Towards Microscopically Enriched and Constrained EDF

Gebremariam Biruk[1] T. Duguet[1,2] S. Bogner[1]

[1]NSCL, Michigan State University

[2]ESNT, DSM/Irfu/SPhN, CEA Saclay

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Outline

Status of current EDFs

- Lack predictive power in unknown regions
- No spectroscopic-quality EDF with the standard parameterization

- What can be missing from current functionals ?
  - no explicit pion physics
  - unclear connection to 3-body (and higher) body forces
  - pairing not treated on same footing
  - no way to estimate theoretical uncertainities

- Both form and couplings might need improvement
- Partial answer: more emphasis on microscopy ?

Derive the complete EDF?

Augment and not derive!

Goal

- EDF from HF+ MBPT with $\chi-$EFT NN/NNN (pion-phys.)

- A quasi-local/Skyrme-like EDF is required
  - Connect with phenomenology
  - Provide improvement to the already existing Skyrme-EDFs
  - Easier to treat numerically

- Non-locality emerges as an interface problem

- At the NN HF level, non-locality due to exchange terms

- Typical exchange terms from HF (NN)
  - From central $\int d\vec{r}_1\, d\vec{r}_2\, V_c(r)\, \rho_q(\vec{r}_1, \vec{r}_2)\, \rho_{q'}(\vec{r}_2, \vec{r}_1)$
  - From central/tensor $\int d\vec{r}_1\, d\vec{r}_2\, V_t(r)\, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{s}_{q'}(\vec{r}_2, \vec{r}_1)$
  - From spin-orbit $\int d\vec{r}_1\, d\vec{r}_2\, V_{so}(r)\, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{r} \times \vec{\nabla}_2\, \rho_{q'}(\vec{r}_2, \vec{r}_1)$

- Three body contributions (HF) typically three non-local/local densities
- A method to approximate the non-locality with local quantities

Outline

The one-body density matrix (DM)

- The normal/anomalous parts of the generalized one-body DM

$$\begin{aligned}\rho(\vec{r}\,\sigma\,q,\vec{r}\,'\sigma'\,q') &= \langle\,\Phi\,|\,c^{\dagger}(\vec{r}\,'\sigma'\,q)\,c\,(\vec{r}\,\sigma\,q)\,|\,\Phi\rangle\\ \kappa(\vec{r}\,\sigma\,q,\vec{r}\,'\bar{\sigma}'\,q') &= \langle\,\Phi\,|\,c(\vec{r}\,'\bar{\sigma}'\,q)\,c\,(\vec{r}\,\sigma\,q)\,|\,\Phi\rangle\end{aligned}$$

- Scalar/Vector $\bigotimes$ Isoscalar/Isovector decomposition e.g.

$$\rho_q(\vec{r}\,\sigma,\vec{r}\,'\sigma') = \frac{1}{4}\left\{\rho_0(\vec{r},\vec{r}\,')\,\delta_{\sigma\sigma'} + \vec{s}_0(\vec{r},\vec{r}\,').\vec{\sigma}_{\sigma\sigma'} + (-1)^{1/2-q}\big[0\to 1\big]\right\}$$

- Dominant leading order MBPT contributions
  - Hartree and Fock diagrams $\to \mathcal{E}\big[\rho\big]$
  - Bogoluibov diagrams $\to \mathcal{E}\big[\kappa,\kappa^*\big]$
- Highly nonlocal, no direct connection to local/Skyrme EDFs

$$\begin{aligned}\mathcal{H}_t(\vec{r}) = {} & \frac{\hbar^2}{2m}\tau_t + \mathcal{C}_t^{\rho\rho}\rho_t^2 + \mathcal{C}_t^{\rho\tau}\rho_t\tau_t + \mathcal{C}_t^{J^2}J_t^2 + \mathcal{C}_t^{\rho\Delta\rho}\rho_t\Delta\rho_t\\ & + \mathcal{C}_t^{\nabla\rho\nabla\rho}\big(\nabla\rho_t\big)^2 + \mathcal{C}_t^{\rho\nabla J}\rho_t\vec{\nabla}\cdot J_t + \mathcal{C}_t^{J\nabla\rho}J_t\cdot\nabla\rho_t\end{aligned}$$

DME objectives and PSA

- Introduced by Negele and Vautherin in 1972

DME in a nutshell

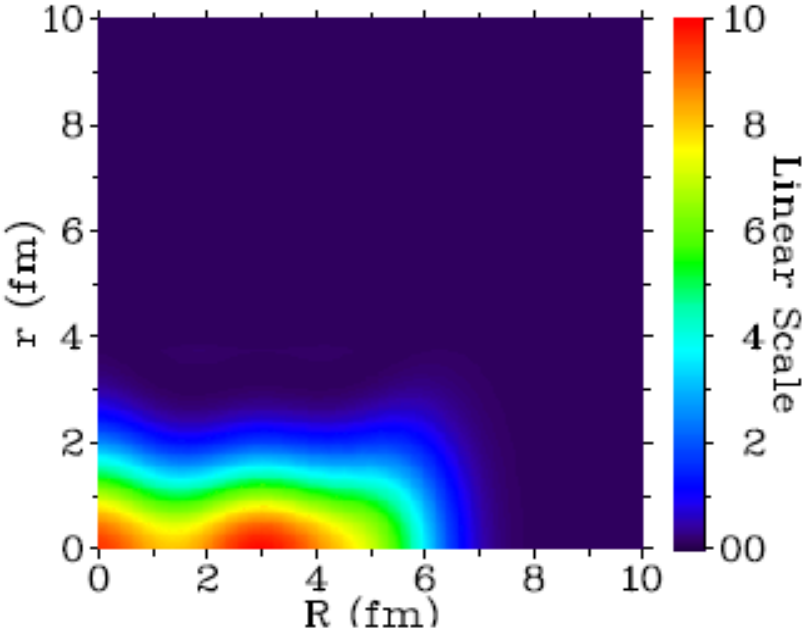
- Expand the DM (scalar/vector) in terms of factorized local densities
  - $\rho_q(\vec{r},\vec{r}') = \sum_n \Pi_n(k_F r)\langle\mathcal{O}_n(\vec{R})\rangle$
  - $\vec{s}_q(\vec{r},\vec{r}') = \sum_n \Pi_n(k_F r)\langle\mathcal{O}_n(\vec{R})\rangle$
  - Local densities $\mathcal{O}_n(\vec{R}) = \left[\rho_q(\vec{R}), \vec{\nabla}\rho_q(\vec{R}), \Delta\rho_q(\vec{R}), \vec{J}_q(\vec{R})...\right]$

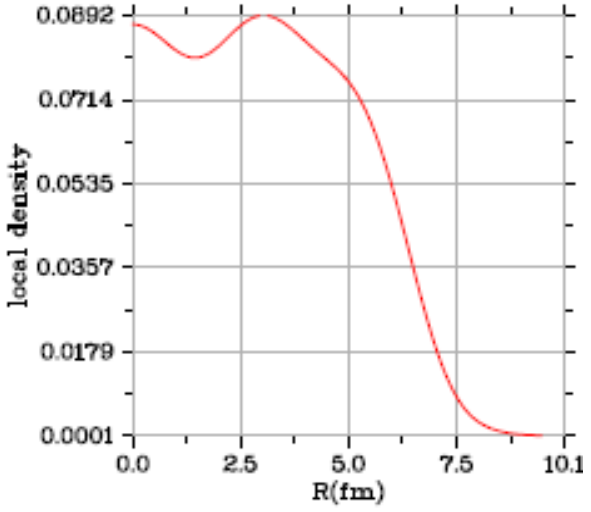
Phase Space Averaging

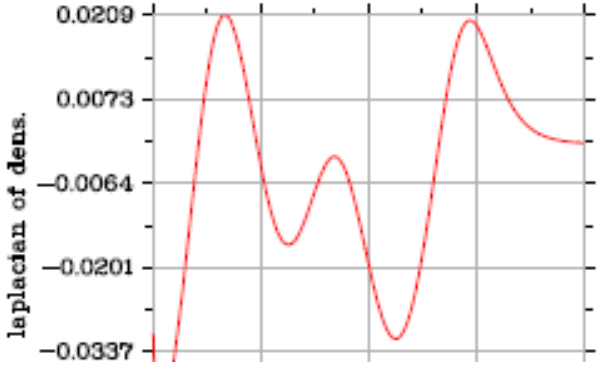
- Constructive method to fix the Π_n functions
  - Isolate the operator that results in the non-locality
  - Average the action of the operator in a model phase space

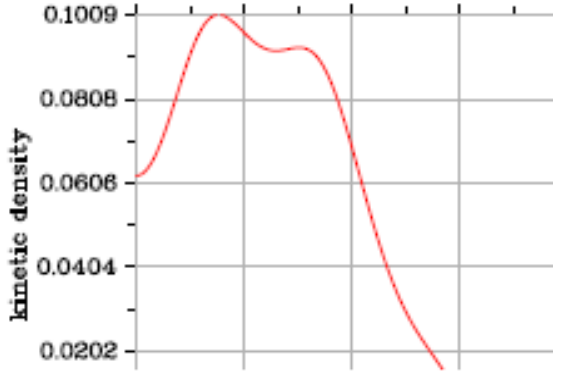
The challenge for the scalar part!

- A separable approximation to $\rho_q(\vec{r}_1, \vec{r}_2)$ with $\rho_q(\vec{R})$, $\tau_q(\vec{R})$, $\Delta\rho_q(\vec{R})$ ...!
- Densities from converged calc. of Pb^{180} using Sly4 functional









PSA for scalar part

- Isolate the operator that results in the non-locality

$$\rho_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) = e^{\vec{r}\cdot\frac{(\vec{\nabla}_1-\vec{\nabla}_2)}{2}} \sum_{i,\sigma}\varphi_i^*(\vec{r}_1\sigma q)\,\varphi_i(\vec{r}_2\sigma q)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

- Angle-averaging over the orientation of $\vec{r}$

$$\rho_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) \simeq \frac{\sinh\left[r\left|\frac{(\vec{\nabla}_1-\vec{\nabla}_2)}{2}\right|\right]}{r\left|\frac{(\vec{\nabla}_1-\vec{\nabla}_2)}{2}\right|}\rho_q(\vec{r}_1,\vec{r}_2)\Big|_{\vec{r}_1=\vec{r}_2=\vec{R}}$$

- Expand operator about arbitrary $-k^2$ rather than 0

$$F\left(\left(\frac{\vec{\nabla}_1-\vec{\nabla}_2}{2}\right)^2\right) = j_0(kr)+\frac{r}{2k}j_1(kr)\left[\left(\frac{\vec{\nabla}_1-\vec{\nabla}_2}{2}\right)^2+k^2\right]+\ldots$$

- What to do with k ?

PSA for scalar part contd.

Phase space model of Negele and Vautherin =INM phase space

- Provides PSA formulation of the original DME (Negele-Vautherin)

$$\rho_q(\vec{R}+\frac{1}{2}\vec{r},\vec{R}-\frac{1}{2}\vec{r}) \quad = \quad \Pi_0^\rho(\Omega)\,\rho_q(\vec{R})+\Pi_2^\rho(\Omega)\left(\frac{1}{4}\Delta\rho_q(\vec{R})-\tau_q(\vec{R})+\frac{3}{5}k_F^2\rho_q(\vec{R})\right)$$

$$\Omega = k_F r \qquad \Pi_0^\rho(k_F r) = \frac{3j_1(k_F r)}{k_F r} \qquad \Pi_2^\rho(k_F r) = \frac{35 j_3(k_F r)}{k_F^3 r}$$

- Finite Fermi systems have smeared out (diffuse) Fermi surface (Durand. et.al.)

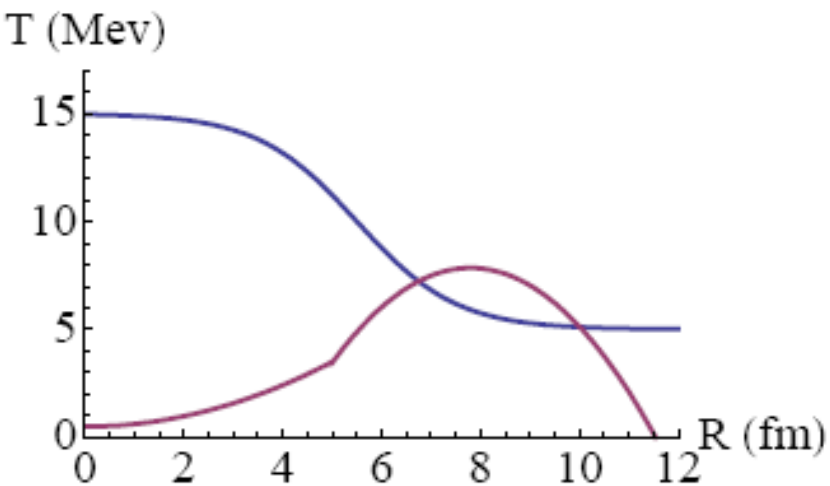


Figure: The effective Fermi energy $\mu(R)$ and the temperature $T(R)$ as deduced by fitting the Fermi function to the momentum distribution in A=184 model nucleus. Around the surface, $T = 7(MeV)$ implies a large effect.
$\tilde{f}(\vec{R},\vec{p}) = \left(1+\exp\{e_p-\mu(R)\}/T(R)\right)^{-1}$
$e_p = p^2/(2m)$

PSA for scalar part contd.

Phase space model for Π−DME =A diffuse Fermi surface

- Realistic phase space distribution for FFS (Fermi function)

$$\rho_q(\vec{R}+\frac{1}{2}\vec{r},\vec{R}-\frac{1}{2}\vec{r}) \quad = \quad \Pi_0^\rho(\Omega)\,\rho_q(\vec{R})+\Pi_2^\rho(\Omega)\left(\frac{1}{4}\Delta\rho_q(\vec{R})-\tau_q(\vec{R})+\frac{3}{5}k_F^2\rho_q(\vec{R})\right)$$

The various $\pi-$functions read

$$\Pi_0^\rho \quad = \quad -\frac{\left(\alpha\,k_F^2r^2-2\beta\,(2\beta+3\alpha)\right)}{2\beta\,(3\alpha+2\beta)}\,e^{-k_F^2r^2/(4\beta)}$$

$$\Pi_2^\rho \quad = \quad \frac{r}{2k_F}\,j_1(k_Fr)$$

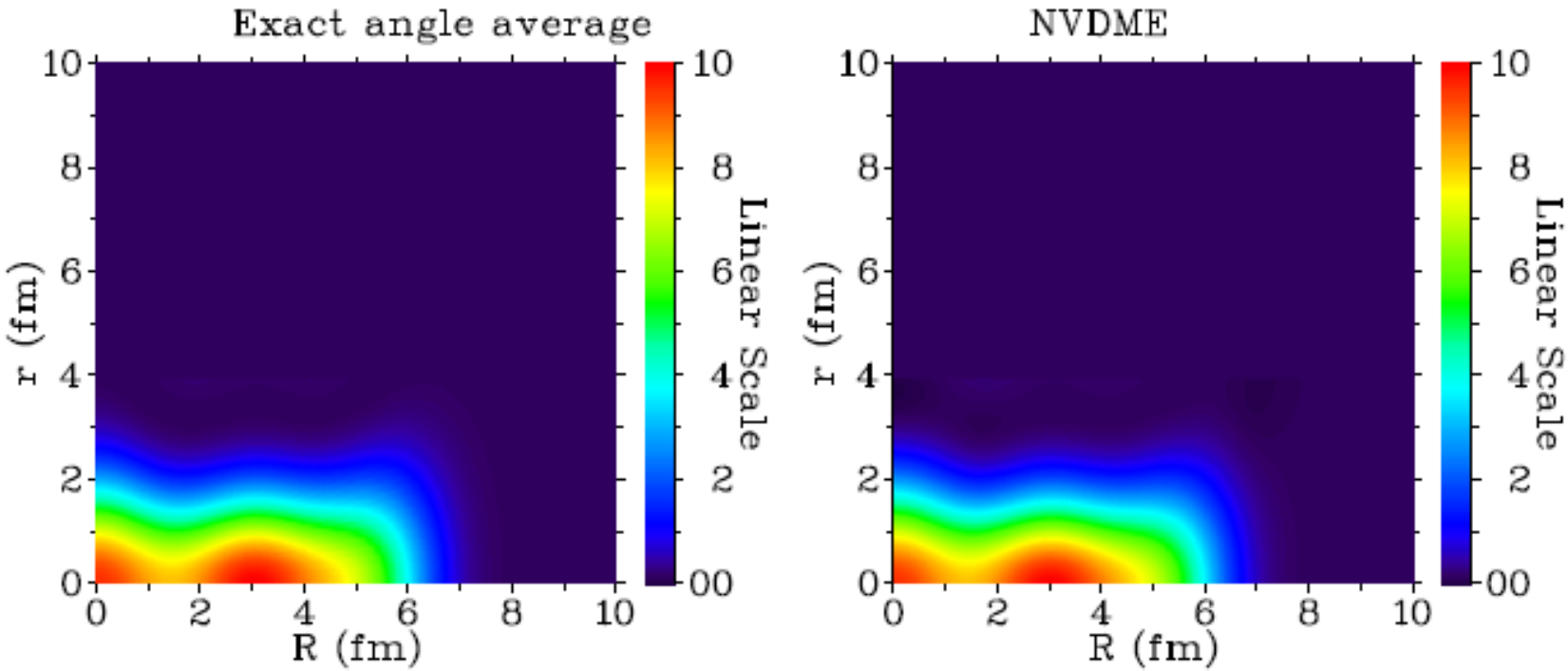
- Parameters α and β characterize the phase space distribution
- Very weak dependence on the number of nucleons

How do the two models compare (non/and with self-consistency)?

- Profile reproductions
- Integrated contributions

Result for the scalar part of the DM

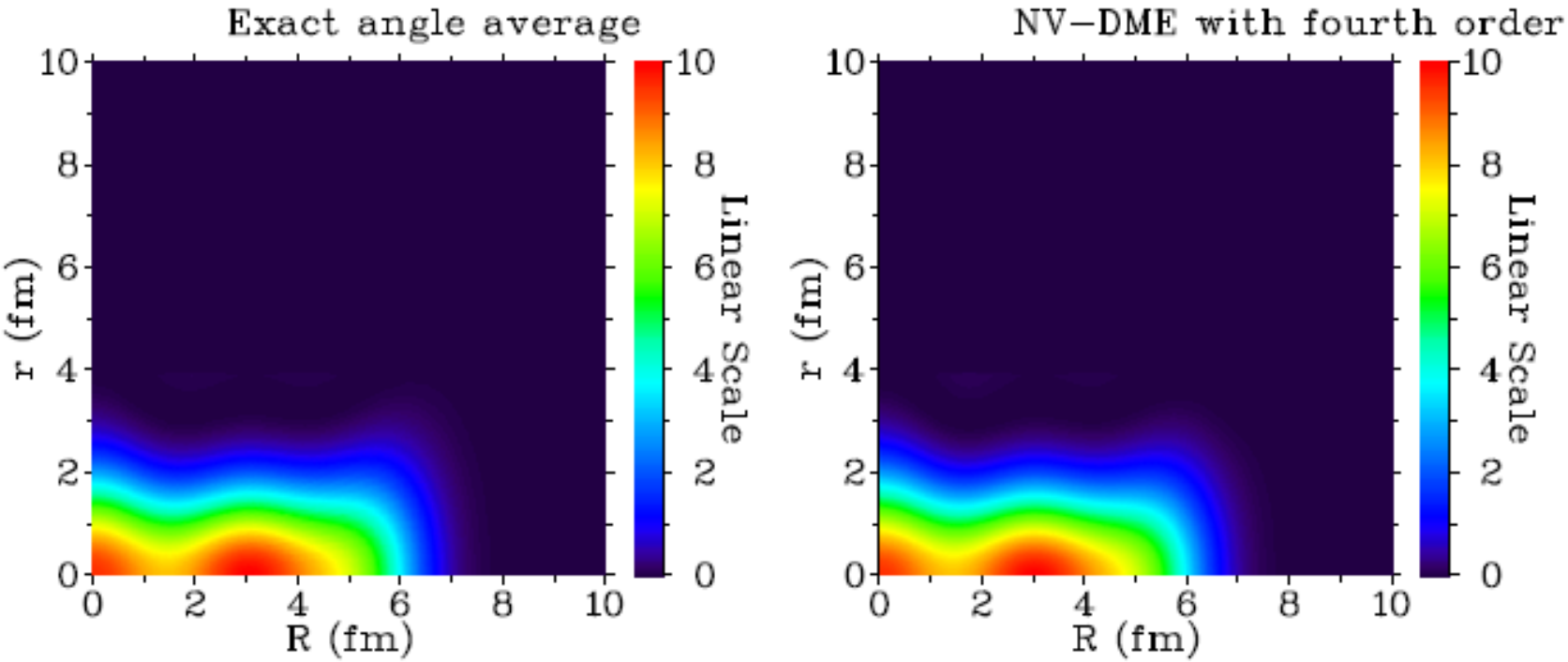
- Comparison of $\int d\Omega_r \, \rho_q(\vec{r}_1, \vec{r}_2) \, \rho_q(\vec{r}_2, \vec{r}_1)$
- Densities from converged calc. of Pb^{180} using Sly4 functional



- Qualitatively, satisfactory agreement!

Result for scalar contd.

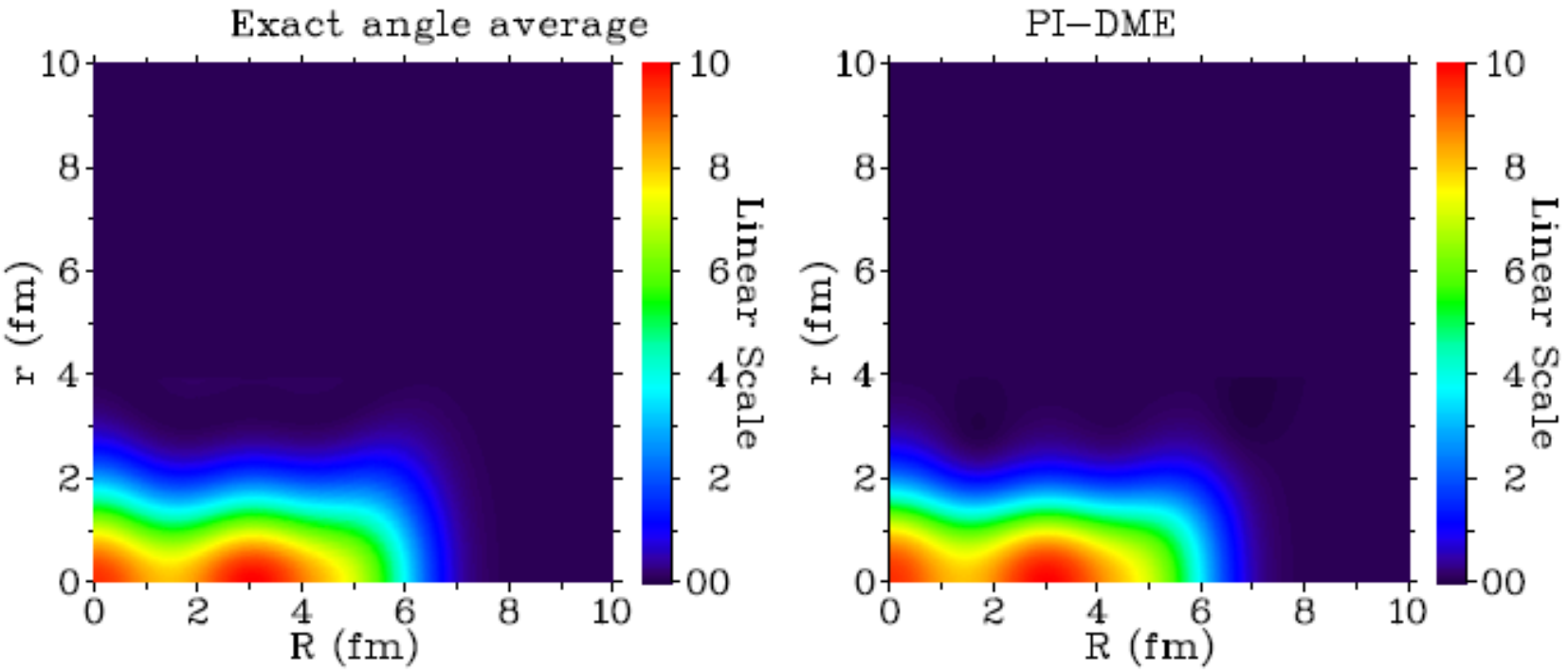
- Comparison of $\int d\Omega_r \, \rho_q(\vec{r}_1, \vec{r}_2) \, \rho_q(\vec{r}_2, \vec{r}_1)$
- Densities from converged calc. of Pb^{180} using Sly4 functional



- Qualitatively, satisfactory agreement!

Result for the scalar contd.

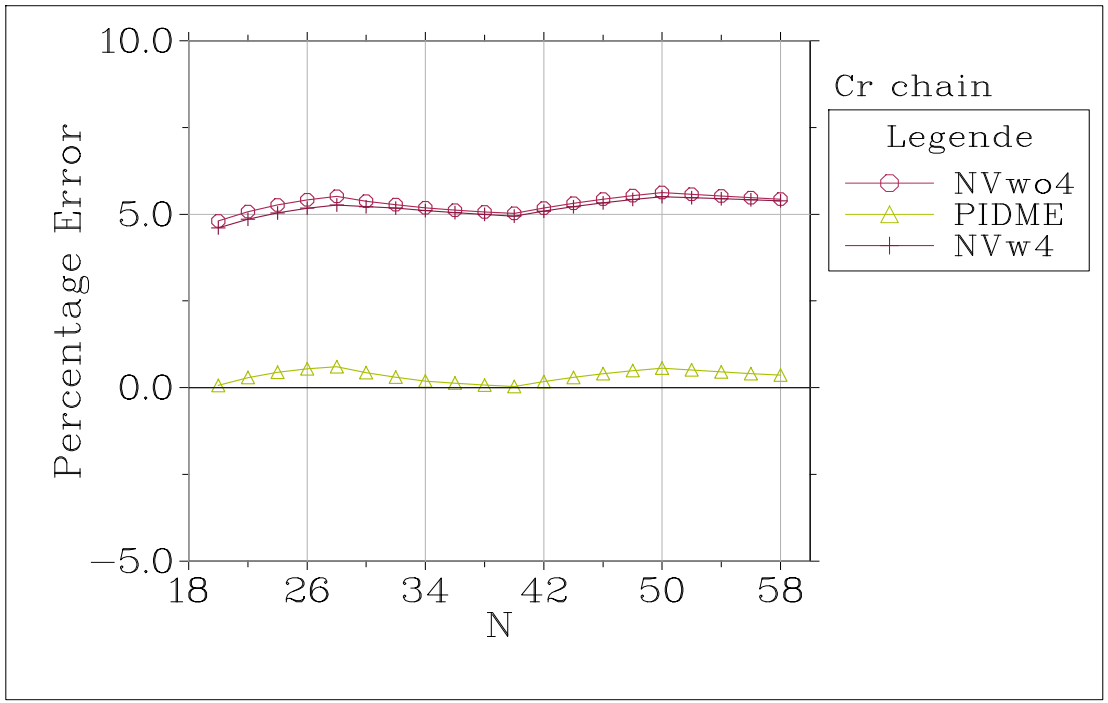
- Comparison of $\int d\Omega_r \, \rho_q(\vec{r}_1, \vec{r}_2) \, \rho_q(\vec{r}_2, \vec{r}_1)$
- Densities from converged calc. of Pb^{180} using Sly4 functional



- Qualitatively, satisfactory agreement!

Result for the scalar contd.

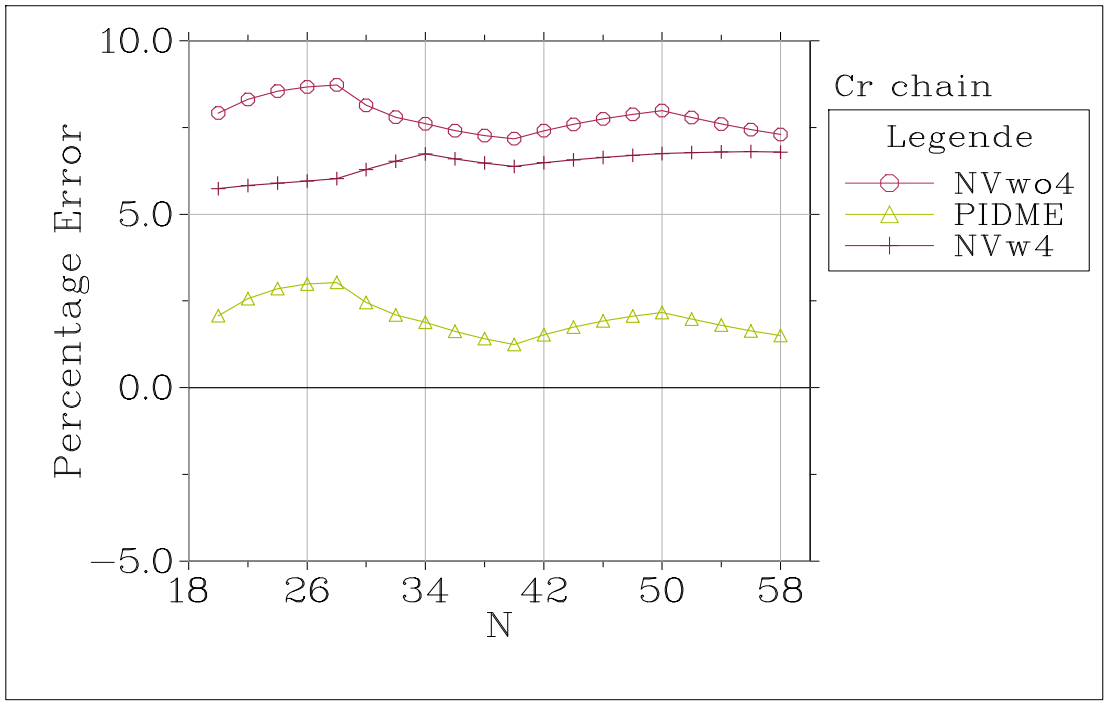
- % error for $\int d\vec{R}\, d\vec{r}\, V(r)\, \rho_q(\vec{r}_1, \vec{r}_2)\rho_q(\vec{r}_2, \vec{r}_1)$ and its DME
- Gogny interaction
- Cr-chain using Sly4 functional



- Slight improvement regarding the integrated contribution
- $\simeq 6-7\%$ residual error for NV-DME
- $\simeq 2-3\%$ residual error for $\Pi-$DME
- Holds throughout the nuclear mass table

Result for the scalar contd.

- % error for $\int d\vec{R}\, d\vec{r}\, V(r)\, \rho_q(\vec{r}_1, \vec{r}_2)\rho_q(\vec{r}_2, \vec{r}_1)$ and its DME
- Pion-exchange potential
- Cr-chain using Sly4 functional



- Slight improvement regarding the integrated contribution
- $\simeq 6-7\%$ residual error for NV-DME
- $\simeq 2-3\%$ residual error for $\Pi-$DME
- Holds throughout the nuclear mass table

Self-consistent DME vs Exchange only DME vs Exact HF (on going!)

Table: E/A for Full DME, Exchange only DME, Exact HF (MeV) for Brink-Boeker force (NV-DME)

element	Full DME	Exchange only DME	Exact HF
^{16}O	-6.204	-5.600	*
^{40}Ca	-8.526	-7.516	*
^{48}Ca	-7.447	-6.625	*
^{90}Zr	-9.339	-8.388	*

- Quoting previous works Error in the binding energy $\approx 10\%$, in exchange only reduces it to $\approx 2\%$, too large radii and smooth density

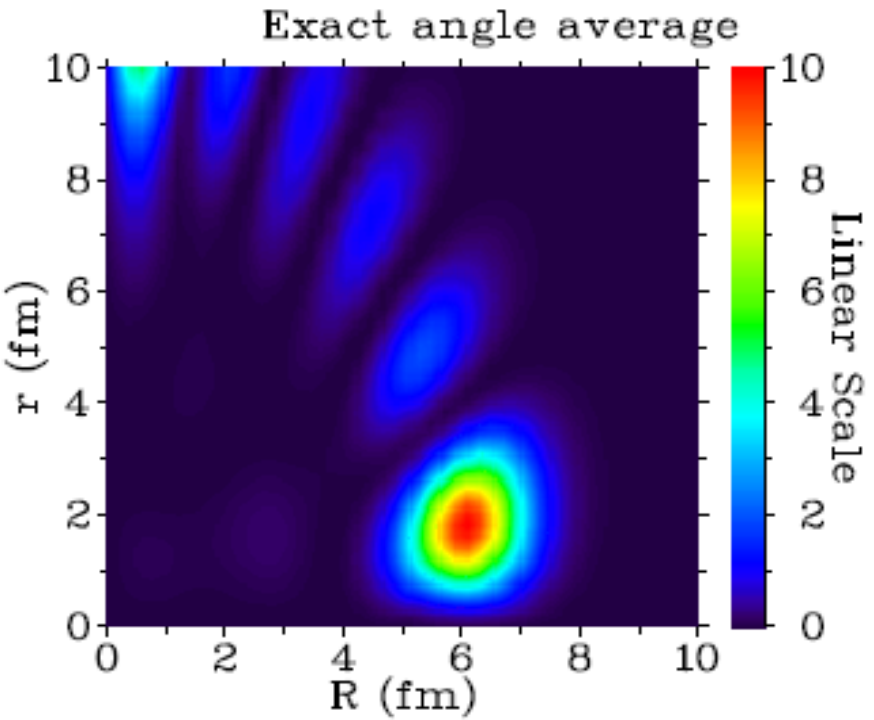
conclusion on DME

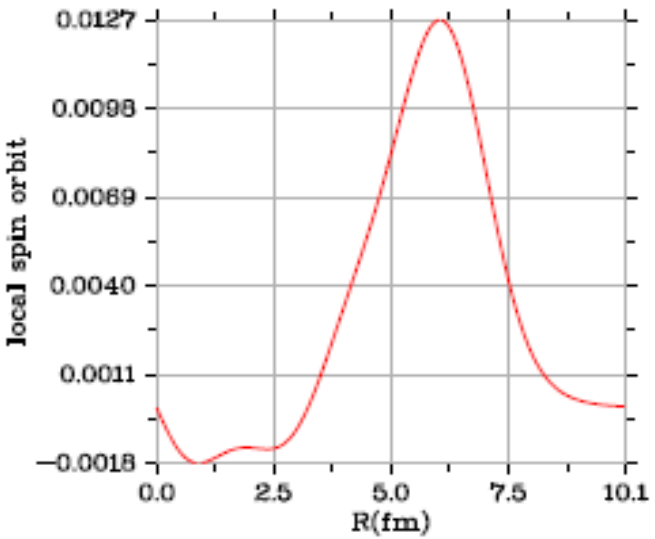
- Quite good for the scalar part (non-local) of the DM
- Not so good for the local scalar density (implication for NNN)

Ongoing work -comparison with complete/realistic interaction!

The challenge for the vector part!

- A separable approximation to $\vec{s}_q(\vec{r}_1, \vec{r}_2)$ with $J_{q,\mu\nu}(\vec{r}_1)$...!
- Densities from converged calc. of Pb^{208} using Sly4 functional





PSA for vector part

- The same set of steps as for the scalar part(with subtle differences)
- Isolate the operator that results in the non-locality

$$\vec{s}_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) = e^{i\vec{r}\cdot\vec{k}}\sum_{i\sigma_1\sigma_2}\langle\sigma_1|\vec{\sigma}|\sigma_2\rangle e^{\vec{r}\cdot\left[\frac{1}{2}(\vec{\nabla}_1-\vec{\nabla}_2)-i\vec{k}\right]}\varphi_i^*(\vec{r}_1\sigma_1 q)\varphi_i(\vec{r}_2\sigma_2 q)$$

where $\vec{k}$ is an arbitrary vector.

- Expand the operator (Taylor series) and keep the first non-zero

$$\begin{aligned}\vec{s}_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) &\simeq \frac{1}{2}e^{i\vec{r}\cdot\vec{k}}\sum_{i\sigma_1\sigma_2}\langle\sigma_1|\vec{\sigma}|\sigma_2\rangle\vec{r}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)\varphi_i^*(\vec{r}_1\sigma_1 q)\varphi_i(\vec{r}_2\sigma_2 q)\\ &= \frac{i}{2}e^{i\vec{r}\cdot\vec{k}}\,\vec{r}\times\vec{J}_q(\vec{R})\end{aligned}$$

- What to do with $\vec{k}$?
- Different choices yield different $\Pi_1^{\vec{s}}$ functions

$$\vec{s}_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) \simeq \frac{i}{2}\,\Pi_1^{\vec{s}}(rk_F)\,\vec{r}\times\vec{J}_q(\vec{R})$$

PSA for vector part contd.

- Dominant contribution from around Fermi surface

Negele and Vautherin

- Average over the orientation of $\vec{k}$
- Set $k = k_F$ (use LDA choice)

$$\vec{s}_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) \simeq \frac{i}{2} j_0(rk_F)\,\vec{r}\times\vec{J}_q(\vec{R})$$

- Finite Fermi systems have anisotropic Fermi surface (Bulgac et. al., Durand et. al.)

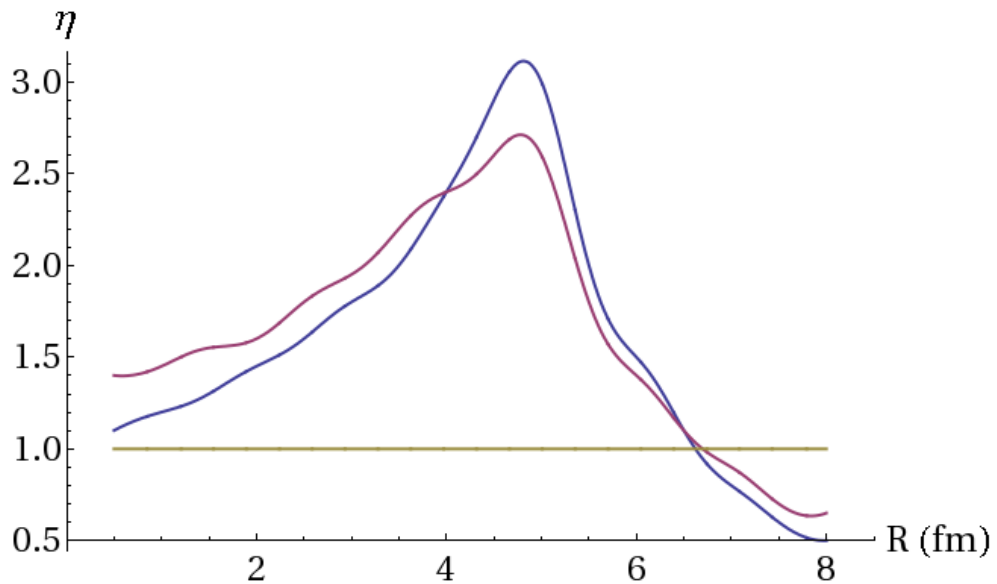


Figure: The anisotropy of momenta as a function of the R for different diffusivities of the potential and model nucleus A=184. Wood's saxon potential diffusivity $a = 0.4$ blue and $a = 0.67$ red curves. $\eta = \Delta P_{||}/\Delta P_{\perp}$.

Phase space model for Π−DME =Anisotropic Fermi surface

- Realistic phase space distribution for FFS (Fermi function)
- Anisotropy quantified by local quadrupolar deformation ($P_2(r)$)

- Use either the Husimi (Bulgac et. al.)/Wigner distributions

$$P_2(r) = \frac{\int d\vec{p}\left[3(\hat{r}.\hat{p}) - \hat{p}^2\right]\mathcal{H}(\vec{r},\vec{p})}{\int d\vec{p}\,\hat{p}^2\,\mathcal{H}(\vec{r},\vec{p})} \simeq \left[\frac{3\sum_{i,\sigma}\left|\left(\hat{r}.\hat{p}\right)^2\varphi_i(\vec{r}\sigma q)\right|^2}{\sum_{i,\sigma}\left|\vec{\nabla}\varphi_i(\vec{r}\sigma q)\right|^2} - 1\right]$$

- Universal feature of $P_2(r)$ in nuclei (FFS)

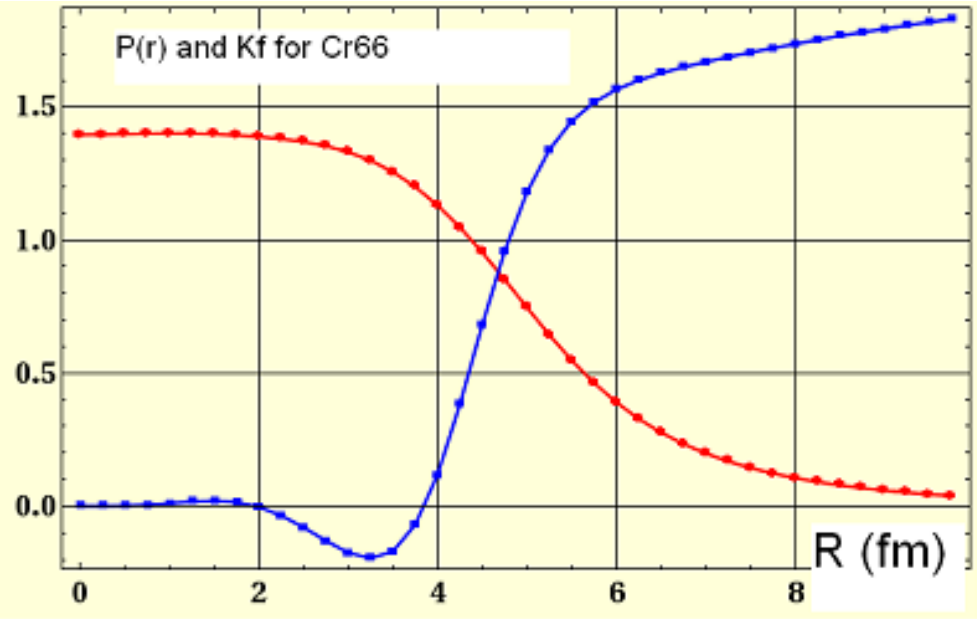


Figure: The quadrupolar deformation (blue) in the momentum distribution of a sample nucleus Cr^{66}. Note the progression from spherical to oblate and then prolate. Universal for all nuclei investigated. K_F (red) plotted for comparison.

PSA for vector part contd.

- Average $\vec{k}$ over a spheroid with quadrupole moment $Q(R) = P_2(R)$
- Spheroid in $\vec{k}$ space with $Q(R)$ fixed at each $\vec{R}$

$$\vec{s}_q\left(\vec{R}+\frac{\vec{r}}{2},\vec{R}-\frac{\vec{r}}{2}\right) \simeq \frac{i}{2}\,\frac{3\,a^2(\vec{R})\,j_1(c(\vec{R})\,k_F\,r)}{c(\vec{R})\,k_F\,r}\,\vec{r}\times\vec{J}_q(\vec{R})$$

where

$$\begin{aligned} a(\vec{R}) &= \frac{1}{\sqrt{c(\vec{R})}} \\ c(\vec{R}) &= \left(\frac{2\big(1+Q(\vec{R})\big)}{\big(2-Q(\vec{R})\big)}\right)^{1/3} \end{aligned}$$

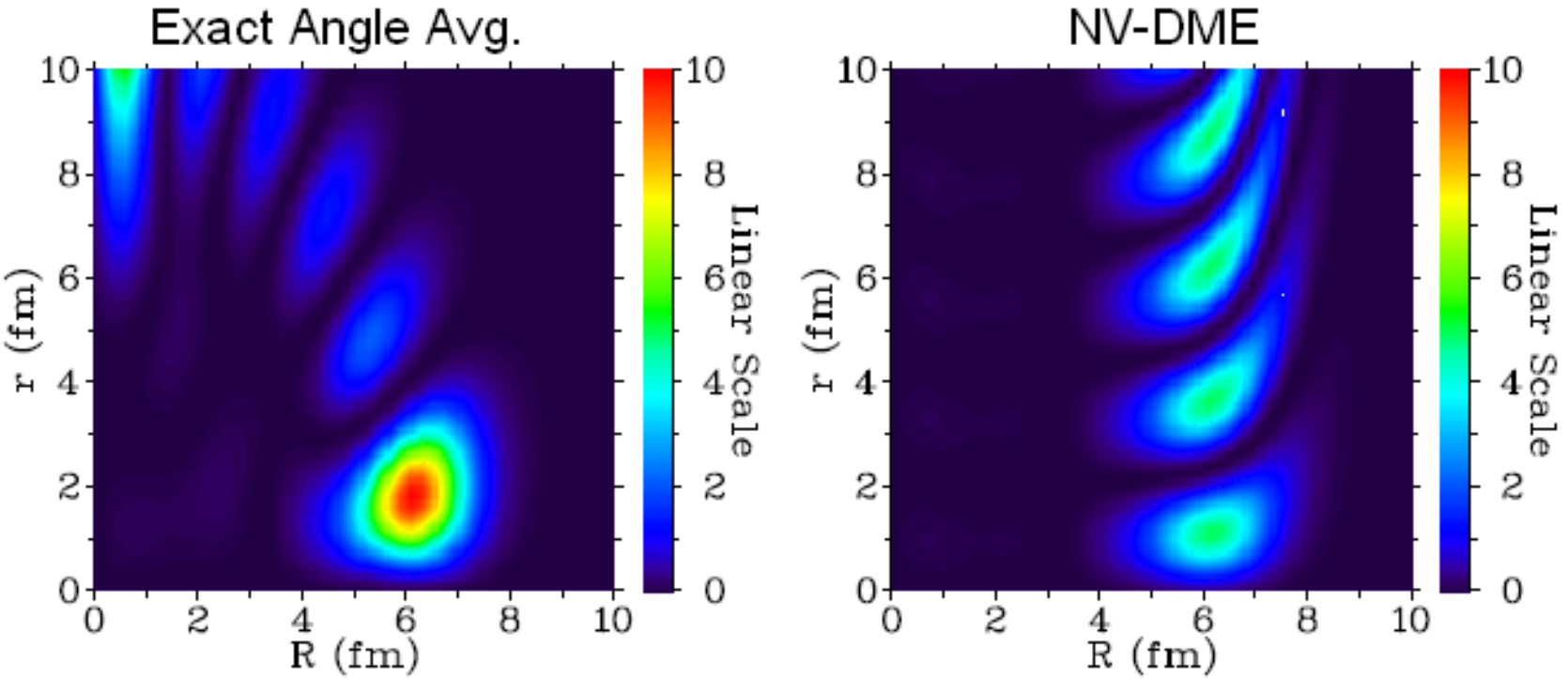
- If spherical Fermi surface at all $\vec{R} \rightarrow Q(\vec{R}) = 0$, $a(\vec{R}) = 1$ and $c(\vec{R}) = 1$

How do the models compare (non/and with self-consistency)?

- Profile reproductions
- Integrated contributions

Result for the vector part of the DM

- Comparison of $\int d\Omega_r \, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{s}_q(\vec{r}_2, \vec{r}_1)$
- Densities from converged calc. of Pb^{208} with Sly4 functional



- NVDME does not work satisfactorly!

Result for the vector part of the DM

- Comparison of $\int d\Omega_r \, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{s}_q(\vec{r}_2, \vec{r}_1)$
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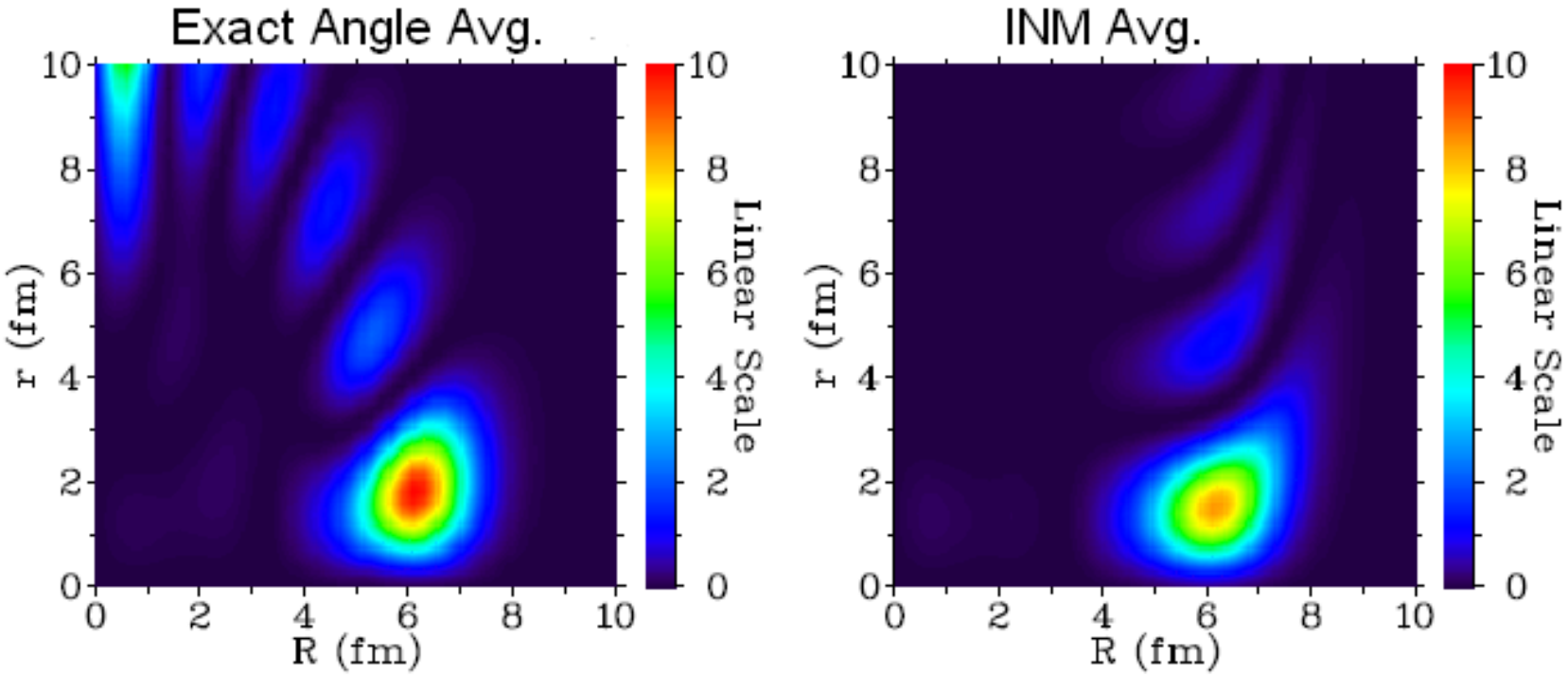
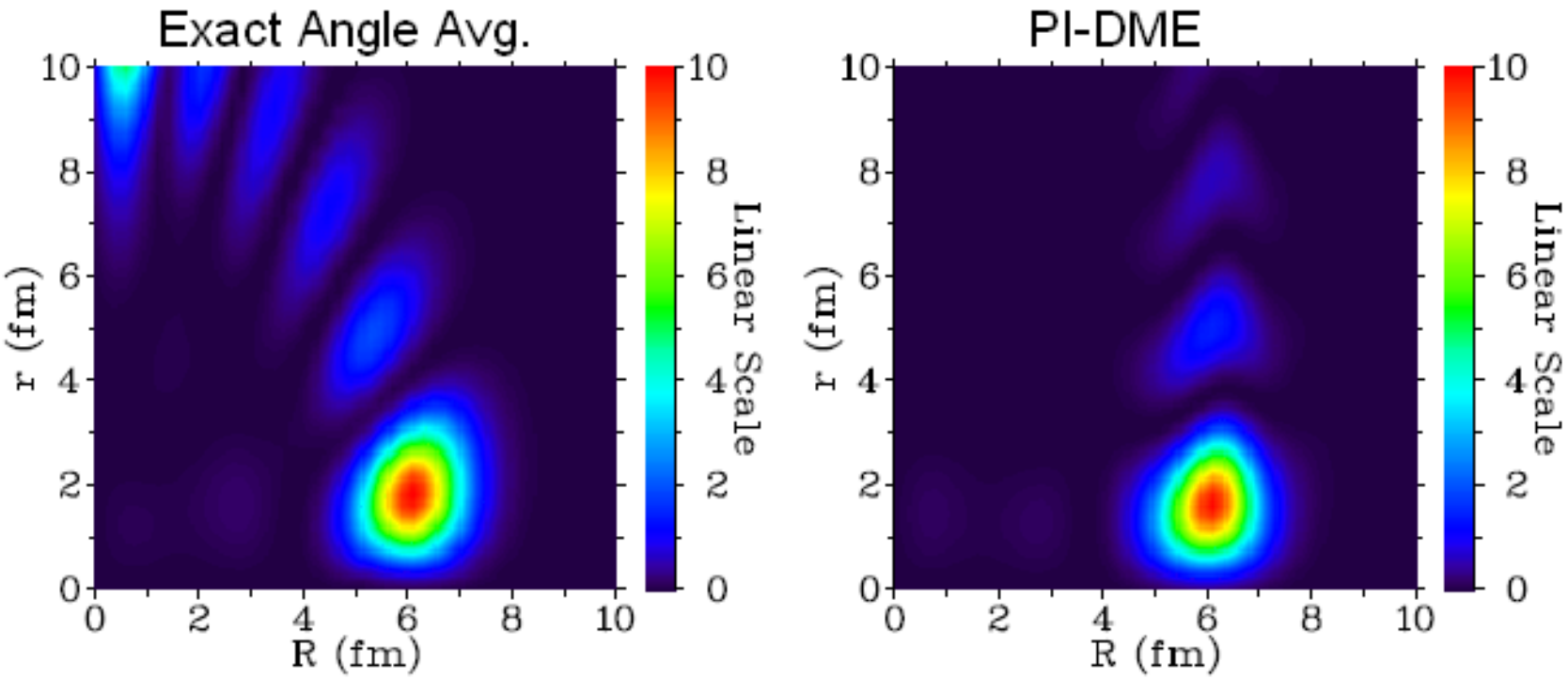


- Significant improvement with INM phase space!

Result for the vector part contd.

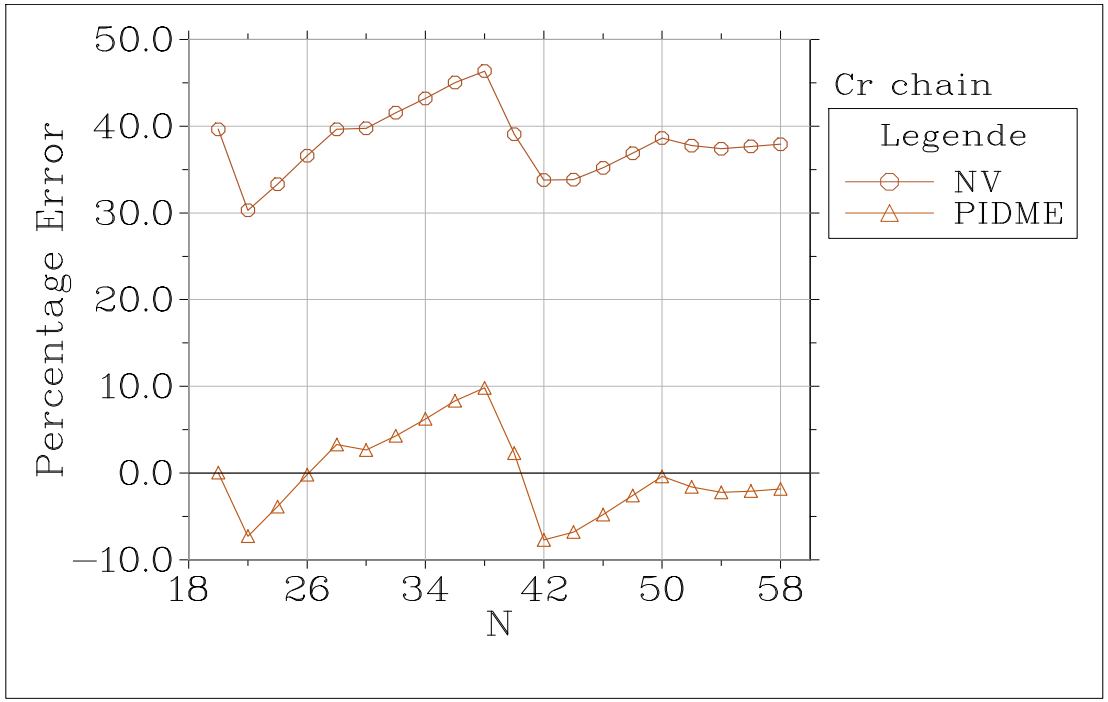
- Comparison of $\int d\Omega_r \, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{s}_q(\vec{r}_2, \vec{r}_1)$
- Densities from converged calc. of Pb^{208} with Sly4 functional



- The most significant/consistent improvement with FFS phase space
- Holds throughout the nuclear mass table

Result for the vector part contd.

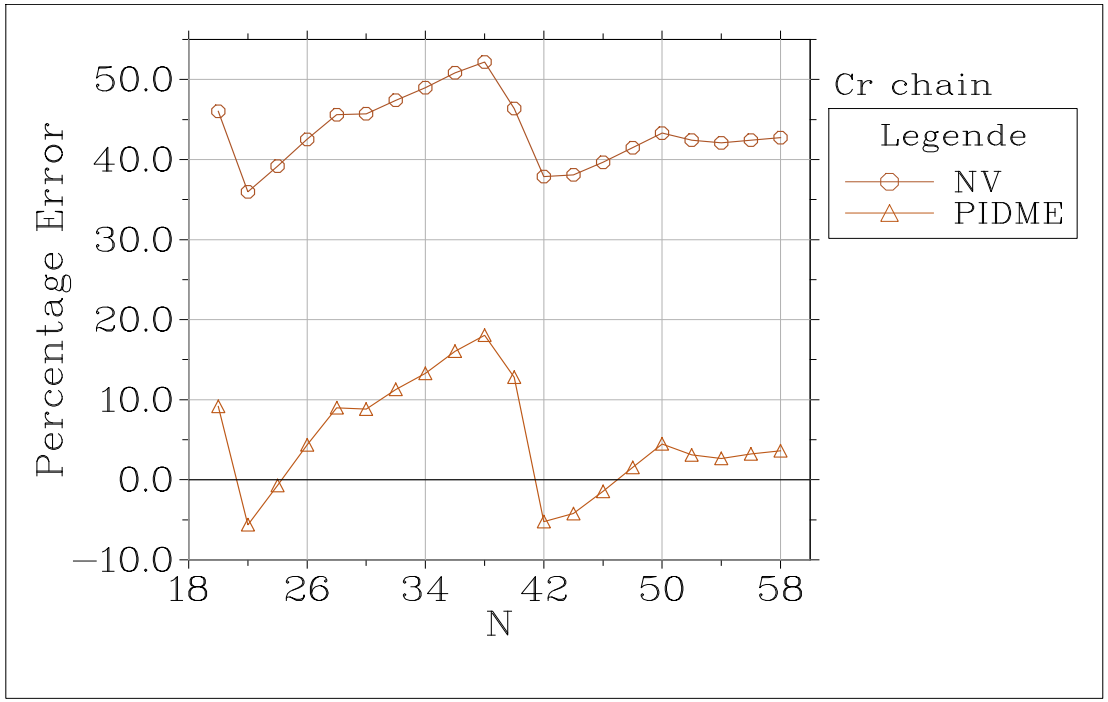
- % error for $\int d\vec{R}\, d\vec{r}\, V(r)\, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{s}_q(\vec{r}_2, \vec{r}_1)$ and its DME
- Gogny interaction
- Cr-chain using Sly4



- Significant improvement regarding the integrated contribution
- Holds throughout the nuclear mass table

Result for the vector part contd.

- % error for $\int d\vec{R}\, d\vec{r}\, V(r)\, \vec{s}_q(\vec{r}_1, \vec{r}_2) \cdot \vec{s}_q(\vec{r}_2, \vec{r}_1)$ and its DME
- Pion-exchange potential
- Cr-chain using Sly4



- Significant improvement regarding the integrated contribution
- Holds throughout the nuclear mass table

Outline

Basic points and hypothesis

- Long-range part of the interaction unmodified by RG evolution
- Add long-range physics using MBPT to existing functionals
- Currently derived lowest order (HF) from NN+NNN at N^2LO

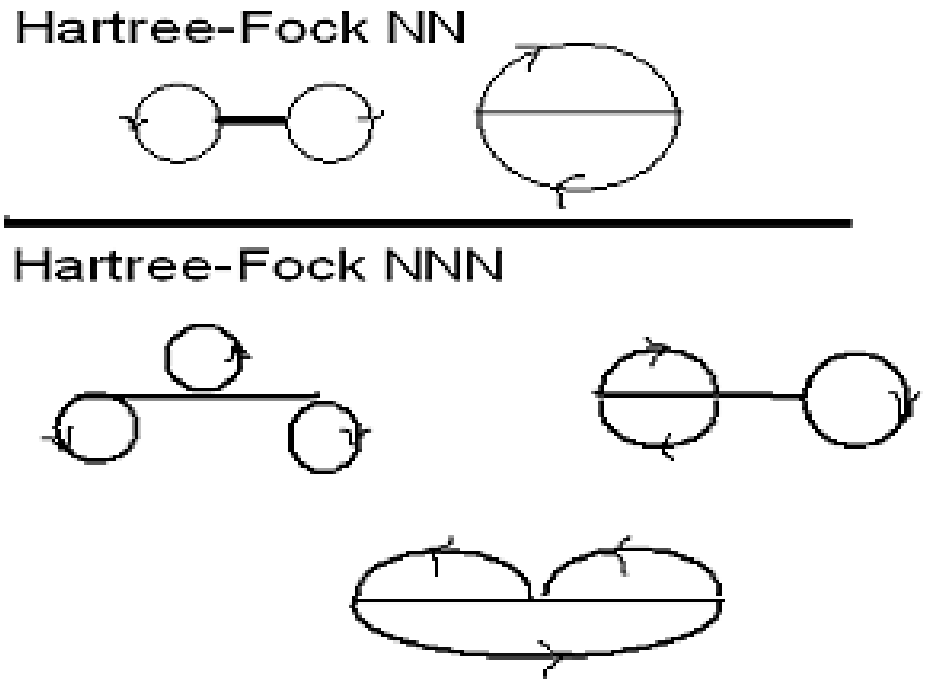


Figure: The set of diagrams currently calculated. Hartree and Fock from NN + NNN.

Basic hypothesis (yet to be tested!)

- Functionals with explicit long-range physics >> current functionals

Application to χ−EFT NN (N^{2}LO)

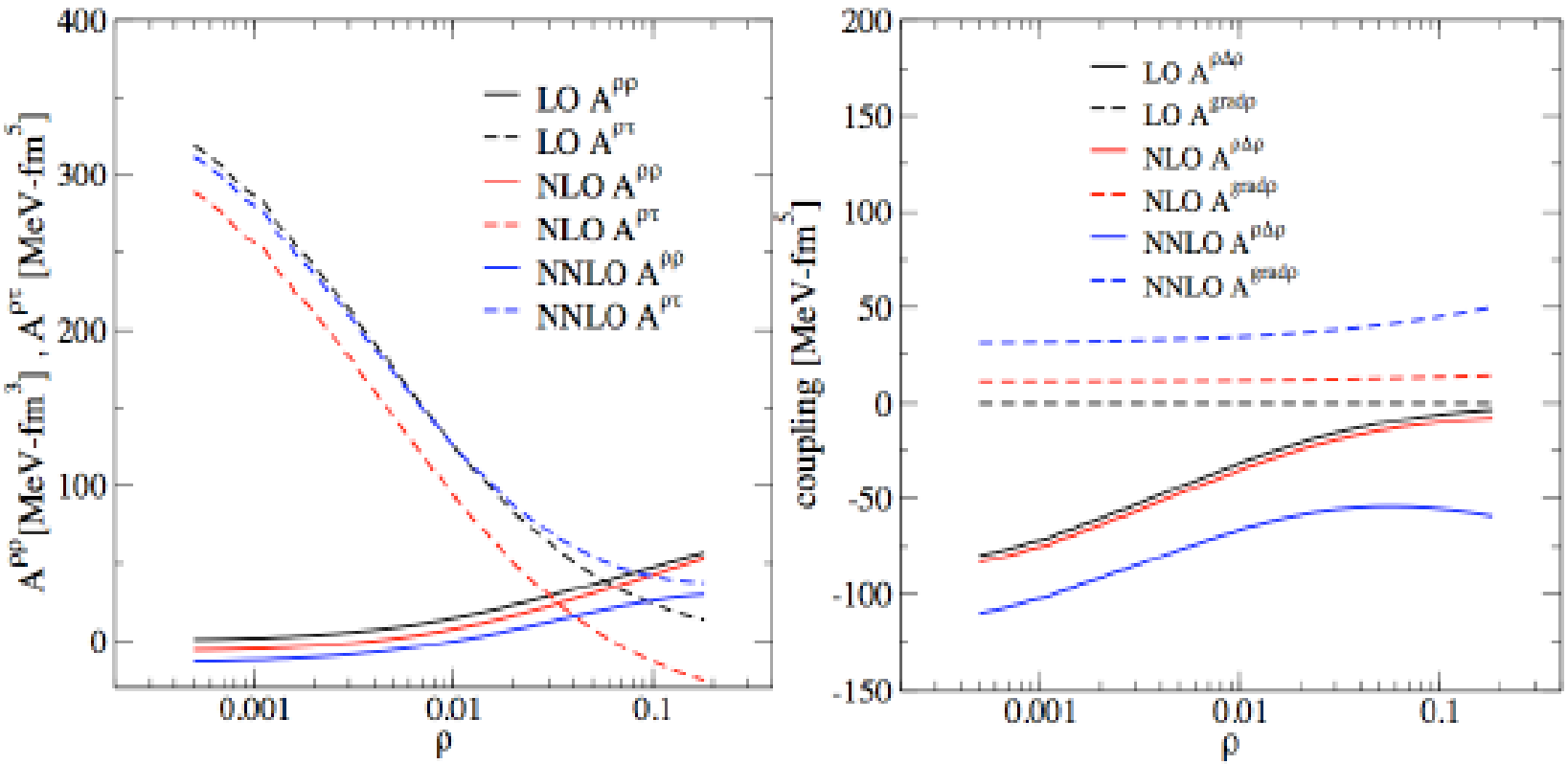
- χ−EFT interactions: $V = V_{\rm cont} + V_\pi$
- EFT NN interaction at N^{2}LO

$$
\begin{aligned}
V_\pi \;=\;& V_C + \tau_1\cdot\tau_2\, W_C + \Big[\, V_S + \tau_1\cdot\tau_2\, W_S \,\Big]\,\vec\sigma_1\cdot\vec\sigma_2 + \Big[\, V_T \\
& + \tau_1\cdot\tau_2\, W_T \,\Big]\,\vec\sigma_1\cdot\vec q\,\vec\sigma_2\cdot\vec q + i\Big[\, V_{LS} + \tau_1\cdot\tau_2\, W_{LS}\,\Big]\,\big(\vec\sigma_1+\vec\sigma_2\big)\cdot\big(\vec q\times\vec k\big)
\end{aligned}
$$

- $\langle\Phi|\, V_\pi\,|\Phi\rangle$ a functional of $\rho_q(\vec r,\vec r\,')$ and $\vec s_q(\vec r,\vec r\,')$
- Direct application of the DME possible (in $\vec p$ space)
- Resulting Skyrme-like functional for TRI

$$
\begin{aligned}
\varepsilon_\pi\big[\rho\big] = \sum_q \int d\vec R\, \Big\{ & A^{\rho\rho}\,\rho_q^2 + A^{\rho\tau}\,\rho_q\,\tau_q + A^{\rho\Delta\rho}\,\rho_q\,\Delta\,\rho_q + A^{\nabla\rho\nabla\rho}\,\vec\nabla\rho_q\cdot\vec\nabla\rho_q \\
& + A^{\nabla\rho J}\,\vec\nabla\rho_q\cdot\vec J_q + A^{J^2}\,\vec J_q\cdot\vec J_q \Big\} \\
+ \sum_{q\neq\bar q} \int d\vec R\, \Big\{ & B^{\rho\rho}\,\rho_q\,\rho_{\bar q} + B^{\rho\tau}\,\rho_q\,\tau_{\bar q} + B^{\rho\Delta\rho}\,\rho_q\,\Delta\,\rho_{\bar q} + B^{\nabla\rho\nabla\rho}\,\vec\nabla\rho_q\cdot\vec\nabla\rho_{\bar q} \\
& + B^{\nabla\rho J}\,\vec\nabla\rho_q\cdot\vec J_{\bar q} + B^{J^2}\,\vec J_q\cdot\vec J_{\bar q} \Big\}
\end{aligned}
$$

Long-range pion exchange contributions to the EDF



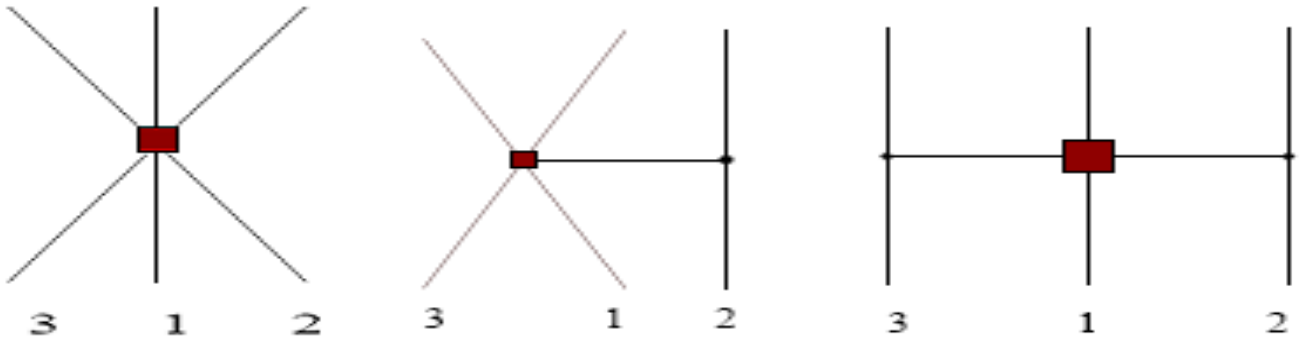
Longest range V <==> Strongest density dependence in EDF

Novel density-dependencies in EDF from 1π and 2π exchanges:

$$\rho^{7/3},\ \rho^{4/3},\ \rho^{2/3},\ \frac{1}{\rho^{2/3}} log(1+c\rho^{2/3}),\ \ldots$$

Application to χ−EFT NNN (N^2LO)

- EFT NNN (N^2LO) contains E, D and C terms



$$\hat{V}_E \equiv E\left(\vec{\tau}_1\cdot\vec{\tau}_2+\vec{\tau}_2\cdot\vec{\tau}_3+\vec{\tau}_3\cdot\vec{\tau}_1\right)$$

$$\hat{V}_D \equiv -\frac{g_A}{4f_\pi^2}\frac{C_D}{f_\pi^2\Lambda_\chi}\left(\frac{\sigma_1\cdot\vec{q}_2\,\sigma_2\cdot\vec{q}_2}{q_2^2+m_\pi^2}\tau_1\cdot\tau_2+\frac{\sigma_2\cdot\vec{q}_3\,\sigma_3\cdot\vec{q}_3}{q_3^2+m_\pi^2}\tau_2\cdot\tau_3 + \frac{\sigma_3\cdot\vec{q}_1\,\sigma_1\cdot\vec{q}_1}{q_1^2+m_\pi^2}\tau_3\cdot\tau_1\right)$$

$$\hat{V}_C \equiv \left(\frac{g_A}{2f_\pi}\right)^2\left(\frac{\sigma_1\cdot\vec{q}_1\,\sigma_2\cdot\vec{q}_2}{(q_1^2+m_\pi^2)(q_2^2+m_\pi^2)}F_{123}^{\alpha\beta}\tau_1^\alpha\tau_2^\beta + \frac{\sigma_2\cdot\vec{q}_2\,\sigma_3\cdot\vec{q}_3}{(q_2^2+m_\pi^2)(q_3^2+m_\pi^2)}F_{231}^{\alpha\beta}\tau_2^\alpha\tau_3^\beta + \frac{\sigma_3\cdot\vec{q}_3\,\sigma_1\cdot\vec{q}_1}{(q_3^2+m_\pi^2)(q_1^2+m_\pi^2)}F_{312}^{\alpha\beta}\tau_3^\alpha\tau_1^\beta\right)$$

Application to $\chi-$EFT NNN (N^{2}LO) contd.

- $\hat{V}_{3N}$ symmetrical w.r.t exchange of two particles
- $\langle\Phi|\, V_{3N}^{HF}\,|\Phi\rangle \equiv \langle\Phi|\, V_{3N}^{HF,dir}\,|\Phi\rangle + \langle\Phi|\, V_{3N}^{HF,1x}\,|\Phi\rangle + \langle\Phi|\, V_{3N}^{HF,2x}\,|\Phi\rangle$
- Using a generalized density matrix: $\varrho^i(\vec{X},\vec{X}') \equiv \varrho(\vec{r}\sigma_i q_i, \vec{r}'\sigma_i q_i)$

$$
\begin{aligned}
\langle V_{3N}^{\mathrm{HF,dir}}\rangle &= \frac{1}{2}\,\mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3 \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, \varrho^1(\vec{X}_1)\,\varrho^2(\vec{X}_2)\,\varrho^3(\vec{X}_3)\,\mathbb{V}_{23} \\
\langle V_{3N}^{\mathrm{HF,1x}}\rangle &= -\,\mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3 \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, \varrho^1(\vec{X}_3,\vec{X}_1)\,\varrho^2(\vec{X}_2)\,\varrho^3(\vec{X}_1,\vec{X}_3)\,\mathbb{V}_{23}\,P_{13}^{\sigma\tau} \\
&\quad -\frac{1}{2}\,\mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3 \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, \varrho^1(\vec{X}_1)\,\varrho^2(\vec{X}_3,\vec{X}_2)\,\varrho^3(\vec{X}_2,\vec{X}_3)\,\mathbb{V}_{23}\,P_{23}^{\sigma\tau} \\
\langle V_{3N}^{\mathrm{HF,2x}}\rangle &= \mathrm{Tr}_1\mathrm{Tr}_2\mathrm{Tr}_3 \int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, \varrho^1(\vec{X}_2,\vec{X}_1)\,\varrho^2(\vec{X}_3,\vec{X}_2)\,\varrho^3(\vec{X}_1,\vec{X}_3) \\
&\quad \mathbb{V}_{23}\,P_{23}^{\sigma\tau}\,P_{12}^{\sigma\tau}\,.
\end{aligned}
$$

Application to $\chi-$EFT NNN (N^{2}LO) contd.

- Calculating $\langle\Phi| V_{3N}^{HF} |\Phi\rangle$ involves tremendous spin-isospin algebra
- Well suited for automation with Mathematica

Three challenges for Mathematica automation

- Automating the spin-isospin algebra
- Rewriting interms of scalar/vector-isoscalar/isovector for DME
- Application of the DME itself

- e.g. Contribution to the exact HF from a piece of the C-term

$$\langle V_{3N}^{\mathrm{HF,CR1,2x}} \rangle = \left(\frac{g_A}{2f_\pi}\right)^2 \frac{c_4}{f_\pi^2}\,\frac{i}{8}\int d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 \int \frac{1}{(2\pi)^6}\, d\vec{q}_2\, d\vec{q}_3\, e^{i\vec{q}_2.(\vec{r}_2-\vec{r}_1)} \times e^{i\vec{q}_3.(\vec{r}_3-\vec{r}_1)}\, \frac{q_2^{\beta_1} q_2^{\beta_2} q_3^{\gamma_1} q_3^{\gamma_2}}{(q_2^2+m_\pi^2)(q_3^2+m_\pi^2)} \Big[\epsilon^{\beta_1\gamma_1\mu_1} \big(-\delta_{\beta_2\gamma_2}\delta_{\mu_2\mu_3} + \delta_{\beta_2\mu_2}\delta_{\gamma_2\mu_3} + \delta_{\beta_2\mu_3}\delta_{\gamma_2\mu_2}\big) \Big(s_1^{\mu_1}(\vec{r}_2,\vec{r}_1) s_1^{\mu_2}(\vec{r}_3,\vec{r}_2) s_0^{\mu_3}(\vec{r}_1,\vec{r}_3) - s_1^{\mu_1}(\vec{r}_2,\vec{r}_1) s_0^{\mu_2}(\vec{r}_3,\vec{r}_2) s_1^{\mu_3}(\vec{r}_1,\vec{r}_3) \Big) + ... \Big]$$

Application to χ−EFT NNN (N^2LO) contd.

Complexities of DME for NNN

- Deal with three non-local/local densities (unlike NN)
- A host of coordinate choices available with differences
- Up to sixth order terms result from the DME
- Exponential increase in the number of terms to simplify

Strategy for coordinate choice

- A coordinate system with known DME expansion
- Avoid expansion of local densities (different length scale than k_F)
- Easier for automation

Not all coordinates are equal!

$$\begin{aligned} \vec{x}_2 &= \vec{r}_2 - \vec{r}_1 \\ \vec{x}_3 &= \vec{r}_3 - \vec{r}_1 \\ \vec{r}_1 &= \vec{r}_1 \end{aligned}$$

Application to $\chi-$EFT NNN (N^2LO) contd.

- Nonlocal densities with three coordinate dependencies appear e.g. $\rho_q(\vec{r}_1+\vec{x}_3,\vec{r}_1+\vec{x}_2)$, $\vec{s}_q(\vec{r}_1+\vec{x}_3,\vec{r}_1+\vec{x}_2)$
- A generic ansatz for the DME of these densities e.g.

$$\begin{aligned}\vec{s}_{0/1}(\vec{r}_1+\vec{x}_3,\vec{r}_1+\vec{x}_2) \quad \simeq \quad & i\Pi^{\vec{s}}_{1,fr}(k,x_2,x_3)\left(1+a_2(\hat{x}_2\cdot\hat{x}_3)^2+a_4(\hat{x}_2\cdot\hat{x}_3)^4\right) \\ & (\vec{x}_3-\vec{x}_2)\otimes\left[\vec{J}_{0/1}(\vec{r}_1)+\frac{1}{2}(\vec{x}_2+\vec{x}_3)\cdot\vec{\nabla}\vec{J}_{0/1}(\vec{r}_1)\right. \\ & \left.+\frac{1}{8}\left((\vec{x}_2+\vec{x}_3)\cdot\vec{\nabla}\right)^2\vec{J}_{0/1}(\vec{r}_1)\right]\end{aligned}$$

- $\Pi-$DME + Taylor series to fix the various functions of this ansatz
- The most important bottleneck to the accuracy of the whole method

Sample EDF from NNN for TRI (N^2LO)

- Even for TRI, a complex/rich function with analytical couplings e.g.

$$
\begin{aligned}
\mathcal{E}^D \quad = \quad & \int d\vec{r} \Big\{ \mathcal{C}_1^{\rho_0^3}\, \rho_0^3(\vec{r}) + \mathcal{C}_1^{\rho_0\rho_1^2}\, \rho_0(\vec{r})\, \rho_1^2(\vec{r}) + \mathcal{C}_1^{\rho_0^2\tau_0}\, \rho_0^2(\vec{r})\, \tau_0(\vec{r}) \\
& + \mathcal{C}_1^{\rho_1^2\tau_0}\, \rho_1^2(\vec{r})\, \tau_0(\vec{r}) + \mathcal{C}_1^{\rho_0\rho_1\tau_1}\, \rho_0(\vec{r})\, \rho_1(\vec{r})\, \tau_1(\vec{r}) \\
& + \mathcal{C}_1^{\rho_1 J_0 J_1}\, \rho_1(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \vec{J}_1(\vec{r}) + \mathcal{C}_1^{\rho_0 J_1^2}\, \rho_0(\vec{r})\, \vec{J}_1(\vec{r}) \cdot \vec{J}_1(\vec{r}) \\
& + \mathcal{C}_1^{\rho_0 J_0 \Delta J_0}\, \rho_0(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \Delta\vec{J}_0(\vec{r}) + \mathcal{C}_1^{\rho_1 J_1 \Delta J_0}\, \rho_1(\vec{r})\, \vec{J}_1(\vec{r}) \cdot \Delta\vec{J}_0(\vec{r}) \\
& + \mathcal{C}_1^{\rho_0 \nabla J_1 \nabla J_1}\, \rho_0(\vec{r}) \left[\vec{\nabla} \cdot \vec{J}_1(\vec{r})\right]^2 + \mathcal{C}_1^{\rho_1 J_0 \Delta J_1}\, \rho_1(\vec{r})\, \vec{J}_0(\vec{r}) \cdot \Delta\vec{J}_1(\vec{r}) \\
& + \ldots \Big\}
\end{aligned}
$$

- Density dependencies from both the three-body and long-range effects

Application to $\chi-$EFT NNN (N^2LO) contd.

A few propaganda statements on the Mathematica code

- Modular Mathematica code
- DME ansatz can be improved independently (accuracy only on DME)
- Complete automation starting from the exact to the DME
- All the resulting terms (up to sixth order) can be accessed
- Easily extensible to both higher order and body $\chi-$EFT interactions
- Makes heavy use of Mathematica's rule processing
  (if anybody is interested!)

Outline

First round implementation-TRI systems

- Constrain form along the standard Skyrme Functional
- Motivated by truncation
  - Second order in derivatives
  - Using k_F e.g. $\rho, \vec{J}, \tau \rightarrow$ third, fourth and fifth orders

$$
\begin{aligned}
\mathcal{H}(\vec{r}) &= \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\vec{r}) + \mathcal{H}_1(\vec{r}), \\
\mathcal{H}_t(\vec{r}) &= \mathcal{G}_t^{\rho\rho}\rho_t^2 + \mathcal{G}_t^{\rho\tau}\rho_t\tau_t + \mathcal{G}_t^{J^2}J_t^2 \\
&\quad + \mathcal{G}_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + \mathcal{G}_t^{\nabla\rho\nabla\rho}\left(\nabla\rho_t\right)^2 + \mathcal{G}_t^{\rho\nabla J}\rho_t\vec{\nabla}\cdot J_t + \mathcal{G}_t^{J\nabla\rho}J_t\cdot\nabla\rho_t
\end{aligned}
$$

where $t = 0, 1$.

- All DME-modified couplings - two terms

$$\mathcal{G}^{\varsigma\varsigma}{}_t = \mathcal{C}^{\varsigma\varsigma}{}_t + g_t^{\varsigma\varsigma}$$

- $g_t^{\varsigma\varsigma}$ analytical - completely fixed by the interaction + DME

Absorb remaining physics with $\mathcal{C}^{\varsigma\varsigma}{}_t$

- Higher order Correlations
- Short-range physics

Example-couplings from $\chi-$EFT NN at LO

- One-pion exchange - the only finite range at LO

$$W_T^{(0)} = -\left(\frac{g_A}{2f_\pi}\right)^2 \frac{1}{q^2+m_\pi^2}$$

- DME length scale set with isoscalar LDA approximation to the Fermi-Momentum

$$K_F(\vec{r}) = \left(\frac{3\pi^2}{2}\rho_0(\vec{r})\right)^{1/3}$$

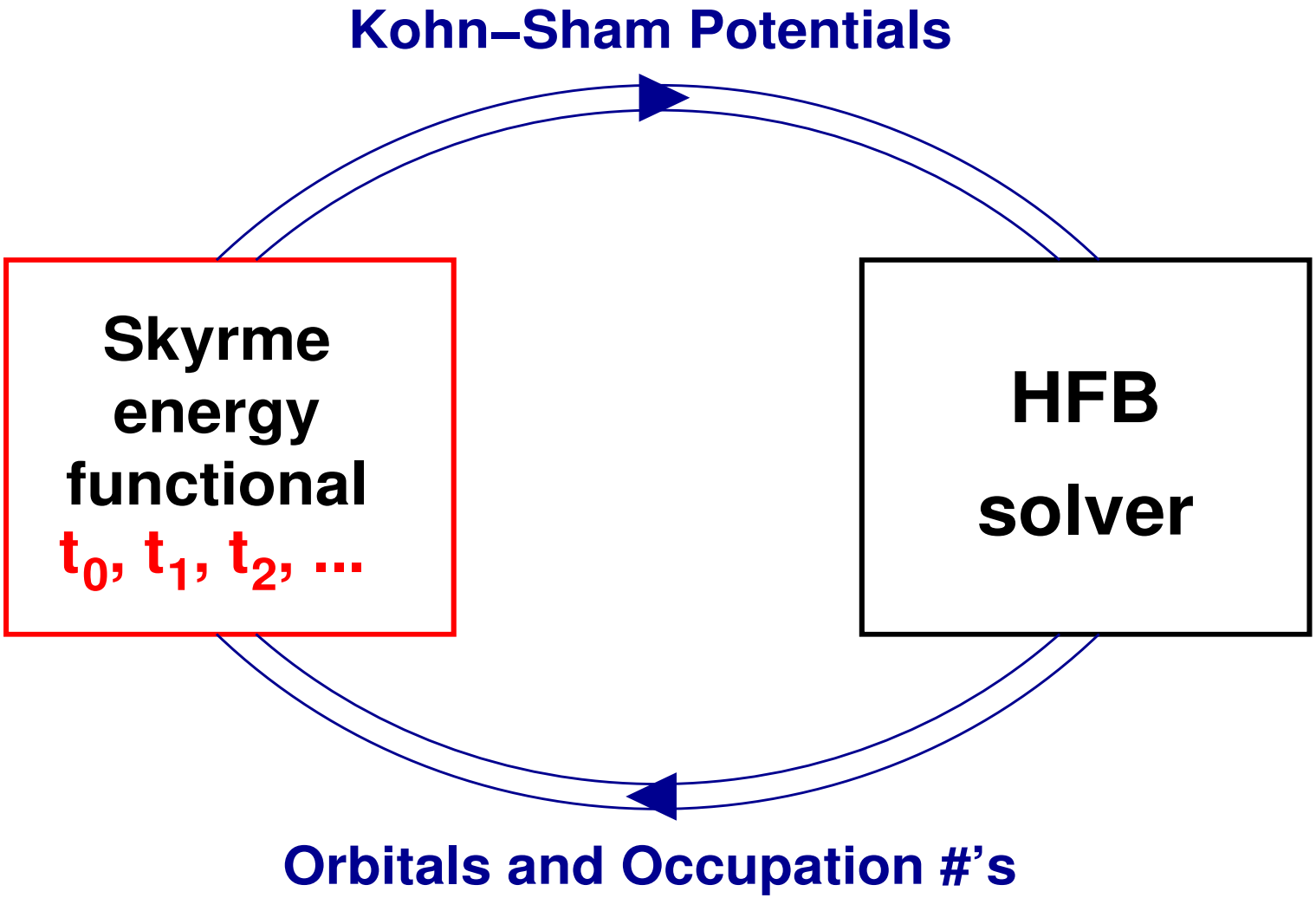
- The non-zero DME-EDF couplings at LO ($u \equiv k_F/m_\pi$)

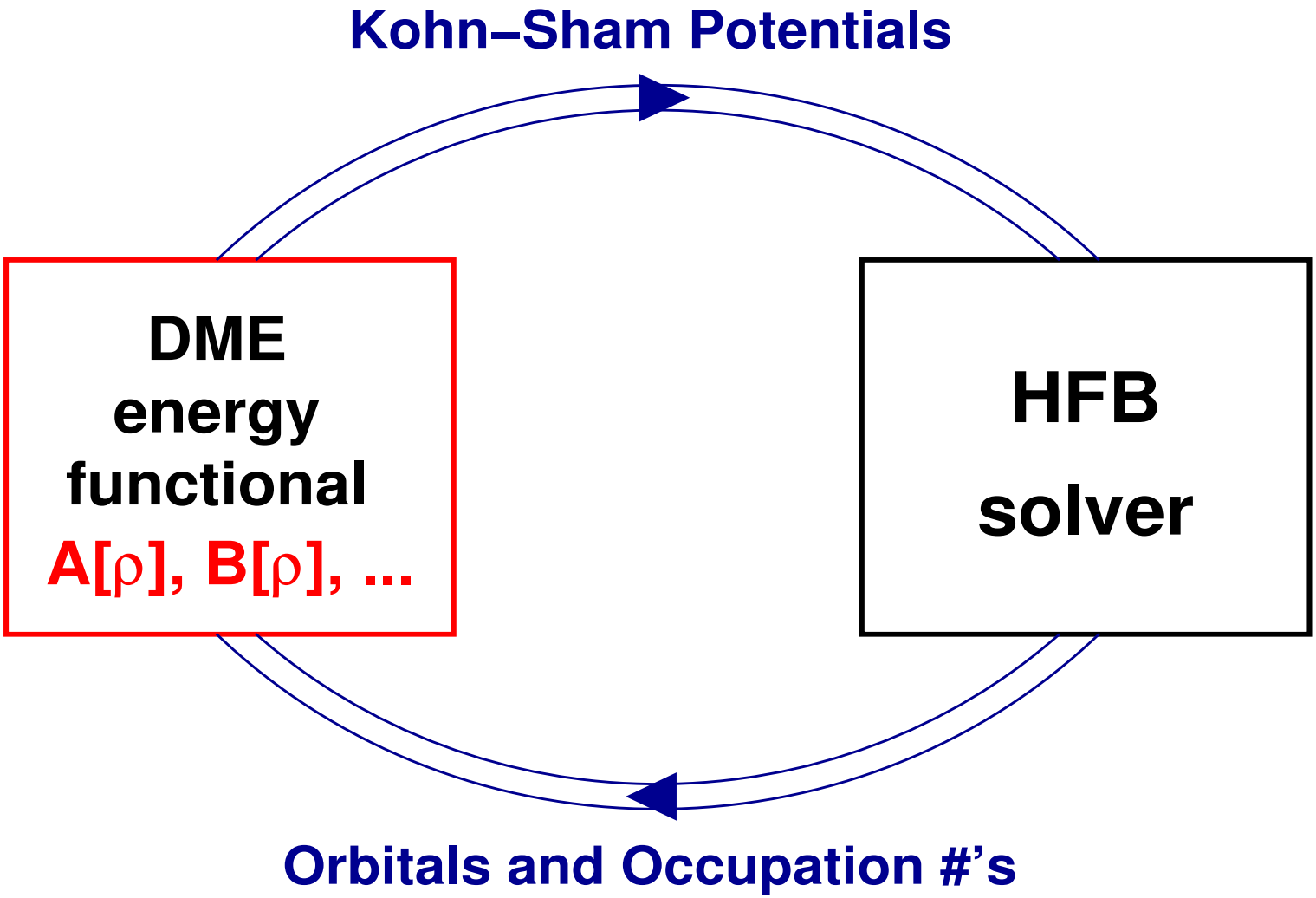
$$\begin{aligned}
A_{(0)}^{\rho\rho} &= -\frac{g_A^2}{256 f_\pi^2 u^6}\left\{\left(-21+498u^2+64u^4-16u^6\right)-12u\left(35+4u^2\right)\arctan(2u)\right. \\
&\quad \left.+\frac{3}{4u^2}\left(7+16u^2(8-9u^2)\right)\log(1+4u^2)\right\} \\
B_{(0)}^{\rho\rho} &= 2A_{(0)}^{\rho\rho} \\
A_{(0)}^{\rho\Delta\rho} &= -\frac{35 g_A^2}{3072 f_\pi^2 m_\pi^2 u^8}\left\{\left(-3+72u^2+4u^4\right)-60u\arctan(2u)\right. \\
&\quad \left.+\frac{1}{4u^2}\left(3+54u^2-72u^4\right)\log(1+4u^2)\right\}
\end{aligned}$$

Example-couplings contd.

$$
\begin{aligned}
A^{\rho\tau}_{(0)} &= -4A^{\rho\Delta\rho}_{(0)} \\
B^{\rho\tau}_{(0)} &= 2A^{\rho\tau}_{(0)} \\
A^{J^2}_{(0)} &= \frac{g_A^2}{48 f_\pi^2 m_\pi^2}\left\{\frac{5+12u^2}{(1+4u^2)^2}+\frac{4}{u^2}\log(1+4u^2)\right\} \\
B^{J^2}_{(0)} &= 2A^{J^2}_{(0)}
\end{aligned}
$$

- No new isovector density dependence from rearrangement terms
- For NN at N^{2}LO, spin-orbit as contact term
- Long-range spin-orbit from two-pion exchange (of NNN)


Kohn–Sham Potentials
Skyrme energy functional
$t_0, t_1, t_2, \ldots$
HFB solver
Orbitals and Occupation #'s


Kohn–Sham Potentials
DME
energy
functional
A[ρ], B[ρ], ...
HFB
solver
Orbitals and Occupation #'s

Outline

Ongoing/Outlook/conclusion

Ready

- A DME for both scalar and vector (DM) with comparable accuracy
- EDF from HF of NN + NNN (at N^2LO)

Ongoing and on the table

- Complete self-consistent test of the DME using local $\chi-$interactions
- Application of the DME to Bogoluibov/pairing contribution
- DME for higher order diagrams, specifically, second order
- Analysis of the couplings

Conclusion

- DME essential for the explicit addition of long-range physics
- Resulting functional the same computational cost as Skyrme
- Adding more diagrams for ever closer to fully microscopic functional
- A long way to go before deriving the functional (if at all!)
- Systematic investigation of DME-enriched functionals required