Skyrme EDF from 2+3+4-body Skyrme pseudo-potential

J. Sadoudi[1] K. Bennaceur[3] T. Duguet[2] R. Jodon[3] J. Meyer[3]

[1] Centre d'Etudes Nucléaires de Bordeaux Gradignan, CNRS/IN2P3
[2] IRFU/SPhN, CEA Saclay
[3] IPNL, Université Lyon 1

28 september 2012

energie atomique • energies alternatives

Outline

1. Introduction
   - Nuclear EDF
   - Model the energy kernel
   - Pathologies
   - Challenges
2. Skyrme pseudo-potential
   - Energy kernel from Skyrme pseudo-potential
   - Two-body case
   - Three-body case
   - Four-body case
3. Implications
   - Parameterizations
   - Results

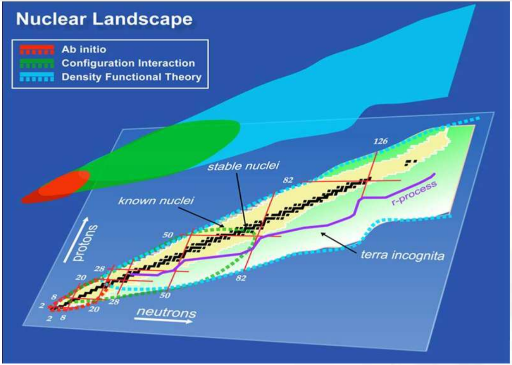
Outline

1. Introduction
   - Nuclear EDF
   - Model the energy kernel
   - Pathologies
   - Challenges
2. Skyrme pseudo-potential
   - Energy kernel from Skyrme pseudo-potential
   - Two-body case
   - Three-body case
   - Four-body case
3. Implications
   - Parameterizations
   - Results

The nuclear Energy Density Functional (EDF) method

Advantages

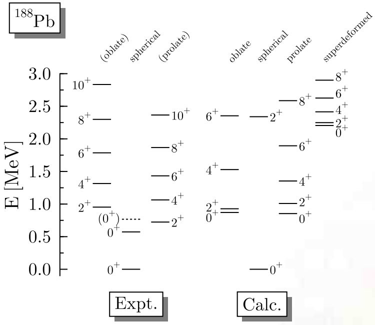
- Tool of choice for the description of medium- and heavy-mass nuclei
- Two step approach : SR-EDF (sym. breaking) and MR-EDF (sym. restoration)
- Addresses both ground-state (SR-EDF) and spectroscopic properties (MR-EDF)
  - ⇒ EDF method has matured into a spectroscopy-oriented method



The nuclear Energy Density Functional (EDF) method

Advantages

- Tool of choice for the description of medium- and heavy-mass nuclei
- Two step approach : SR-EDF (sym. breaking) and MR-EDF (sym. restoration)
- Addresses both ground-state (SR-EDF) and spectroscopic properties (MR-EDF)
  - ➥ EDF method has matured into a spectroscopy-oriented method



[M. Bender, unpublished]

The nuclear Energy Density Functional (EDF) method

Advantages

- Tool of choice for the description of medium- and heavy-mass nuclei
- Two step approach : SR-EDF (sym. breaking) and MR-EDF (sym. restoration)
- Addresses both ground-state (SR-EDF) and spectroscopic properties (MR-EDF)
  - ➥ EDF method has matured into a spectroscopy-oriented method

Disadvantage

- Existing param. (Gogny, Skyrme, ...) successful but lack predictive power

Challenges

- Towards EDF parameterizations with enhanced predictive power
  - ➥ EDF is meant to strongly overlap with *ab-initio* methods in the next 10 years
- Extend the reach of EDF calculations, e.g. odd-even and odd-odd nuclei

➾ **New : Current EDF parameterizations contain spurious contributions**

The nuclear Energy Density Functional (EDF) method

Advantages

- Tool of choice for the description of medium- and heavy-mass nuclei
- Two step approach : SR-EDF (sym. breaking) and MR-EDF (sym. restoration)
- Addresses both ground-state (SR-EDF) and spectroscopic properties (MR-EDF)
  - ➥ EDF method has matured into a spectroscopy-oriented method

Disadvantage

- Existing param. (Gogny, Skyrme, ...) successful but lack predictive power

Challenges

- Towards EDF parameterizations with enhanced predictive power
  - ➥ EDF is meant to strongly overlap with *ab-initio* methods in the next 10 years
- Extend the reach of EDF calculations, e.g. odd-even and odd-odd nuclei

➾ **New : Current EDF parameterizations contain spurious contributions**

The nuclear Energy Density Functional (EDF) method : Basic ingredients

- The key object is 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
  - ➥ $|\Phi(g)\rangle = \prod_\mu \beta_\mu^{(g)}|0\rangle \Rightarrow$ Bogoliubov product states

- $E[g',g]$ **not necessarily related to an (effective) Hamiltonian**

Model the off-diagonal energy kernel : general EDF method

Quasi-local Skyrme EDF

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

- Skyrme family
  - s.p. basis (i) = position $(\vec{r}) \otimes$ spin $(\sigma) \otimes$ isospin (q) s.p. basis
  - near diagonal $\Rightarrow$ local densities

$$\rho_q^{g'g}(\vec{r}) \equiv \sum_\sigma \rho_{\vec{r}\sigma q\vec{r}\sigma q}^{g'g}$$ Matter

$$\tau_q^{g'g}(\vec{r}) \equiv \sum_\sigma \vec{\nabla} \cdot \vec{\nabla}' \rho_{\vec{r}\sigma q\vec{r}'\sigma q}^{g'g}\Big|_{\vec{r}=\vec{r}'}$$ Kinetic

$$j_{q,\mu}^{g'g}(\vec{r}) \equiv \frac{i}{2} \sum_{\sigma\sigma'} \left(\nabla' - \nabla\right)_\mu \rho_{\vec{r}\sigma q\vec{r}'\sigma q}^{g'g}\Big|_{\vec{r}=\vec{r}'}$$ Current

Model the off-diagonal energy kernel : general EDF method

Quasi-local Skyrme EDF

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

- Skyrme family
  - s.p. basis (i) = position $(\vec{r}) \otimes$ spin $(\sigma) \otimes$ isospin (q) s.p. basis
  - near diagonal $\Rightarrow$ local densities

$$s_{q,\nu}^{g'g}(\vec{r}) \equiv \sum_\sigma \rho_{\vec{r}\sigma q \vec{r}\sigma' q}^{g'g} \sigma_\nu^{\sigma'\sigma}$$ Spin

$$T_{q,\nu}^{g'g}(\vec{r}) \equiv \sum_\sigma \vec{\nabla}\cdot\vec{\nabla}'\, \rho_{\vec{r}\sigma q \vec{r}'\sigma' q}^{g'g} \sigma_\nu^{\sigma'\sigma}\Big|_{\vec{r}=\vec{r}'}$$ Spin-kinetic

$$J_{q,\mu\nu}^{g'g}(\vec{r}) \equiv \frac{i}{2}\sum_{\sigma\sigma'} \left(\nabla' - \nabla\right)_\mu \rho_{\vec{r}\sigma q \vec{r}'\sigma' q}^{g'g}\, \sigma_\nu^{\sigma'\sigma}\Big|_{\vec{r}=\vec{r}'}$$ Spin-current

Model the off-diagonal energy kernel : general EDF method

Quasi-local Skyrme EDF

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

- Skyrme family
  - s.p. basis (i) = position $(\vec{r}) \otimes$ spin $(\sigma) \otimes$ isospin (q) s.p. basis
  - near diagonal $\Rightarrow$ local densities $\Rightarrow$ simplified case

$$\rho_q^{g'g}(\vec{r}) \equiv \sum_\sigma \rho_{\vec{r}\sigma q \vec{r}\sigma q}^{g'g}$$ Matter

$$s_{q,\nu}^{g'g}(\vec{r}) \equiv \sum_\sigma \rho_{\vec{r}\sigma q \vec{r}\sigma' q}^{g'g} \sigma_\nu^{\sigma'\sigma}$$ Spin

Ex: purely local Skyrme bilinear kernel without gradients, isospin and pairing

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

- $C^{\rho\rho}$ and C^{ss} are the free parameters to adjust phenomenologically

Model the off-diagonal energy kernel : pseudo-potential-based EDF

Quasi-local Skyrme EDF

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

- Skyrme family
  - s.p. basis (i) = position $(\vec{r}) \otimes$ spin $(\sigma) \otimes$ isospin (q) s.p. basis
  - near diagonal $\Rightarrow$ local densities $\Rightarrow$ simplified case

$$\rho_q^{g'g}(\vec{r}) \equiv \sum_\sigma \rho^{g'g}_{\vec{r}\sigma q\vec{r}\sigma q} \qquad \text{Matter}$$

$$s_{q,\nu}^{g'g}(\vec{r}) \equiv \sum_\sigma \rho^{g'g}_{\vec{r}\sigma q\vec{r}\sigma' q}\sigma_\nu^{\sigma'\sigma} \qquad \text{Spin}$$

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

- $H_{\text{pseudo}} = \frac{1}{2}\sum v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$ with $v_{\vec{r}_1\vec{r}_2\vec{r}_1\vec{r}_2} = t_0\,\delta(\vec{r}_1 - \vec{r}_2)$

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

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

Model the off-diagonal energy kernel : density-dependent interaction

Quasi-local Skyrme EDF

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

- Skyrme family
  - s.p. basis (i) = position $(\vec{r}) \otimes$ spin $(\sigma) \otimes$ isospin (q) s.p. basis
  - near diagonal $\Rightarrow$ local densities $\Rightarrow$ simplified case

$\rho^{g'g}_{q}(\vec{r}) \equiv \sum_\sigma \rho^{g'g}_{\vec{r}\sigma q\vec{r}\sigma q}$ Matter

$s^{g'g}_{q,\nu}(\vec{r}) \equiv \sum_\sigma \rho^{g'g}_{\vec{r}\sigma q\vec{r}\sigma' q}\sigma^{\sigma'\sigma}_{\nu}$ Spin

Ex: purely local Skyrme (quasi) bilinear kernel

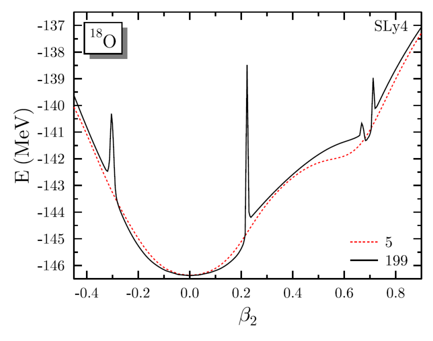
$$E^{\text{ex}}[g',g] \equiv \int d\vec{r}\left\{A^{\rho\rho}[\rho^{g'g}(\vec{r})]\rho^{g'g}(\vec{r})\rho^{g'g}(\vec{r}) + A^{ss}[\rho^{g'g}(\vec{r})]\vec{s}^{g'g}(\vec{r})\cdot\vec{s}^{g'g}(\vec{r})\right\}$$

- EDF method with density-dependent interaction is **not** a pseudo-potential-based EDF

➥ Empirical density dependence breaks the **Pauli principle** = **self-interaction**

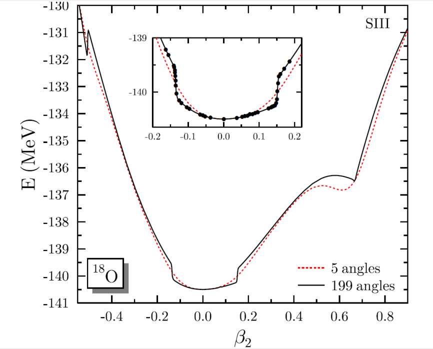
Particle number restoration pathologies

$E^{Z=8,N=10}$ for $E[\rho\rho\rho^{1/6}]$



[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

$E^{Z=8,N=10}$ for $E[\rho\rho\rho]$

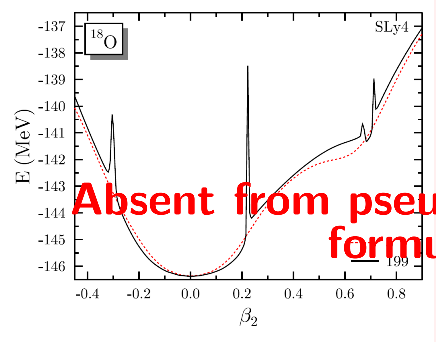


[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

- Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
- Using general approach to $E[g, g']$ unsafe a priori [D. Lacroix *et al.*, PRC79 (2009) 044318]
- Originates from self interaction in the EDF kernel [D. Lacroix *et al.*, PRC79 (2009) 044318]

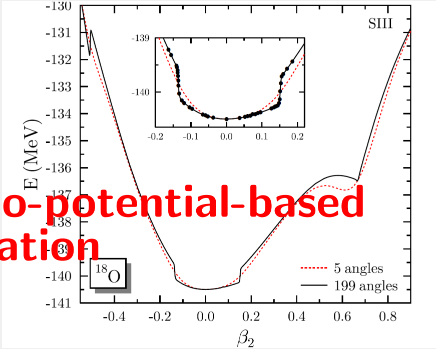
Particle number restoration pathologies

$E^{Z=8,N=10}$ for $E[\rho\rho\rho^{1/6}]$



[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

$E^{Z=8,N=10}$ for $E[\rho\rho\rho]$



[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

Absent from pseudo-potential-based formulation

- Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
- Using general approach to $E[g, g']$ unsafe a priori [D. Lacroix *et al.*, PRC79 (2009) 044318]
- Originates from self interaction in the EDF kernel [D. Lacroix *et al.*, PRC79 (2009) 044318]

Motivations : General-EDF vs pseudo-potential-based-EDF

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

Challenges

General-EDF

- General-EDF formulation provides good phenomenology at the SR level

Pseudo-potential-based EDF

- ✖ How to get **high-quality EDF parameterizations** in such a restricted formulation?
- ➥ According to previous (limited) attempt, it is a challenge
- ➥ 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

Outline

1. Introduction
   - Nuclear EDF
   - Model the energy kernel
   - Pathologies
   - Challenges

2. Skyrme pseudo-potential
   - Energy kernel from Skyrme pseudo-potential
   - Two-body case
   - Three-body case
   - Four-body case

3. Implications
   - Parameterizations
   - Results

A new Skyrme pseudo-potential

- Two-body Skyrme pseudo-potential **without density dependence**
- Replace density dependence by gradient-less three-body Skyrme pseudo-potential
  - Known as unsufficient
- Add three-body (central) Skyrme pseudo-potential up to second order in gradients
- Add four-body gradient-less Skyrme pseudo-potential
- The same pseudo-potential should be used in the normal and pairing channel

Energy kernel from Skyrme pseudo-potential

Skyrme pseudo-Hamiltonian : 2+3+4-body

$$
\begin{aligned}
H_{\text{pseudo}} \equiv & + \frac{1}{2!} \sum_{ijkl} \langle \hat{v}_{12} \rangle_{ijkl} \; a_i^\dagger a_j^\dagger a_l a_k \\
& + \frac{1}{3!} \sum_{ijklmn} \langle \hat{v}_{123} \rangle_{ijklmn} \; a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \\
& + \frac{1}{4!} \sum_{ijklmnop} \langle \hat{v}_{1234} \rangle_{ijklmnop} \; a_i^\dagger a_j^\dagger a_k^\dagger a_l^\dagger a_p a_o a_n a_m
\end{aligned}
$$

Energy kernel

- Energy kernel through $\langle \Phi(g) | H_{\text{pseudo}}(\{t_i\}) | \Phi(g) \rangle$ and Standard Wick Theorem

$$
E_H[\rho_{ij}, \kappa_{ij}, \kappa^*_{ij}] = E_H^{\rho\rho} + E_H^{\kappa\kappa} + E_H^{\rho\rho\rho} + E_H^{\kappa\kappa\rho} + E_H^{\rho\rho\rho\rho} + E_H^{\kappa\kappa\rho\rho} + E_H^{\kappa\kappa\kappa\kappa}
$$

where

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

Energy kernel from Skyrme pseudo-potential

$$E_H^{\rho\rho} = \frac{1}{2} \sum_{ijkl} \langle \hat{v}_{12} \mathcal{A}_{12} \rangle_{ijkl} \, \rho_{ki} \, \rho_{lj}$$

$$E_H^{\kappa\kappa} = \frac{1}{2} \sum_{ijkl} \langle \hat{v}_{12} \rangle_{ijkl} \, \kappa^{\dagger}_{ij} \kappa_{kl}$$

$$E_H^{\rho\rho\rho} = \frac{1}{6} \sum_{ijklmn} \langle \hat{v}_{123} \mathcal{A}_{123} \rangle_{ijklmn} \, \rho_{li} \, \rho_{mj} \, \rho_{nk}$$

$$E_H^{\kappa\kappa\rho} = \frac{1}{6} \sum_{ijklmn} \langle \mathcal{A}^{12}_{123} \, \hat{v}_{123} \mathcal{A}^{12}_{123} \rangle_{ijklmn} \, \kappa^{\dagger}_{ij} \kappa_{lm} \rho_{nk}$$

$$E_H^{\rho\rho\rho\rho} = \frac{1}{24} \sum_{ijklmnop} \langle \hat{v}_{1234} \mathcal{A}_{1234} \rangle_{ijklmnop} \, \rho_{mi} \, \rho_{nj} \, \rho_{ok} \, \rho_{pl}$$

$$E_H^{\kappa\kappa\rho\rho} = \frac{1}{24} \sum_{ijklmnop} \langle \mathcal{A}^{12S}_{1234} \, \hat{v}_{1234} \mathcal{A}^{12}_{1234} \rangle_{ijklmnop} \, \kappa^{\dagger}_{ij} \kappa_{mn} \rho_{ok} \rho_{pl}$$

$$E_H^{\kappa\kappa\kappa\kappa} = \frac{1}{24} \sum_{ijklmnop} \langle \mathcal{A}^{12}_{123} \, \hat{v}_{1234} \mathcal{A}^{12}_{123} \rangle_{ijklmnop} \, \kappa^{\dagger}_{ij} \kappa^{\dagger}_{kl} \kappa_{mn} \kappa_{op}$$

- Pauli principle $\Rightarrow$ antisymmetrizers, exchange operators

Construction of the Skyrme pseudo-potential

Skyrme pseudo-potential ingredients

- Aim : Construct the most general $\hat{v}_{12}$, $\hat{v}_{123}$ and $\hat{v}_{1234}$ Skyrme pseudo-potentials
  - ➥ i.e. identify all 2-, 3- and 4-body operators providing independent EDF terms
- Kronecker, gradients and exchange operators
  - ➥ $\hat{\delta}_{r_i r_j}$, $\hat{\vec{k}}_{ij} = -\frac{i}{2}(\hat{\vec{\nabla}}_i - \hat{\vec{\nabla}}_j)$, P^r_{ij}, P^σ_{ij}, P^τ_{ij} with $i \neq j \in \{1,2,3,4\}^2$

Energy functional derivation

- Two- and three-body central potential up to second order in gradients
- Two-body spin-orbit and four-body gradient-less potentials
  - ➥ Generates around 120 parameters/different terms a priori
- Derivation straightforward but almost impossible by hand for 120 terms
- Development of a **formal computation code**
- Identification of correlated terms via Singular Value Decomposition

Two-body case (known)

Skyrme pseudo-potential

- Two-body Skyrme operators providing independent terms in $E_H^{\rho\rho}$ and $E_H^{\kappa\kappa}$

$$\hat{v}_{12} = t_0 \left(1 + x_0 P_{12}^{\sigma}\right) \hat{\delta}_{r_1 r_2} + \frac{t_1}{2} \left(1 + x_1 P_{12}^{\sigma}\right) \left(\hat{\vec{k}}_{12}'^{2} + \hat{\vec{k}}_{12}^{2}\right) \hat{\delta}_{r_1 r_2}$$
$$+ t_2 \left(1 + x_2 P_{12}^{\sigma}\right) \hat{\vec{k}}_{12}' \cdot \hat{\vec{k}}_{12}\, \hat{\delta}_{r_1 r_2} + iW_0 \left(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2\right) \hat{\vec{k}}_{12}' \wedge \hat{\vec{k}}_{12}$$

Bilinear Skyrme functional (energy density)

$$\mathcal{E}_{H,\text{even}}^{\rho\rho}(\vec{r}) = \sum_{t=0,1} A_t^{\rho} \rho_t^2 + A_t^{\tau} \rho_t \tau_t + A_t^{\nabla\rho} \vec{\nabla}\rho_t \cdot \vec{\nabla}\rho_t + \sum_{\mu\nu} A_t^{J} J_{t,\mu\nu} J_{t,\mu\nu} + A_t^{\nabla J} \rho_t \vec{\nabla} \cdot \vec{J}_t$$

$$\mathcal{E}_{H,\text{odd}}^{\rho\rho}(\vec{r}) = \sum_{t=0,1} A_t^{s} \vec{s}_t^{\,2} + A_t^{T} \vec{s}_t \vec{T}_t + \sum_{\mu\nu} A_t^{\nabla s} \nabla_\mu s_{t,\nu} \nabla_\mu s_{t,\nu} + A_t^{j} \vec{j}_t \cdot \vec{j}_t + A_t^{\nabla j} \vec{s}_t \cdot \vec{\nabla} \times \vec{j}_t$$

$$\mathcal{E}_{H}^{\kappa\kappa}(\vec{r}) = \sum_{t=0,1} A_t^{\tilde{\rho}} \tilde{\rho}_t^2 + A_t^{\tilde{\tau}} \tilde{\rho}_t \tilde{\tau}_t + A_t^{\nabla\tilde{\rho}} \vec{\nabla}\tilde{\rho}_t \cdot \vec{\nabla}\tilde{\rho}_t + \sum_{\mu\nu} A_t^{\tilde{J}} \tilde{J}_{t,\mu\nu} \tilde{J}_{t,\mu\nu}$$
$$+ \sum_{\mu\nu} A_t^{\tilde{J}W} \left(\tilde{J}_{t,\mu\mu} \tilde{J}_{t,\nu\nu} - \tilde{J}_{t,\mu\nu} \tilde{J}_{t,\nu\mu}\right)$$

Three-body case (new)

Skyrme pseudo-potential

- Final three-body Skyrme pseudo-potential

$$
\begin{aligned}
\hat{v}_{123} = & \, u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right) \\
& + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{12} \right] \left(\hat{\vec{k}}_{12} \cdot \hat{\vec{k}}_{12} + \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
& + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{31} \right] \left(\hat{\vec{k}}_{31} \cdot \hat{\vec{k}}_{31} + \hat{\vec{k}}'_{31} \cdot \hat{\vec{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
& + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{23} \right] \left(\hat{\vec{k}}_{23} \cdot \hat{\vec{k}}_{23} + \hat{\vec{k}}'_{23} \cdot \hat{\vec{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\
& + u_2 \left[1 + y_{21} P^{\sigma}_{12} + y_{22} (P^{\sigma}_{13} + P^{\sigma}_{23}) \right] \left(\hat{\vec{k}}_{12} \cdot \hat{\vec{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
& + u_2 \left[1 + y_{21} P^{\sigma}_{31} + y_{22} (P^{\sigma}_{32} + P^{\sigma}_{12}) \right] \left(\hat{\vec{k}}_{31} \cdot \hat{\vec{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
& + u_2 \left[1 + y_{21} P^{\sigma}_{23} + y_{22} (P^{\sigma}_{21} + P^{\sigma}_{31}) \right] \left(\hat{\vec{k}}_{23} \cdot \hat{\vec{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}
\end{aligned}
$$

Three-body case (new)

Skyrme pseudo-potential

Trilinear Skyrme functional (energy density) : Normal part

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

$$+ B^{\tau}_{10}\rho_1\rho_1\tau_0 + B^{\nabla\rho}_{10}\rho_1\vec{\nabla}\rho_1\cdot\vec{\nabla}\rho_0 + \sum_{\mu\nu} B^{J}_{10}\rho_1 J_{1,\mu\nu}J_{0,\mu\nu}$$

$$\mathcal{E}^{\rho\rho\rho}_{H,\text{odd}} = \sum_{t=0,1} \Big\{ B^{s}_{t}\rho_0\vec{s}^{\,2}_t + B^{T}_{t}\rho_0\vec{s}_t\cdot\vec{T}_t + \sum_{\mu\nu} B^{\nabla s}_{t}\rho_0\nabla_\mu s_{t,\nu}\nabla_\mu s_{t,\nu} + B^{j}_{t}\rho_0\vec{j}_t\cdot\vec{j}_t$$

$$+B^{T}_{t\bar{t}}\rho_1\vec{s}_t\cdot\vec{T}_{\bar{t}} + B^{\tau s}_{t}\vec{s}_0\vec{s}_t\tau_t + \sum_{\mu\nu}\Big[B^{\nabla\rho s}_{t} s_{0,\nu}\nabla_\mu\rho_t\nabla_\mu s_{t,\nu}$$

$$+B^{\nabla\rho s}_{t\bar{t}} s_{1,\nu}\nabla_\mu\rho_t\nabla_\mu s_{\bar{t},\nu} + B^{Js}_{t} s_{0,\nu}j_{t,\mu}J_{t,\mu\nu} + B^{Js}_{t\bar{t}} s_{1,\nu}j_{t,\mu}J_{\bar{t},\mu\nu}\Big]$$

$$+ \sum_{\mu\nu\lambda k}\epsilon_{\nu\lambda k}\Big[B^{\nabla sJ}_{t} s_{0,k}\nabla_\mu s_{t,\nu}J_{t,\mu\lambda} + B^{\nabla sJ}_{t\bar{t}} s_{1,k}\nabla_\mu s_{t,\nu}J_{\bar{t},\mu\lambda}\Big]\Big\}$$

$$+B^{s}_{10}\rho_1\vec{s}_1\cdot\vec{s}_0 + B^{\nabla s}_{10}\rho_1\nabla_\mu s_{1,\nu}\nabla_\mu s_{0,\nu} + B^{j}_{10}\rho_1\vec{j}_1\cdot\vec{j}_0 + B^{\tau s}_{10}\vec{s}_1\vec{s}_1\tau_0$$

Three-body case (new)

Skyrme pseudo-potential

Trilinear Skyrme functional (energy density) : Pairing part

$$\mathcal{E}_H^{\kappa\kappa\rho} = \sum_{t=0,1} \Big\{ B_{tt}^{\tilde\rho}\, \rho_0 \tilde\rho_t^2 + B_{t\bar t}^{\tilde\rho}\, \rho_1 \tilde\rho_{\bar t} \tilde\rho_t + B_{tt}^{\tau\tilde\rho}\, \tau_0 \tilde\rho_t^2 + B_{t\bar t}^{\tau\tilde\rho}\, \tau_1 \tilde\rho_{\bar t} \tilde\rho_t$$
$$+ B_{tt}^{\nabla\tilde\rho}\, \rho_0 \vec\nabla\tilde\rho_t \cdot \vec\nabla\tilde\rho_t + B_{t\bar t}^{\nabla\tilde\rho}\, \rho_1 \vec\nabla\tilde\rho_{\bar t} \cdot \vec\nabla\tilde\rho_t + B_{tt}^{\tilde\rho\nabla\tilde\rho}\, \vec\nabla\rho_0 \cdot \vec\nabla\tilde\rho_t \tilde\rho_t$$
$$+ B_{t\bar t}^{\tilde\rho\nabla\tilde\rho}\, \vec\nabla\rho_1 \cdot \vec\nabla\tilde\rho_{\bar t}\tilde\rho_t + \sum_{\mu\nu} B_{tt}^{\tilde J}\, \rho_0 \tilde J_{t,\mu\nu} \tilde J_{t,\mu\nu} + \sum_{\mu\nu} B_{t\bar t}^{\tilde J}\, \rho_1 \tilde J_{\bar t,\mu\nu} \tilde J_{t,\mu\nu}$$
$$+ \sum_{\mu\nu} B_{tt}^{J\tilde J}\, J_{0,\mu\nu} \tilde\rho_t \tilde J_{t,\mu\nu} + \sum_{\mu\nu} B_{t\bar t}^{J\tilde J}\, J_{1,\mu\nu} \tilde\rho_{\bar t} \tilde J_{t,\mu\nu} \Big\}$$

Four-body case (new)

Skyrme pseudo-potential

- Final three-body Skyrme pseudo-potential

$$\hat{v}_{1234} = v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \hat{\delta}_{r_1 r_2} \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_2 r_4} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \hat{\delta}_{r_1 r_4} + \cdots \right)$$

Bilinear Skyrme functional (energy density) : normal and pairing part

$$\mathcal{E}^{\rho\rho\rho\rho}_{H,\text{even}}(\vec{r}) = \sum_{t=0,1} C^{\rho}_{t} \rho^{4}_{t} + C^{\rho}_{01} \rho^{2}_{0} \rho^{2}_{1}$$

$$\mathcal{E}^{\rho\rho\rho\rho}_{H,\text{odd}}(\vec{r}) = \sum_{t=0,1} \left\{ C^{s}_{t} \vec{s}^{\,4}_{t} + C^{\rho s}_{tt} \rho^{2}_{t} \vec{s}^{\,2}_{t} + C^{\rho s}_{t\bar{t}} \rho^{2}_{\bar{t}} \vec{s}^{\,2}_{t} \right\} + C^{\rho\rho s s} \rho_0 \rho_1 \vec{s}_0 \vec{s}_1 + C^{s}_{01} \vec{s}^{\,2}_{0} \vec{s}^{\,2}_{1}$$

$$\mathcal{E}^{\kappa\kappa\rho\rho}_{H}(\vec{r}) = \sum_{t=0,1} \left\{ C^{\tilde{\rho}\rho}_{tt} \rho^{2}_{t} \tilde{\rho}^{2}_{t} + C^{\tilde{\rho}\rho}_{t\bar{t}} \rho^{2}_{\bar{t}} \tilde{\rho}^{2}_{t} \right\} + C^{\rho\rho\tilde{\rho}\tilde{\rho}} \rho_0 \rho_1 \tilde{\rho}_0 \tilde{\rho}_1$$

$$\mathcal{E}^{\kappa\kappa\kappa\kappa}_{H}(\vec{r}) = \sum_{t=0,1} \left\{ C^{\tilde{\rho}\tilde{\rho}}_{tt} \tilde{\rho}^{4}_{t} + C^{\tilde{\rho}\tilde{\rho}}_{t\bar{t}} \tilde{\rho}^{2}_{\bar{t}} \tilde{\rho}^{2}_{t} \right\}$$

Outline

1. Introduction
   - Nuclear EDF
   - Model the energy kernel
   - Pathologies
   - Challenges
2. Skyrme pseudo-potential
   - Energy kernel from Skyrme pseudo-potential
   - Two-body case
   - Three-body case
   - Four-body case
3. Implications
   - Parameterizations
   - Results

Parameterizations

General-EDF : good-quality parameterizations

- Quasi-bilinear functional (density-dependent interaction) : 7+2+1 param. ⇒ **SLy4**
  - Parameterization of reference

Pseudo-potential-based EDF : as good-quality as general-EDF parameterizations?

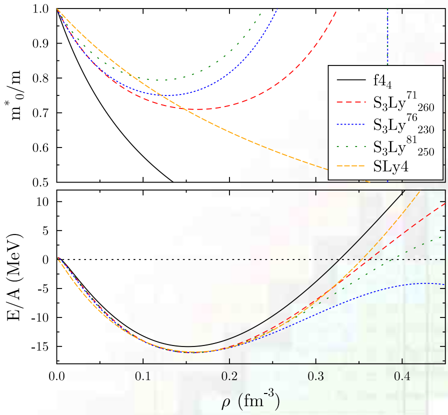
- Three-body pseudo-potential : 7+6+1 param. ⇒ $\mathbf{S_3Ly}^{71}_{260}$, $\mathbf{S_3Ly}^{76}_{230}$, $\mathbf{S_3Ly}^{81}_{250}$
  - Not pseudo-potential-based : two-body contact for pairing part
- Three and four-body gradient-less pseudo-potential : 7+2 param. ⇒ $\mathbf{f}4_4$
  - **pseudo-potential-based** : same potential for normal and pairing part
  - Much more constrained : pairing and instabilities
  - Aim : safely usable for MR-EDF

Results

Symmetric Nuclear Matter : equation of states

Parametrizations	$f4_4$	$S_3Ly^{71}_{260}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
E/A	-15.041	-16.088	-16.062	-16.079	-15.972
ρ_{sat}	0.152	0.157	0.157	0.157	0.160

	m_0^*/m	K_∞	a_{sym}
$f4_4$	0.47	264.2	23
$S_3Ly^{71}_{260}$	0.71	259,8	32
$S_3Ly^{76}_{230}$	0.76	230.0	32
$S_3Ly^{81}_{250}$	0.81	249.9	32
SLy4	0.695	229.9	32

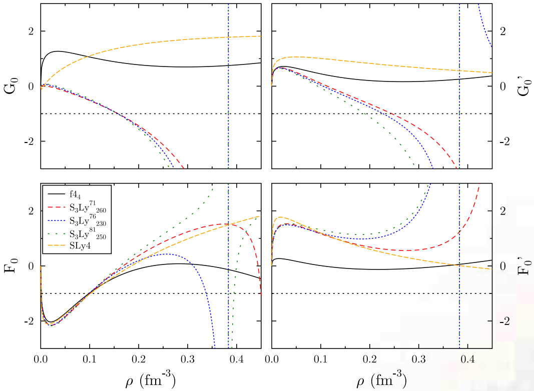


Results

Symmetric Nuclear Matter

Landau parameters : infinite-wavelength instabilities

- Instabilities $F_l < -(2l+1)$, $G_l < -(2l+1)$



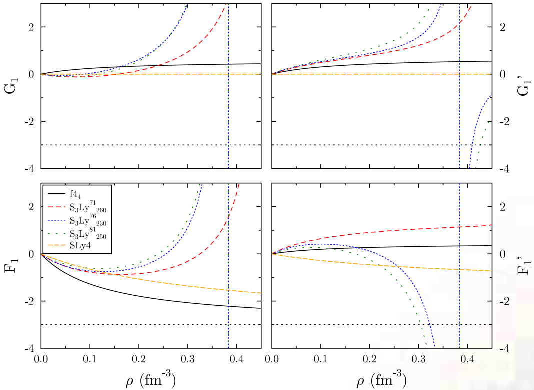
➥ **The weak point** ⇒ known for gradient-less 3B potential [B. D. Chang, PLB56 (1975) 205]

Results

Symmetric Nuclear Matter

Landau parameters : infinite-wavelength instabilities

- Instabilities $F_l < -(2l+1)$, $G_l < -(2l+1)$



➥ **The weak point** $\Rightarrow$ known for gradient-less 3B potential [B. D. Chang, PLB56 (1975) 205]

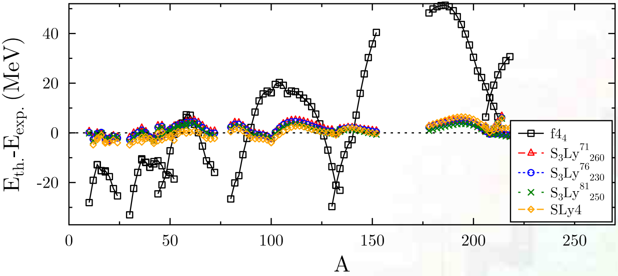
Results

Symmetric Nuclear Matter

Spin instabilities

Systematics : binding energies

Parametrizations	$f4_4$	$S_3Ly^{71}_{260}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotopic chains				
$\bar{\Delta}_E$ (MeV)	4.52	1.97	1.62	1.06	0.21
$\bar{\Delta}_{\|E\|}$ (MeV)	17.54	2.64	2.36	2.02	2.48
σ_E (MeV)	21.67	2.44	2.32	2.12	3.02



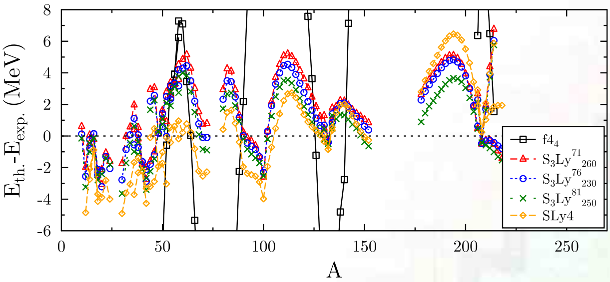
Results

Symmetric Nuclear Matter

Spin instabilities

Systematics : binding energies

Parametrizations	f4_4	$S_3Ly^{71}_{260}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotonic chains				
$\bar{\Delta}_E$ (MeV)	-2.99	0.49	0.21	-0.03	-0.75
$\bar{\Delta}_{\|E\|}$ (MeV)	16.57	1.66	1.50	1.39	1.68
σ_E (MeV)	18.62	1.94	1.83	1.70	1.98



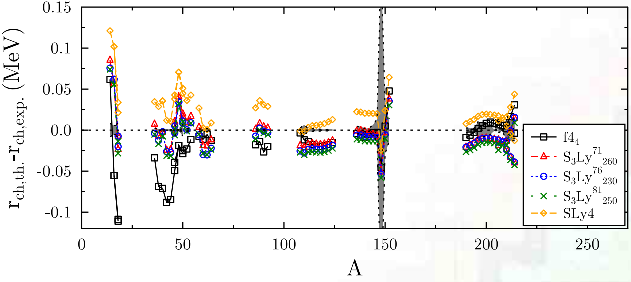
Results

Symmetric Nuclear Matter

Spin instabilities

Systematics : radii

Parametrizations	f4_4	$S_3Ly^{71}_{260}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotopic chains				
$\bar{\Delta}_{r_c}$ (10^{-2} fm)	-2.3	-0.8	-1.3	-1.6	1.9
$\bar{\Delta}_{\lvert r_c \rvert}$ (10^{-2} fm)	2.6	1.8	2.1	2.3	2.0
σ_{r_c} (10^{-2} fm)	3.1	1.9	2.0	1.9	2.2



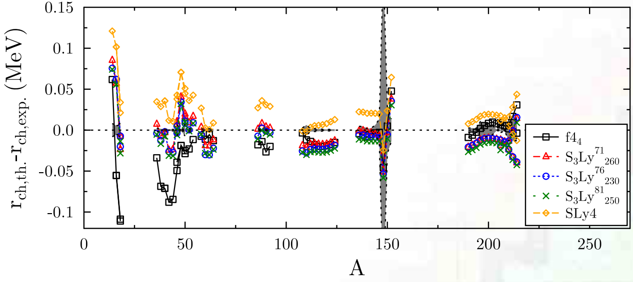
Results

Symmetric Nuclear Matter

Spin instabilities

Systematics : radii

Parametrizations	$f4_4$	$S_3Ly^{71}_{260}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotonic chains				
$\bar{\Delta}_{r_c}$ (10^{-2} fm)	-2.0	0.5	0.1	-0.2	3.6
$\bar{\Delta}_{\vert r_c \vert}$ (10^{-2} fm)	3.0	1.6	1.5	1.7	3.7
σ_{r_c} (10^{-2} fm)	3.4	2.4	2.3	2.3	2.5



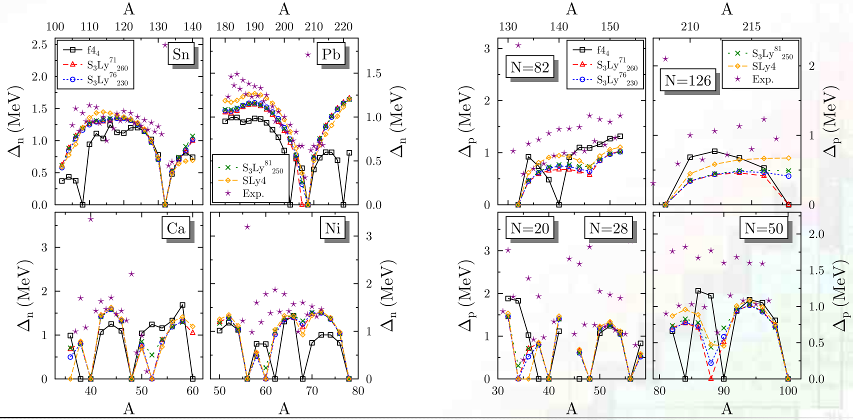
Results

Symmetric Nuclear Matter

Spin instabilities

Systematics : gaps

- Pairing : ULBS (two-body contact interaction) for S_3Ly and SLy4
- Pairing : same pseudo-potential in the normal and pairing channel for $f4_4$



Results

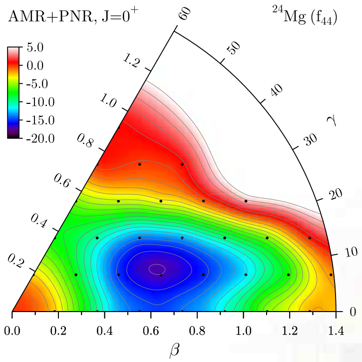
Symmetric Nuclear Matter

Spin instabilities

Binding energies, radii and gaps systematics

Angular momentum and particule number restoration

- Pseudo-potential-based MR-EDF computation possible using f4_4 parameterization



Results

Symmetric Nuclear Matter

Spin instabilities

Binding energies, radii and gaps systematics

Angular momentum and particule number restoration

Conclusions

- **First viable pseudo-potential-based EDF parameterizations**
  - ➥ **Spurious free spectroscopy calculation doable**
  - ➥ **As good phenomenology as modern EDFs ?**

Outlooks

- **Complete central three-body + four-body gradient-less** pseudo-potential param.
- Spin-orbit and tensor three-body pseudo-potential-based functional almost derived
- Post-analysis of the free parameters
- Make use of pseudo-potential-based parameterizations for deformed nuclei
- **Make use of future good parameterizations in MR-EDF calculations**

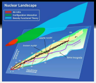
Appendices

Low-energy nuclear physics interests

- Spectrum of $H\,|\Psi_i^A\rangle = E_i^A\,|\Psi_i^A\rangle$ for all $A = N + Z$
- Observables for each state, e.g. $r^2 \equiv \langle\Psi_i^A|\,\sum_k^A \hat{r}_k^2\,|\Psi_i^A\rangle/A$
- Decays between $|\Psi_i\rangle$, i.e. nuclear, electromagnetic, electro-weak

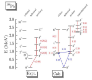
Ground state

Mass, deformation



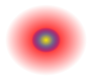
Spectroscopy

Excitations modes



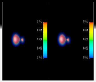
Limits

Drip-lines, halos



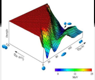
Reaction properties

Fusion, transfer...



Heavy elements

Fission, fusion, SHE



Astrophysics

NS, SN, r-process

Low-energy nuclear physics interests

- Spectrum of $H\,|\Psi_i^A\rangle = E_i^A\,|\Psi_i^A\rangle$ for all $A\!=\!N\!+\!Z$
- Observables for each state, e.g. $r^2 \equiv \langle\Psi_i^A|\sum_k^A \hat{r}_k^2\,|\Psi_i^A\rangle/A$
- Decays between $|\Psi_i\rangle$, i.e. nuclear, electromagnetic, electro-weak

Goals for low-energy nuclear theory

- Model the unknown nuclear Hamiltonian H
- Solve A-body problem and describe properties of nuclei
- Understand states of nuclear matter in astrophysical environments

SR- and MR-EDF steps

Single-Reference EDF : Static collective correlations

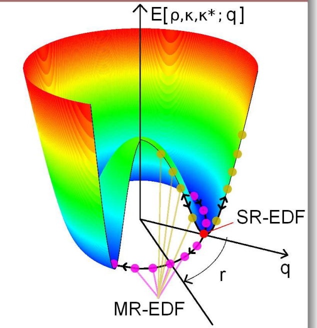
- Invokes single $|\Phi(g)\rangle$ and diagonal energy kernel $E_q^{\text{SR}} \equiv \text{Min}_{|\Phi(g)\rangle} E[g,g]$
- $|\Phi(g)\rangle$ can break symmetries $\Rightarrow$ deformation parameter $g = qe^{ir}$
- Provides first approximation to binding energies, $\langle r^2_{\text{ch}}\rangle$, $\rho(\vec{r})$, β_2 and ESPE $\{\epsilon_i\}$

Multi-Reference : Dynamical collective correlations

- Mixes off-diagonal energy kernels

$$E_k^{MR} \equiv \text{Min}_{\{f_q^k\}} \frac{\sum_{g'g} f_g^{k*} f_{g'}^{k*} E[g',g]\langle\Phi(g')|\Phi(g)\rangle}{\sum_{g'g} f_g^{k*} f_{g'}^{k*} \langle\Phi(g')|\Phi(g)\rangle}$$

- Restores broken symmetries r
- Treats collective vibrations q
  - ➥ Includes associated G.S. correlations
  - ➥ Provides associated collective excitations
- QRPA, Bohr-Hamiltonian are approximations



SR- and MR-EDF steps

Single-Reference EDF : Static collective correlations

- Invokes single $|\Phi(g)\rangle$ and diagonal energy kernel $E_q^{\text{SR}} \equiv \text{Min}_{|\Phi(g)\rangle} E[g,g]$
- $|\Phi(g)\rangle$ can break symmetries $\Rightarrow$ deformation parameter $g = qe^{ir}$
- Provides first approximation to binding energies, $\langle r^2_{\text{ch}}\rangle$, $\rho(\vec{r})$, β_2 and ESPE $\{\epsilon_i\}$

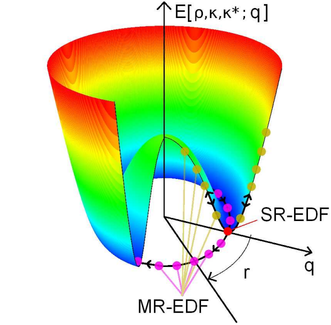
Multi-Reference : Dynamical collective correlations

- Symmetry group $\mathcal{G} = \{R(r)\}$
- Rotate symmetry breaking state

$$|\Phi(r)\rangle = R(r)|\Phi(0)\rangle$$

- Projected energy is obtained thanks to

$$E^{\lambda} = \frac{1}{c^{*}_{\lambda b}c_{\lambda a}}\frac{d_{\lambda}}{v_{\mathcal{G}}}\int_{\mathcal{G}} dm(r) S^{\lambda *}_{ab}(r) E[0,r]$$



SR- and MR-EDF steps

Single-Reference EDF : Static collective correlations

- Invokes single $|\Phi(g)\rangle$ and diagonal energy kernel $E_q^{\text{SR}} \equiv \text{Min}_{|\Phi(g)\rangle} E[g,g]$
- $|\Phi(g)\rangle$ can break symmetries $\Rightarrow$ deformation parameter $g = qe^{ir}$
- Provides first approximation to binding energies, $\langle r^2_{\text{ch}} \rangle$, $\rho(\vec{r})$, β_2 and ESPE $\{\epsilon_i\}$

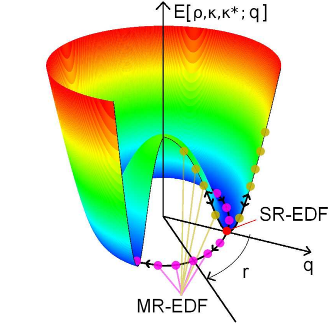
Multi-Reference : Dynamical collective correlations

- Symmetry group $\mathcal{G} = \{R(r)\}$
- Rotate symmetry breaking state

$$|\Phi(r)\rangle = R(r)|\Phi(0)\rangle$$

- Projected energy is obtained thanks to

$$E[0,r]\langle\Phi(0)|\Phi(r)\rangle = \sum_{\lambda ab} c^*_{\lambda b} c_{\lambda a} E^{\lambda} S^{\lambda *}_{ab}(r)$$



➥ Spurious contaminations? Need to focus on the strategy followed to **build** $E[g', g]$

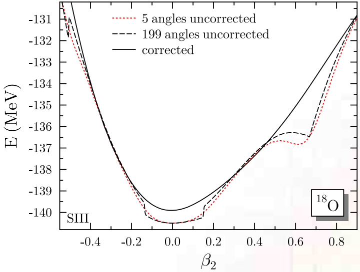
Regularization of EDF kernel

[D. Lacroix *et al.*, PRC79 (2009) 044318] [M. Bender *et al.* PRC79 (2009) 044319] [T. Duguet *et al.* PRC79 (2009) 044320]

Regularized MR calculations

$$E_{\text{REG}} \equiv E[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'\,*}] - E_C[\langle\Phi_{g'}|;|\Phi_g\rangle]$$

- ✔ E^λ is free from divergencies/steps
- ✔ Does not change diagonal EDF kernel
- ✖ Only for integer power of the density



Expansion on $U(1)$ Irreps

$$E[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]\,\langle\Phi_0|\Phi_\varphi\rangle \quad = \quad \sum_{A\in\mathbb{Z}} c_A^2\; E^A\; e^{iA(\varphi)}$$

- $c_A^2 E^A \neq 0$ for $A \leq 0$ $\Rightarrow$ general-EDF formulation
- Regularization restores $c_A^2 E^A = 0$ for $A \leq 0$
- ✖ **Other corrections maybe necessary**

Correction coming from angular momentum restoration

Expansion on $SO(3)$ Irreps

$$E[\rho^{0\Omega}, \kappa^{0\Omega}, \kappa^{\Omega 0\,*}]\, \langle \Phi(0)|\Phi(\Omega)\rangle = \sum_{lmk} c^{*}_{lm} c_{lk}\; E^{l}\; D^{l}_{mk}(\Omega)$$

Pseudo-potential-based EDF method

- Mathematical property of the angular-momentum-restored density potential energy

$$E^{l}_{H} = \frac{1}{2} \int d\vec{R}\, d\vec{r}\; V(r)\, \rho^{[2]}_{lmlm}(\vec{R},\vec{r}) = \int d\vec{R} \sum_{l'=0}^{2l} \mathcal{V}^{l'0}_{l}(R)\;\; C^{lm}_{lml'0} Y^{0}_{l'}(\hat{R})$$

[T. Duguet, J. Sadoudi, J.Phys.G 37 (2010) 064009]

General EDF method

- Correction on general EDF kernel to ensure such property still do be derived

Energy kernel from Skyrme pseudo-potential

Skyrme pseudo-Hamiltonian : 2+3+4-body

$$H_{\text{pseudo}} \equiv + \frac{1}{2!} \sum_{ijkl} \langle \hat{v}_{12} \rangle_{ijkl} \, a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{3!} \sum_{ijklmn} \langle \hat{v}_{123} \rangle_{ijklmn} \, a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l + \frac{1}{4!} \sum_{ijklmnop} \langle \hat{v}_{1234} \rangle_{ijklmnop} \, a_i^\dagger a_j^\dagger a_k^\dagger a_l^\dagger a_p a_o a_n a_m \; ,$$

where

$$\langle \hat{O}_{12} \rangle_{ijkl} \equiv \langle ij | \hat{O}_{12} | kl \rangle$$
$$\langle \hat{O}_{123} \rangle_{ijklmn} \equiv \langle ijk | \hat{O}_{123} | lmn \rangle$$
$$\langle \hat{O}_{1234} \rangle_{ijklmnop} \equiv \langle ijkl | \hat{O}_{1234} | mnop \rangle$$

Energy kernel from Skyrme pseudo-potential

Skyrme pseudo-Hamiltonian : 2+3+4-body

Energy kernel

- Energy kernel through $\langle \Phi(g) | H_{\text{pseudo}} | \Phi(g) \rangle$ and Standard Wick Theorem

Normal part

$$E_H^{\rho\rho} = \frac{1}{2} \sum_{ijkl} \langle \hat{v}_{12} \mathcal{A}_{12} \rangle_{ijkl} \, \rho_{ki} \, \rho_{lj}$$

$$E_H^{\rho\rho\rho} = \frac{1}{6} \sum_{ijklmn} \langle \hat{v}_{123} \mathcal{A}_{123} \rangle_{ijklmn} \, \rho_{li} \, \rho_{mj} \, \rho_{nk}$$

$$E_H^{\rho\rho\rho\rho} = \frac{1}{24} \sum_{ijklmnop} \langle \hat{v}_{1234} \mathcal{A}_{1234} \rangle_{ijklmnop} \, \rho_{mi} \, \rho_{nj} \, \rho_{ok} \, \rho_{pl}$$

- Pauli principle $\Rightarrow$ antisymmetrizers

$$\mathcal{A}_{12} \equiv 1 - P_{12}$$
$$\mathcal{A}_{123} \equiv (1 - P_{13} - P_{23}) \mathcal{A}_{12}$$
$$\mathcal{A}_{1234} \equiv (1 - P_{14} - P_{24} - P_{34}) \mathcal{A}_{123}$$

Energy kernel from Skyrme pseudo-potential

Skyrme pseudo-Hamiltonian : 2+3+4-body

Energy kernel

- Energy kernel through $\langle\Phi(g)|H_{\text{pseudo}}|\Phi(g)\rangle$ and Standard Wick Theorem

Pairing part

$$E_H^{\kappa\kappa} = \frac{1}{2}\sum_{ijkl}\langle\hat{v}_{12}\rangle_{ijkl}\;\kappa^{\dagger}_{ij}\kappa_{kl}$$

$$E_H^{\kappa\kappa\rho} = \frac{1}{6}\sum_{ijklmn}\langle\mathcal{A}^{12}_{123}\,\hat{v}_{123}\mathcal{A}^{12}_{123}\rangle_{ijklmn}\;\kappa^{\dagger}_{ij}\kappa_{lm}\rho_{nk}$$

$$E_H^{\kappa\kappa\rho\rho} = \frac{1}{24}\sum_{ijklmnop}\langle\mathcal{A}^{12S}_{1234}\,\hat{v}_{1234}\mathcal{A}^{12}_{1234}\rangle_{ijklmnop}\;\kappa^{\dagger}_{ij}\kappa_{mn}\rho_{ok}\rho_{pl}$$

$$E_H^{\kappa\kappa\kappa\kappa} = \frac{1}{24}\sum_{ijklmnop}\langle\mathcal{A}^{12}_{123}\,\hat{v}_{1234}\mathcal{A}^{12}_{123}\rangle_{ijklmnop}\;\kappa^{\dagger}_{ij}\kappa^{\dagger}_{kl}\kappa_{mn}\kappa_{op}$$

- Pauli principle $\Rightarrow$ exchange operators

$$\mathcal{A}^{12}_{123} \equiv (1 - P_{13} - P_{23}) \qquad \mathcal{A}^{12}_{1234} \equiv (1 - P_{14} - P_{24} - P_{34})\mathcal{A}^{12}_{123}$$

$$\mathcal{A}^{12S}_{1234} \equiv (1 - P_{13} - P_{23} - P_{14} - P_{24} - P_{34})$$

Construction of the Skyrme pseudo-potential

Symmetry under particles exchange

- Pseudo-potentials have to be symmetric under particles exchange, i.e.

$$\hat{v}_{12} = \hat{v}_{\overline{12}} = \hat{v}_{\overline{21}} \quad \rightarrow \quad \langle \hat{v}_{12} \rangle_{ijkl} = \langle \hat{v}_{12} \rangle_{jilk}$$
$$\hat{v}_{123} = \hat{v}_{\overline{123}} = \hat{v}_{\overline{213}} = \hat{v}_{\overline{132}} = \hat{v}_{\overline{321}} = \hat{v}_{\overline{312}} = \hat{v}_{\overline{231}}$$
$$\hat{v}_{1234} = \hat{v}_{\overline{1234}} = \hat{v}_{\overline{2134}} = \hat{v}_{\overline{1324}} = \hat{v}_{\overline{3214}} = \hat{v}_{\overline{3124}} = \hat{v}_{\overline{2314}} = \cdots$$

- We will make use of two-body symmetric operators $(\hat{\delta}_{r_i r_j}, \hat{\vec{k}}_{ij}, \hat{\vec{k}}'_{ij}, \hat{P}^{\sigma}_{ij})$
- Three-body and four-body potential can be defined following

$$\begin{aligned}
\hat{v}_{123} &\equiv \hat{v}_{\overline{123}} + \hat{v}_{\overline{132}} + \hat{v}_{\overline{231}} \\
\hat{v}_{1234} &\equiv \hat{v}_{\overline{1234}} + \hat{v}_{\overline{1243}} + \hat{v}_{\overline{1342}} + \hat{v}_{\overline{2341}} \\
&\equiv \hat{v}_{\overline{1234}} + \hat{v}_{\overline{1324}} + \hat{v}_{\overline{2314}} + \hat{v}_{\overline{1243}} + \hat{v}_{\overline{1423}} + \hat{v}_{\overline{2413}} \\
&\quad + \hat{v}_{\overline{1342}} + \hat{v}_{\overline{1432}} + \hat{v}_{\overline{3412}} + \hat{v}_{\overline{2341}} + \hat{v}_{\overline{2431}} + \hat{v}_{\overline{3421}}
\end{aligned}$$

- One just have to define $\hat{v}_{\overline{12}}$, $\hat{v}_{\overline{123}}$ and $\hat{v}_{\overline{1234}}$ to get $\hat{v}_{12}$, $\hat{v}_{123}$ and $\hat{v}_{1234}$

Construction of the Skyrme pseudo-potential

Symmetry under particles exchange

- One just have to define $\hat{v}_{\overline{12}}$, $\hat{v}_{\overline{123}}$ and $\hat{v}_{\overline{1234}}$ to get $\hat{v}_{12}$, $\hat{v}_{123}$ and $\hat{v}_{1234}$

Skyrme pseudo-potential ingredients

- Aim : Construct the most general $\hat{v}_{\overline{12}}$, $\hat{v}_{\overline{123}}$ and $\hat{v}_{\overline{1234}}$ Skyrme pseudo-potentials
  - ➥ i.e. identify all 2-, 3- and 4-body operators providing independent EDF terms
- Kronecker operators
  - ➥ $\hat{\delta}_{r_i r_j}$ with $i \neq j \in \{1,2,3,4\}^2$
- Gradients operators
  - ➥ $\hat{\vec{k}}_{ij} = -\frac{i}{2}(\hat{\vec{\nabla}}_i - \hat{\vec{\nabla}}_j)$, $\hat{\vec{k}}'_{ij} = \frac{i}{2}(\hat{\vec{\nabla}}'_i - \hat{\vec{\nabla}}'_j)$ with $i \neq j \in \{1,2,3,4\}^2$
- Exchange operators
  - ➥ P^r_{ij}, P^σ_{ij}, P^τ_{ij} with $i \neq j \in \{1,2,3,4\}^2$
- Generates all possibilities which are hermitian

Construction of the Skyrme pseudo-potential

Symmetry under particles exchange

- One just have to define $\hat{v}_{\overline{12}}$, $\hat{v}_{\overline{123}}$ and $\hat{v}_{\overline{1234}}$ to get $\hat{v}_{12}$, $\hat{v}_{123}$ and $\hat{v}_{1234}$

Skyrme pseudo-potential ingredients

- Aim : Construct the most general $\hat{v}_{\overline{12}}$, $\hat{v}_{\overline{123}}$ and $\hat{v}_{\overline{1234}}$ Skyrme pseudo-potentials
- Using : Kronecker, gradients and exchange operators
- Generates all possibilities which are hermitian

Energy functional derivation

- The third and fourth particle provides many possibilities a priori
- Two- and three-body central potential up to second order in gradients
- Two-body spin-orbit and four-body gradient-less potentials
  - ➥ Generates around 120 parameters/different terms a priori
- Derivation straightforward but almost impossible by hand for 120 terms
- Development of a **formal computation code**
- Identification of correlated terms via Singular Value Decomposition

Two-body case (known)

Skyrme pseudo-potential

- Two-body Skyrme operators providing independent terms in $E_H^{\rho\rho}$ and $E_H^{\kappa\kappa}$

$$
\begin{aligned}
\hat{v}_{12} = & \; t_0 \left(1 + x_0 P^{\sigma}_{12}\right) \hat{\delta}_{r_1 r_2} \\
& + \frac{t_1}{2} \left(1 + x_1 P^{\sigma}_{12}\right) \left(\hat{\vec{k}}'^{2}_{12} + \hat{\vec{k}}^{2}_{12}\right) \hat{\delta}_{r_1 r_2} \\
& + t_2 \left(1 + x_2 P^{\sigma}_{12}\right) \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}_{12} \, \hat{\delta}_{r_1 r_2} \\
& + i W_0 \left(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2\right) \hat{\vec{k}}'_{12} \wedge \hat{\vec{k}}_{12}
\end{aligned}
$$

Bilinear Skyrme functional (energy density) : Normal part

$$
\mathcal{E}^{\rho\rho}_{H,\text{even}}(\vec{r}) = \sum_{t=0,1} A^{\rho}_t \rho_t^2 + A^{\tau}_t \rho_t \tau_t + A^{\nabla\rho}_t \vec{\nabla}\rho_t \cdot \vec{\nabla}\rho_t + \sum_{\mu\nu} A^{J}_t J_{t,\mu\nu} J_{t,\mu\nu} + A^{\nabla J}_t \rho_t \vec{\nabla} \cdot \vec{J}_t
$$

$$
\mathcal{E}^{\rho\rho}_{H,\text{odd}}(\vec{r}) = \sum_{t=0,1} A^{s}_t \vec{s}_t^{\,2} + A^{T}_t \vec{s}_t \vec{T}_t + \sum_{\mu\nu} A^{\nabla s}_t \nabla_\mu s_{t,\nu} \nabla_\mu s_{t,\nu} + A^{j}_t \vec{j}_t \cdot \vec{j}_t + A^{\nabla j}_t \vec{s}_t \cdot \vec{\nabla} \times \vec{j}_t
$$

Two-body case (known)

Skyrme pseudo-potential

- Two-body Skyrme operators providing independent terms in $E_H^{\rho\rho}$

$$\hat{v}_{12} = t_0\left(1 + x_0 P_{12}^{\sigma}\right)\hat{\delta}_{r_1 r_2} + \frac{t_1}{2}\left(1 + x_1 P_{12}^{\sigma}\right)\left(\hat{\vec{k}}_{12}^{\prime 2} + \hat{\vec{k}}_{12}^{2}\right)\hat{\delta}_{r_1 r_2} + t_2\left(1 + x_2 P_{12}^{\sigma}\right)\hat{\vec{k}}_{12}^{\prime} \cdot \hat{\vec{k}}_{12}\,\hat{\delta}_{r_1 r_2} + iW_0\,(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2)\hat{\vec{k}}_{12}^{\prime} \wedge \hat{\vec{k}}_{12}$$

Bilinear Skyrme functional (energy density) : Pairing part

$$\mathcal{E}_H^{\kappa\kappa}(\vec{r}) = \sum_{t=0,1} A_t^{\tilde{\rho}}\tilde{\rho}_t^2 + A_t^{\tilde{\tau}}\tilde{\rho}_t\tilde{\tau}_t + A_t^{\nabla\tilde{\rho}}\vec{\nabla}\tilde{\rho}_t \cdot \vec{\nabla}\tilde{\rho}_t + \sum_{\mu\nu} A_t^{\tilde{J}}\tilde{J}_{t,\mu\nu}\tilde{J}_{t,\mu\nu} + \sum_{\mu\nu} A_t^{\tilde{J}W}\left(\tilde{J}_{t,\mu\mu}\tilde{J}_{t,\nu\nu} - \tilde{J}_{t,\mu\nu}\tilde{J}_{t,\nu\mu}\right)$$

Two-body case (known)

Skyrme pseudo-potential

Bilinear Skyrme functional (derived by code)

Bilinear functional coefficients (derived by code)

		t_0	t_0x_0	t_1	t_1x_1	t_2	t_2x_2	W_0
A_0^ρ	$=$	$+\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$
A_1^ρ	$=$	$-\frac{1}{8}$	$-\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
A_0^τ	$=$	$+0$	$+0$	$+\frac{3}{16}$	$+0$	$+\frac{5}{16}$	$+\frac{1}{4}$	$+0$
A_1^τ	$=$	$+0$	$+0$	$-\frac{1}{16}$	$-\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+0$
$A_0^{\nabla\rho}$	$=$	$+0$	$+0$	$+\frac{9}{64}$	$+0$	$-\frac{5}{64}$	$-\frac{1}{16}$	$+0$
$A_1^{\nabla\rho}$	$=$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{32}$	$-\frac{1}{64}$	$-\frac{1}{32}$	$+0$
A_0^J	$=$	$+0$	$+0$	$+\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$+0$
$\vdots$		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Three-body case (new)

Skyrme pseudo-potential

- Final three-body Skyrme pseudo-potential

$$
\begin{aligned}
\hat{v}_{123} &\equiv \hat{v}_{\overline{123}} + \hat{v}_{\overline{132}} + \hat{v}_{\overline{231}} \\
\hat{v}_{\overline{123}} &= u_0 \; \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
&\quad + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{12}\right] \left(\hat{\vec{k}}_{12} \cdot \hat{\vec{k}}_{12} + \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}'_{12}\right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
&\quad + u_2 \left[1 + y_{21} P^{\sigma}_{12} + y_{22} (P^{\sigma}_{13} + P^{\sigma}_{23})\right] \left(\hat{\vec{k}}_{12} \cdot \hat{\vec{k}}'_{12}\right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3}
\end{aligned}
$$

Three-body case (new)

Skyrme pseudo-potential

- Final three-body Skyrme pseudo-potential

$$\begin{aligned}
\hat{v}_{123} = & \, u_0 \left(\hat{\delta}_{r_1 r_3}\hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2}\hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1}\hat{\delta}_{r_3 r_1}\right) \\
& + \frac{u_1}{2}\left[1 + y_1 P^{\sigma}_{12}\right]\left(\hat{\vec{k}}_{12}\cdot\hat{\vec{k}}_{12} + \hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}'_{12}\right)\hat{\delta}_{r_1 r_3}\hat{\delta}_{r_2 r_3} \\
& + \frac{u_1}{2}\left[1 + y_1 P^{\sigma}_{31}\right]\left(\hat{\vec{k}}_{31}\cdot\hat{\vec{k}}_{31} + \hat{\vec{k}}'_{31}\cdot\hat{\vec{k}}'_{31}\right)\hat{\delta}_{r_3 r_2}\hat{\delta}_{r_1 r_2} \\
& + \frac{u_1}{2}\left[1 + y_1 P^{\sigma}_{23}\right]\left(\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}_{23} + \hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}'_{23}\right)\hat{\delta}_{r_2 r_1}\hat{\delta}_{r_3 r_1} \\
& + u_2\left[1 + y_{21} P^{\sigma}_{12} + y_{22}(P^{\sigma}_{13} + P^{\sigma}_{23})\right]\left(\hat{\vec{k}}_{12}\cdot\hat{\vec{k}}'_{12}\right)\hat{\delta}_{r_1 r_3}\hat{\delta}_{r_2 r_3} \\
& + u_2\left[1 + y_{21} P^{\sigma}_{31} + y_{22}(P^{\sigma}_{32} + P^{\sigma}_{12})\right]\left(\hat{\vec{k}}_{31}\cdot\hat{\vec{k}}'_{31}\right)\hat{\delta}_{r_3 r_2}\hat{\delta}_{r_1 r_2} \\
& + u_2\left[1 + y_{21} P^{\sigma}_{23} + y_{22}(P^{\sigma}_{21} + P^{\sigma}_{31})\right]\left(\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{23}\right)\hat{\delta}_{r_2 r_1}\hat{\delta}_{r_3 r_1}
\end{aligned}$$

Three-body case (new)

Skyrme pseudo-potential

Trilinear Skyrme functional (energy density) : Normal part

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

$$+ B^{\tau}_{10} \rho_1 \rho_1 \tau_0 + B^{\nabla\rho}_{10} \rho_1 \vec{\nabla}\rho_1 \cdot \vec{\nabla}\rho_0 + \sum_{\mu\nu} B^{J}_{10} \rho_1 J_{1,\mu\nu} J_{0,\mu\nu}$$

$$\mathcal{E}^{\rho\rho\rho}_{H,\text{odd}} = \sum_{t=0,1} \Big\{ B^{s}_{t} \rho_0 \vec{s}_t^{\,2} + B^{T}_{t} \rho_0 \vec{s}_t \cdot \vec{T}_t + \sum_{\mu\nu} B^{\nabla s}_{t} \rho_0 \nabla_\mu s_{t,\nu} \nabla_\mu s_{t,\nu} + B^{j}_{t} \rho_0 \vec{j}_t \cdot \vec{j}_t$$

$$+ B^{T}_{t\bar{t}} \rho_1 \vec{s}_t \cdot \vec{T}_{\bar{t}} + B^{\tau s}_{t} \vec{s}_0 \vec{s}_t \tau_t + \sum_{\mu\nu} \Big[B^{\nabla\rho s}_{t} s_{0,\nu} \nabla_\mu \rho_t \nabla_\mu s_{t,\nu}$$

$$+ B^{\nabla\rho s}_{t\bar{t}} s_{1,\nu} \nabla_\mu \rho_t \nabla_\mu s_{\bar{t},\nu} + B^{Js}_{t} s_{0,\nu} j_{t,\mu} J_{t,\mu\nu} + B^{Js}_{t\bar{t}} s_{1,\nu} j_{t,\mu} J_{\bar{t},\mu\nu} \Big]$$

$$+ \sum_{\mu\nu\lambda k} \epsilon_{\nu\lambda k} \Big[B^{\nabla s J}_{t} s_{0,k} \nabla_\mu s_{t,\nu} J_{t,\mu\lambda} + B^{\nabla s J}_{t\bar{t}} s_{1,k} \nabla_\mu s_{t,\nu} J_{\bar{t},\mu\lambda} \Big] \Big\}$$

$$+ B^{s}_{10} \rho_1 \vec{s}_1 \cdot \vec{s}_0 + B^{\nabla s}_{10} \rho_1 \nabla_\mu s_{1,\nu} \nabla_\mu s_{0,\nu} + B^{j}_{10} \rho_1 \vec{j}_1 \cdot \vec{j}_0 + B^{\tau s}_{10} \vec{s}_1 \vec{s}_1 \tau_0$$

Three-body case (new)

Skyrme pseudo-potential

Trilinear Skyrme functional (energy density) : Pairing part

$$\mathcal{E}_H^{\kappa\kappa\rho} = \sum_{t=0,1} \Big\{ B_{tt}^{\tilde\rho}\,\rho_0\tilde\rho_t^2 + B_{t\bar t}^{\tilde\rho}\,\rho_1\tilde\rho_{\bar t}\tilde\rho_t + B_{tt}^{\tau\tilde\rho}\,\tau_0\tilde\rho_t^2 + B_{t\bar t}^{\tau\tilde\rho}\,\tau_1\tilde\rho_{\bar t}\tilde\rho_t$$

$$+ B_{tt}^{\nabla\tilde\rho}\,\rho_0\vec\nabla\tilde\rho_t\cdot\vec\nabla\tilde\rho_t + B_{t\bar t}^{\nabla\tilde\rho}\,\rho_1\vec\nabla\tilde\rho_{\bar t}\cdot\vec\nabla\tilde\rho_t + B_{tt}^{\tilde\rho\nabla\tilde\rho}\,\vec\nabla\rho_0\cdot\vec\nabla\tilde\rho_t\tilde\rho_t$$

$$+ B_{t\bar t}^{\tilde\rho\nabla\tilde\rho}\,\vec\nabla\rho_1\cdot\vec\nabla\tilde\rho_{\bar t}\tilde\rho_t + \sum_{\mu\nu} B_{tt}^{\tilde J}\,\rho_0\tilde J_{t,\mu\nu}\tilde J_{t,\mu\nu} + \sum_{\mu\nu} B_{t\bar t}^{\tilde J}\,\rho_1\tilde J_{\bar t,\mu\nu}\tilde J_{t,\mu\nu}$$

$$+ \sum_{\mu\nu} B_{tt}^{J\tilde J}\,J_{0,\mu\nu}\tilde\rho_t\tilde J_{t,\mu\nu} + \sum_{\mu\nu} B_{t\bar t}^{J\tilde J}\,J_{1,\mu\nu}\tilde\rho_{\bar t}\tilde J_{t,\mu\nu} \Big\}$$

Three-body case (new)

Skyrme pseudo-potential

Trilinear Skyrme functional (derived by code)

Trilinear functional coefficients (derived by code)

		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}	=	$+0$	$-\frac{1}{16}$	$-\frac{1}{32}$	$+\frac{1}{32}$	$+\frac{1}{16}$	$-\frac{1}{16}$
$B_0^{\nabla\rho}$	=	$+0$	$+\frac{15}{128}$	$+0$	$-\frac{15}{256}$	$-\frac{3}{64}$	$-\frac{3}{128}$
$B_{10}^{\nabla\rho}$	=	$+0$	$-\frac{5}{64}$	$+\frac{1}{32}$	$+\frac{5}{128}$	$+\frac{1}{32}$	$+\frac{7}{64}$
$B_1^{\nabla\rho}$	=	$+0$	$-\frac{5}{128}$	$-\frac{1}{32}$	$-\frac{7}{256}$	$-\frac{1}{32}$	$-\frac{5}{128}$
	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Four-body case (new)

Skyrme pseudo-potential

- Final three-body Skyrme pseudo-potential

$$\begin{aligned}\hat{v}_{1234} \equiv\, & \hat{v}_{\overline{12}34} + \hat{v}_{\overline{13}24} + \hat{v}_{\overline{23}14} + \hat{v}_{\overline{12}43} + \hat{v}_{\overline{14}23} + \hat{v}_{\overline{24}13} \\ & + \hat{v}_{\overline{13}42} + \hat{v}_{\overline{14}32} + \hat{v}_{\overline{34}12} + \hat{v}_{\overline{23}41} + \hat{v}_{\overline{24}31} + \hat{v}_{\overline{34}21} \\ \hat{v}_{\overline{12}34} =\, & v_0\, \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4}\end{aligned}$$

Four-body case (new)

Skyrme pseudo-potential

- Final three-body Skyrme pseudo-potential

$$\hat{v}_{1234} = v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \hat{\delta}_{r_1 r_2} \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_2 r_4} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \hat{\delta}_{r_1 r_4} + \cdots \right)$$

Bilinear Skyrme functional (energy density) : normal and pairing part

$$\mathcal{E}^{\rho\rho\rho\rho}_{H,\text{even}}(\vec{r}) = \sum_{t=0,1} C^{\rho}_{t} \rho_t^4 + C^{\rho}_{01} \rho_0^2 \rho_1^2$$

$$\mathcal{E}^{\rho\rho\rho\rho}_{H,\text{odd}}(\vec{r}) = \sum_{t=0,1} \left\{ C^{s}_{t} \vec{s}_t^{\,4} + C^{\rho s}_{tt} \rho_t^2 \vec{s}_t^{\,2} + C^{\rho s}_{t\bar{t}} \rho_{\bar{t}}^2 \vec{s}_t^{\,2} \right\} + C^{\rho\rho s s} \rho_0 \rho_1 \vec{s}_0 \vec{s}_1 + C^{s}_{01} \vec{s}_0^{\,2} \vec{s}_1^{\,2}$$

$$\mathcal{E}^{\kappa\kappa\rho\rho}_{H}(\vec{r}) = \sum_{t=0,1} \left\{ C^{\tilde{\rho}\rho}_{tt} \rho_t^2 \tilde{\rho}_t^2 + C^{\tilde{\rho}\rho}_{t\bar{t}} \rho_{\bar{t}}^2 \tilde{\rho}_t^2 \right\} + C^{\rho\rho\tilde{\rho}\tilde{\rho}} \rho_0 \rho_1 \tilde{\rho}_0 \tilde{\rho}_1$$

$$\mathcal{E}^{\kappa\kappa\kappa\kappa}_{H}(\vec{r}) = \sum_{t=0,1} \left\{ C^{\tilde{\rho}\tilde{\rho}}_{tt} \tilde{\rho}_t^4 + C^{\tilde{\rho}\tilde{\rho}}_{t\bar{t}} \tilde{\rho}_{\bar{t}}^2 \tilde{\rho}_t^2 \right\}$$

Four-body case (new)

Skyrme pseudo-potential

Bilinear Skyrme functional

Bilinear functional coefficients

		v_0
C_0^ρ	$=$	$+\frac{3}{64}$
C_1^ρ	$=$	$+\frac{3}{64}$
C_{01}^ρ	$=$	$-\frac{3}{32}$
C_0^s	$=$	$+\frac{3}{64}$
C_1^s	$=$	$+\frac{3}{64}$
$C_{00}^{\rho s}$	$=$	$-\frac{3}{32}$
$C_{11}^{\rho s}$	$=$	$-\frac{3}{32}$
$C_{10}^{\rho s}$	$=$	$-\frac{3}{32}$
$C_{01}^{\rho s}$	$=$	$-\frac{3}{32}$
	$\vdots$	$\vdots$

Motivation

General-EDF

- Good-quality EDF parameterization of reference : **SLy4**

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

Pseudo-potential-based EDF

- Aim : Get a pseudo-potential parameterization as good as **SLy4**
  - ➥ Similar fitting procedure used

➘ 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

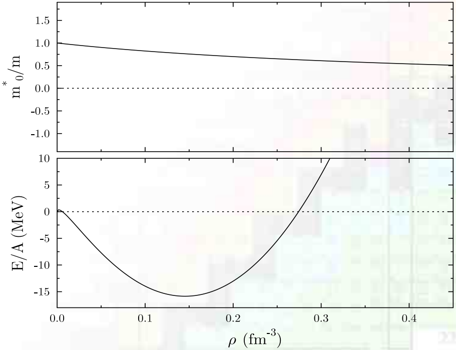
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\, \rho_0^{2/3} + \frac{3}{8} t_0\, \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{16} u_0\, \rho_0^2$$

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

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

SIII parameterization

- $\rho_{\mathrm{sat}} = 0.145\ (0.16 \pm 0.002)$ 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

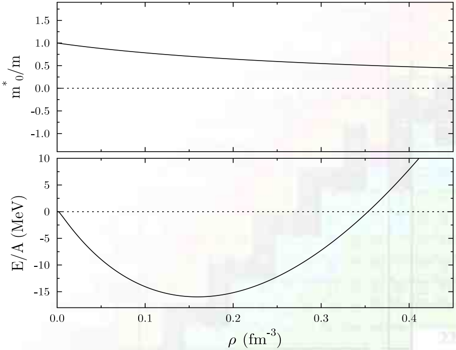
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\, \rho_0^{2/3} + \frac{3}{8} t_0\, \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{1}{16} u_0\, \rho_0^{1+\alpha}$$

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

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

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

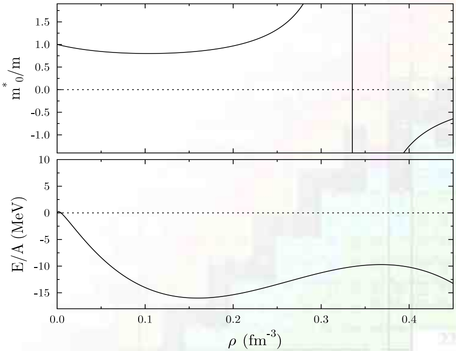
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{16} u_0 \rho_0^2 + \frac{3}{80} c_s \Theta_{3s} \rho_0^{8/3}$$

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

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

Our parameterization

- $\rho_{\text{sat}} = 0.16\ (0.16 \pm 0.002)\ \text{fm}^{-3}$
- ➥ $\frac{E}{A} = -16\ (-16.0 \pm 0.2)$ 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

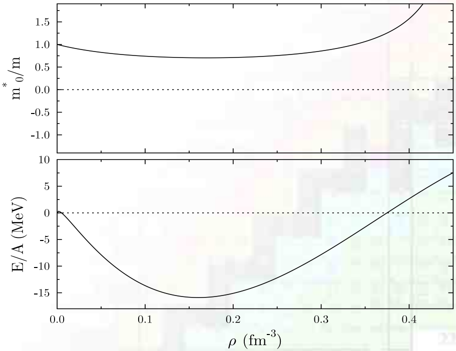
$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_s\, \rho_0^{2/3} + \frac{3}{8} t_0\, \rho_0 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{16} u_0\, \rho_0^2 + \frac{3}{80} c_s \Theta_{3s} \rho_0^{8/3}$$

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

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

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

Set of parameterizations

- Produce a set of parameterizations

➥ $S_3Ly^{71}_{260}$ ➥ $S_3Ly^{73}_{250}$ ➥ $S_3Ly^{76}_{230}$ ➥ $S_3Ly^{81}_{250}$

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