Non-empirical energy functionals from low-momentum interactions

III. Many-body perturbation theory and non-empirical energy functionals

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Lecture series

Outline

1. Introduction to energy density functional methods
2. Low-momentum interactions from renormalization group methods
3. The building of non-empirical energy functionals
   - Time-ordered Many-body perturbation theory (MBPT)
   - Formal connection between single-reference EDF and MBPT
   - The density matrix expansion
   - First application to the pairing part of the EDF

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1. Introduction
   - Some questions raised about EDF methods
   - Ab-initio many-body methods
2. Time-ordered many-body perturbation theory
   - Elements of formalism
   - Application to symmetric nuclear matter
   - Application to doubly-magic nuclei
3. Towards non-empirical energy functionals
   - Comparison between Skyrme EDF and MBPT expressions
   - Basics of the density matrix expansion
   - First calculations with non-empirical pairing energy functional
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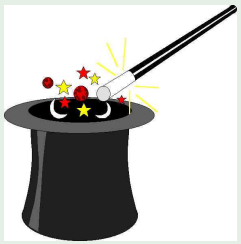
Constructing non-empirical EDFs for nuclei

Long term objective

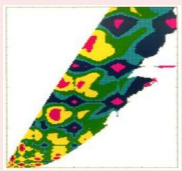
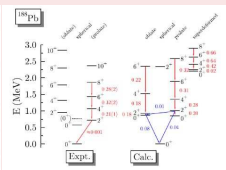
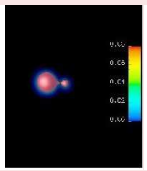
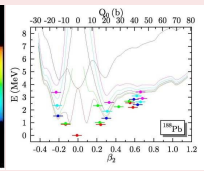
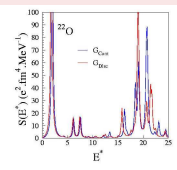
Build non-empirical EDF in place of existing models

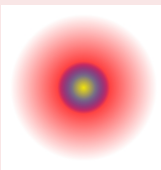
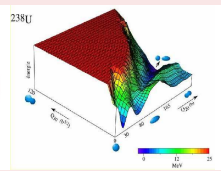
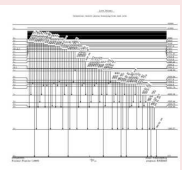
Empirical



Predictive?

Finite nuclei and extended nuclear matter

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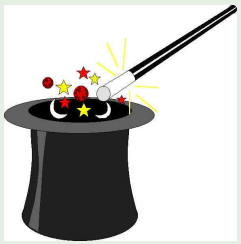
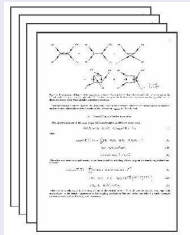


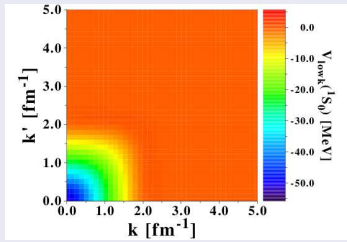
Predictive?

Non-empirical

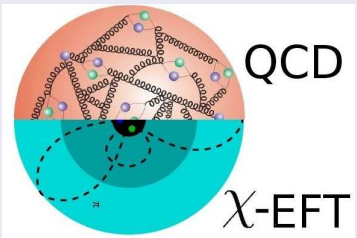


Predictive...

Low-k NN+NNN



QCD / χ-EFT



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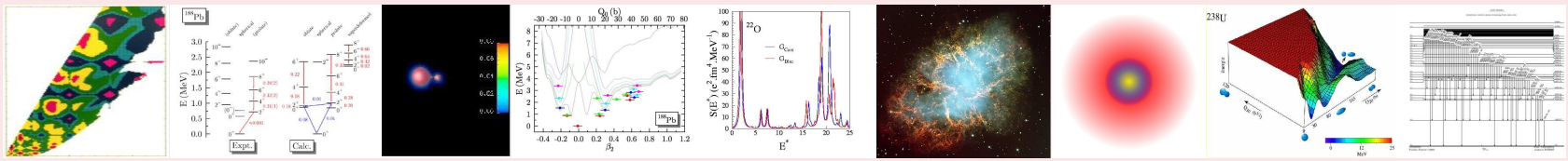

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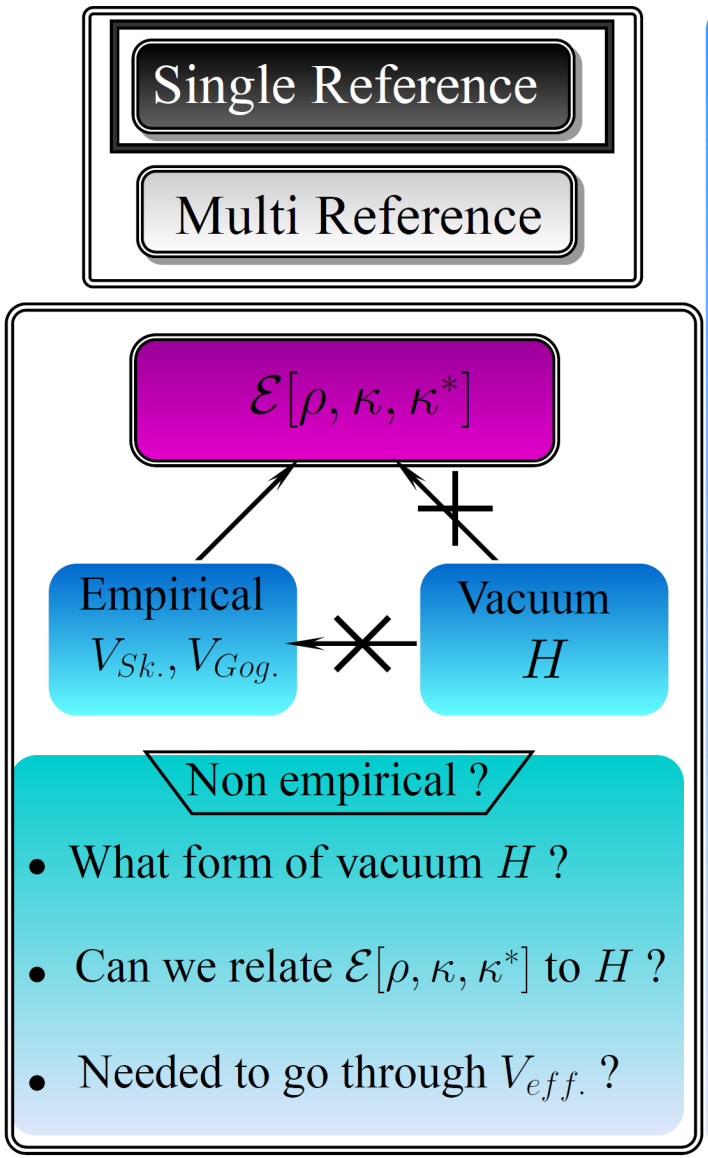
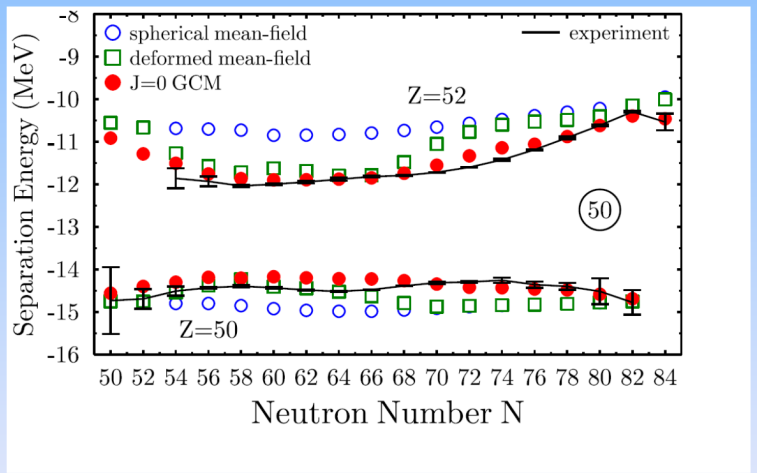
Energy Density Functional method: some relevant questions



Empirical knowledge

- $\mathcal{E}[\rho, \kappa, \kappa^*]$ built empirically so far
- Effective separation of scales for correlations
  - Bulk $\sim$ 800 Mev $\propto$ A
  - Collective def. $\leq$ 20 Mev $= F(N_{val}, G_{deg})$
  - Collective fluct. $\leq$ 4 MeV $= G(N_{val}, G_{deg})$
- Observables impacted by correlation
  - Symmetry breaking
  - Collective fluctuation



Take-away message

Time-ordered many-body perturbation theory

1. Many-body problem (seems to) becomes perturbative with $H(\Lambda_{\text{low}})$
2. First applications in INM and doubly-magic nuclei confirm so
3. MBPT with $H(\Lambda_{\text{low}})$ = good ab-initio scheme to build non-empirical EDF

Towards (extended) energy functionals

1. MBPT too expensive for heavy open-shell nuclei
2. Approximate methods, e.g. the DME, to put it under a bearable form
3. Controlled refit of Λ-dependent couplings to reach desired accuracy

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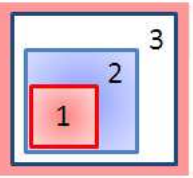
A-initio methods to solve the nuclear A-body problem

Currently used ab-initio methods

- Solve the N-body problem in terms of point-like nucleons+$H(\Lambda)$

Name	Short description	Variational	Scale as	Up to
Few-body (Faddeev...)	$H\Psi = E\Psi$ 	Yes	M^A	A = 2-4
Green-Function Monte-Carlo (GFMC)	$\Psi(\tau) = e^{-(H-E_0)\tau}\Psi_T$, $= [e^{-(H-E_0)\Delta\tau}]^n \Psi_T$ + auxiliary field 	Yes	$\frac{M!}{(M-A)!A!}$	A <12
No-core Shell Model	$H\Psi = E\Psi$ 	Yes	4^A	A <16
Coupled-Cluster (CC)	$\|\Psi\rangle = e^S \|\Psi_0\rangle$ $S = S_1 + S_2 + \cdots$ 	No	$(M-A)^4 A^2$	A <100 Only doubly-magic for now

M : configuration space size

From D. Lacroix

- Many-body perturbation theory is missing; why!?

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Many-body perturbation theory (no pairing, V^{NN} only)

Unperturbed (reference) vacuum

- Reference Slater determinant $|\Phi\rangle = \prod_{i=1}^{N} a_i^+ |0\rangle$
- Associated one-body density matrix $\rho_{\alpha\beta} = \delta_{\alpha i}\,\delta_{\beta i}$
  1. Greek indices $\alpha, \ldots$ = arbitrary s.p. states
  2. Roman indices $i, \ldots$ = occupied ("hole") s.p. states
  3. Roman indices $a, \ldots$ = empty ("particle") s.p. states
- Excited Slater determinants $|\Phi_{ij\ldots}^{ab\cdots}\rangle$, e.g. 2p-2h state $|\Phi_{ij}^{ab}\rangle = a_a^+ a_b^+ a_j a_i |\Phi\rangle$

Hartree-Fock s.p. basis a_α^+ / ψ_α

- $h^{HF}\,\psi_\alpha = \epsilon_\alpha\,\psi_\alpha$
- $h_{\alpha\gamma}^{HF} \equiv t_{\alpha\gamma} + \sum_{\beta\delta} \bar{V}_{\alpha\beta\gamma\delta}^{NN}\,\rho_{\delta\beta}$

Matrix elements of V^{NN}

- $V_{\alpha\beta\gamma\delta}^{NN} \equiv \langle 1:\alpha; 2:\beta | V^{NN} | 1:\gamma; 2:\delta \rangle$
- $\bar{V}_{\alpha\beta\alpha\beta}^{NN} \equiv V_{\alpha\beta\gamma\delta}^{NN} - V_{\alpha\beta\delta\gamma}^{NN}$

Hartree-Fock energy from Wick theorem with respect to $|\Phi\rangle$

$$E^{HF} \equiv \langle \Phi | H | \Phi \rangle = \sum_i t_{ii} + \frac{1}{2} \sum_{ij} \bar{V}_{ijij}^{NN}$$

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Many-body perturbation theory (no pairing, V^{NN} only)

$H(\Lambda)$ in normal-ordered form

- Using Wick's theorem with respect to $|\Phi\rangle$

$$H(\Lambda) = E^{HF} + \sum_{\alpha} \epsilon_\alpha : a_\alpha^+ a_\alpha : + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{V}^{NN}_{\alpha\beta\gamma\delta} : a_\alpha^+ a_\beta^+ a_\delta a_\gamma : \equiv H_0 + V_{\rm res}$$

- H_0 denotes the unperturbed Hamiltonian and $V_{\rm res}$ the residual interaction
  - $H_0|\Phi^{ab\ldots}_{ij\ldots}\rangle = E^{ab\ldots}_{ij\ldots}|\Phi^{ab\ldots}_{ij\ldots}\rangle$ with $E^{ab\ldots}_{ij\ldots} = E^{HF} + (\epsilon_a + \epsilon_b + \ldots - \epsilon_i - \epsilon_j - \ldots)$
  - $\langle\Phi| V_{\rm res}|\Phi\rangle = \langle\Phi| V_{\rm res}|\Phi^a_i\rangle = 0$

Correlations (always defined with respect to a given reference!)

- True ground-state energy of $|\Psi\rangle$ is $E \equiv E^{HF} + \Delta E^{HF}$

1. Can minimize ΔE^{HF} through symmetry breaking (N, J, $\pi\ldots$)
   - Includes correlations with respect to symmetry restricted E^{HF}!
2. Not enough as "bulk" correlations are missing in the first place
   - Cf. Infinite Nuclear Matter and doubly magic nuclei below...

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Time-ordered (Goldstone) MBPT from Gell-Man Low theorem

- ΔE^{HF} expanded as a power series in V_{res}

$$\Delta E^{HF} = \sum_{n=0} \langle \Phi | V_{\text{res}} \left(\frac{1}{E^{HF} - H_0} V_{\text{res}} \right)^n | \Phi \rangle_{\text{connected}}$$

- Summing all terms provides the exact ground-state energy

Perturbative approach

- If it makes sense
  1. Meaningful answer obtained from a finite number of terms
  2. Contributions decreases as n increases
  3. May need to define H_0 ($|\Phi\rangle$) differently to speed up convergence
- Counter examples
  1. Cooper instability = need to expand around a Bogoliubov vacuum
  2. $H(\Lambda_{\text{high}})$ = need to sum pp ladders and expand in (hole-lines)^n
- What about using $H(\Lambda_{\text{low}})$ rather than $H(\Lambda_{\text{high}})$?

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Many-body perturbation theory (no pairing, V^{NN} only)

Computation procedure = 1st version

1. Truncate expansion to given order $n_{\max}$
2. Insert (quasi) completeness relationship of $\mathcal{H}_N$ in between each operator

$$\mathbb{1}_N - |\Phi\rangle\langle\Phi| = \sum_{\substack{a \\ i}} |\Phi_i^a\rangle\langle\Phi_i^a| + \left(\tfrac{1}{2!}\right)^2 \sum_{\substack{a,b \\ i,j}} |\Phi_{ij}^{ab}\rangle\langle\Phi_{ij}^{ab}| + \left(\tfrac{1}{3!}\right)^2 \sum_{\substack{a,b,c \\ i,j,k}} |\Phi_{ijk}^{abc}\rangle\langle\Phi_{ijk}^{abc}| + \dots$$

3. Apply each resolvent operator $(E^{HF} - H_0)^{-1}$ to extract energy denominators
4. Compute each matrix elements of V_{res}

Example: second order ($n_{\max} = 1$)

$$\begin{aligned} \Delta E^{HF}(2) &= \frac{1}{4} \sum_{i,j,a,b} \frac{|\langle\Phi| V_{\text{res}} |\Phi_{ij}^{ab}\rangle|^2}{E^{HF} - E_{ij}^{ab}} \\ &= \frac{1}{4} \sum_{i,j,a,b} \frac{|\bar{V}_{ijab}^{NN}|^2}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} < 0 \end{aligned}$$

Needed matrix elements

1. $\langle\Phi| V_{\text{res}} |\Phi_i^a\rangle = 0$
2. $\langle\Phi| V_{\text{res}} |\Phi_{ij}^{ab}\rangle = \bar{V}_{ijab}^{NN}$
3. $\langle\Phi| V_{\text{res}} |\Phi_{ijk\dots}^{abc\dots}\rangle = 0$

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Many-body perturbation theory (no pairing, V^{NN} only)

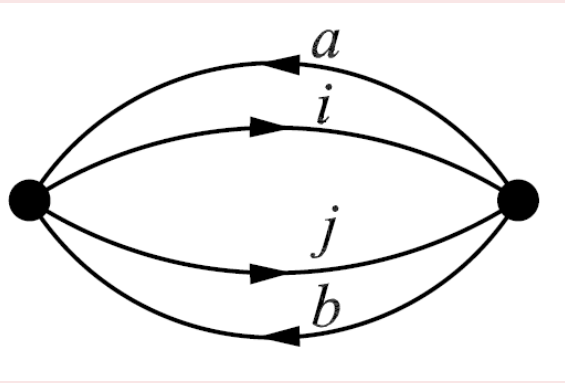
Computation procedure = 2nd version

1. Matrix elements $\langle \Phi^{a'b'c'\dots}_{i'j'k'\dots} | V_{\rm res} | \Phi^{abc\dots}_{ijk\dots} \rangle$ cumbersome to compute
2. Develop systematic approach = diagrammatic techniques
3. Rules to compute Hugenholtz/Golsdtone diagrams

Example: second order ($n_{\rm max} = 1$)

$$\Delta E^{HF}(2) = \frac{1}{4} \sum_{i,j,a,b} \frac{|\bar{V}^{NN}_{ijab}|^2}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

Diagram



Remark

1. Hole state $\Leftrightarrow$ factor $\rho_{\alpha\alpha}$ in $\sum$
2. Particle state $\Leftrightarrow$ factor $1-\rho_{\alpha\alpha}$ in $\sum$

Many-body perturbation theory (no pairing, V^{NN} only)

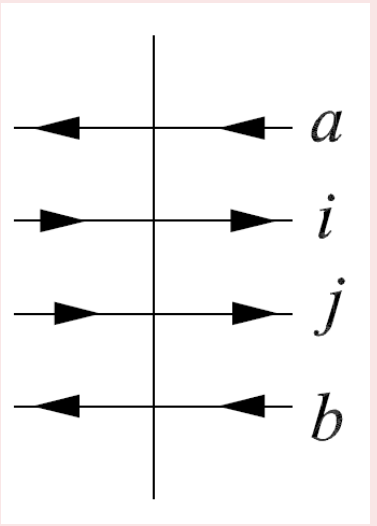
Computation procedure = 2nd version

1. Matrix elements $\langle \Phi^{a'b'c'\ldots}_{i'j'k'\ldots} | V_{\rm res} | \Phi^{abc\ldots}_{ijk\ldots} \rangle$ cumbersome to compute
2. Develop systematic approach = diagrammatic techniques
3. Rules to compute Hugenholtz/Golsdtone diagrams

Energy denorminator

$$(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)^{-1}$$

Diagram



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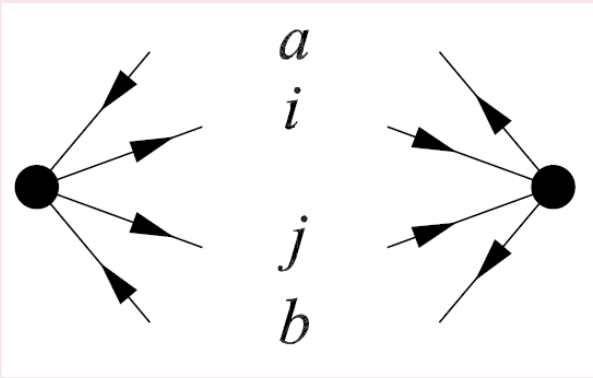
Matrix elements

$$V^{NN}_{ijab} \times V^{NN}_{abij}$$

Diagram



Plus some extra rules

- Sum over internal lines, pre-factor, sign...

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Infinite nuclear matter

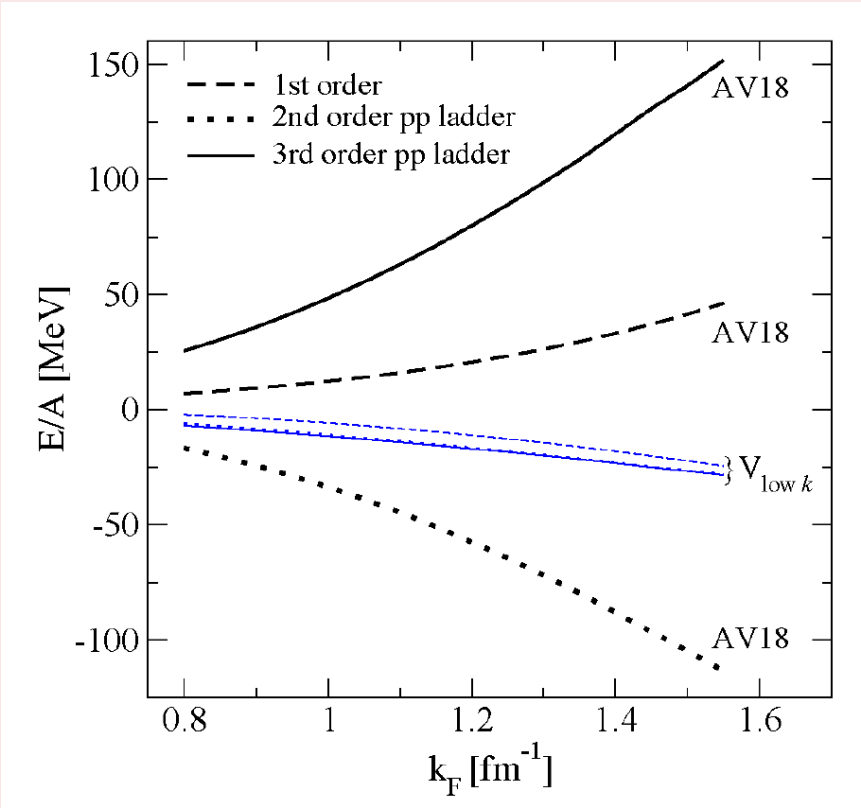
Is nuclear matter perturbative?

- Not with $H(\Lambda_{\text{high}})$
- Seems to be with $H(\Lambda_{\text{low}})$
- New paradigm!?

Saturation mechanism

- V^{NNN} plays an essential
- Coester line with V^{NN} only

EOS of symmetric nuclear matter



[S. K. Bogner *et al.*, NPA 763, 59]

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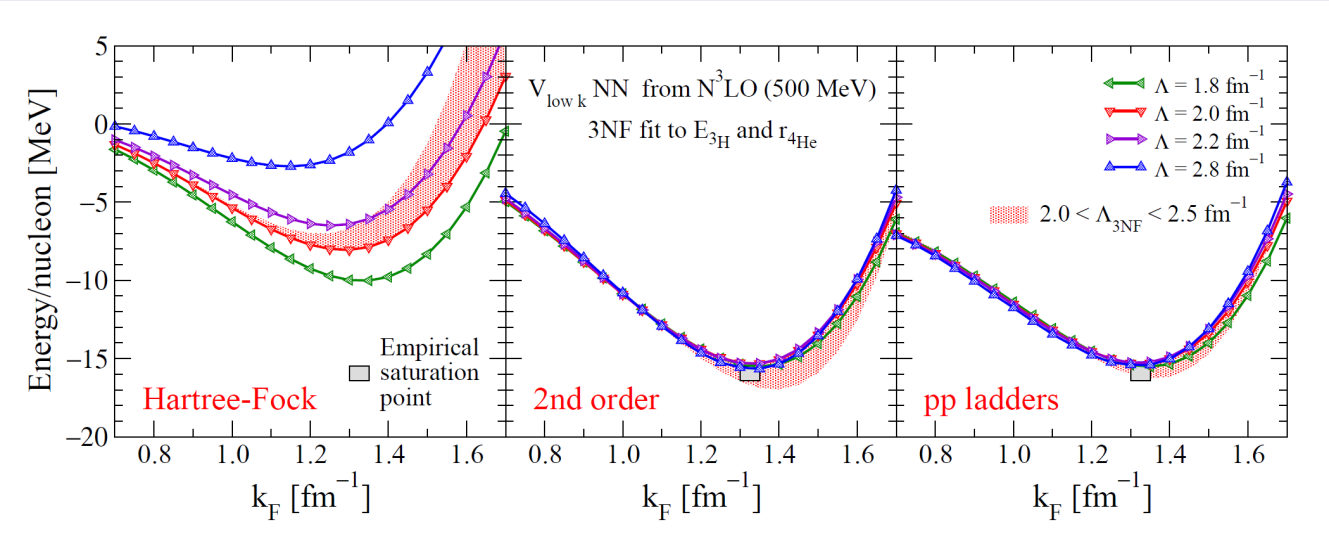

[S. K. Bogner *et al.*, arXiv:0903.3366]

MBPT with low-momentum interactions

- How much goes into each order depends on (Λ of) H but not the full answer!
- EOS is converged at 2^{nd} order (at least in pp channel) for $\Lambda \in [1.8; 2.8]$ fm^{-1}
- Good reproduction of the empirical saturation point

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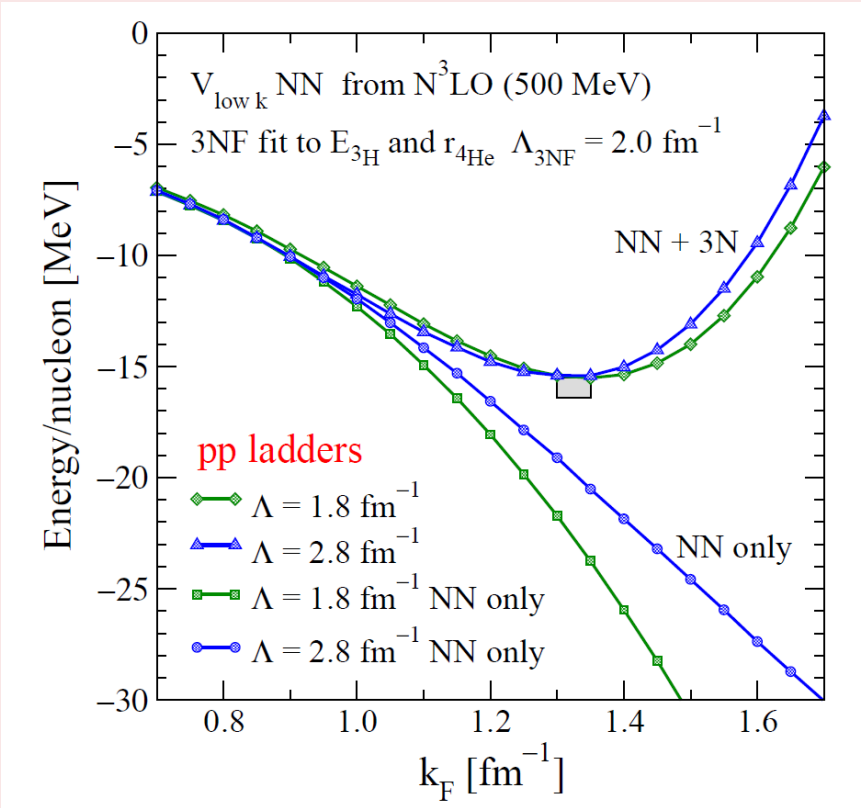

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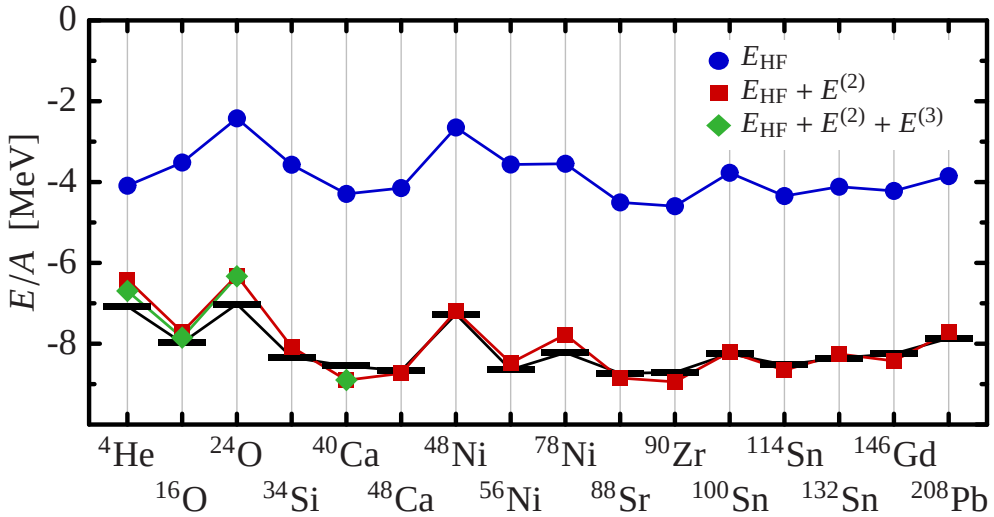
Finite nuclei

Doubly-magic nuclei

- Do not spontaneously break N, Z, J
- Good testing ground for symmetry conserving HF+MBPT (except for $\vec{P}$)
- Performed with V_{UCOM}^{NN} and no V^{NNN}



[R. Roth *et al.*, PRC73 (2006) 044312]

Binding energy (per particle)

- HF provides correct trend with A but underbinds tremendously
- Second-order MBPT provides good account of missing bulk correlations

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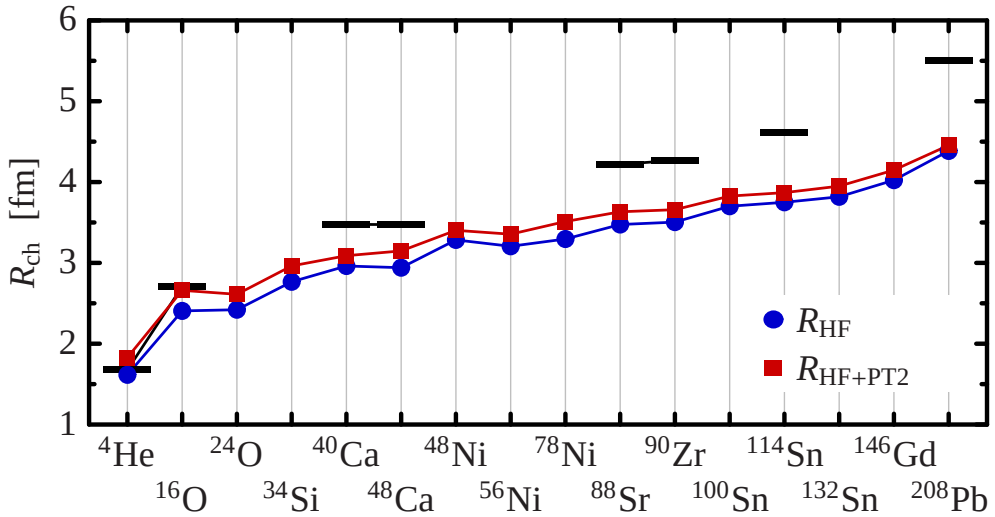

[R. Roth *et al.*, PRC73 (2006) 044312]

Charge radii

- HF underestimates significantly in heavy nuclei
- Second-order improves the situation but it is not enough (V^{NNN}?)

Heavy nuclei from $H(\Lambda)$ at $\Lambda \approx 2$ fm^{-1}

Conclusions

1. Doubly magic nuclei
   - Second-order MBPT provides bulk of correlations ≈ -8 MeV$/A$
   - Need to study effect of $V^{NNN}(\Lambda)$ on $r_{\rm ch}$ and spin-orbit splittings
   - Accuracy requires to add collective fluctuations (MR)
2. Open-shell nuclei
   - Should break N, Z, J^2 to add about $f(N_{\rm val}, \nu_{\rm val}) \times 20$ MeV correlations
   - Second-order MBPT very costly, i.e. scales as $N^5_{\rm basis}$

What is the plan? Connect to EDF methods

1. Controlled approximation to (second-order) MBPT
   - A priori justification to empirical energy functionals
   - Educated guess for extended energy functionals
   - Estimates of coupling with uncertainty through Λ dependence
2. Controlled refit of "educated couplings"
   - Compensates for missing accuracy (leaving out MR correlations)

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Skyrme EDF in canonical basis ($\rho_{\alpha\beta} = \rho_{\alpha\alpha}\,\delta_{\alpha\beta}$)

Trilinear Skyrme EDF in coordinate space (no pairing)

$$\mathcal{E}[\rho] = \int d\vec{r} \sum_q \frac{\hbar^2}{2m}\,\tau_q(\vec{r}) + \sum_{qq'} \Big[C^{\rho\rho}_{qq'}\,\rho_q(\vec{r})\,\rho_{q'}(\vec{r}) + \ldots + C^{\rho\rho\rho}_{qqq'}\,\rho^2_q(\vec{r})\,\rho_{q'}(\vec{r}) + \ldots \Big]$$

Local densities

- $f_q(\vec{r}) \equiv \sum_\alpha W^f_{\alpha\alpha}(\vec{r}q)\,\rho_{\alpha\alpha}$

Form factors for $f \in \{\rho, \tau, \vec{J}\}$

- $W^\rho_{\alpha\alpha}(\vec{r}q) = \psi^\dagger_\alpha(\vec{r}q)\,\psi_\alpha(\vec{r}q)$
- $W^\tau_{\alpha\alpha}(\vec{r}q) = \nabla\psi^\dagger_\alpha(\vec{r}q)\cdot\nabla\psi_\alpha(\vec{r}q)$
- $W^J_{\alpha\alpha}(\vec{r}q) = -\frac{i}{2}\{\psi^\dagger_{\alpha\mu}(\vec{r}q)\big[\nabla\times\hat{\sigma}\,\psi_\alpha(\vec{r}q)\big] - \text{h.c.}\}$

Trilinear Skyrme EDF in canonical basis

$$\mathcal{E}[\rho] \;=\; \sum_\alpha t_{\alpha\alpha}\,\rho_{\alpha\alpha} + \frac{1}{2}\sum_{\alpha\beta}\bar{v}^{\rho\rho}_{\alpha\beta\alpha\beta}\,\rho_{\alpha\alpha}\,\rho_{\beta\beta} + \frac{1}{6}\sum_{\alpha\beta\gamma}\bar{v}^{\rho\rho\rho}_{\alpha\beta\gamma\alpha\beta\gamma}\,\rho_{\alpha\alpha}\,\rho_{\beta\beta}\,\rho_{\gamma\gamma}$$

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Matrix elements of effective vertices

- $t_{\alpha\alpha} \equiv \int d\vec{r}\,\frac{\hbar^2}{2m}\,W^{\tau}_{\alpha\alpha}(\vec{r}q)$
- $\bar{v}^{\rho\rho}_{\alpha\beta\alpha\beta} \equiv 2\int d\vec{r} \sum_{ff'} C^{ff'}_{qq'}\,W^{f}_{\alpha\alpha}(\vec{r}q)\,W^{f'}_{\beta\beta}(\vec{r}q')$
- $\bar{v}^{\rho\rho\rho}_{\alpha\beta\gamma\alpha\beta\gamma} \equiv 6\int d\vec{r} \sum_{ff'f''} C^{ff'f''}_{qq'}\,W^{f}_{\alpha\alpha}(\vec{r}q)\,W^{f'}_{\beta\beta}(\vec{r}q')\,W^{f''}_{\gamma\gamma}(\vec{r}q'')$

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MBPT energy in canonical basis (no pairing, V^{NN} only)

MBPT energy at second order

$$
\begin{aligned}
E^{HF} + \Delta E^{HF}(2) &= \sum_{\alpha} t_{\alpha\alpha}\, \rho_{\alpha\alpha} \\
&+ \frac{1}{2} \sum_{\alpha\beta} \bar{V}^{NN}_{\alpha\beta\alpha\beta}\, \rho_{\alpha\alpha}\, \rho_{\beta\beta} \\
&+ \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \frac{|\,\bar{V}^{NN}_{\alpha\beta\gamma\delta}|^2}{\epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta}\, \rho_{\alpha\alpha}\, \rho_{\beta\beta}\, (1-\rho_{\gamma\gamma})(1-\rho_{\delta\delta})
\end{aligned}
$$

Non-empirical, generalized, nuclear EDF

1. Defines an energy functional $\mathcal{E}[\rho;\{\epsilon_\alpha\}]$ of fourth order in ρ
   - Can introduce effective vertices $\bar{v}^{\rho\rho}$, $\bar{v}^{\rho\rho\rho}$ and $\bar{v}^{\rho\rho\rho\rho}$
2. Depends on $\{\epsilon_\alpha\}$ for $n_{\max} > 0$ = traces back to non-locality in time
3. Very non-local in space as $n_{\max}$ increases
   - Quadruple $\int d\vec{r}$ at second order versus single $\int d\vec{r}$ for Skyrme

MBPT energy in canonical basis (no pairing, V^{NN} only)

Choice of the self-energy, i.e. of H_0

$$h_{\alpha\beta} \equiv t_{\alpha\beta} + \Sigma_{\alpha\beta} \equiv t_{\alpha\beta} + \sum_{\gamma\delta} \overline{v}^{ph}_{\alpha\gamma\beta\delta}\, \rho_{\delta\gamma}$$

I. Use Σ^{HF} for all $n_{\max}$

$$\overline{v}^{ph}_{\alpha\gamma\beta\delta} = \bar{V}^{NN}_{\alpha\gamma\beta\delta}$$

- Choice made above
- Energy-independent
- ϵ_α has no meaning

II. Dress Σ according to $\mathcal{E}$

$$h_{\alpha\beta} \equiv \frac{\delta\mathcal{E}}{\delta\rho_{\beta\alpha}}$$

- As for EDF method
- Energy-dependent
- $\epsilon_\alpha \approx$ sep. energies

III. Local Σ through OEP

$$\Sigma(\vec{r}) \equiv \frac{\delta[\mathcal{E}-\mathcal{T}]}{\delta\rho(\vec{r})}$$

- Approach of DFT
- Energy-independent
- $\epsilon_F \approx$ sep. energy

All the above can be repeated with pairing

- MBPT with both normal (ρ) and anomalous (κ) contractions
- Definition of the anomalous self-energy $\Delta_{\alpha\beta}$

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MBPT in coordinate representation (central V^{NN}, no spin, no isospin)

Zeroth-order (HF) energy

$$E^{HF} \subset \int\int d\vec{r}_1\, d\vec{r}_2\; V^{NN}(|\vec{r}_1 - \vec{r}_2|)\, \rho_{\vec{r}_1\vec{r}_2}\, \rho_{\vec{r}_2\vec{r}_1}$$

1. Non-local through functional of the non-local density matrix $\rho_{\vec{r}_1\vec{r}_2}$
2. Good starting point for the density matrix expansion (DME)

Second-order energy

$$\Delta E^{HF}(2) \subset \int\int\int\int d\vec{r}_{1234} \Bigg[\sum_{\alpha\beta\gamma\delta} \psi^*_\alpha(\vec{r}_1)\psi^*_\beta(\vec{r}_2)\, V^{NN}(|\vec{r}_1 - \vec{r}_2|)\psi_\gamma(\vec{r}_1)\psi_\delta(\vec{r}_2)$$
$$\psi^*_\gamma(\vec{r}_3)\psi^*_\delta(\vec{r}_4)\, V^{NN}(|\vec{r}_3 - \vec{r}_4|)\psi_\alpha(\vec{r}_3)\psi_\delta(\vec{r}_4) \Bigg] \frac{\rho_{\alpha\alpha}\,\rho_{\beta\beta}\,(1-\rho_{\gamma\gamma})\,(1-\rho_{\delta\delta})}{\epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta}$$

1. Highly non-local + not even a functional of $\rho_{\vec{r}_1\vec{r}_2}$
2. Extension of the DME beyond HF needed [V. Rotival *et al.*, unpublished]

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Ideas underlying the DME for E^{HF}

Expand the density matrix in terms of local densities

- Look for separable expansion into relative $\vec{r}$ and center of mass $\vec{R}$ coordinates

$$\rho_{\vec{r}_1\,\vec{r}_2} \quad \approx \quad \sum_{k=0}^{k_{\max}} \Pi_k^{\rho}\big(k_F(\vec{R})\,r\big)\,\mathcal{O}_k(\vec{R})$$

where $\mathcal{O}_k(\vec{R}) \in \{\rho_q(\vec{R}), \vec{\nabla}\rho_q(\vec{R}), \Delta\rho_q(\vec{R})\}$

Insert back into E^{HF} for $k_{\max} = 2$

- E^{HF} takes the form of a generalized Skyrme EDF

$$E^{HF} \quad \subset \quad \int d\vec{R}\Big[C^{\rho\rho}(\vec{R})\,\rho(\vec{R})\,\rho(\vec{R}) + C^{\rho\Delta\rho}(\vec{R})\,\rho(\vec{R})\,\Delta\rho(\vec{R}) + C^{\rho\tau}(\vec{R})\,\rho(\vec{R})\,\tau(\vec{R})\Big]$$

- Non-empirical, position/density dependent couplings $C^{ff'}(\vec{R})$, e.g.

$$C^{\rho\rho}(\vec{R}) \equiv 4\pi \int r^2\,dr\; V^{NN}(r)\left[\Pi_0^{\rho}(k_F(\vec{R})r)\right]^2$$

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How to determine quantitative Π_k functions?

Expansion of $\rho_{\vec{r}_1\,\vec{r}_2}$ [J. Negele, D. Vautherin, PRC5, 1472]

1. Truncated Bessel expansion of non-locality operator $e^{\frac{1}{2}\vec{r}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)}$
2. First term $k=0$ provides exact limit in INM
3. Sufficient for spin-saturated nuclei only
4. Analytical expressions of $\Pi^{\rho}_{k}(k_F(\vec{R}))$

Expansion of $\vec{s}_{\vec{r}_1\,\vec{r}_2}$ [B. Gebremariam, T. D., S. Bogner, in preparation]

1. Taylor expansion of non-locality operator and phase-space averaging of $\vec{k}$

$$\vec{s}_{\vec{R}+\frac{\vec{r}}{2}\,\vec{R}-\frac{\vec{r}}{2}} = e^{i\vec{r}\cdot\vec{k}}\; e^{\frac{\vec{r}}{2}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)-i\vec{r}\cdot\vec{k}} \sum_{\alpha} \psi^{\dagger}_{\alpha}(\vec{r}_1)\,\vec{\sigma}\,\psi_{\alpha}(\vec{r}_2)\,\rho_{\alpha\alpha}\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

2. Opens up DME for all spin-unsaturated nuclei!
3. Analytical expressions of $\Pi^{s}_{k}(k_F(\vec{R}))$
4. Few % error on E^{HF} from full fledged $V^{NN}(\Lambda_{\text{low}})$ (central, tensor, spin-orbit)

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The density matrix expansion

Work under completion [B. Gebremariam, T. D., S. Bogner, in preparation]

1. EDF at HF level from π-exchanges of χ-EFT $V^{NN} + V^{NNN}$ at N^{2}LO
   - Automatized Mathematica derivation of coupling constants from V^{NNN}
   - Ready-to use Mathematica handbook for EDF solvers
2. Educated guess for empirical fitting (with UNEDF collaboration)
   - Add (quasi) density-independent Skyrme EDF to be fitted

Near future [B. Gebremariam, T. D., S. Bogner, in preparation]

1. Empirical work
   - Systematic study of DME couplings and role of pion-physics/V^{NNN}
   - Full fledged fitting of "augmented/educated" Skyrme-like EDF
2. Formalism
   - Extend DME to non-locality in time and apply to second-order in MBPT
   - Extend DME to pairing channel including ultra-violet renormalization

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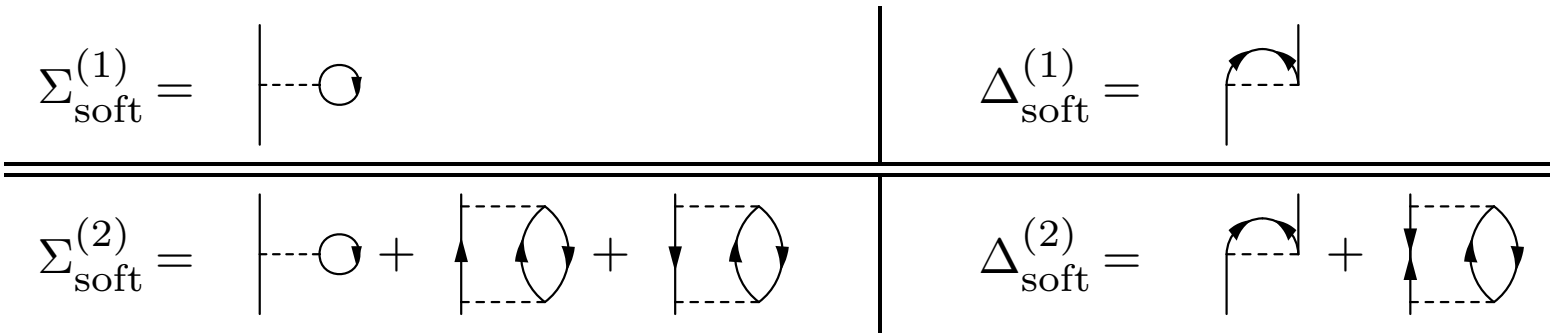
Pairing part of the EDF

Motivations

- Empirical schemes lack predictive power
- Microscopic origin of $(T=1, J=0)$ superfluidity in finite nuclei?
  - Direct term of V^{NN} ($^1S_0$, $^3P_1$, $^1D_2$) and V^{NNN}?
  - Coupling to density, spin, isospin fluctuations: 40%?



First step: v^{pp} built at 1st order in V^{NN} (nuclear + Coulomb)

- Starts with $^1S_0$ only as it dominates at sub-nuclear densities
- Virtual state at $E \simeq 0$ makes V^{NN} almost separable in $^1S_0$

Finite nuclei calculations

$V_{\text{low k}}$ is given as tables of numbers

Produce analytical operator representation

- Why?
  - Interest to understand encoded operator structure
  - Perform integrals analytically in codes
- Which representation?
  - V_{NN} (quasi) separability in ${}^1S_0$ channel provides an incentive
  - Sum of separable terms is efficient for pairing part of the EDF

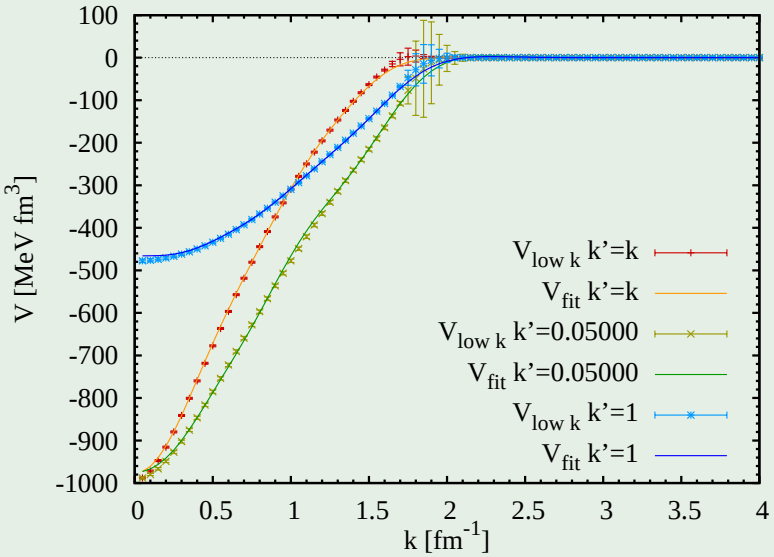
Separable representation of $V_{\text{low k}}(\Lambda) + V_{\text{Coul}}$

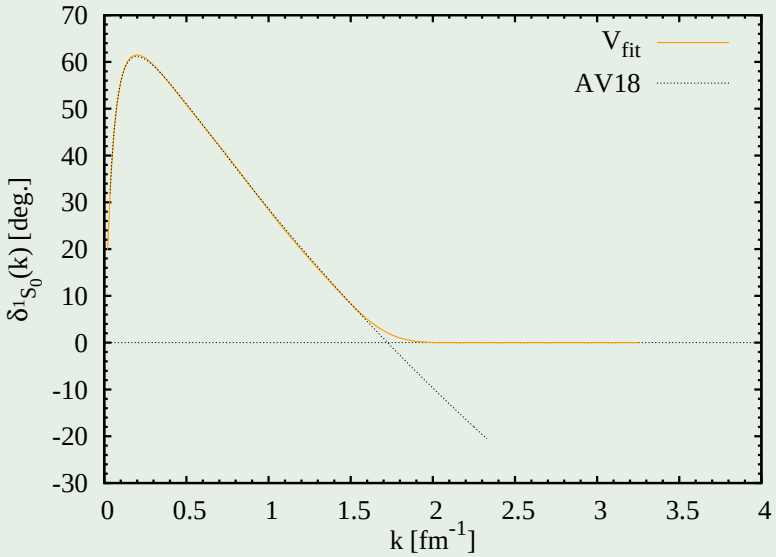
High precision separable representation of rank n

$$V_n^{^1S_0}(k,k',\Lambda) \quad = \quad \sum_{\alpha,\beta=1}^{n} g_\alpha(k)\ \lambda_{\alpha\beta}\ g_\beta(k')$$

- Fit $g_\alpha(k)$ and $\lambda_{\alpha\beta}$ to $V_{\text{low k}}^{^1S_0}(k,k',\Lambda)$ and $\delta^{^1S_0}(k)$

For $\Lambda = 1.8/4.0/\text{“}\infty\text{”}$ fm^{-1} (rank 3/4/15) and smooth cutoff





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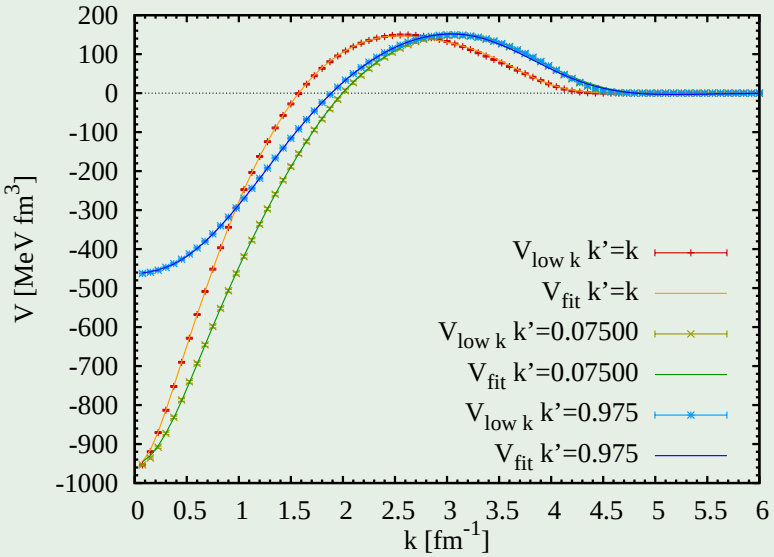

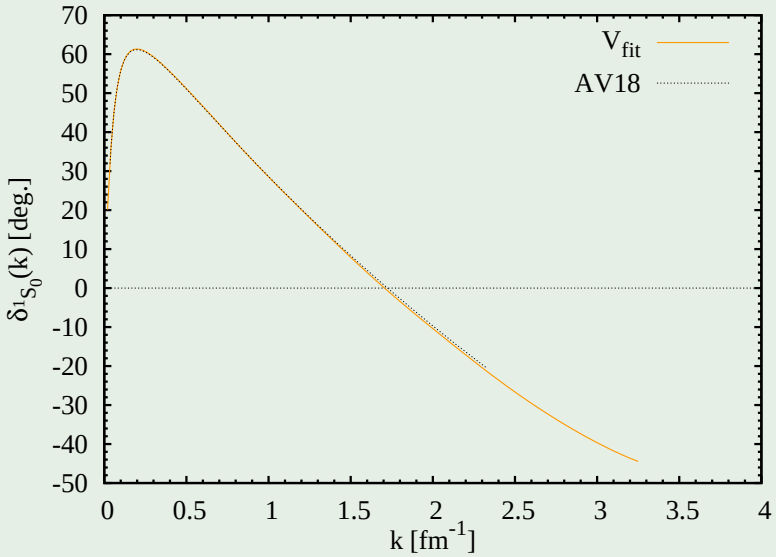

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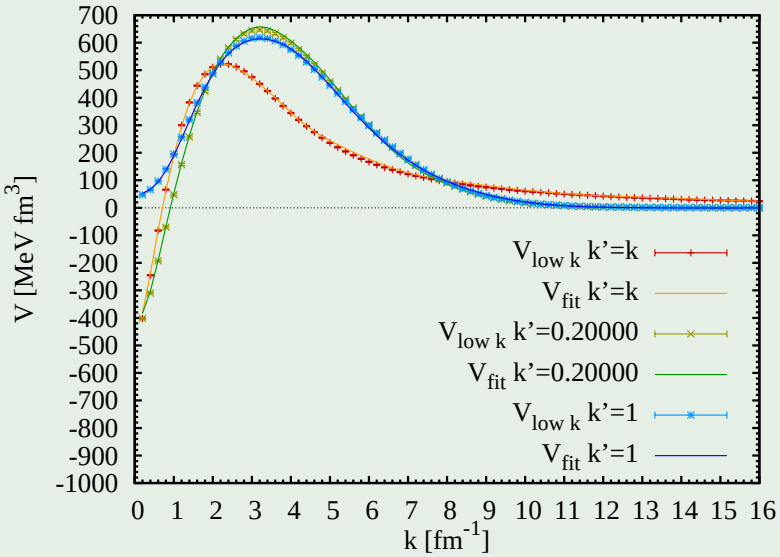
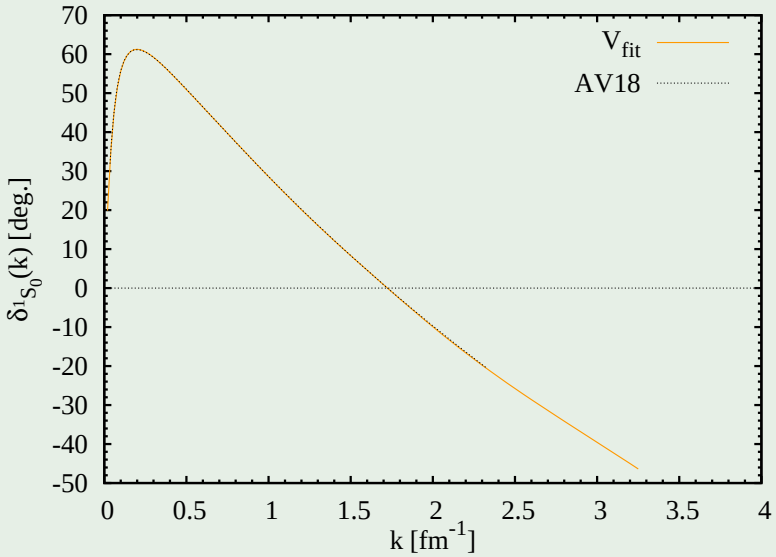




Coulomb interaction

Need to incorporate Coulomb effects on proton gaps

- Only one such published calculation so far: Madrid group (Gogny)
- Simplified treatment of e.m. interaction (Coulomb)

Truncated Coulomb interaction at $r = a > 2R_{\text{nucleus}}$

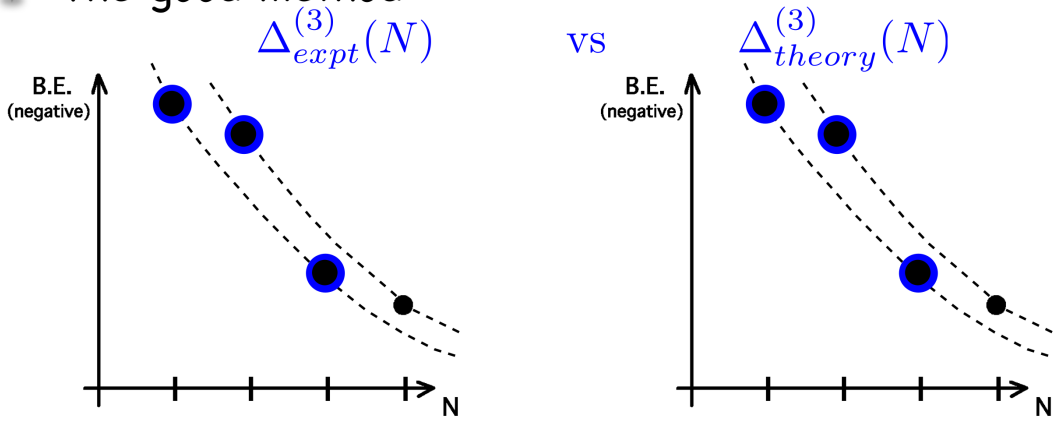
- A separable expansion exists (S-wave part here)

$$
\begin{aligned}
V^{a}_{\text{Coul},\ell=0}(k,k') &= 4\pi e^2 a^2 \sum_{n=0}^{\infty} (2n+1)\, j_n^2\left(\frac{ak}{2}\right)\, j_n^2\left(\frac{ak'}{2}\right), \\
\lambda_{\alpha\beta} &= e^2 a^2 (2\alpha+1)\,\delta_{\alpha\beta} \\
g_\alpha(k) &= \sqrt{4\pi}\, j_\alpha^2\left(\frac{ak}{2}\right) \\
G_\alpha(r) &= \frac{1}{\sqrt{\pi}\, a^2 r}\, P_\alpha\left(1-2(\tfrac{r}{a})^2\right) \text{ for } r \le a
\end{aligned}
$$

- ~ 15 terms needed (peanuts !)

Comparing theoretical and experimental "pairing gaps"

The good method

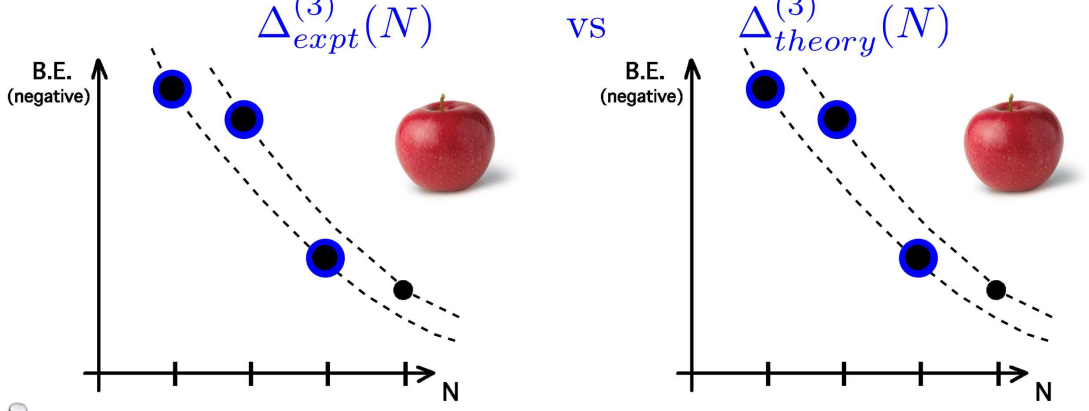


$$\Delta^{(3)}_{\mathrm{nexp/th}}(N) = \frac{(-1)^N}{2}\left[E_0(N+1) - 2E_0(N) - E_0(N-1)\right]$$

Comparing theoretical and experimental "pairing gaps"

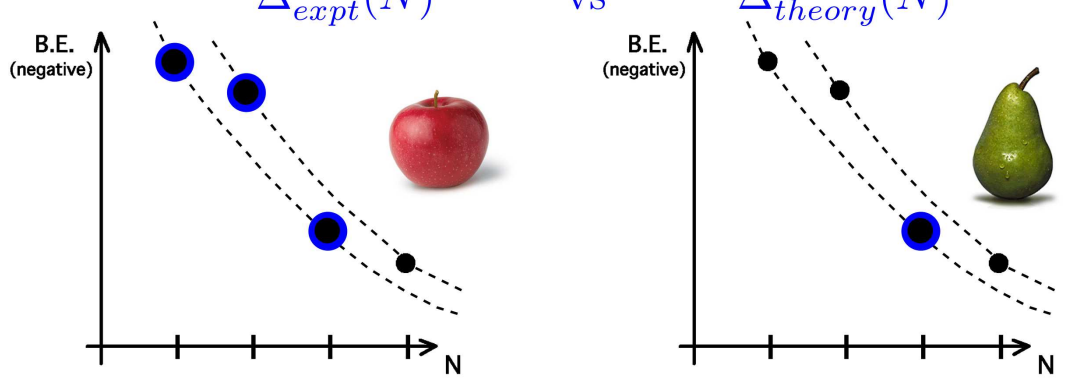
The good method

$\Delta^{(3)}_{expt}(N)$ vs $\Delta^{(3)}_{theory}(N)$



The actual method

$\Delta^{(3)}_{expt}(N)$ vs $\Delta^{LCS}_{theory}(N)$



$\Delta^{(3)}_{q,\mathrm{exp}}(\mathrm{odd})$ versus $\Delta^{\mathrm{q}}_{\mathrm{LCS}}(\mathrm{even}) = \Delta^{q}_{\epsilon_F}$ in even-N nucleus

EDF calculations in spherical nuclei

Spherical code BSLHFB (T. Lesinski, unpublished)

- Handles highly non-local pairing EDF in systematic calculations
- Calculations almost as cheap as for a local pairing EDF
- Spherical Bessel basis $j_\ell(kr)$
- Well suited for drip-line physics

Calculations

- Results for 470 nuclei predicted spherical (Gogny-D1S)
- $k_{\max} \sim 4.0$ fm^{-1}, $R_{box} = 20$ fm, $j_{max} = 45/2$
- Pairing complemented with (SLy4) Skyrme EDF : $m_0^* = 0.7m$
- ✔ Reminder: nothing in the pairing channel is adjusted in nuclei

[T. D., T. Lesinski, Eur. Phys. J. Special Topics **156** (2008) 207]

[T. Lesinski, T. D., K. Bennaceur, J. Meyer, EPJA 40 (2009) 121]

[K. Hebeler, T. D., T. Lesinski, A. Schwenk, arXiv:0904.3152]

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Pairing gaps ($^1S_0$) from $v^{pp} = V^{NN} + V_{\rm Coul}$

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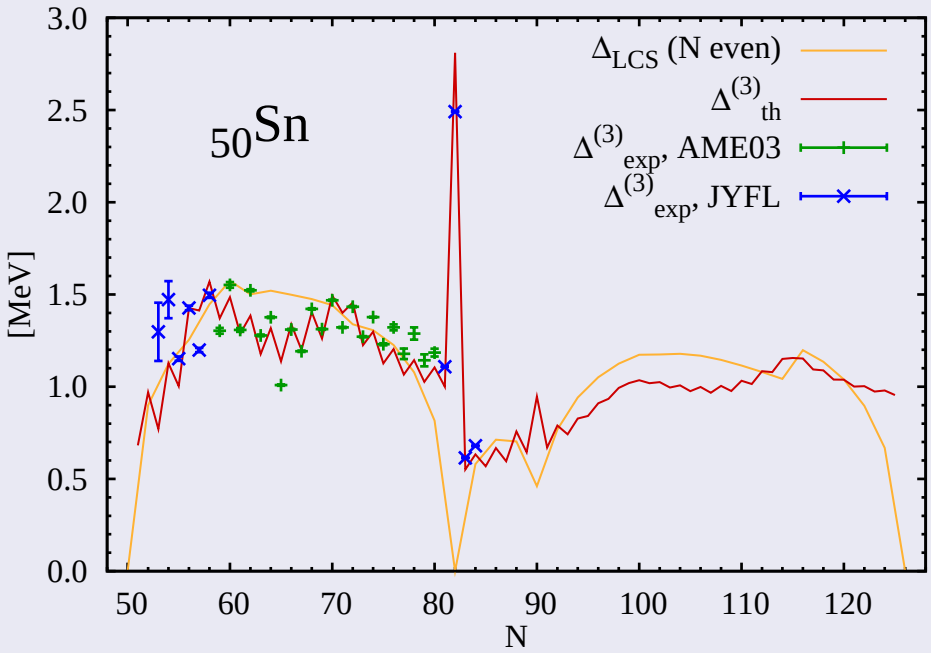
$\Delta^{(3)}_{n,\rm exp}(N)$ versus $\Delta^{(3)}_{n,\rm th}(N)$ (self-consistent qp filling approximation)



- Deepening around $N \approx 115$ arises from blocking of $\Delta_{\rm LCS}$(odd)
- $\Delta^{(3)}$ well described close to $N = 82$ without LN, proj. or pairing vib.
- New masses towards or beyond shell closure very valuable to confront theory

Pairing gaps ($^1S_0$) from $v^{pp} = V^{NN} + V_{\rm Coul}$

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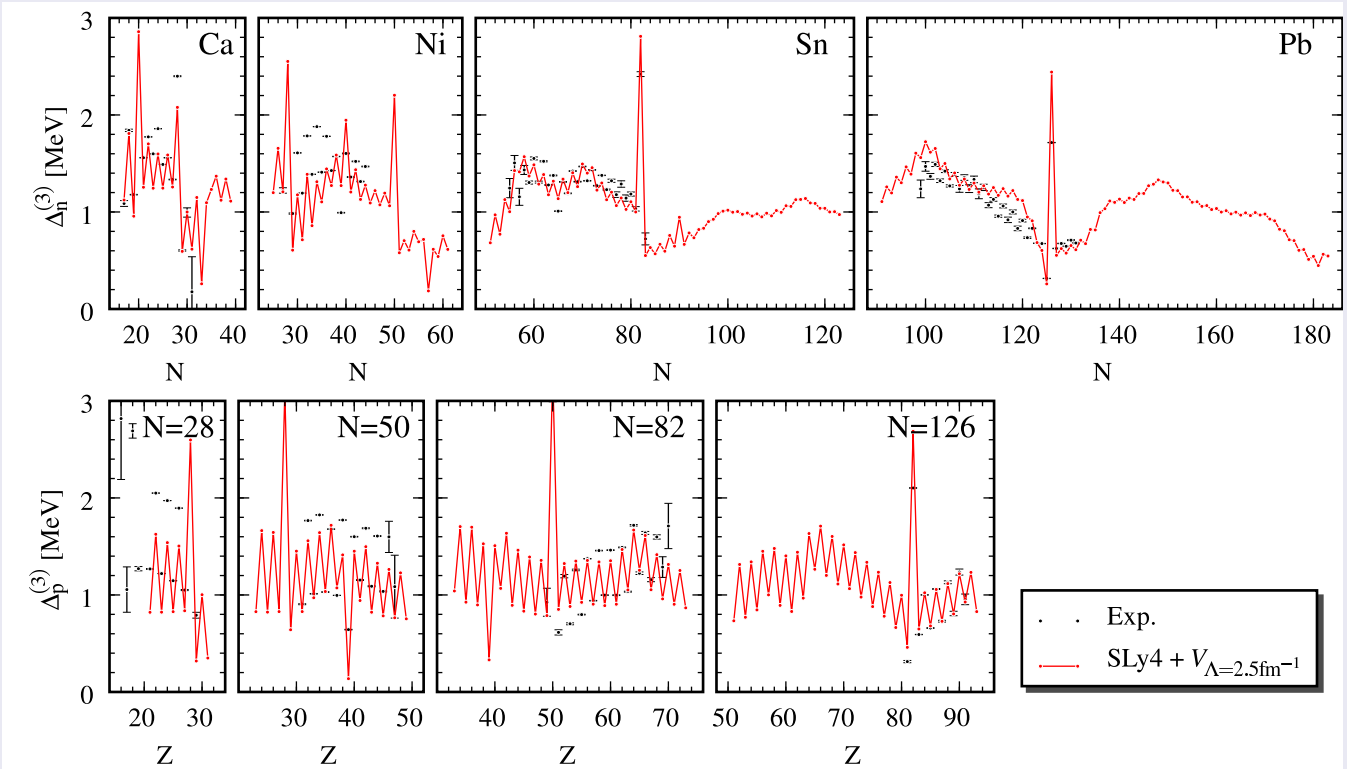
$\Delta^{(3)}_{q,\,\rm exp}$ versus $\Delta^{(3)}_{q,\,\rm th}$ (self-consistent qp filling approximation)



- Neutron and proton gaps consistent with experiment
- Large oscillation of $\Delta^{(3)}_p$ due to Coulomb in ph

Non-empirical pairing energy functional

Work under completion [T. Lesinski, T. D., K. Bennaceur, J. Meyer, in preparation]

1. Addition of χ-EFT $V^{NN\langle N\rangle}(\Lambda)$ at N^{2}LO
2. Set up of $v_{eff} \approx V^{NN+NN\langle N\rangle}(\Lambda)$ for 3D code

Near future [S. Baroni, A. Pastore, T. D., A. Schwenk, in preparation]

- Add coupling to density, spin and isospin fluctuations
  1. Self-energies at second order
  2. Coupling to collective QRPA modes

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Selected bibliography


P. Nozières,
Theory of interacting Fermi systems, 1964, Westview press, Advanced Book Classics


R. Roth, P. Papakonstantinou, N. Paar, H. Hergert, T. Neff, H. Feldmeier,
Phys. Rev. C73 (2006) 044312


J. E. Drut, R. J. Furnstahl, L. Platter,
arXiv:0906.1463


J. Negele, D. Vautherin,
Phys. Rev. C5 (1972) 1472


B. Gebremariam, T. Duguet, S. Bogner,
in preparation


T. Lesinski, T. Duguet, K. Bennaceur, J. Meyer,
Eur. Phys. J. A40 (2009) 121


T. Duguet, T. Lesinski,
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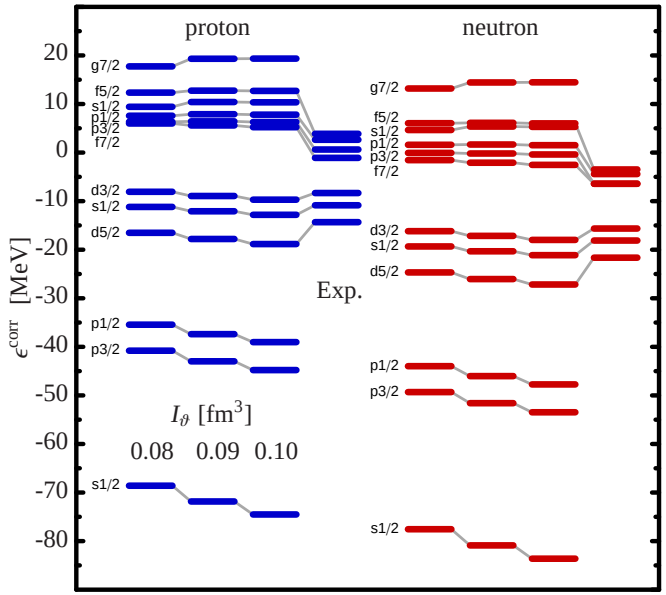
HF single-particle energies

Doubly-magic nuclei

- Do not spontaneously break N, Z, J
- Good testing ground for symmetry conserving HF (except for $\vec{P}$)



[R. Roth *et al.*, PRC73 (2006) 044312]

Single-particle energies ϵ_k in ^{40}Ca

- Ordering is correct but density of states is too low