Pseudo-potential-based Skyrme EDF kernel

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Outline

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General EDF method : Basic ingredients

Key object : the off-diagonal energy kernel

$$E[g',g] \equiv E[\langle\Phi(g')|;|\Phi(g)\rangle] \equiv E[\rho_{ij}^{g'g}, \kappa_{ij}^{g'g}, \kappa_{ij}^{gg'\,*}]$$

which is a functional of one-body *transition* density matrices

$$\rho_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j^\dagger a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle} \quad ; \quad \kappa_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle}$$

- $\{a_i^\dagger\}$ = arbitrary single-particle basis
- $|\Phi(g)\rangle$ = Bogoliubov product state with collective label g

Ex: purely local Skyrme bilinear kernel without isospin and pairing

$$E^{\text{ex}}[g',g] \equiv \int d\vec{r}\,\left\{C^{\rho\rho}\rho^{g'g}(\vec{r})\rho^{g'g}(\vec{r}) + C^{ss}\vec{s}^{g'g}(\vec{r})\cdot\vec{s}^{g'g}(\vec{r})\right\}$$

- $\{\rho^{g'g}(\vec{r}),\ \vec{s}^{g'g}(\vec{r})\}$ = set of one-body *local* transition densities
- $C^{\rho\rho}$ and C^{ss} are the free parameters to adjust phenomenologically

Particular case : pseudo-potential-based EDF

Key object : the off-diagonal energy kernel

$$E_H[g',g]\,\langle\Phi(g')|\Phi(g)\rangle \;\equiv\; \langle\Phi(g')|H_{\text{pseudo}}(\{t_i\})|\Phi(g)\rangle \overset{\text{GWT}}{=} E_H[\rho_{ij}^{g'g},\kappa_{ij}^{g'g},\kappa_{ij}^{gg'\,*}]$$

which is a functional of one-body *transition* density matrices

$$\rho_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j^\dagger a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle} \quad ; \quad \kappa_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle}$$

- $\{a_i^\dagger\}$ = arbitrary single-particle basis
- $|\Phi(g)\rangle$ = Bogoliubov product state with collective label g

Ex: purely local Skyrme bilinear kernel derived from two-body pseudo-potential

- $H_{\text{pseudo}} = t_0\,\delta(\vec{r}_1-\vec{r}_2)$

$$E_H^{\text{ex}}[g',g] = \int d\vec{r}\,\left\{A^{\rho\rho}\rho^{g'g}(\vec{r})\rho^{g'g}(\vec{r}) + A^{ss}\vec{s}^{\,g'g}(\vec{r})\cdot\vec{s}^{\,g'g}(\vec{r})\right\}$$

- $A^{\rho\rho}$ and A^{ss} are related through a single parameter $t_0 \Rightarrow$ **Pauli principle**

EDF method : density-dependent interaction

Key object : the off-diagonal energy kernel

$$E[g',g]\,\langle\Phi(g')|\Phi(g)\rangle \equiv \langle\Phi(g')|\text{“}H\text{”}(\{t_i\},\rho^{g'g}(\vec{r}))|\Phi(g)\rangle \overset{\text{”GWT”}}{=} E[\rho_{ij}^{g'g},\kappa_{ij}^{g'g},\kappa_{ij}^{gg'\,*}]$$

which is a functional of one-body transition density matrices

$$\rho_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j^\dagger a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle} \quad ; \quad \kappa_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle}$$

- $\{a_i^\dagger\}$ = arbitrary single-particle basis
- $|\Phi(g)\rangle$ = Bogoliubov product state with collective label g

Ex: purely local Skyrme (quasi) bilinear kernel

$$E^{\text{ex}}[g',g] \equiv \int d\vec{r}\,\left\{A^{\rho\rho}\rho^{g'g}(\vec{r})\rho^{g'g}(\vec{r})\rho^{g'g}(\vec{r}) + A^{ss}\rho^{g'g}(\vec{r})\vec{s}^{\,g'g}(\vec{r})\cdot\vec{s}^{\,g'g}(\vec{r})\right\}$$

- Empirical density dependence breaks the **Pauli principle** = **self-interaction**
- EDF method with density-dependent interaction is **not** a pseudo-potential-based EDF

Motivations

General-EDF vs pseudo-potential-based-EDF

- ✘ General-EDF formulation break **Pauli principle** *a priori*
- ✔ Pseudo-potential-based EDF one case free from such problem
  - ➥ The pseudo-potential must not depend on the system
- ✘ Symmetry restoration for general-EDF ⇒ problematic *a priori*
  - ✘ Can design regularization method but non trivial
  - ✔ Pseudo-potential-based-EDF ⇒ free from any problem

Outline

Challenges

Pseudo-potential-based EDF

- ✗ How to get **high-quality EDF parameterizations** in such a restricted formulation?
- ➥ According to previous (limited) attempt, this is not easy
- ➥ Develop rich enough pseudo-potential to provide good phenomenology
- ➥ Develop simple enough pseudo-potential whose fitting remains bearable
- ✗ The analytical derivation of the energy kernel can be tedious

A new Skyrme pseudo-potential

- Two-body Skyrme pseudo-potential **without density dependence (unsufficient)**
- The most general three-body Skyrme pseudo-potential at second order in gradients
- The same pseudo-potential should be used in the normal and pairing channel
- ✗ Present study : normal part of the functional only

Construction of the three-body Skyrme Pseudo-potential

- Pseudo-potential ⇒ compute $E[g,g]$ and $E[g',g]$ strictly follows
- Three-body kernel through Standard Wick Theorem

$$E_{H}^{\rho\rho\rho} = \frac{1}{6} \sum_{ijklmn} \langle ijk|\hat{v}^3_{123}\mathcal{A}_{123}|lmn\rangle \, \rho_{li}\, \rho_{mj}\, \rho_{nk}$$

Antisymmetrizer : $\mathcal{A}_{123} = 1 - P_{12} - P_{13} - P_{23} + P_{12}P_{23} + P_{13}P_{23}$

- Aim : Construct the most general Skyrme three-body pseudo-potential
  - ➥ i.e. identify all three-body operators providing independent EDF terms

Skyrme pseudo-potential ingredients

- $\hat{v}^3_{123} = \hat{v}^3_{\underline{123}} + \hat{v}^3_{\underline{312}} + \hat{v}^3_{\underline{231}}$: develop and derive the energy functional only for $\hat{v}^3_{\underline{123}}$
- Kronecker operators : $\hat{\delta}_{r_i r_j}$ with $i \neq j \in \{1,2,3\}^2$
- Gradients operators : $\hat{\vec{k}}_{ij}$, $\hat{\vec{k}}'_{ij}$ with $i \neq j \in \{1,2,3\}^2$, $\quad \hat{\vec{k}}_{ij} = -\frac{i}{2}(\hat{\vec{\nabla}}_i - \hat{\vec{\nabla}}_j)$
- Exchange operators : P^r_{ij}, P^σ_{ij}, P^τ_{ij} with $i \neq j \in \{1,2,3\}^2$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}'_{kl} \qquad \text{or} \qquad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}'_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}_{kl}$$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^{3}_{123} \; : \quad \hat{\vec{k}}_{12} \cdot \hat{\vec{k}}_{12} + \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}'_{12} \qquad \text{or} \qquad \hat{\vec{k}}_{12} \cdot \hat{\vec{k}}'_{12}$$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^{3}_{\overline{31}2} \;:\quad \hat{\vec{k}}_{13}\cdot\hat{\vec{k}}_{13}+\hat{\vec{k}}'_{13}\cdot\hat{\vec{k}}'_{13} \qquad \text{or} \qquad \hat{\vec{k}}_{13}\cdot\hat{\vec{k}}'_{13}$$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^{3}_{231} \;:\quad \hat{\vec{k}}_{23} \cdot \hat{\vec{k}}_{23} + \hat{\vec{k}}'_{23} \cdot \hat{\vec{k}}'_{23} \qquad \text{or} \qquad \hat{\vec{k}}_{23} \cdot \hat{\vec{k}}'_{23}$$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^{3}_{\overline{12}3} \;:\quad \hat{\vec{k}}_{23} \cdot \hat{\vec{k}}_{13} + \hat{\vec{k}}'_{23} \cdot \hat{\vec{k}}'_{13} \qquad \text{or} \qquad \hat{\vec{k}}_{13} \cdot \hat{\vec{k}}'_{23} + \hat{\vec{k}}'_{13} \cdot \hat{\vec{k}}_{23}$$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^{3}_{\underline{12}3} \; : \quad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}'_{kl} \qquad \text{or} \qquad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}'_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}_{kl}$$

- Function of exchange operators $P^{\{x\}}_{\underline{12}3}$ multiplies each spatial structure listed above

$$P^{\{x_i\}}_{\underline{12}3} = t_i \left[1 + x_i \, P^{\sigma}_{12} \right] \quad ??$$

Construction of the three-body Skyrme Pseudo-potential

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Construction of the three-body Skyrme Pseudo-potential

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  - ➥ $P^{r}_{ij} = \pm 1$ only when applied with gradient terms $\hat{\vec{k}}_{ij}$, $\hat{\vec{k}}'_{ij}$

Construction of the three-body Skyrme Pseudo-potential

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- Function of exchange operators $P^{\{x\}}_{123}$ multiplies each spatial structure listed above

$$P^{\{x_i\}}_{123} = t_i \left[1 + x_i^1 \, P^{\sigma}_{12} + x_i^2 \, (P^{\sigma}_{13} + P^{\sigma}_{23}) + x_i^3 \, P^{\tau}_{12} + \cdots \right]$$

  - ➥ $P^{r}_{ij} = \pm 1$ only when applied with gradient terms $\hat{\vec{k}}_{ij}$, $\hat{\vec{k}}'_{ij}$
  - ➥ Starts with 100 parameters

Construction of the three-body Skyrme Pseudo-potential

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- Function of exchange operators $P^{\{x\}}_{123}$ multiplies each spatial structure listed above

$$P^{\{x_i\}}_{123} = t_i \left[1 + x_i^1 \ P^{\sigma}_{12} + x_i^2 \ (P^{\sigma}_{13} + P^{\sigma}_{23}) + x_i^3 \ P^{\tau}_{12} + \cdots \right]$$

  - $P^r_{ij} = \pm 1$ only when applied with gradient terms $\hat{\vec{k}}_{ij}$, $\hat{\vec{k}}'_{ij}$
  - Starts with 100 parameters
- Derivation of the trilinear EDF : straightforward but cumbersome
  - Development of a formal computation code
  - Identification of correlated terms via SVD

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^3_{123} \;:\quad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}'_{kl} \qquad \text{or} \qquad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}'_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}_{kl}$$

- Function of exchange operators $P^{\{x\}}_{123}$ multiplies each spatial structure listed above

$$P^{\{x_i\}}_{123} = t_i \left[1 + x^1_i \; P^{\sigma}_{12} + x^2_i \; (P^{\sigma}_{13} + P^{\sigma}_{23}) + x^3_i \; P^{\tau}_{12} + \cdots \right]$$

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- Derivation of the trilinear EDF : straightforward but cumbersome
  - ➥ Development of a formal computation code
  - ➥ Identification of correlated terms via SVD
- Final three-body Skyrme pseudo-potential

$$\begin{aligned}
\hat{v}^3_{123} &= u_0 \; \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
&+ \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{12} \right] \left(\hat{\vec{k}}_{12} \cdot \hat{\vec{k}}_{12} + \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
&+ u_2 \left[1 + y_{21} P^{\sigma}_{12} + y_{22} (P^{\sigma}_{13} + P^{\sigma}_{23}) \right] \left(\hat{\vec{k}}_{12} \cdot \hat{\vec{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3}
\end{aligned}$$

Construction of the three-body Skyrme Pseudo-potential

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- Function of exchange operators $P^{\{x\}}_{\underline{123}}$ multiplies each spatial structure listed above

$$P^{\{x_i\}}_{\underline{123}} = t_i \left[1 + x_i^1 \; P^\sigma_{12} + x_i^2 \; (P^\sigma_{13} + P^\sigma_{23}) + x_i^3 \; P^\tau_{12} + \cdots \right]$$

  - ➥ $P^r_{ij} = \pm 1$ only when applied with gradient terms $\hat{\vec{k}}_{ij}$, $\hat{\vec{k}}'_{ij}$
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- Derivation of the trilinear EDF : straightforward but cumbersome
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- Final three-body Skyrme pseudo-potential

$$\begin{aligned}
\hat{v}^3_{\underline{312}} &= u_0 \; \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
&+ \frac{u_1}{2} \left[1 + y_1 P^\sigma_{31} \right] \left(\hat{\vec{k}}_{31} \cdot \hat{\vec{k}}_{31} + \hat{\vec{k}}'_{31} \cdot \hat{\vec{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
&+ u_2 \left[1 + y_{21} P^\sigma_{31} + y_{22} (P^\sigma_{32} + P^\sigma_{12}) \right] \left(\hat{\vec{k}}_{31} \cdot \hat{\vec{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2}
\end{aligned}$$

Construction of the three-body Skyrme Pseudo-potential

- Hermiticity implies that gradient operators combine according to

$$\hat{v}^3_{123} \quad : \quad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}'_{kl} \qquad \text{or} \qquad \hat{\vec{k}}_{ij} \cdot \hat{\vec{k}}'_{kl} + \hat{\vec{k}}'_{ij} \cdot \hat{\vec{k}}_{kl}$$

- Function of exchange operators $P^{\{x\}}_{123}$ multiplies each spatial structure listed above

$$P^{\{x_i\}}_{123} = t_i \left[1 + x^1_i \; P^\sigma_{12} + x^2_i \; (P^\sigma_{13} + P^\sigma_{23}) + x^3_i \; P^\tau_{12} + \cdots \right]$$

  - ➥ $P^r_{ij} = \pm 1$ only when applied with gradient terms $\hat{\vec{k}}_{ij}$, $\hat{\vec{k}}'_{ij}$
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- Derivation of the trilinear EDF : straightforward but cumbersome
  - ➥ Development of a formal computation code
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- Final three-body Skyrme pseudo-potential

$$\begin{aligned}
\hat{v}^3_{231} &= u_0 \; \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\
&+ \frac{u_1}{2} \left[1 + y_1 P^\sigma_{23} \right] \left(\hat{\vec{k}}_{23} \cdot \hat{\vec{k}}_{23} + \hat{\vec{k}}'_{23} \cdot \hat{\vec{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\
&+ u_2 \left[1 + y_{21} P^\sigma_{23} + y_{22} (P^\sigma_{21} + P^\sigma_{31}) \right] \left(\hat{\vec{k}}_{23} \cdot \hat{\vec{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}
\end{aligned}$$

Trilinear part of the EDF

Functional of the one-body local densities

$$\mathcal{E}^{\rho\rho\rho}_{\text{even}} = \sum_{t=0,1} \left\{ B^{\rho}_{t} \rho_0 \rho_t^2 + B^{\tau}_{t} \rho_0 \rho_t \tau_t + B^{\nabla\rho}_{t} \rho_0 \vec{\nabla}\rho_t \cdot \vec{\nabla}\rho_t + \sum_{\mu\nu} B^{J}_{t} \rho_0 J_{t,\mu\nu} J_{t,\mu\nu} \right\}$$
$$+ B^{\tau}_{10} \rho_1 \rho_1 \tau_0 + B^{\nabla\rho}_{10} \rho_1 \vec{\nabla}\rho_1 \cdot \vec{\nabla}\rho_0 + \sum_{\mu\nu} B^{J}_{10} \rho_1 J_{1,\mu\nu} J_{0,\mu\nu}$$

$$\mathcal{E}^{\rho\rho\rho}_{\text{odd}} = \sum_{t=0,1} \left\{ B^{s}_{t} \rho_0 \vec{s}_t^{\,2} + B^{T}_{t} \rho_0 \vec{s}_t \cdot \vec{T}_t + \sum_{\mu\nu} B^{\nabla s}_{t} \rho_0 \nabla_\mu s_{t,\nu} \nabla_\mu s_{t,\nu} + B^{j}_{t} \rho_0 \vec{j}_t \cdot \vec{j}_t \right.$$
$$+ B^{T}_{t\bar{t}} \rho_1 \vec{s}_t \cdot \vec{T}_{\bar{t}} + B^{\tau s}_{t} \vec{s}_0 \vec{s}_t \tau_t + \sum_{\mu\nu} \left[B^{\nabla\rho s}_{t} s_{0,\nu} \nabla_\mu \rho_t \nabla_\mu s_{t,\nu} \right.$$
$$\left. + B^{\nabla\rho s}_{t\bar{t}} s_{1,\nu} \nabla_\mu \rho_t \nabla_\mu s_{\bar{t},\nu} + B^{Js}_{t} s_{0,\nu} j_{t,\mu} J_{t,\mu\nu} + B^{Js}_{t\bar{t}} s_{1,\nu} j_{t,\mu} J_{\bar{t},\mu\nu} \right]$$
$$\left. + \sum_{\mu\nu\lambda k} \epsilon_{\nu\lambda k} \left[B^{\nabla sJ}_{t} s_{0,k} \nabla_\mu s_{t,\nu} J_{t,\mu\lambda} + B^{\nabla sJ}_{t\bar{t}} s_{1,k} \nabla_\mu s_{t,\nu} J_{\bar{t},\mu\lambda} \right] \right\}$$
$$+ B^{s}_{10} \rho_1 \vec{s}_1 \cdot \vec{s}_0 + B^{\nabla s}_{10} \rho_1 \nabla_\mu s_{1,\nu} \nabla_\mu s_{0,\nu} + B^{j}_{10} \rho_1 \vec{j}_1 \cdot \vec{j}_0 + B^{\tau s}_{10} \vec{s}_1 \vec{s}_1 \tau_0$$

Trilinear part of the EDF

Functional of the one-body local densities

$$\mathcal{E}^{\rho\rho\rho}_{\text{even}} = \sum_{t=0,1} \Big\{ B^{\rho}_{t} \rho_0 \rho_t^2 + B^{\tau}_{t} \rho_0 \rho_t \tau_t + B^{\nabla\rho}_{t} \rho_0 \vec{\nabla}\rho_t \cdot \vec{\nabla}\rho_t + \sum_{\mu\nu} B^{J}_{t} \rho_0 J_{t,\mu\nu} J_{t,\mu\nu} \Big\}$$
$$+ B^{\tau}_{10} \rho_1 \rho_1 \tau_0 + B^{\nabla\rho}_{10} \rho_1 \vec{\nabla}\rho_1 \cdot \vec{\nabla}\rho_0 + \sum_{\mu\nu} B^{J}_{10} \rho_1 J_{1,\mu\nu} J_{0,\mu\nu}$$

$$\mathcal{E}^{\rho\rho\rho}_{\text{odd}} = \sum_{t=0,1} \Big\{ B^{s}_{t} \rho_0 \vec{s}_t^{\,2} + B^{T}_{t} \rho_0 \vec{s}_t \cdot \vec{T}_t + \sum_{\mu\nu} B^{\nabla s}_{t} \rho_0 \nabla_\mu s_{t,\nu} \nabla_\mu s_{t,\nu} + B^{j}_{t} \rho_0 \vec{j}_t \cdot \vec{j}_t$$
$$+ B^{T}_{t\bar{t}} \rho_1 \vec{s}_t \cdot \vec{T}_{\bar{t}} + B^{\tau s}_{t} \vec{s}_0 \vec{s}_t \tau_t + \sum_{\mu\nu} \Big[B^{\nabla\rho s}_{t} s_{0,\nu} \nabla_\mu \rho_t \nabla_\mu s_{t,\nu}$$
$$+ B^{\nabla\rho s}_{t\bar{t}} s_{1,\nu} \nabla_\mu \rho_t \nabla_\mu s_{\bar{t},\nu} + B^{Js}_{t} s_{0,\nu} j_{t,\mu} J_{t,\mu\nu} + B^{Js}_{t\bar{t}} s_{1,\nu} j_{t,\mu} J_{\bar{t},\mu\nu} \Big]$$
$$+ \sum_{\mu\nu\lambda k} \epsilon_{\nu\lambda k} \Big[B^{\nabla sJ}_{t} s_{0,k} \nabla_\mu s_{t,\nu} J_{t,\mu\lambda} + B^{\nabla sJ}_{t\bar{t}} s_{1,k} \nabla_\mu s_{t,\nu} J_{\bar{t},\mu\lambda} \Big] \Big\}$$
$$+ B^{s}_{10} \rho_1 \vec{s}_1 \cdot \vec{s}_0 + B^{\nabla s}_{10} \rho_1 \nabla_\mu s_{1,\nu} \nabla_\mu s_{0,\nu} + B^{j}_{10} \rho_1 \vec{j}_1 \cdot \vec{j}_0 + B^{\tau s}_{10} \vec{s}_1 \vec{s}_1 \tau_0$$

Trilinear part of the EDF

Time-even functional coefficients

		u_0	u_1	$u_1 y_1$	u_2	$u_2 y_{21}$	$u_2 y_{22}$
B_0^{ρ}	$=$	$+\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
B_1^{ρ}	$=$	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
B_0^{τ}	$=$	$+0$	$+\frac{3}{32}$	$+0$	$+\frac{15}{64}$	$+\frac{3}{16}$	$+\frac{3}{32}$
B_{10}^{τ}	$=$	$+0$	$-\frac{1}{32}$	$+\frac{1}{32}$	$-\frac{5}{64}$	$-\frac{1}{16}$	$-\frac{7}{32}$
B_1^{τ}	$=$	$+0$	$-\frac{1}{16}$	$-\frac{1}{32}$	$+\frac{1}{32}$	$+\frac{1}{16}$	$-\frac{1}{16}$
$B_0^{\nabla\rho}$	$=$	$+0$	$+\frac{15}{128}$	$+0$	$-\frac{15}{256}$	$-\frac{3}{64}$	$-\frac{3}{128}$
$B_{10}^{\nabla\rho}$	$=$	$+0$	$-\frac{5}{64}$	$+\frac{1}{32}$	$+\frac{5}{128}$	$+\frac{1}{32}$	$+\frac{7}{64}$
$B_1^{\nabla\rho}$	$=$	$+0$	$-\frac{5}{128}$	$-\frac{1}{32}$	$-\frac{7}{256}$	$-\frac{1}{32}$	$-\frac{5}{128}$
B_0^{J}	$=$	$+0$	$+\frac{1}{32}$	$-\frac{1}{16}$	$-\frac{7}{64}$	$-\frac{1}{8}$	$+\frac{1}{32}$
B_{10}^{J}	$=$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{1}{32}$	$+0$	$+\frac{3}{16}$
B_1^{J}	$=$	$+0$	$+\frac{1}{32}$	$+0$	$-\frac{7}{64}$	$-\frac{1}{16}$	$-\frac{1}{32}$

Conclusions

Three-body pseudo-potential in the literature

- Time-even and time-odd EDF from u_0 [Beiner *et al.* NPA, **238**, (1975), 29]
- Time-even EDF from u_0, u_1 [Waroquier *et al.* PRC, **19**, (1979), 1983]
- Time-even EDF from u_0, u_1, y_1, u_2, y_{21} [Liu *et al.* NPA, **534**, (1991), 1] (incorrect)

➥ Performing MR-EDF, i.e. using $E[g', g]$, necessitates time-odd part

Complete energy functional

- The **pairing functional** must be computed from the same pseudo-potential
  - ➥ Under progress

➪ Spin-orbit and tensor three-body pseudo-potential in development

Outline

1. Introduction
2. Three-body Skyrme pseudo-potential
   - Construction of the pseudo-potential
   - Trilinear part of the EDF
3. Fitting protocol
   - Symmetric Nuclear Matter
   - SLyX Fitting protocol
4. Results
   - SNM properties
   - Landau parameters
   - Binding energies and radii systematics
5. Conclusions

Motivation

- Aim :
  1. Overcome known difficulty for pure $t_0\ \hat{\delta}_{\vec{r}_1\vec{r}_2}\ \hat{\delta}_{\vec{r}_2\vec{r}_3}$
  2. Get a pseudo-potential parameterization as good as **SLy4**

  ➥ Similar fitting procedure used

- How many parameters?

  ➥ Usual bilinear functional (density-dependent interaction) : 7+2 parameters

  ➥ Two-body plus three-body pseudo-potential : (9-2)+6 parameters = 4 more

Fitting protocol : Symmetric Nuclear Matter

SNM properties : **gradient-less** three-body pseudo-potential

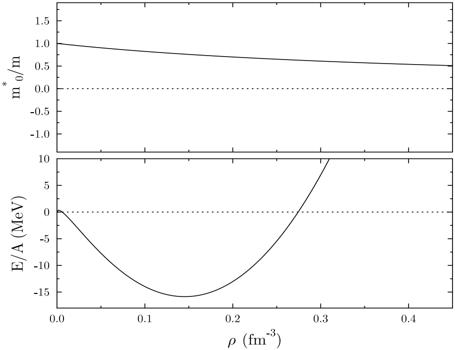
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\, \rho_0^{2/3} + \frac{3}{8} t_0\, \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{16} u_0\, \rho_0^2$$

$$K_\infty = -\frac{6}{5}\frac{\hbar^2}{2m} c_s\, \rho_{\text{sat}}^{2/3} + \frac{3}{8} c_s \Theta_s \rho_{\text{sat}}^{5/3} + \frac{27}{8} u_0\, \rho_{\text{sat}}^2$$

$$\frac{m_0^*}{m} = \left[1 + \frac{1}{16}\frac{2m}{\hbar^2}(\Theta_s \rho_0)\right]^{-1}$$

SIII parameterization

- $\rho_{\text{sat}} = 0.145\ (0.16 \pm 0.002)\ \text{fm}^{-3}$
- ➥ $\frac{E}{A} = -15.853\ (-16.0 \pm 0.2)$ MeV
- ➥ $\frac{m_0^*}{m} = 0.763\ (0.85 \pm 0.05)$
- ➥ $K_\infty = 355.373\ (230 \pm 20)$ MeV



Fitting protocol : Symmetric Nuclear Matter

SNM properties : usual functional (general EDF framework)

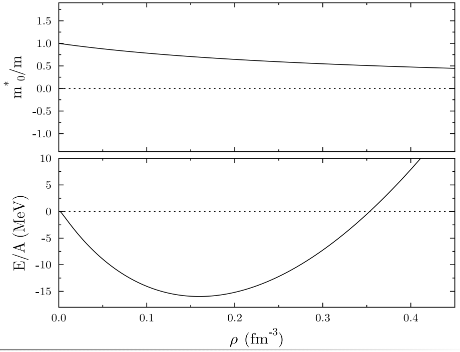
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\, \rho_0^{2/3} + \frac{3}{8} t_0\, \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{1}{16} u_0\, \rho_0^{1+\alpha}$$

$$K_\infty = -\frac{6}{5}\frac{\hbar^2}{2m} c_s\, \rho_{\text{sat}}^{2/3} + \frac{3}{8} c_s \Theta_s \rho_{\text{sat}}^{5/3} + \frac{9}{16}\alpha(1+\alpha)\, u_0\, \rho_{\text{sat}}^{1+\alpha}$$

$$\frac{m_0^*}{m} = \left[1 + \frac{1}{16}\frac{2m}{\hbar^2}(\Theta_s \rho_0)\right]^{-1}$$

SLy4 parameterization ($\alpha = 1/6$)

- $\rho_{\text{sat}} = 0.16\ (0.16 \pm 0.002)$ fm^{-3}
- ➥ $\frac{E}{A} = -15.972\ (-16.0 \pm 0.2)$ MeV
- ➥ $\frac{m_0^*}{m} = 0.695\ (0.85 \pm 0.05)$
- ➥ $K_\infty = 229.901\ (230 \pm 20)$ MeV



Fitting protocol : Symmetric Nuclear Matter

SNM properties : Our three-body pseudo-potential

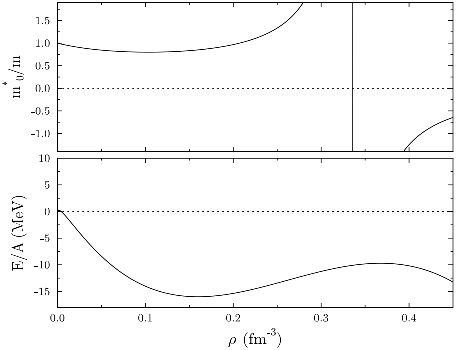
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\,\rho_0^{2/3} + \frac{3}{8} t_0\,\rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{16} u_0\,\rho_0^2 + \frac{3}{80} c_s \Theta_{3s} \rho_0^{8/3}$$

$$K_\infty = -\frac{6}{5}\frac{\hbar^2}{2m} c_s\,\rho_{\mathsf{sat}}^{2/3} + \frac{3}{8} c_s \Theta_s \rho_{\mathsf{sat}}^{5/3} + \frac{27}{8} u_0\,\rho_{\mathsf{sat}}^2 + \frac{3}{2} c_s \Theta_{3s} \rho_{\mathsf{sat}}^{8/3}$$

$$\frac{m_0^*}{m} = \left[1 + \frac{1}{16}\frac{2m}{\hbar^2}\left(\Theta_s \rho_0 + \Theta_{3s}\rho_0^2\right)\right]^{-1}$$

Our parameterization

- $\rho_{\mathsf{sat}} = 0.16 \; (0.16 \pm 0.002) \; \mathsf{fm}^{-3}$
- ➥ $\frac{E}{A} = -16 \; (-16.0 \pm 0.2)$ MeV
- ➥ $\frac{m_0^*}{m} = 0.85 \; (0.85 \pm 0.05)$
- ➥ $K_\infty = 230 \; (230 \pm 20)$ MeV



Fitting protocol : Symmetric Nuclear Matter

SNM properties : Our three-body pseudo-potential

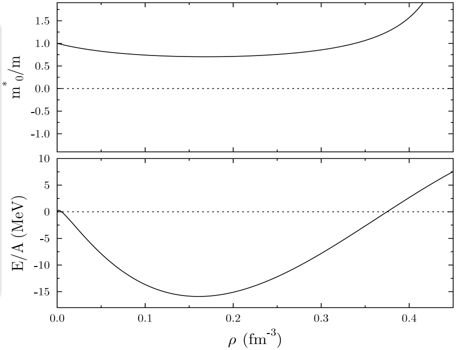
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\, \rho_0^{2/3} + \frac{3}{8} t_0\, \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{16} u_0\, \rho_0^2 + \frac{3}{80} c_s \Theta_{3s} \rho_0^{8/3}$$

$$K_\infty = -\frac{6}{5}\frac{\hbar^2}{2m} c_s\, \rho_{\text{sat}}^{2/3} + \frac{3}{8} c_s \Theta_s \rho_{\text{sat}}^{5/3} + \frac{27}{8} u_0\, \rho_{\text{sat}}^2 + \frac{3}{2} c_s \Theta_{3s} \rho_{\text{sat}}^{8/3}$$

$$\frac{m_0^*}{m} = \left[1 + \frac{1}{16}\frac{2m}{\hbar^2}\left(\Theta_s \rho_0 + \Theta_{3s} \rho_0^2\right)\right]^{-1}$$

Our parameterization 2

- $\rho_{\text{sat}} = 0.1606\ (0.16 \pm 0.002)\ \text{fm}^{-3}$
- $\frac{E}{A} = -15.901\ (-16.0 \pm 0.2)$ MeV
- $\frac{m_0^*}{m} = 0.7045\ (0.85 \pm 0.05)$
- $K_\infty = 255.496\ (230 \pm 20)$ MeV



SLyX Fitting protocol

Which impact those two behaviors (ρ_{cr},ρ_{infl}) have?

- Produce a set of parameterizations varying
  - K_∞ : $\{230, 240, 250, 260, 270\}$
  - $\frac{m_0^*}{m}$: $\{0.70, 0.71, \cdots, 0.80, 0.81\}$
  - Parameterizations (preliminary) name : $S_3Ly^{10m_0^*/m}_{K_\infty}$

Fitted nuclear properties

- Fit on **pure neutron matter** equation of state
  - As for SLy4 parameterization : Wiringa *ab-initio* data
- Symmetry energy $a_{\text{sym}} = 32$ MeV
- Binding energies and radii of doubly magic nuclei (if exist):

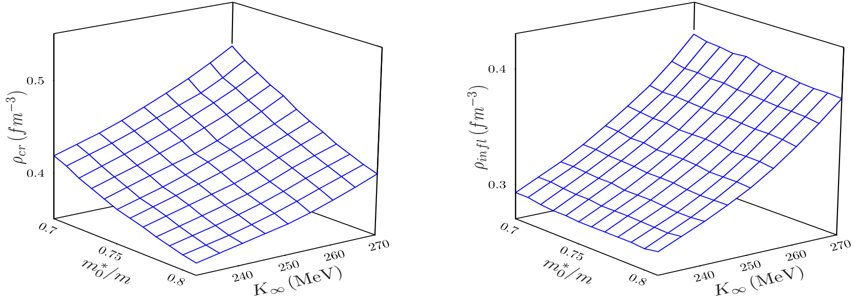
$$^{40}\text{Ca},\ ^{48}\text{Ca},\ ^{56}\text{Ni},\ ^{100}\text{Sn},\ ^{132}\text{Sn},\ ^{208}\text{Pb}$$

- Neutron spin-orbit splitting $\epsilon_{3p} \equiv \epsilon_{\nu 3p_{1/2}} - \epsilon_{\nu 3p_{3/2}}$ in ^{208}Pb

Outline

S_3Ly parameterizations

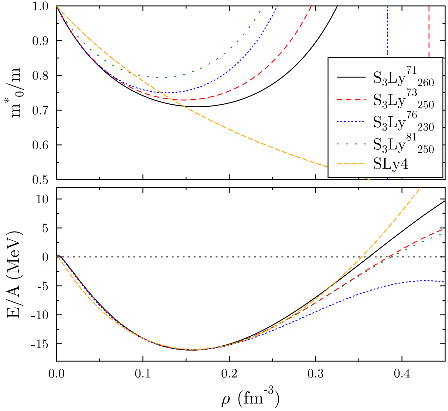
- Is S_3Ly parameterizations high-quality EDFs?
  - ➥ Choice of four S_3Ly parameterizations + SLy4
  - ➥ $S_3Ly^{71}_{260}$, $S_3Ly^{73}_{250}$, $S_3Ly^{76}_{230}$, $S_3Ly^{81}_{250}$



$S_3Ly^{10\,m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
ρ_{cr}	0.464	0.431	0.383	0.383	*
ρ_{infl}	0.362	0.333	0.289	0.327	*

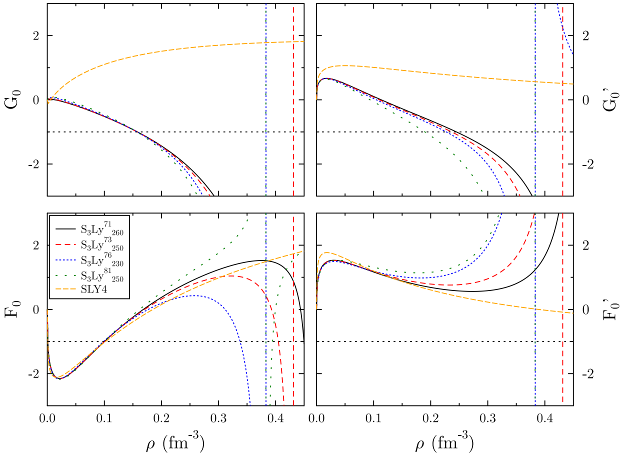
SNM properties

$\mathrm{S_3Ly}^{10\,m_0^*/m}_{K_\infty}$	$\mathrm{S_3Ly}^{71}_{260}$	$\mathrm{S_3Ly}^{73}_{250}$	$\mathrm{S_3Ly}^{76}_{230}$	$\mathrm{S_3Ly}^{81}_{250}$	SLy4
E/A	-16.088	-16.087	-16.062	-16.079	-15.972
ρ_{sat}	0.157	0.157	0.157	0.157	0.160
m_0^*/m	0.710	0.730	0.760	0.810	0.695
K_∞	259.829	250.208	230.049	249.894	229.901



Landau parameters

- Spin instabilities around saturation density, i.e. $G_0 \leq -1$
  - Known from [Chang, PLB, **56**, (1975), 205] ⇒ gradient-less 3B potential
- **Weak point** of present parameterizations ⇒ need for higher-order terms?



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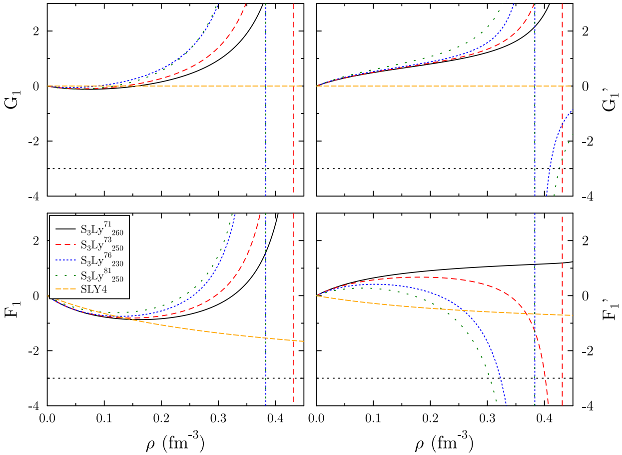
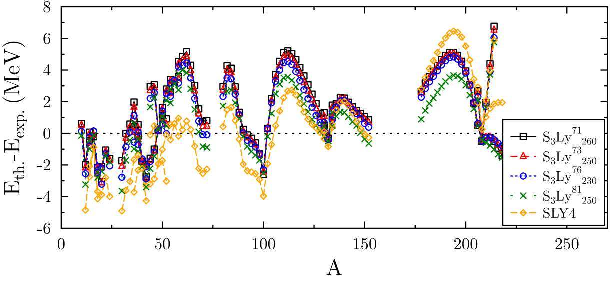


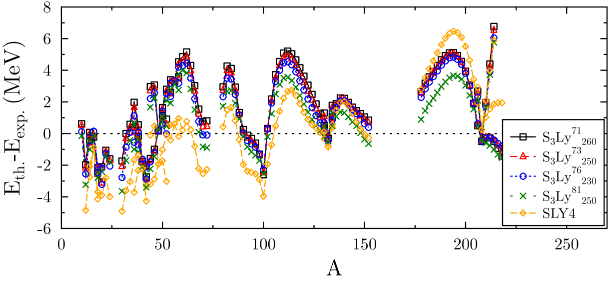
Binding energies systematic

$\mathrm{S_3Ly}^{10\,m_0^*/m}_{K_\infty}$	$\mathrm{S_3Ly}^{71}_{260}$	$\mathrm{S_3Ly}^{73}_{250}$	$\mathrm{S_3Ly}^{76}_{230}$	$\mathrm{S_3Ly}^{81}_{250}$	SLy4
	Isotopic chains				
$\bar{\Delta}_E$ (MeV)	2.18	2.02	1.79	1.19	0.75
$\bar{\Delta}_{\|E\|}$ (MeV)	2.74	2.61	2.42	2.01	2.63
σ_E (MeV)	2.40	2.36	2.28	2.05	3.12



Binding energies systematic

$S_3Ly^{10\,m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotonic chains				
$\bar{\Delta}_E$ (MeV)	0.73	0.63	0.47	0.05	-0.54
$\bar{\Delta}_{\|E\|}$ (MeV)	1.63	1.56	1.46	1.38	1.67
σ_E (MeV)	1.87	1.82	1.76	1.70	2.03



Binding energies systematic

$S_3Ly^{10\ m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotonic chains				
$\bar{\Delta}_E$ (MeV)	0.73	0.63	0.47	0.05	-0.54
$\bar{\Delta}_{\|E\|}$ (MeV)	1.63	1.56	1.46	1.38	1.67
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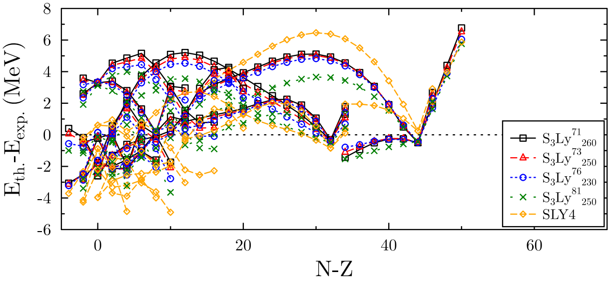
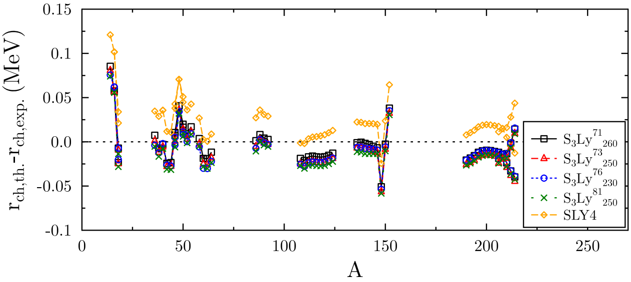


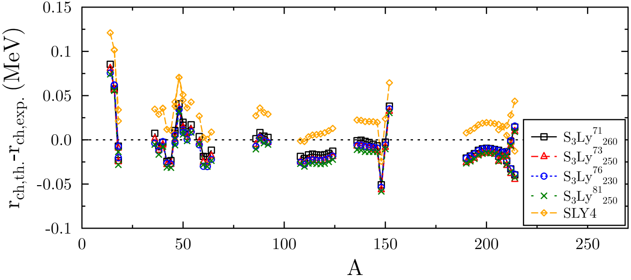
Radii systematic

$S_3Ly^{10\,m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotopic chains				
$\bar{\Delta}_{r_c}$ (10^{-2} fm)	-1.0	-1.6	-1.4	-1.8	1.7
$\bar{\Delta}_{\|r_c\|}$ (10^{-2} fm)	1.8	2.2	2.0	2.4	1.9
σ_{r_c} (10^{-2} fm)	1.8	1.9	1.9	1.8	2.2



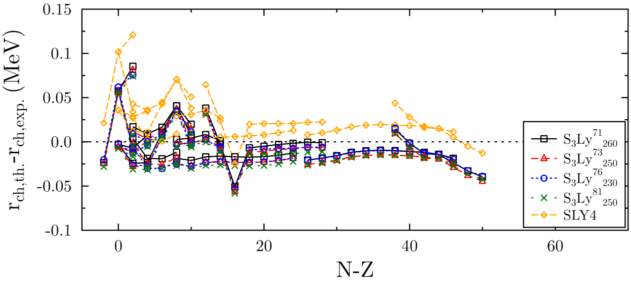
Radii systematic

$S_3Ly^{10\, m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotonic chains				
$\bar{\Delta}_{r_c}$ $(10^{-2}$ fm)	0.5	0.0	0.1	-0.3	3.5
$\bar{\Delta}_{\|r_c\|}$ $(10^{-2}$ fm)	1.6	1.7	1.5	1.8	3.6
σ_{r_c} $(10^{-2}$ fm)	2.5	2.5	2.4	2.5	2.7



Radii systematic

$S_3Ly^{10\, m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotonic chains				
$\bar{\Delta}_{r_c}$ (10^{-2} fm)	0.5	0.0	0.1	-0.3	3.5
$\bar{\Delta}_{\lvert r_c \rvert}$ (10^{-2} fm)	1.6	1.7	1.5	1.8	3.6
σ_{r_c} (10^{-2} fm)	2.5	2.5	2.4	2.5	2.7



Outline

Conclusions and outlooks

- Possible to get **as good phenomenology as usual EDFs** with pseudo-potential
- Still spin-instabilities remain a problem

Functional form

- Pairing functional must be computed to be in a true pseudo-potential formulation
- Four-body gradient-less pseudo-potential might help to control spin-instabilities
- S-O and tensor three-body pseudo-potential?

Adjustment procedure

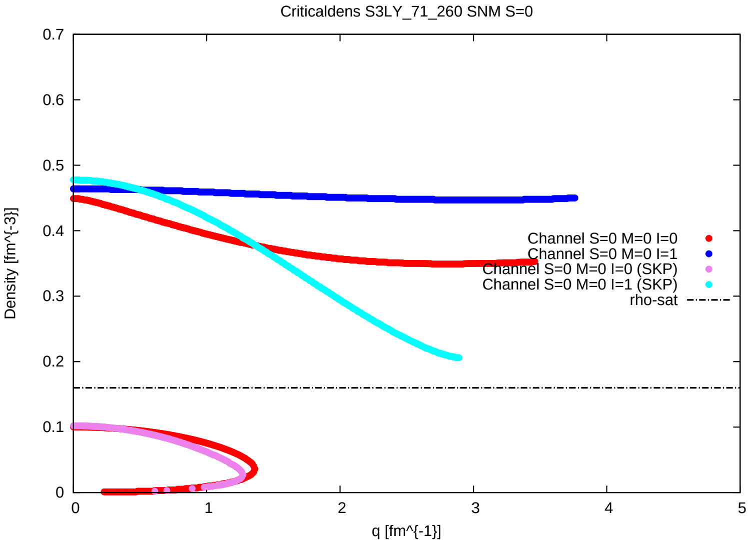
- Use of modern INM equation of states
- Control finite-size instabilities of trilinear parameterizations

Post-fit analysis

- Determine which free parameters are under or over constrained
- **Make use of future spurious free parameterizations in MR-EDF calculations**

Finite-size instabilities

- Finite-size instabilities through RPA code : A. Pastore



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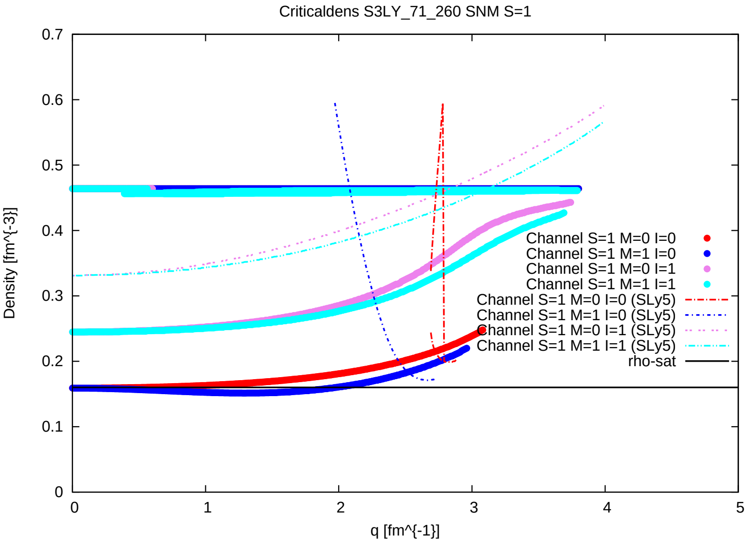

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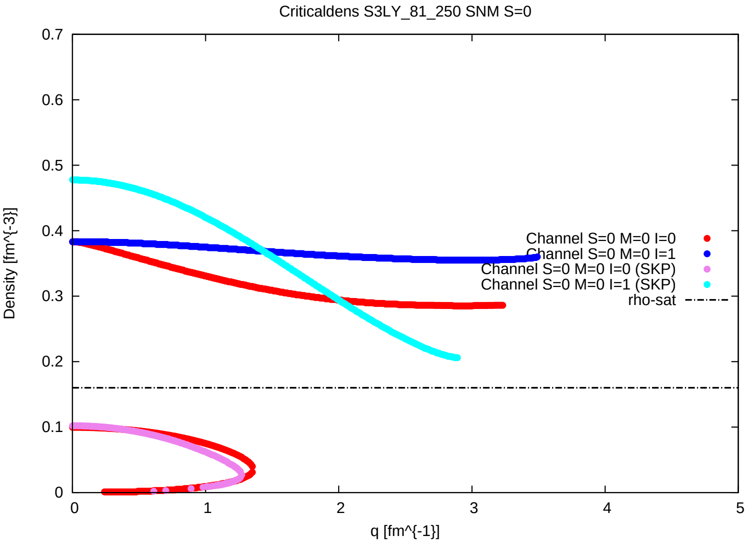

Finite-size instabilities

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