Non-empirical nuclear EDF from low-momentum interactions

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EFES-LIA workshop on the Nuclear Energy Density Functional method,
RIKEN, Feb. 25th - 26th, 2010

Outline

Outline

Long term project and collaboration

Design *non-empirical* Energy Density Functionals

- Bridge with *ab-initio* many-body techniques
- Calculate properties of heavy/complex nuclei from NN+NNN
- Controlled calculations with theoretical error bars

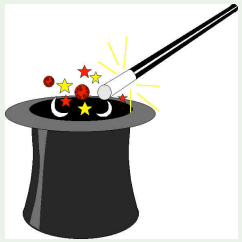
SPhN	T. Duguet, J. Sadoudi, V. Soma
IPNL	K. Bennaceur, J. Meyer
TRIUMF	A. Schwenk, K. Hebeler, S. Baroni
NSCL	S. K. Bogner, B. Gebremariam
OSU	R. J. Furnstahl, L. Platter
ORNL	T. Lesinski
Julich	A. Nogga
Jyvaskyla	A. Pastore

Constructing non-empirical EDFs for nuclei

Long term objective

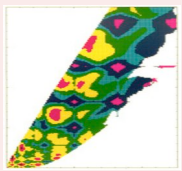
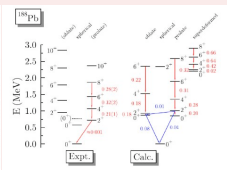
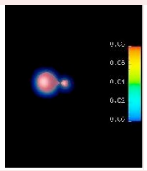
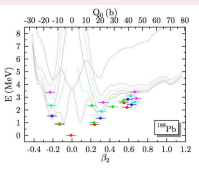
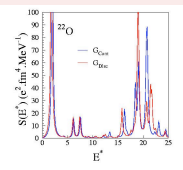
Build non-empirical EDF in place of existing models

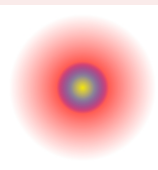
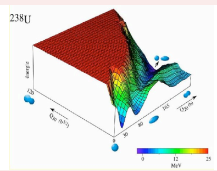
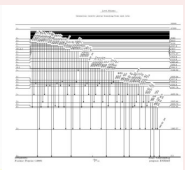
Empirical



Predictive?

Finite nuclei and extended nuclear matter

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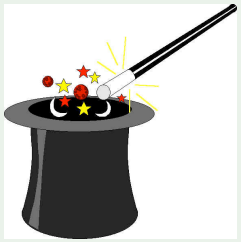
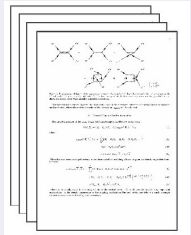


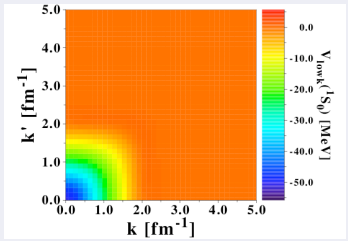
Predictive?

Non-empirical

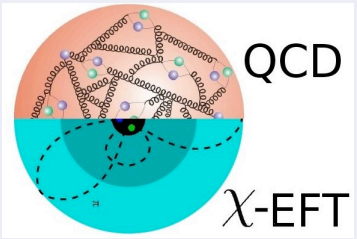


Predictive...

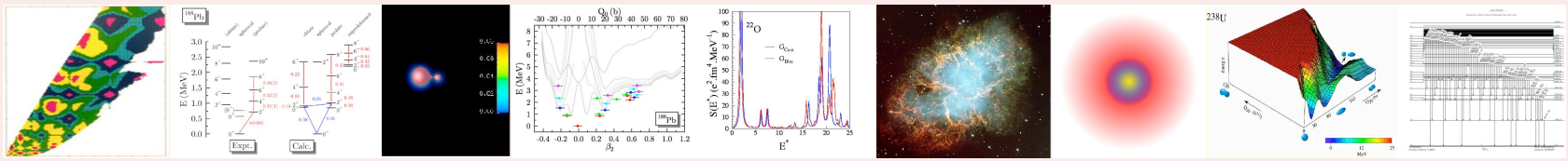
Low-k NN+NNN



QCD / χ-EFT



Finite nuclei and extended nuclear matter



Non-empirical energy density functional

Many-body scheme

$$H(\Lambda) = T + V^{NN}(\Lambda) + V^{NNN}(\Lambda) + \ldots \quad \text{at} \quad \Lambda \approx 2 \text{ fm}^{-1}$$
$$+$$
Many-Body Perturbation Theory (Gorkov propagators)

$$\begin{aligned}
\mathcal{E}[\{\rho_{ij}\},\{\kappa_{ij}\},\{\kappa^*_{ij}\};\{E_k\}] \quad &\equiv \quad \sum_{ij} t_{ij}\,\rho_{ji} \\
&+ \quad \frac{1}{2}\sum_{ijkl} \bar{v}^{\rho\rho}_{ijkl}\,\rho_{ki}\,\rho_{lj} + \frac{1}{4}\sum_{ijkl} \bar{v}^{\kappa\kappa}_{ijkl}\,\kappa^*_{ij}\,\kappa_{kl} \\
&+ \quad \frac{1}{6}\sum_{ijklmn} \bar{v}^{\rho\rho\rho}_{ijklmn}\,\rho_{li}\,\rho_{mj}\,\rho_{nk} + \ldots
\end{aligned}$$

Relevant questions

1. How reducing momentum dependencies associated with spatial non-localities?
2. What about energy dependencies associated with time non-localities?
3. Energy dependencies versus multi-reference extension?
4. What accuracy one can aim at and how to use the Λ (in)dependence?

Outline

Non-empirical pairing

Work accomplished so far (T. Lesinski *et al.*)

1. $V^{NN}(\Lambda)$ and $V^{NN\langle N\rangle}(\Lambda)$ at lowest order (SLyX in s.p. field h)
   - New HFB spherical code - expansion on bessel functions basis
   - Efficient handling of finite-range/non-local (separable) vertex
2. Set up of $v_{eff} \approx V^{NN+NN\langle N\rangle}(\Lambda)$ for 3D code

Results

- Gaps at lowest order in $V^{NN}(\Lambda)$ close to data
- Coulomb decreases proton gaps by $\sim 15\%$
- $V^{NN\langle N\rangle}(\Lambda)$ decreases gaps by $\sim 30\%$
- Essential to compute actual odd-even mass differences

Near future (S. Baroni, A. Pastore, V. Soma *et al.*)

- Add coupling to density, spin and isospin fluctuations
  1. Approximate second-order self energies
  2. Coupling to collective QRPA modes
  3. Self-consistent second-order Green's function (Gorkov) calculations

Outline

The density matrix expansion

Work accomplished so far (B. Gebremariam *et al.*)

1. Extension of Negele-Vautherin DME for spin-unsaturated systems
   - Use momentum phase-space averaging techniques
   - Use local momentum distribution of finite Fermi systems
2. 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
3. Educated guess for empirical fitting (with UNEDF collaboration)
   - Add (quasi) density-independent Skyrme EDF to be fitted

Near future (B. Gebremariam *et al.*)

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

Outline

Outline

Nuclear interactions and the Renormalization Group

Approach

- $V(\vec{k},\vec{k}',\Lambda=\infty) = V^{\text{hard}}(\vec{k},\vec{k}')$
- Run down Λ
- Keep $\delta^{^{S}L_{J}}(k)$ and E_{Deuteron}

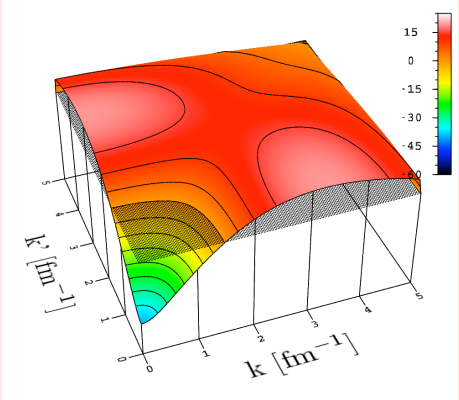
General Properties

- Vacuum interaction
- Universal $V_{NN}(\Lambda \approx 2) \equiv V_{\text{low k}}$
- $V_{\text{low k}}$ is perturbative

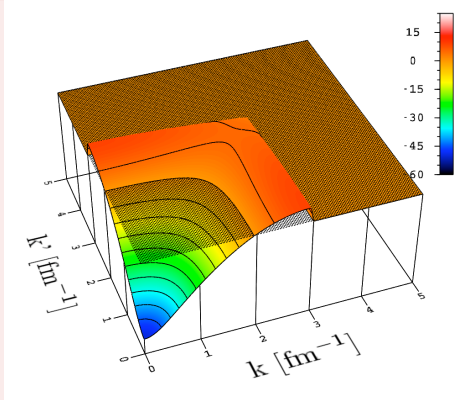
Crucial points

- $H = V_{NN}(\Lambda) + V_{NNN}(\Lambda) + \ldots$
- $\partial_\Lambda A \neq 0 \Rightarrow$ missing pieces
- Ex: omitted NNN(Λ)

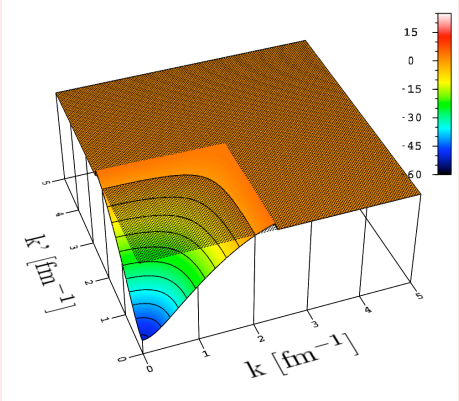
Convergence of the RG flow



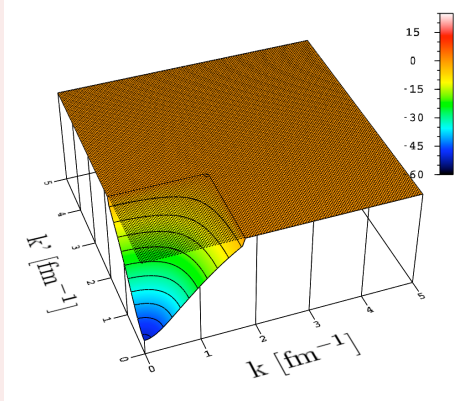
$\Lambda = 5.0$ fm^{-1}



$\Lambda = 3.0$ fm^{-1}



$\Lambda = 2.4$ fm^{-1}



$\Lambda = 1.8$ fm^{-1}

Outline

Many-body perturbation theory

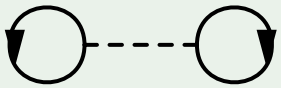
Gell-Man Low theorem and Goldstone MBPT

- $E = E^{HF} + \Delta E^{HF}$ with ΔE^{HF} in powers of $V_{\rm res}$ (from normal ordering)

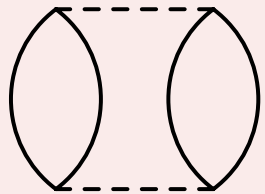
$$\Delta E^{HF} = \sum_{n=0} \langle \Phi | V_{\rm res} \left(\frac{1}{E^{HF} - H_0} V_{\rm res} \right)^n | \Phi \rangle_{\rm connected}$$

- Summing all terms provides exact ground-state energy
- The game is to optimize the reference vacuum ($|\Phi\rangle$) + summing few terms
- May redefine vacuum (HFB + symmetry breaking) to speed-up convergence

First order: $n = 0$

$E_0^{HF} = T^{HF} +$ 

Second order $n = 1, \ldots$

$\Delta E_0^{HF} =$  $+ \ldots$

Many-body perturbation theory

Energy functional at second order

- Energy functional goes up to sixth order in ρ_{ij} and κ_{ij}

$$\begin{aligned}\mathcal{E}[\{\rho_{ij}\},\{\kappa_{ij}\},\{\kappa^*_{ij}\};\{E_k\}] \equiv & \sum_{ij} t_{ij}\,\rho_{ji} \\ & + \frac{1}{2}\sum_{ijkl}\bar{v}^{\rho\rho}_{ijkl}\,\rho_{ki}\,\rho_{lj} + \frac{1}{4}\sum_{ijkl}\bar{v}^{\kappa\kappa}_{ijkl}\,\kappa^*_{ij}\,\kappa_{kl} \\ & + \frac{1}{6}\sum_{ijklmn}\bar{v}^{\rho\rho\rho}_{ijklmn}\,\rho_{li}\,\rho_{mj}\,\rho_{nk} + \ldots\end{aligned}$$

- Effective vertices $\bar{v}^{\rho\rho}_{ijkl}$, $\bar{v}^{\kappa\kappa}_{ijkl}\ldots$ expressed in terms of V^{NN}, $V^{NNN}\ldots$ and E_k

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- Effective vertices $\bar{v}^{\rho\rho}_{ijkl}$, $\bar{v}^{\kappa\kappa}_{ijkl}\ldots$ expressed in terms of V^{NN}, $V^{NNN}\ldots$ and E_k
  - Ex: in absence of pairing and omitting V^{NNN}

$$\bar{v}^{\rho\rho\rho\rho}_{ijklijkl} \equiv 6\,\frac{\left|\bar{V}^{NN}_{ijkl}\right|^2}{\epsilon_i+\epsilon_j-\epsilon_k-\epsilon_l} \quad ; \quad \bar{v}^{\rho\rho\rho}_{ijkijk} \equiv \frac{1}{2}\sum_l \bar{v}^{\rho\rho\rho\rho}_{ijklijkl} \quad ; \quad \bar{v}^{\rho\rho}_{ijij} \equiv \bar{V}^{NN}_{ijij} + \frac{1}{6}\sum_k \bar{v}^{\rho\rho\rho}_{ijkijk}$$

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- Effective vertices $\bar{v}^{\rho\rho}_{ijkl}$, $\bar{v}^{\kappa\kappa}_{ijkl}\ldots$ expressed in terms of V^{NN}, $V^{NNN}\ldots$ and E_k

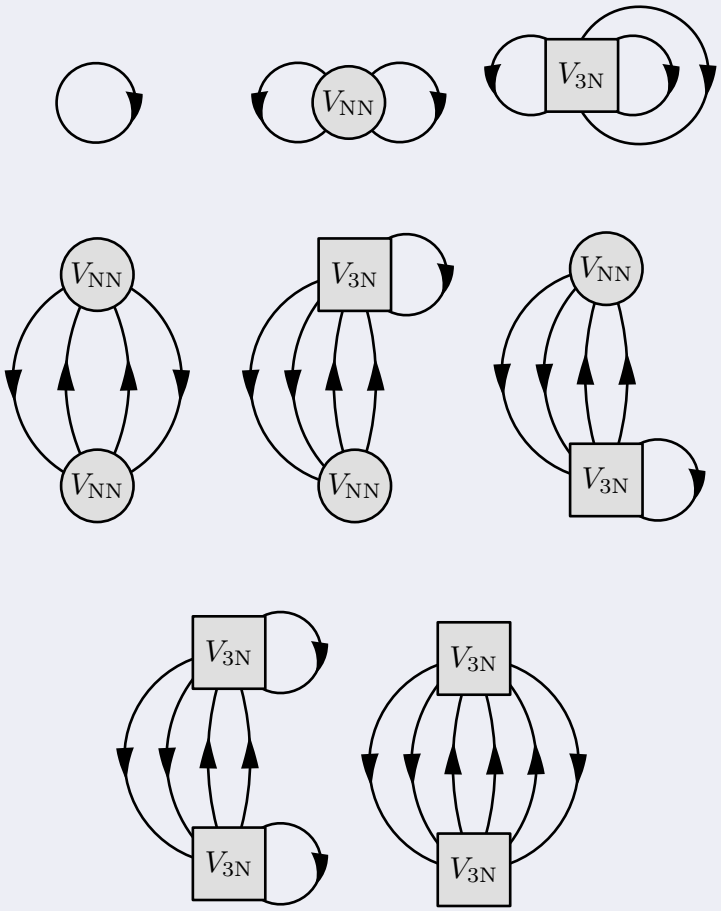
Self-energies and effective kernels

- There is freedom as to how to define the one-body fields, e.g.

$$h_{ij} \equiv \frac{\delta\mathcal{E}}{\delta\rho_{ji}} \equiv t_{ij} + \Sigma_{ij} \equiv t_{ij} + \sum_{kl}\bar{v}^{ph}_{ikjl}\,\rho_{lk} \quad ; \quad \Delta_{ij} \equiv \frac{\delta\mathcal{E}}{\delta\kappa^*_{ij}} \equiv \frac{1}{2}\sum_{kl}\bar{v}^{pp}_{ijkl}\,\kappa_{kl}$$

Equation of state of infinite nuclear matter

Set of diagrams



(Λ-dependent) questions of interest

1. Is INM perturbative?
2. What is the role of V^{NNN}?
3. What is the saturation mechanism?
4. Is phenomenology accounted for?

Calculation scheme

- Hamiltonian $H(\Lambda)$
  - $V^{NN}(\Lambda)$ from RG
  - $V^{NNN}_{\mathrm{N^2LO}}$ with (c_D, c_E) fitted at Λ
- E/A at 2^{nd} order
  - Use of $V_{NNN} \Longrightarrow V_{NN\langle N\rangle}$
  - Last diagram omitted
- Self-energy at 1^{st} order $\Sigma^{(1)}(k)$

Equation of state of infinite nuclear matter

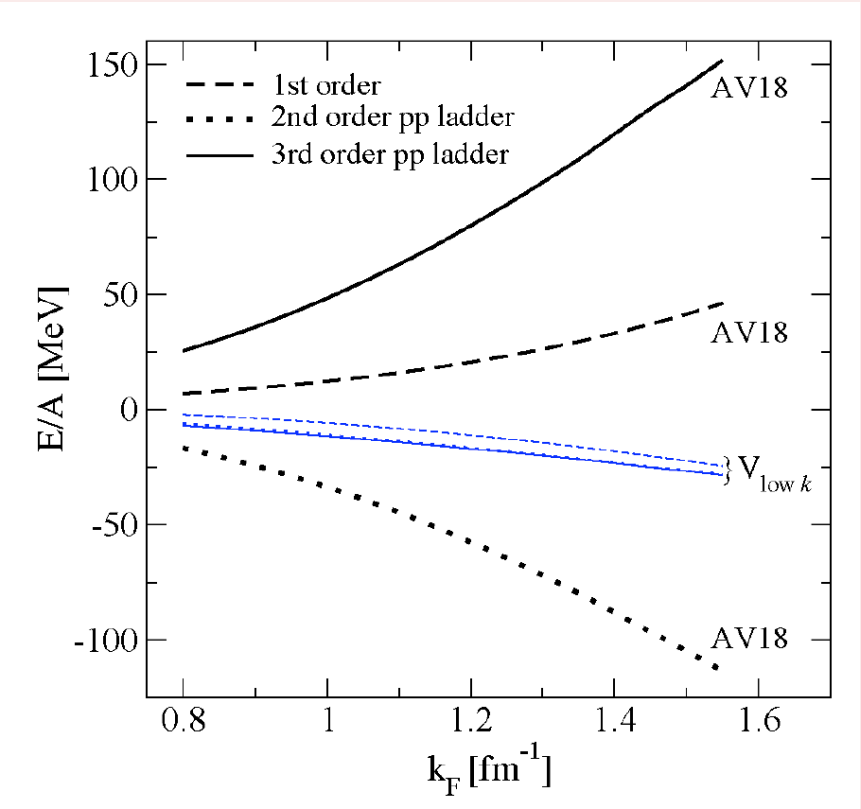
Is nuclear matter perturbative?

- 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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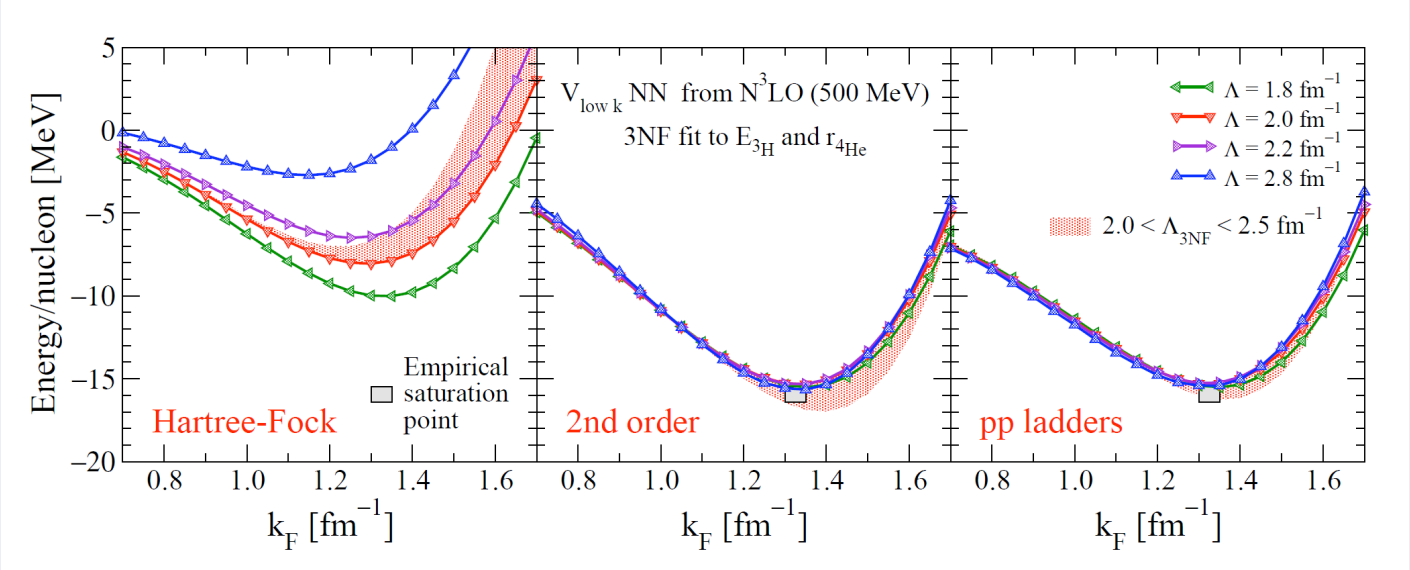


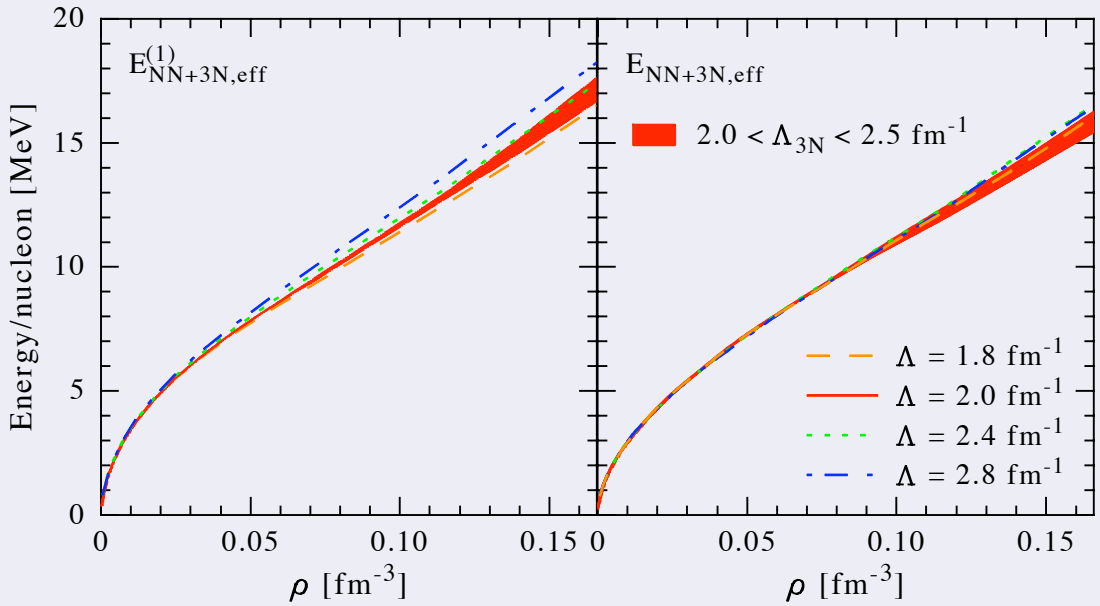
[S. K. Bogner *et al.*, arXiv:0903.3366]

MBPT with low-momentum interactions

- Importance of each order depends on (Λ of) H but not the full answer!
- 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

Equation of state of infinite nuclear matter

EOS of pure neutron matter



[K. Hebeler, A. Schwenk, arXiv:0911.0483]

MBPT with low-momentum interactions

- Little contribution from 2^{nd} order for $\Lambda_{NN} \in [1.8; 2.8]$ fm^{-1}
- Little dependence on RG cut-offs Λ_{NN} and Λ_{3N}
- Larger uncertainty from c_3 entering the long-range 2π-exchange V_C^{NNN}

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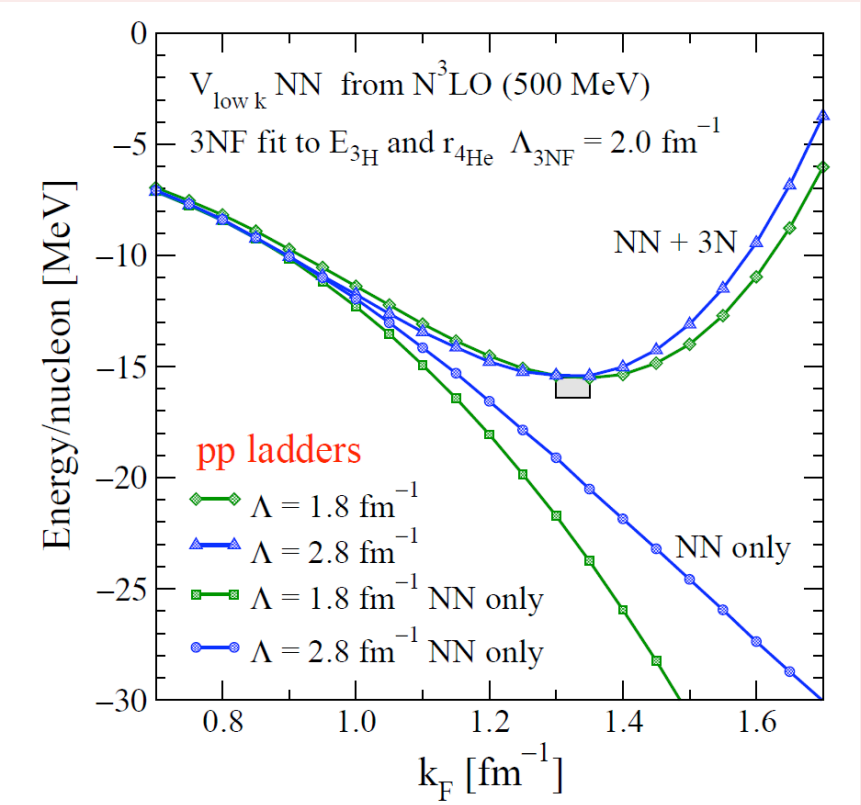
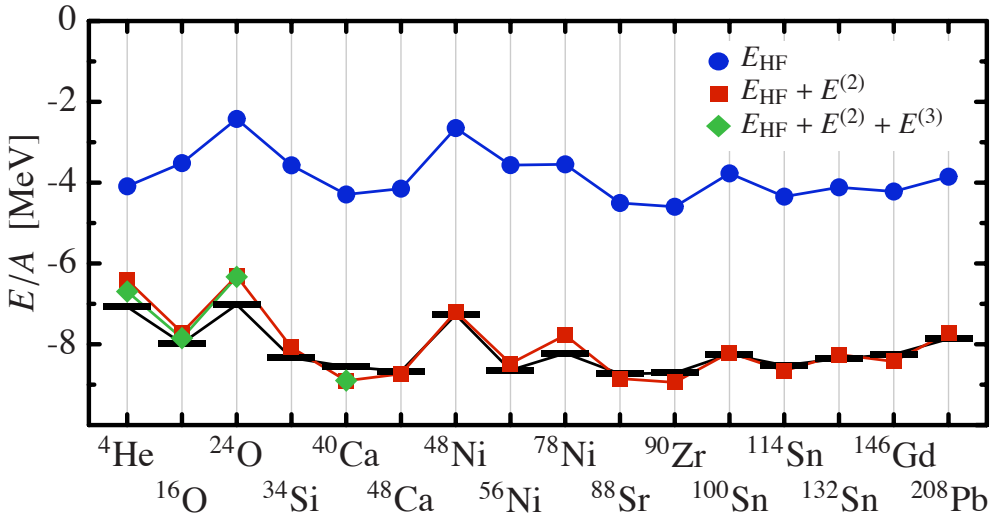


[S. K. Bogner *et al.*, arXiv:0903.3366]

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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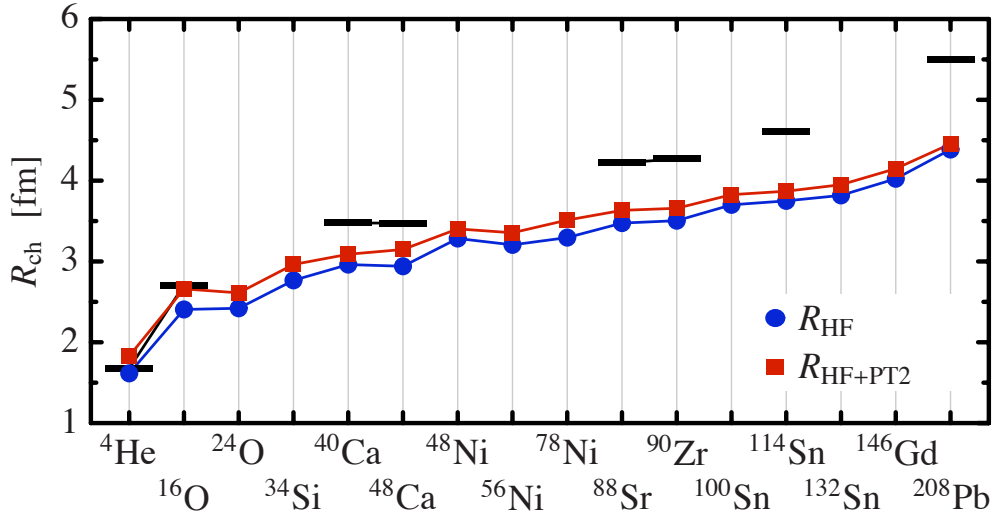

[R. Roth *et al.*, PRC73 (2006) 044312]

Charge radii

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

HF single-particle energies

Doubly-magic nuclei

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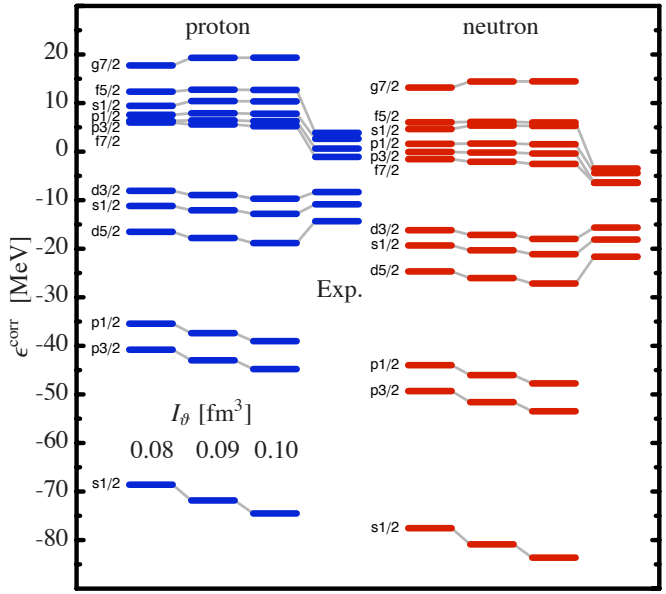

[R. Roth *et al.*, PRC73 (2006) 044312]

Single-particle energies ϵ_k in ^{40}Ca

- Ordering is correct but density of states is too low

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 remains very costly, i.e. scales as $N_{\rm basis}^5$

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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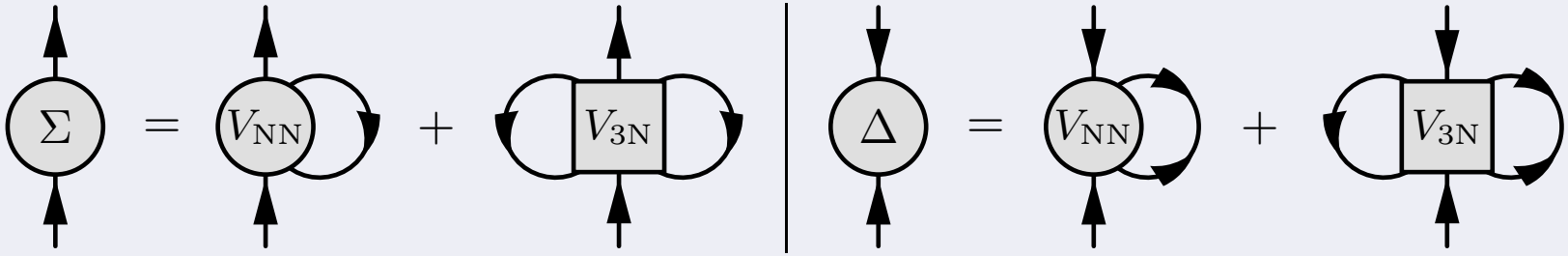
Energy functional at lowest-order in V_{NN} and $V_{NN\langle N\rangle}$

Motivations

- Empirical schemes lack predictive power
- Microscopic origin of $(T=1, J=0)$ superfluidity in finite nuclei?
  - Direct term of V_{NN} and $V_{NN\langle N\rangle}$ ($^1S_0$, $^3P_1$, $^1D_2$)?
  - Coupling to density, spin, isospin fluctuations: 40%?
- For now: build Σ^q and Δ^q at lowest-order in V_{NN} and $V_{NN\langle N\rangle}$



At this point in time

- v^{pp}: microscopically built from V_{NN} and $V_{NN\langle N\rangle}$
- v^{ph}: semi-empirical from constrained Skyrme EDF

Finite nuclei calculations

Low-momentum interactions for finite nuclei calculations

- Vacuum interactions with renormalized short-distance physics
- Good starting point for structure calculations through EDF method?

V_{NN} and $V_{NN\langle N\rangle}$ given as numerical matrices in (k, k') and (k, k', k_F^n, k_F^p)

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
  - New separable expansion of Coulomb

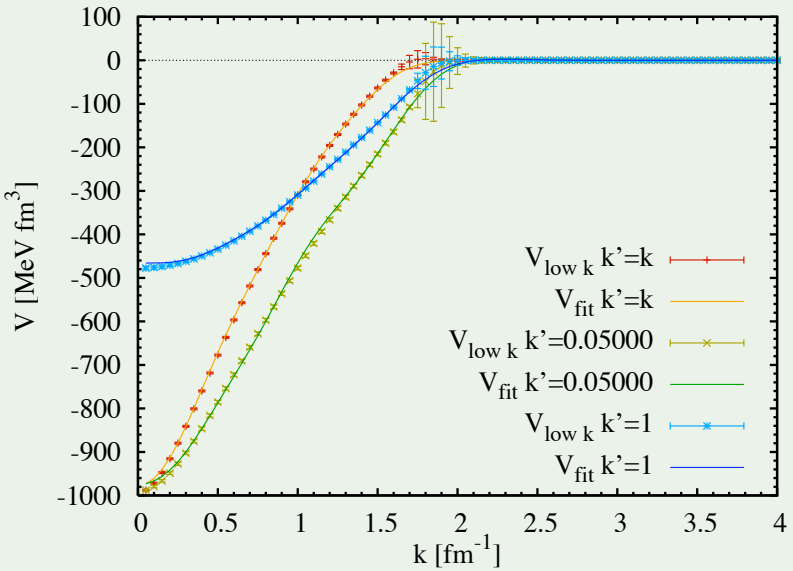
Rank-n high-precision separable representation of $V_{NN}(\Lambda)$

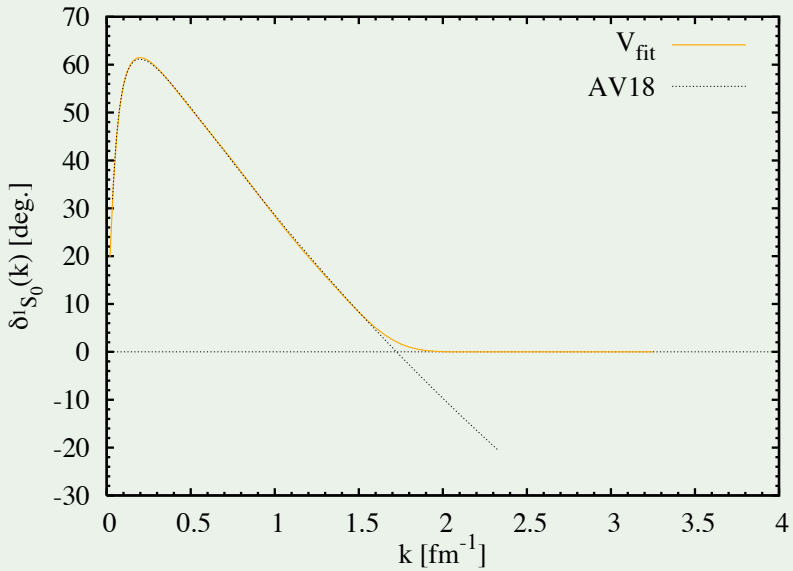
Focus on $^1S_0$ as it dominates at sub-nuclear densities

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

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

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





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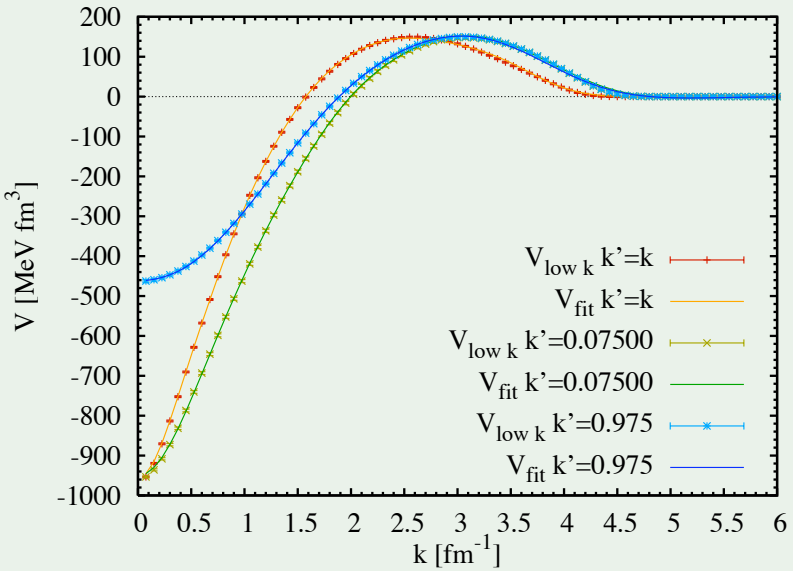

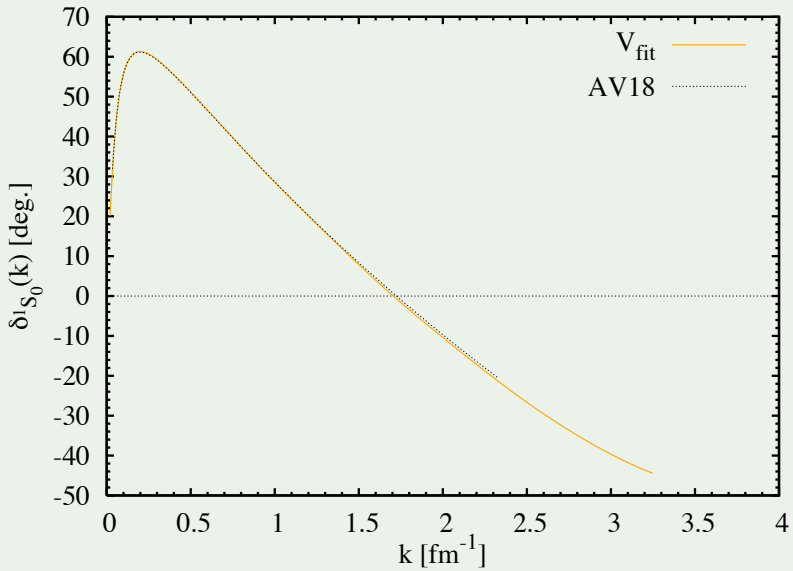

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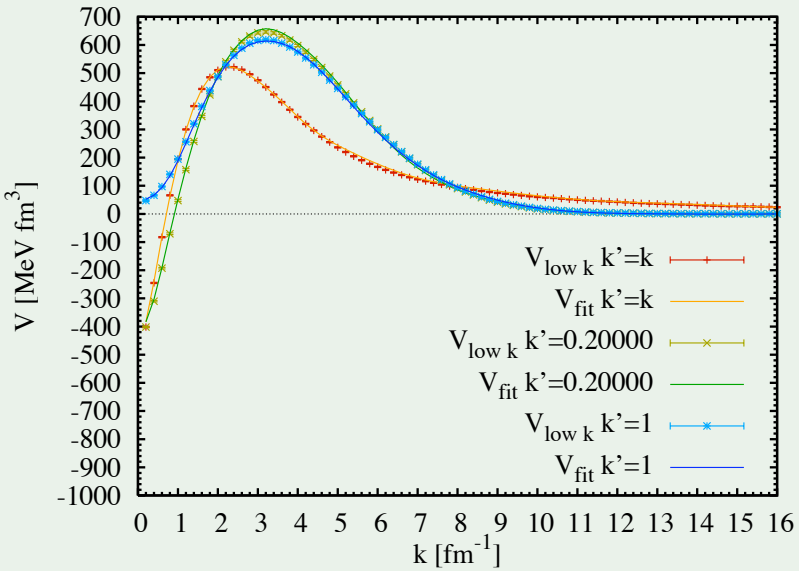
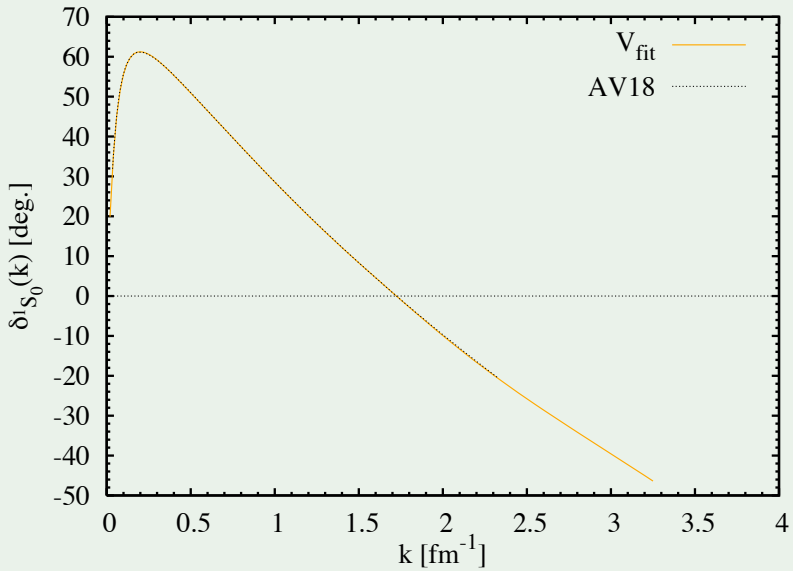




Separable representation of $V_{\rm Coul}$

Coulomb effects on proton-proton pairing

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

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

- Exact separable expansion (S-wave part here)

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

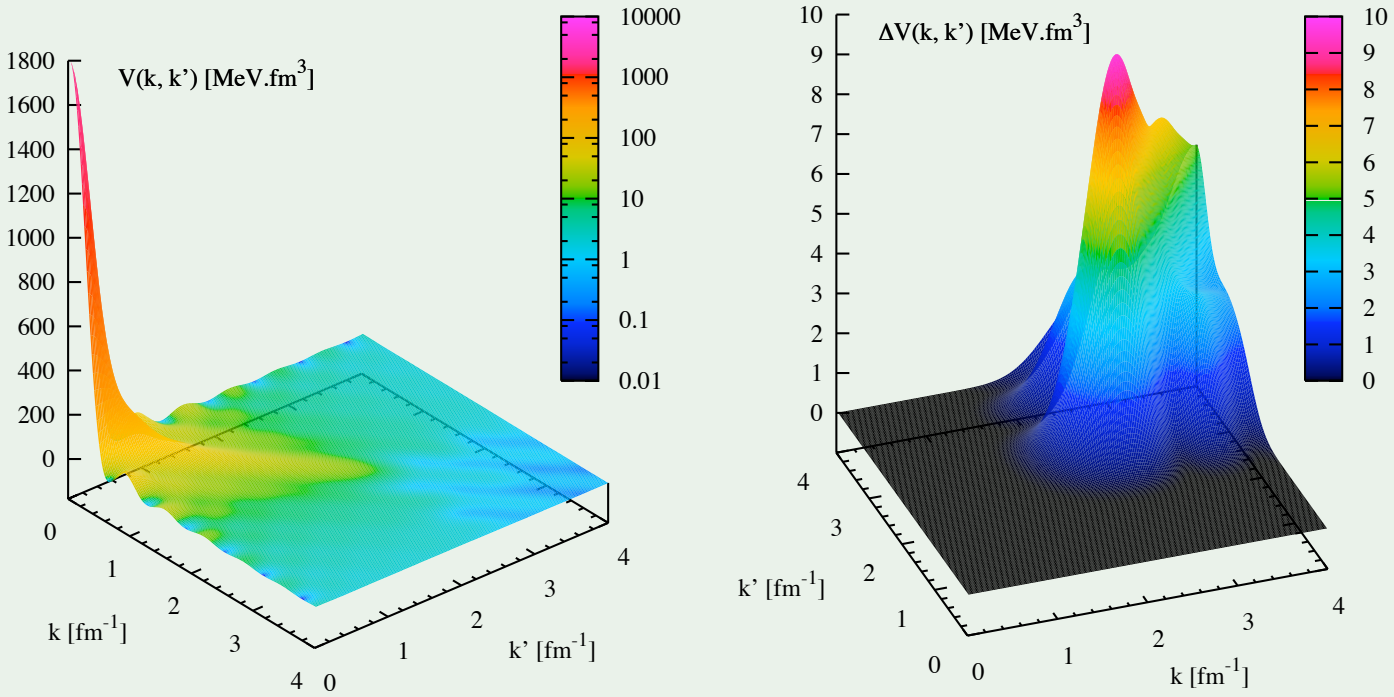
- Separable expansion exists for higher partial waves

Separable representation of V_{Coul}

Coulomb effects on proton-proton pairing

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

Tests for $a = 10$ fm and truncated expansion at $N_{\mathrm{Coul}} = 10$



- $N_{\mathrm{Coul}} \sim 15$ in practice (peanuts !)

Rank-n separable representation of $V_{NN\langle N\rangle}(\Lambda)$

Focus on ${}^1S_0$ partial-wave

- Rank-n separable anzatz

$$V^{{}^1S_0}_{qq\langle q'\rangle}(k,k';k_F^{q'}) = \sum_{\alpha,\beta=1}^{n} g_\alpha^{qq\langle q'\rangle}(k)\ \lambda_{\alpha\beta}^{qq\langle q'\rangle}(k_F^{q'})\ g_\beta^{qq\langle q'\rangle}(k')$$

- Parameterized density dependence

$$\lambda_{\alpha\beta}^{qq\langle q'\rangle}(k_F^{q'}) \quad = \quad \sum_{i\in\mathbb{N}} \lambda_{\alpha\beta}^{qq\langle q'\rangle}(i)\,(k_F^{q'})^i$$

- Fit $g_\alpha^{qq\langle q'\rangle}(k)$ and $\lambda_{\alpha\beta}^{qq\langle q'\rangle}(k_F^{q'})$ to $V^{{}^1S_0}_{qq\langle q'\rangle}(k,k';k_F^{q'})$ from INM

- Local Density Approximation (LDA)

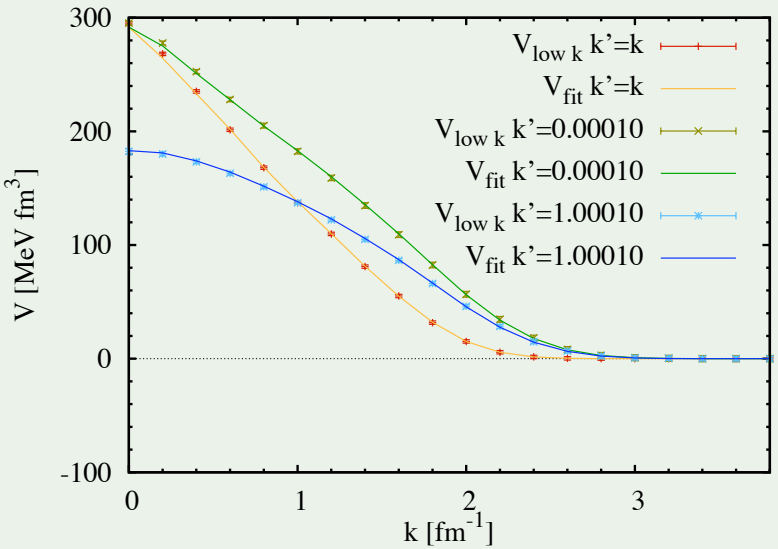
$$\lambda_{\alpha\beta}\left(k_F^{q'}\right) \to \lambda_{\alpha\beta}\left(k_F^{q'}(\mathbf{R})\right) \qquad \text{with} \qquad k_F^{q'}(\mathbf{R}) \equiv \left(3\pi^2\rho_{q'}(\mathbf{R})\right)^{1/3}$$

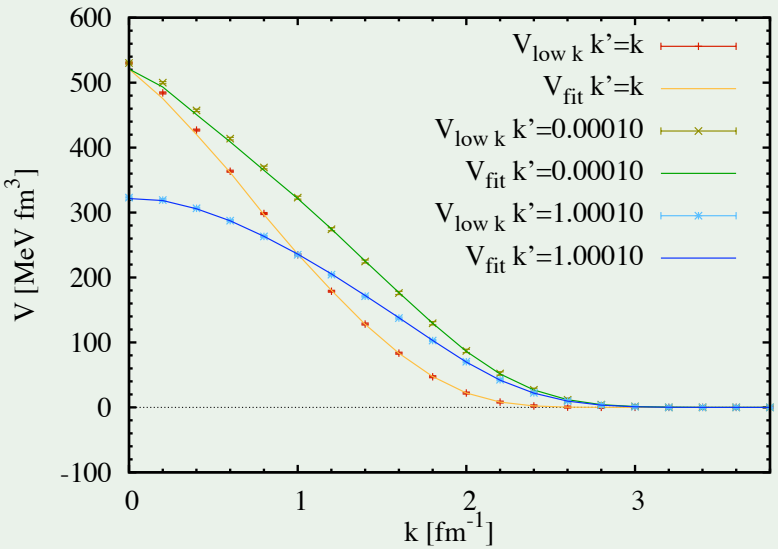
Rank-n separable representation of $V_{NN\langle N\rangle}(\Lambda)$

Focus on $^1S_0$ partial-wave

- Rank-n separable anzatz
- Parameterized density dependence
- Fit $g_\alpha^{qq\langle q'\rangle}(k)$ and $\lambda_{\alpha\beta}^{qq\langle q'\rangle}(k_F^{q'})$ to $V_{qq\langle q'\rangle}^{^1S_0}(k,k';k_F^{q'})$ from INM
- Local Density Approximation (LDA)

Fit at $k_F^{q'} = 1.2/1.4$ fm^{1} (left/right) for $\Lambda = 2.0$ fm^{1}, $n = 4$ and $i = 3,4$





EDF calculations in spherical nuclei

Benefice from using rank-n separable representation

- Separable force in coordinate-space $[\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2]$

$$\langle \mathbf{r}_1' \mathbf{r}_2' | \, V_{qq}^{^1S_0} | \mathbf{r}_1 \mathbf{r}_2 \rangle \quad = \quad \sum_{\alpha,\beta}^{\mathrm{n}} G_\alpha(r') \; \lambda_{\alpha\beta} \; G_\beta(r) \; \delta(\mathbf{R}' - \mathbf{R}),$$

  where $G_\alpha(r) =$ fourier transform of $g_\alpha(k)$

- The pairing energy functional reads

$$\mathcal{E}^{\kappa\kappa} \quad = \quad \sum_q \frac{1}{2} \int d^3\mathbf{R} \sum_{\alpha,\beta=1}^{\mathrm{n}} \breve{\tilde{\rho}}_\alpha^{q\,*}(\mathbf{R}) \; \lambda_{\alpha\beta} \; \breve{\tilde{\rho}}_\beta^{q}(\mathbf{R})$$

Cost of interaction's finite-range and non-locality

- Induce non-local pairing field and density
- BUT the functional depends only on *local* effective pair densities

$$\breve{\tilde{\rho}}_\alpha^{q}(\mathbf{R}) \quad = \quad \int d^3\mathbf{r} \; G_\alpha(r) \sum_\sigma (-)^{\frac{1}{2}-\sigma} \; \kappa^q \left(\mathbf{R} + \mathbf{r}/2, \sigma; \mathbf{R} - \mathbf{r}/2, -\sigma\right)$$

EDF calculations in spherical nuclei

Building of the pairing-field matrix

- Define reduced two-body wave-functions (spin-singlet part)

$$\breve{\Psi}^{q\,\alpha}_{ij}(\mathbf{R}) \equiv \int d^3\mathbf{r}\; G_\alpha(r)\,\Psi^q_{ij}(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2)$$

$$\Psi^q_{ij}(\mathbf{r},\mathbf{r}') \equiv \sum_\sigma (-)^{s-\sigma}\phi_i(\mathbf{r},\sigma,q)\phi_j(\mathbf{r}',-\sigma,q).$$

  from basis functions $\phi_i \Rightarrow \breve{\Psi}^{q\,\alpha}_{ij}(\mathbf{R})$ are computed once

- Build densities and pairing field matrix elements

$$\breve{\Delta}^q_\alpha(\mathbf{R}) \equiv \frac{1}{2}\sum_\beta^n \lambda_{\alpha\beta}\,\breve{\rho}^q_\beta(\mathbf{R}) \equiv \frac{1}{2}\sum_\beta^n \lambda_{\alpha\beta}\sum_{ij}\breve{\Psi}^{q\,\beta}_{ij}(\mathbf{R})\,\kappa^q_{ij}$$

$$\Delta^q_{ij} = \sum_\alpha^n \int d^3\mathbf{R}\;\breve{\Psi}^{q,\alpha}_{ij}(\mathbf{R})\,\breve{\Delta}^q_\alpha(\mathbf{R})$$

➡ Pseudo-local pairing problem!

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, PRC80 (2009) 044321]

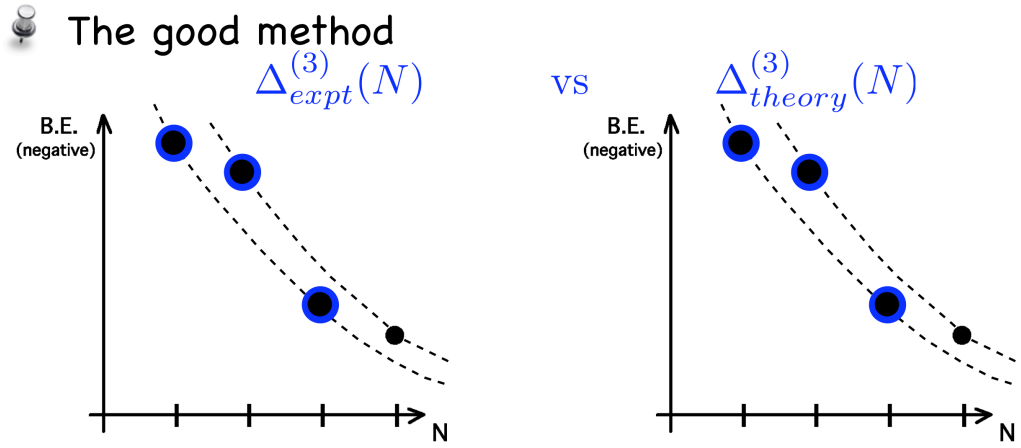
[T. D., T. Lesinski, AIP Conf. Proc. 1165 (2009) 243]

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

Pairing gap

Odd-even mass staggering

- Lack of binding of odd nucleus vs even neighbors measures pairing gap



Three-point mass difference

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

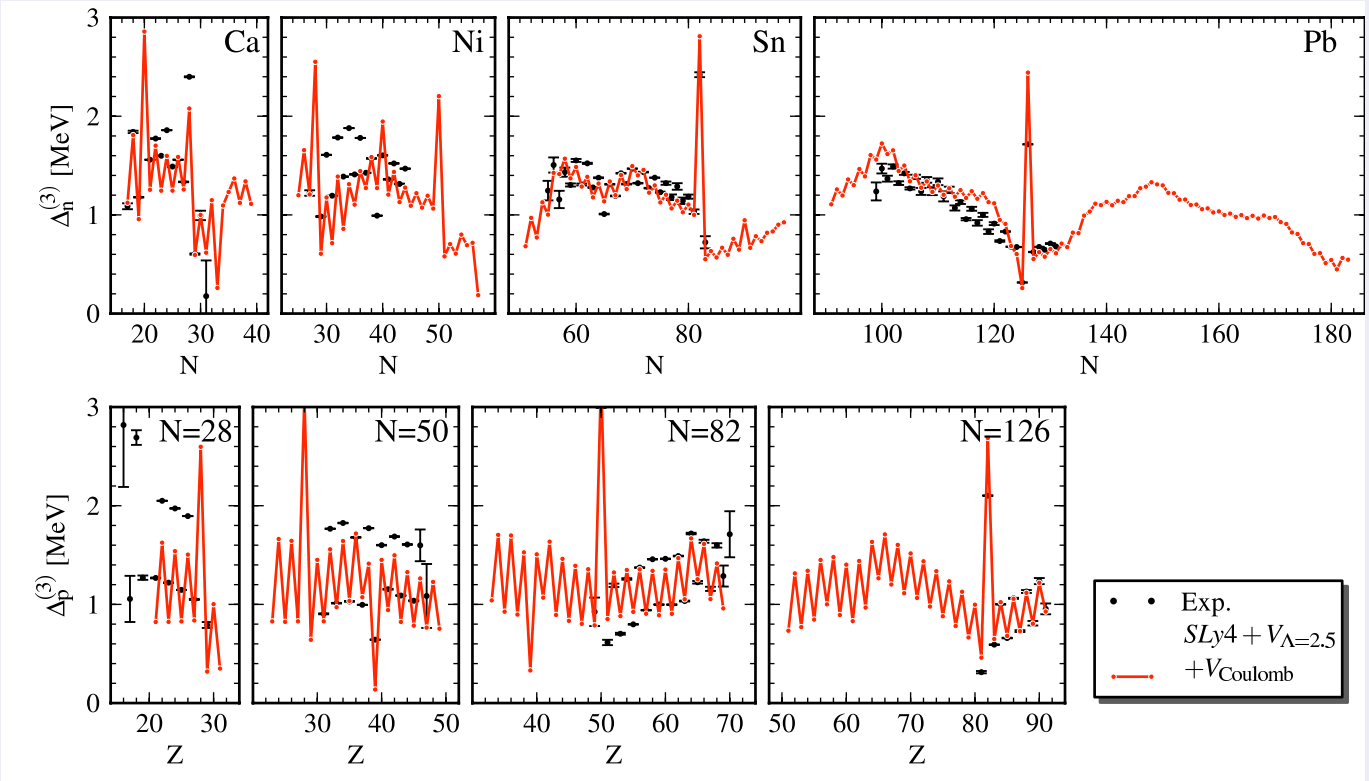
- Interplay with shell structure must be disentangled

  [T. D. *et al.*, PRC65 (2001) 014310 and 014311]

Pairing gaps

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

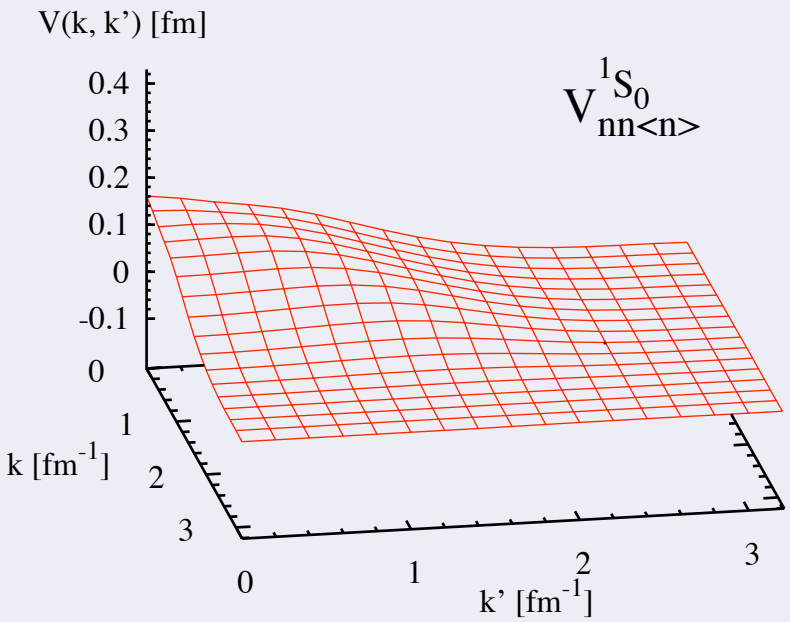
$\Delta_q^{(3)}$ from $v^{pp} = V_{NN} + V_{\mathrm{Coul}}$ ($^1S_0$)

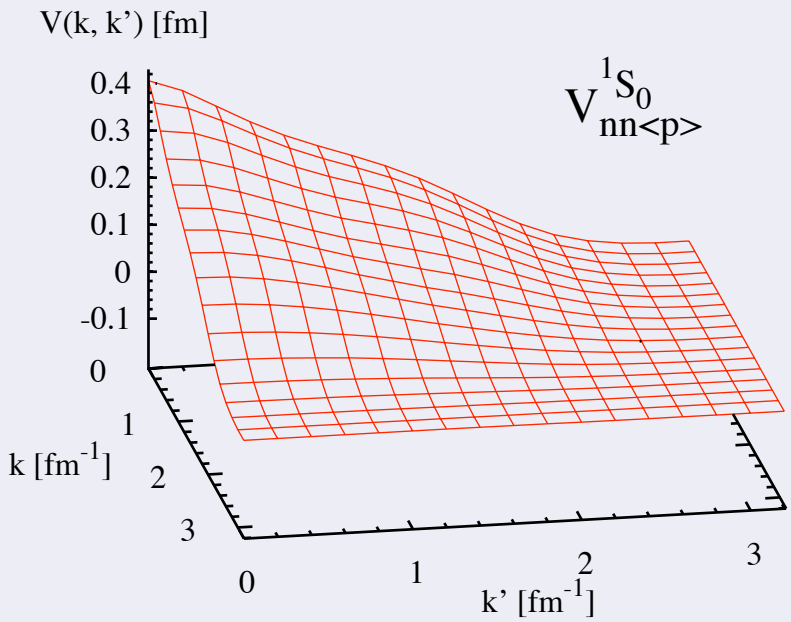


- Pairing gaps consistent with experiment
- Large oscillation of $\Delta_p^{(3)}$ due to Coulomb in ph

${}^1S_0$ matrix elements of $V_{NN\langle N\rangle}$

Dependence of $V^{{}^1S_0}_{qq\langle q'\rangle}$ over isospin of q' ($k_F^{q'}$=1.2 fm^{-1})

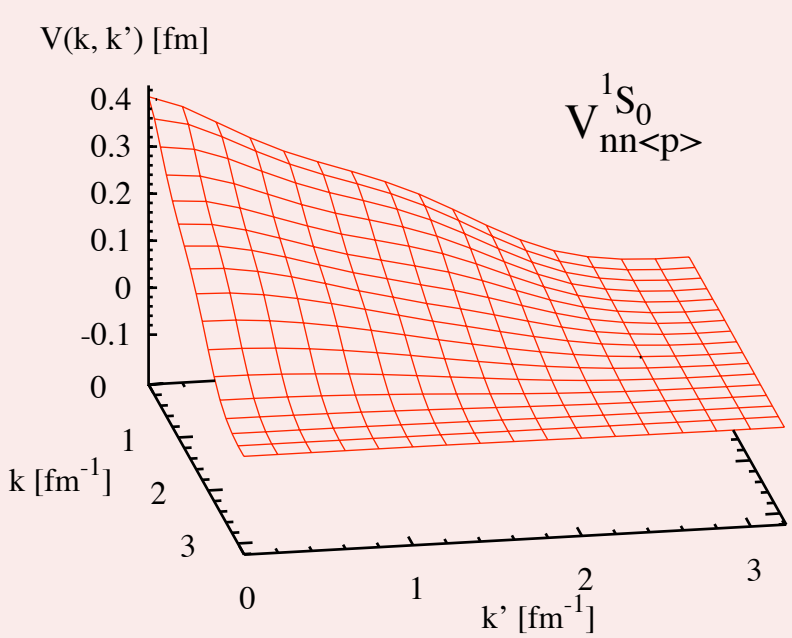


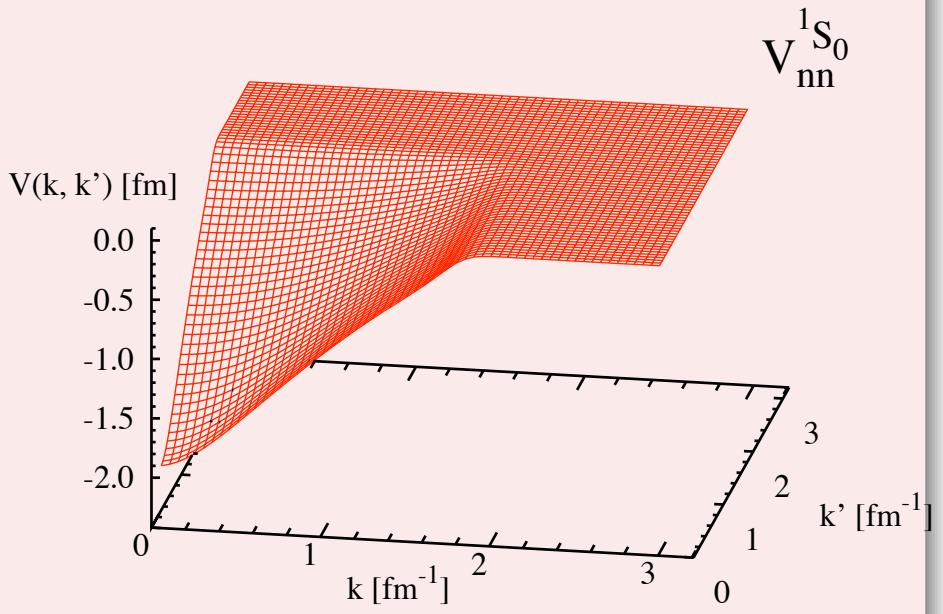


1. $V^{{}^1S_0}_{qq\langle q'\rangle}$ repulsive at all $k_F^{q'}$
2. Averaged force stronger in SNM than in PNM
3. $V^{{}^1S_0}_{qq\langle \bar{q}\rangle}$ more repulsive than $V^{{}^1S_0}_{qq\langle q\rangle}$

$^1S_0$ matrix elements of $V_{NN\langle N\rangle}$

Comparison between $V_{NN}^{^1S_0}$ and $V_{NN\langle N\rangle}^{^1S_0}$



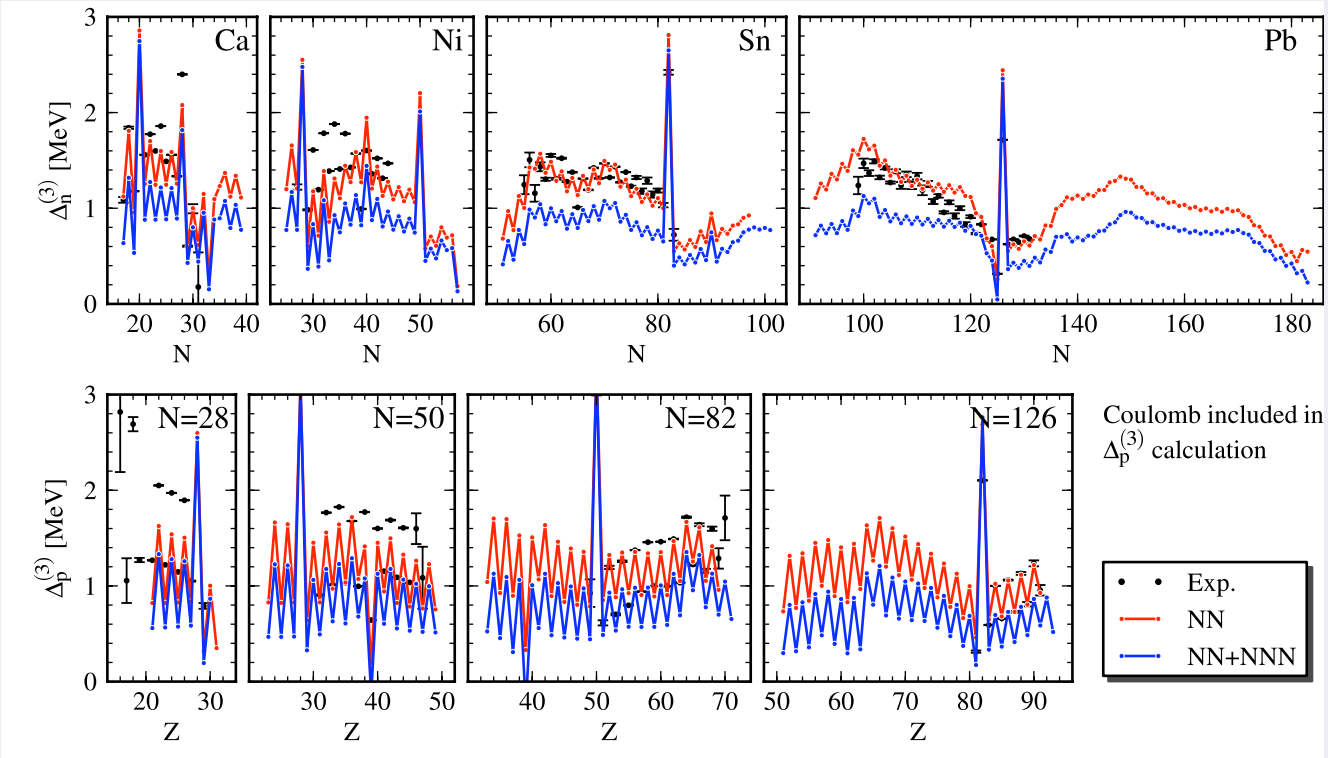


- $V_{qq\langle q'\rangle}^{^1S_0}$ (≥ 0) quite weaker than $V_{qq}^{^1S_0}$ (≤ 0) up to $k_F^{\rm sat}$
- Pairing gaps based on $V_{NN}^{^1S_0}$ expected to decrease ; but by how much!?

Pairing gaps

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

$\Delta_q^{(3)}$ from $v^{pp} = V_{NN} + V_{\mathrm{Coul}}$ ($^1S_0$)



- $\Delta_q^{(3)}$ decreased by 20% with slight isovector trend ($|\,V^{\,^1S_0}_{qq\langle\bar{q}\rangle}\,| > |\,V^{\,^1S_0}_{qq\langle q\rangle}\,|$)
- Leave $\sim 20-30\%$ for coupling to (collective) fluctuations

Outlook

Study pairing and shell structure interplay

- Systematic of OEMS and QP excitation spectra [with T. Lesinski *et al.*]
- Systematic of charge radii with focus on NNN [with T. Lesinski *et al.*]

Extend to deformed nuclei

- Tractable finite-range interaction [with V. Hellemans *et al.*]
- Map onto a quasi-local EDF [with B. Gebremariam *et al.*]

Add coupling to density, spin and isospin fluctuations

- Self-energies at second order [with S. Baroni *et al.*]
- Coupling to collective QRPA modes [with A. Pastore *et al.*]
  - e.g. [A. Pastore, F. Barranco, R. A. Broglia, E. Vigezzi, PRC78 (2008) 024315]
- Self-consistent Green's function (Gorkov) calculations [with V. Soma *et al.*]

Outline

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

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

With $f \in \{\rho, \tau, \vec{J}\}$

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

Trilinear Skyrme EDF in canonical basis

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

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

Trilinear Skyrme EDF in coordinate space (no pairing)

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

Matrix elements of effective vertices

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

Trilinear Skyrme EDF in canonical basis

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

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

Zeroth-order (HF) energy

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

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

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

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]

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

Zeroth-order (HF) energy

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

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

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

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]

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^f 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 $\Pi_k^\rho(k_F(\vec{R}))$

Expansion of $\vec{s}_{\vec{r}_1\vec{r}_2}$ [B. Gebremariam, T. D., S. K. Bogner, arXiv:0910.4979]

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

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

2. Opens up DME for all spin-unsaturated nuclei!
3. Analytical expression for $\Pi_k^s(k_F(\vec{R}))$
4. Recovers $\Pi_k^\rho(k_F(\vec{R}))$ of Negele and Vautherin
5. Few % error on E^F from full fledged $V^{NN}(\Lambda_{\text{low}})$ (central, tensor, spin-orbit)

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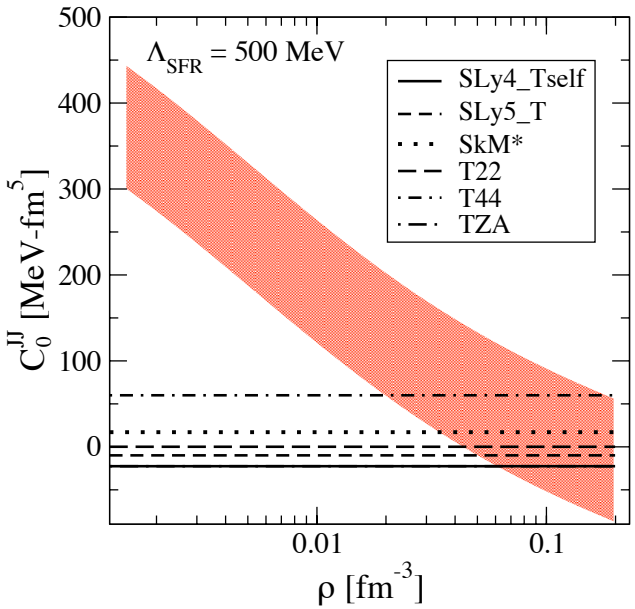
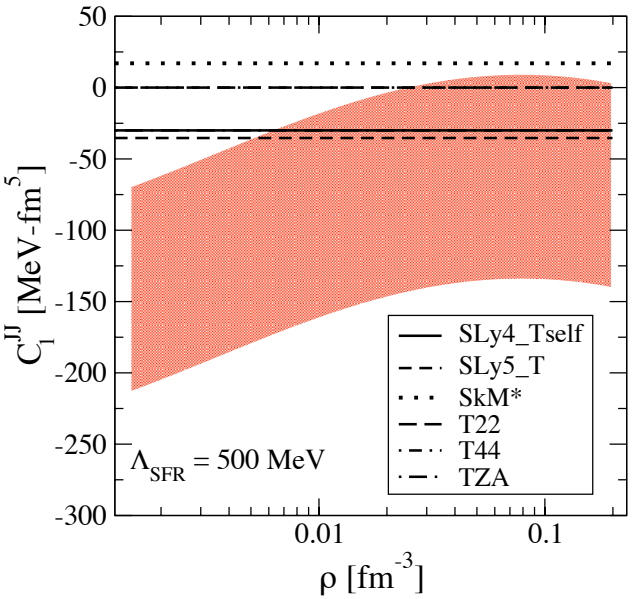
The density matrix expansion

Under completion [B. Gebremariam, S. K. Bogner, T. D., 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. Comparison with phenomenology
   - Study of Fock DME couplings and role of pion-physics/ V^{NNN}

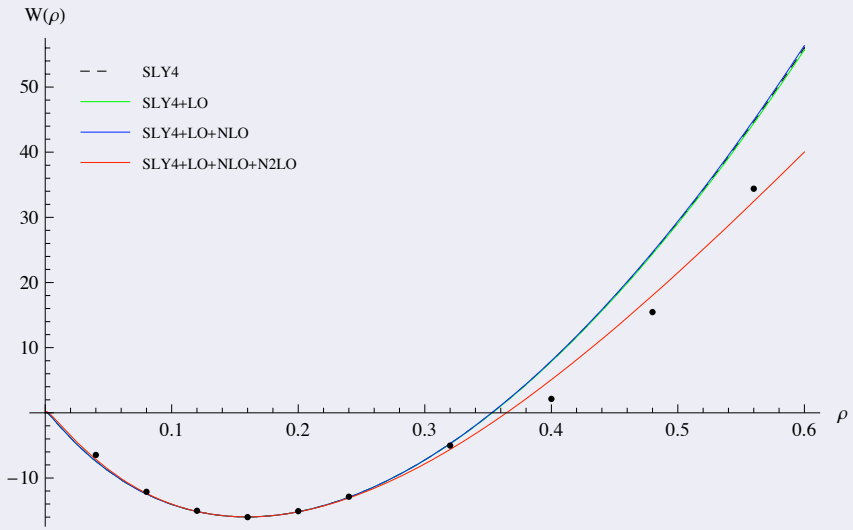


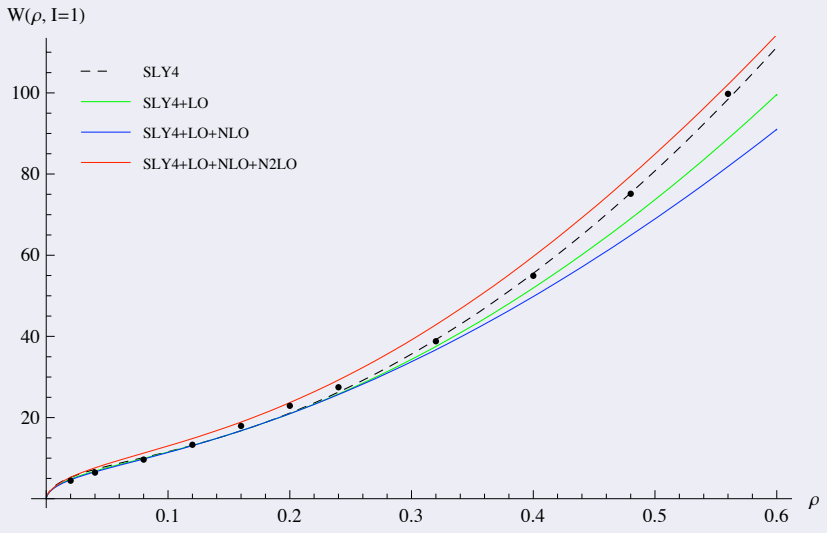


The density matrix expansion

Near future

1. Educated guess for empirical fitting [M. Stoitsov *et al.*, under progress]
   - Take DME coulings (keeping exact Hartree from V^{NN})
   - Add (quasi) density-independent Skyrme EDF and refit





2. Formalism [V. Rotival *et al.*, under progress]
   - Extend DME to non-locality in time and apply to second-order in MBPT
   - Extend DME to pairing channel including ultra-violet renormalization