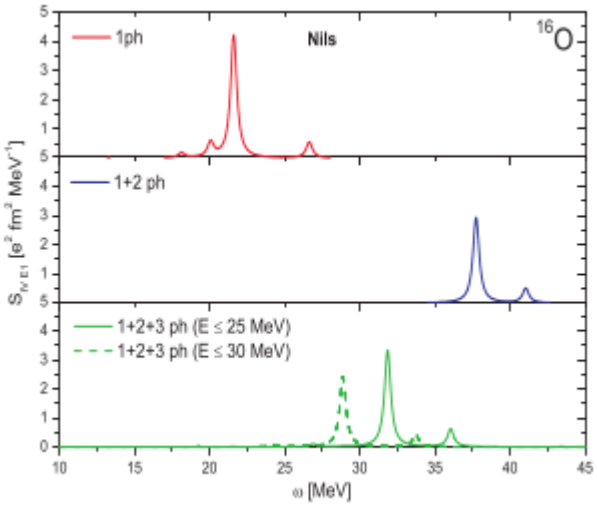
Possible improvements:

- more efficient computations (better use of paralel computing)

- **importance truncation**

- formulate **EoM** directly on the **correlated g.s.** ??





Summary

- **Quantum many-body probem** remain **unsolved** for decades
- In atomic nuclei **QMB** even more **complicated**, description of **interaction** is **open problem** too
- Several **model dependent approaches** to **QMB**, no one precise
- We discussed **DFT**, nuclear **mean-field**, **EMPM** approaches – **open problems** call for solution and further effort!!

Thank you for attention!