Generator coordinate method with variational basis generation

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Multi-reference EDF method with variational basis generation

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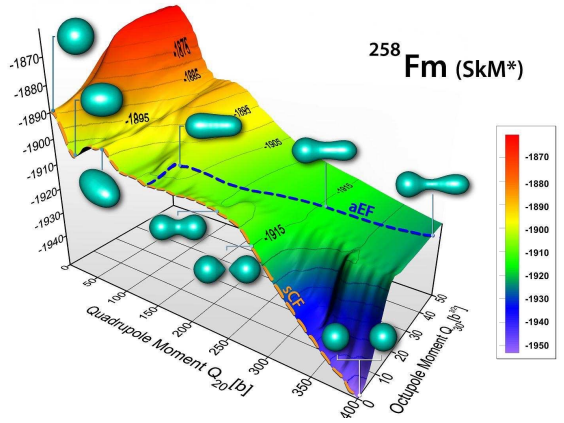
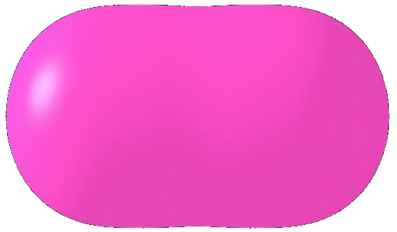
Nuclear collective motion

J. Dobaczewski, J. Phys.: Conf. Ser. **312** 092002 (2011).

Collectivity plays an important role in nuclear many-body physics





Ex.) Nuclear fission

Our goal is fundamental:

Develop better method to describe **collective motion** in **microscopic** way

all nucleons are treated as dynamical degrees of freedom

Conventional method

Basis: a priori selected

$$|\Psi\rangle = f_1 \left|\ \right\rangle + f_2 \left|\ \right\rangle + f_3 \left|\ \right\rangle + f_4 \left|\ \right\rangle + \cdots$$

Weight functions are variational parameter

Details in next slide

Generator Coordinate Method

Trial many-body wave function

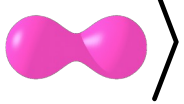
$$|\Psi\rangle = \sum_a f_a |\Phi_a\rangle$$

basis: a priori selected SD

Weight function f are variational parameters

How to prepare appropriate bases ???

$|\Psi_a\rangle = |\Psi(a)\rangle$ a: properly chosen “collective” coordinates

$|\Psi\rangle = f_1 |$  $\rangle + f_2 |$  $\rangle + f_3 |$  $\rangle + f_4 |$  $\rangle + \cdots$

Collective coordinates: deformation parameter Q_2

Generator Coordinate Method

Trial many-body wave function

$$|\Psi\rangle = \sum_a f_a |\Phi_a\rangle$$

basis: a priori selected SD

Weight function f are variational parameters

How to prepare appropriate bases ???

$|\Psi_a\rangle = |\Psi(a)\rangle$ a: properly chosen “collective” coordinates

Problem: Arbitrariness / needs careful physical consideration to determine collective coordinates

Our idea

Trial many-body wave function

$$|\Psi\rangle = \sum_a f_a |\Phi_a\rangle$$

Both bases and weight functions are variational parameters

How to prepare appropriate bases ???

Not necessary to choose collective coordinates !!!

- ✓ Basis states are optimized automatically
- ✓ May produce more suitable bases

Variational basis optimization

Trial function:

$$|\Psi\rangle = \sum_a f_a |\Phi_a\rangle \qquad \Phi_a = \mathcal{A}[\varphi_1^{(a)} \varphi_2^{(a)} \cdots \varphi_N^{(a)}]$$

Slater determinant — Single particle states (orthonormal set)

Total energy to be minimized:

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\sum_{ab} f_a^* f_b H_{ab}}{\sum_{ab} f_a^* f_b N_{ab}}$$

$$\begin{aligned}
H_{ab} &= \langle\Phi_a|H|\Phi_b\rangle && : \text{Hamiltonian kernel} \\
N_{ab} &= \langle\Phi_a|\Phi_b\rangle && : \text{Norm kernel} \\
\rho^{(ab)}_{\beta\alpha} &= \frac{\langle\Phi_a|\, a^\dagger_\alpha a_\beta \,|\Phi_b\rangle}{\langle\Phi_a|\Phi_b\rangle} && : \text{Transition density} \\
E^{(ab)} &= E[\rho^{(ab)}] && : \text{EDF} \\
h^{(ab)}_{\alpha\beta} &= \frac{\delta E[\rho^{(ab)}]}{\delta \rho^{(ab)}_{\beta\alpha}} && : \text{HF Hamiltnian}
\end{aligned}$$

Variational basis optimization

Gradient of Energy

- Single particle states

  Variation restricted to particle-hole direction $\left\langle \varphi_i^{(a)} \right| \to \left\langle \varphi_i^{(a)} \right| + \left\langle \delta\varphi_i^{(a)} \right| (1-\rho^{(a)})$

$$\frac{\delta E}{\delta \langle \varphi_i^{(a)}|_{ph}} = \sum_b \frac{f_a^* N_{ab} f_b}{\langle \Psi|\Psi\rangle} \left(1-\rho^{(ab)}\right) \left[E - E^{(ab)} + h^{(ab)}\rho^{(ab)}\right] |\varphi_i^{(a)}\rangle$$

- Weight function

$$\frac{\partial E}{\partial f_a^*} = \frac{1}{\langle \Psi|\Psi\rangle} \sum_b (H_{ab} - E N_{ab}) f_b$$

(=0 Hill-Wheeler eq.)

$$\begin{aligned}
H_{ab} &= \langle \Phi_a | H | \Phi_b \rangle && : \text{Hamiltonian kernel} \\
N_{ab} &= \langle \Phi_a | \Phi_b \rangle && : \text{Norm kernel} \\
\rho^{(ab)}_{\beta\alpha} &= \frac{\langle \Phi_a | \, a_\alpha^\dagger a_\beta \, | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle} && : \text{Transition density} \\
E^{(ab)} &= E[\rho^{(ab)}] && : \text{EDF} \\
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\end{aligned}$$

Set up

Volkov interaction No.1 A. B. Volkov, Nucl. Phys. 74 (1965).

$$V(r) = \sum_{i=1,2} (W_i - M_i P_\sigma P_\tau) e^{-r^2/r_i^2}$$: effective nuclear force

No Coulomb interaction

Axial / reflection / time-reversal symmetry

Basis expansion with axial harmonic oscillator

^{20}Ne

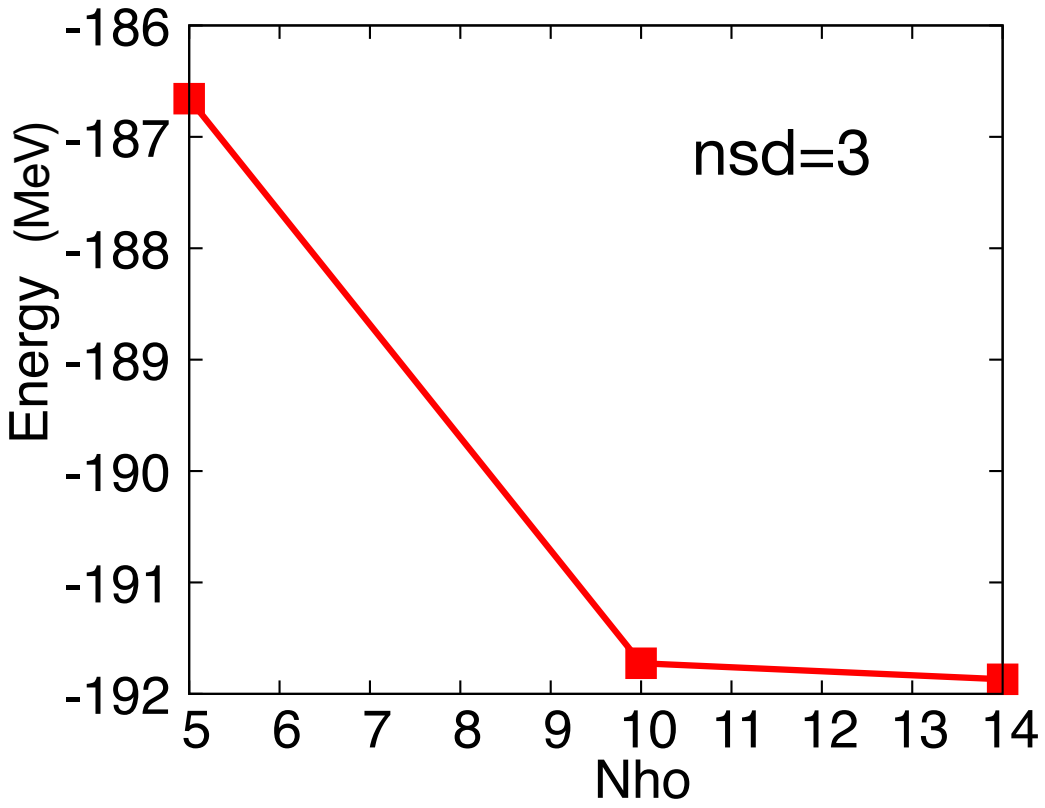
Initial states: Woods-Saxon potentials with different deformations

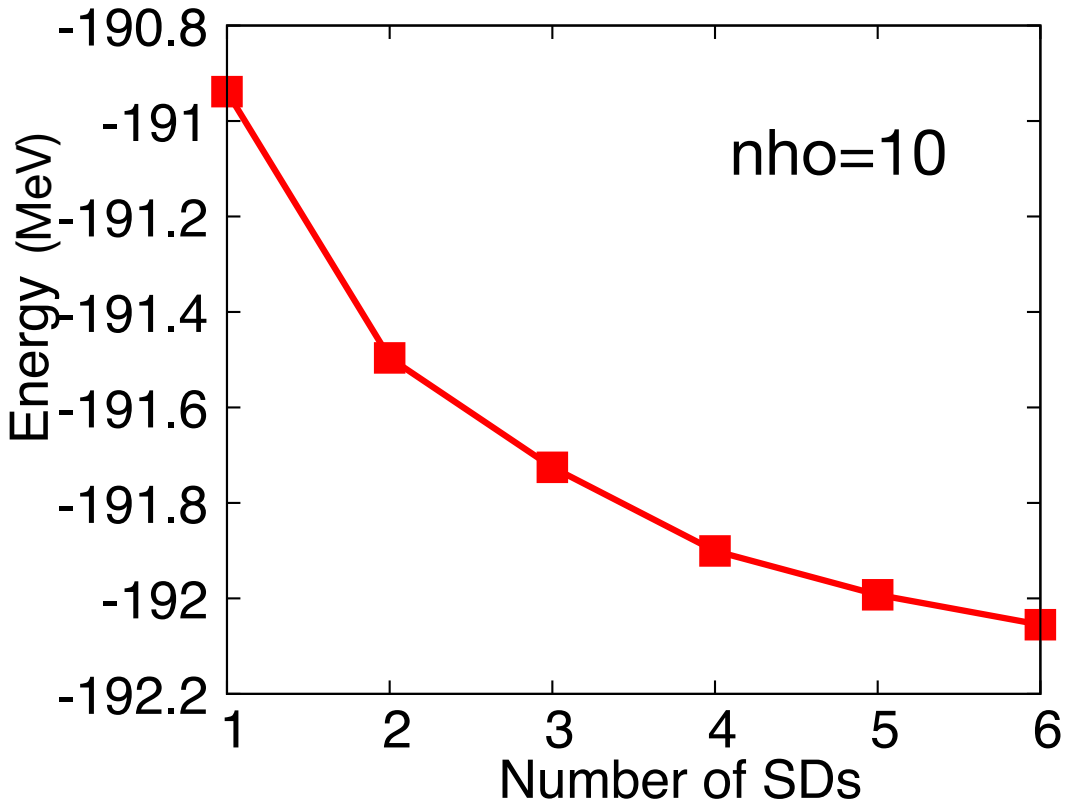
nho: number of major shells of the basis HO

nsd: number of Slater determinants

Results

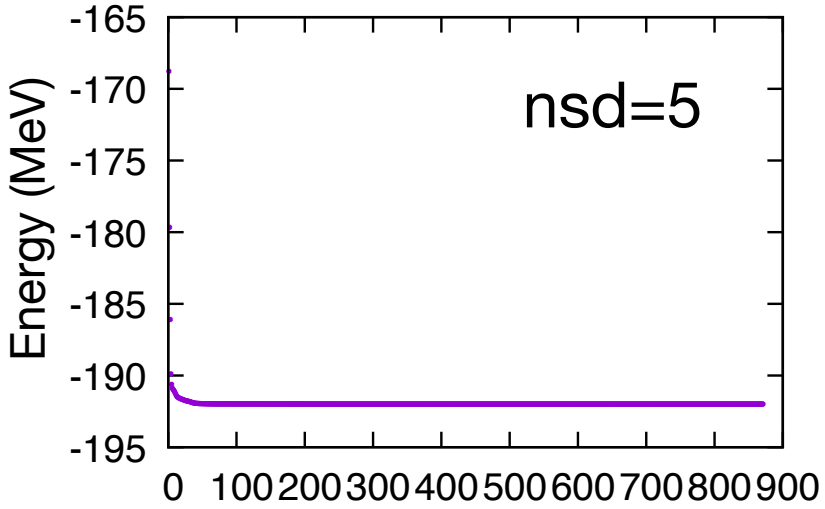
nho / nsd dependence of energy of ^{20}Ne

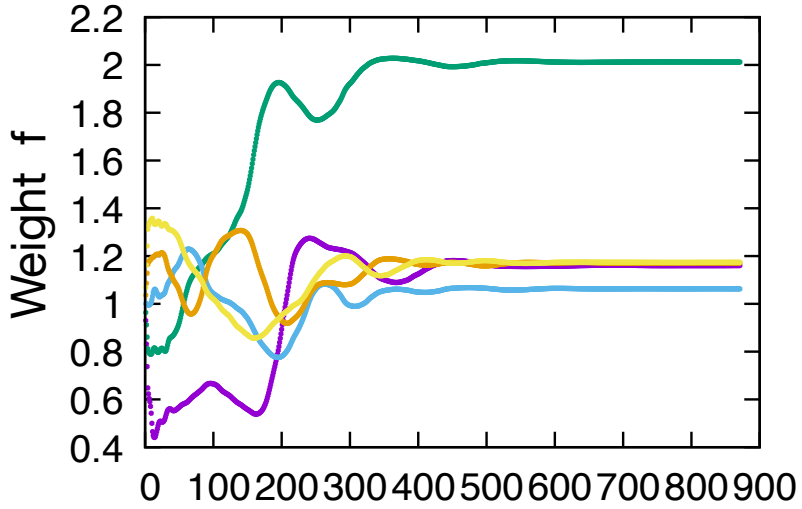




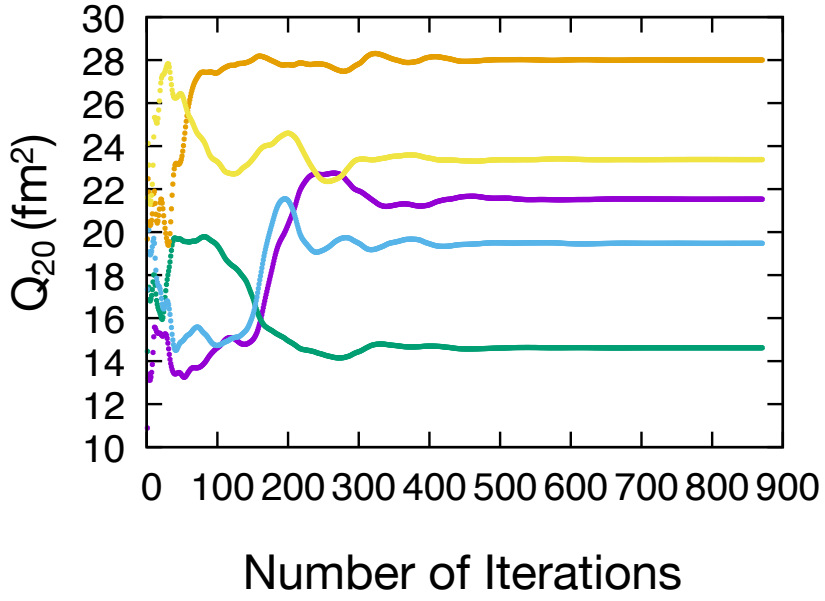
✓ Tendency of convergence

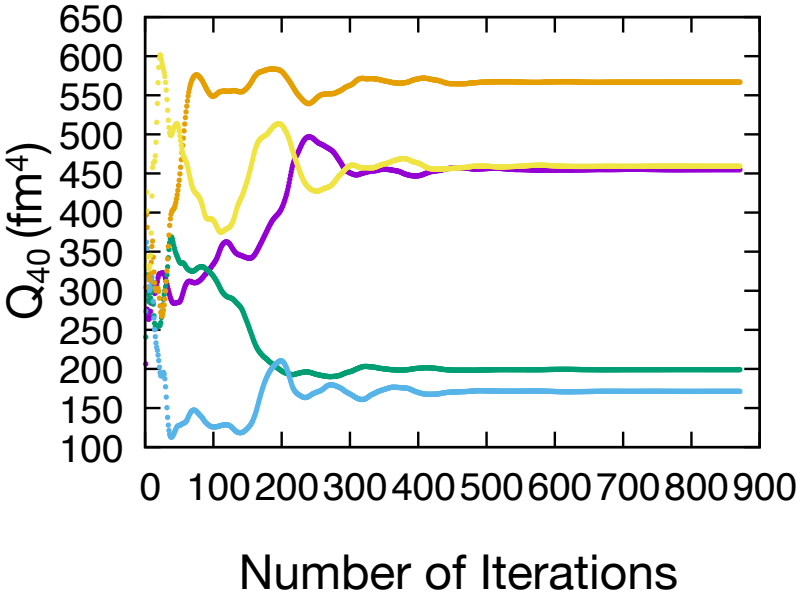
Results

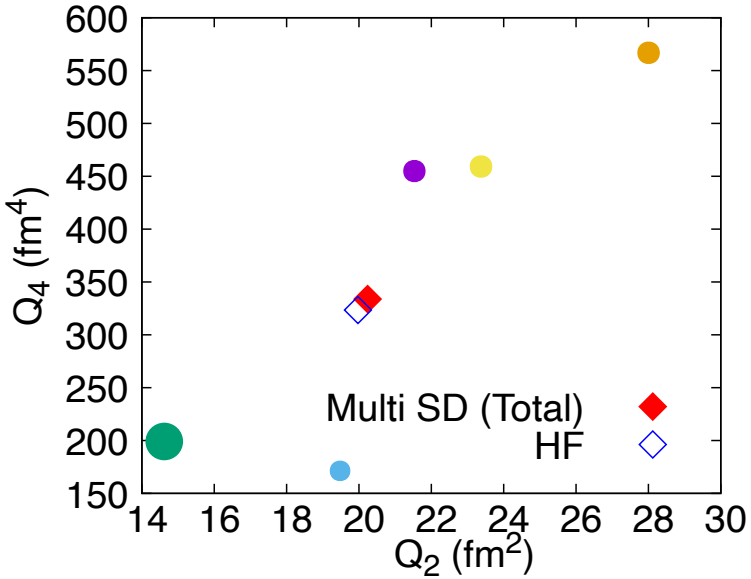




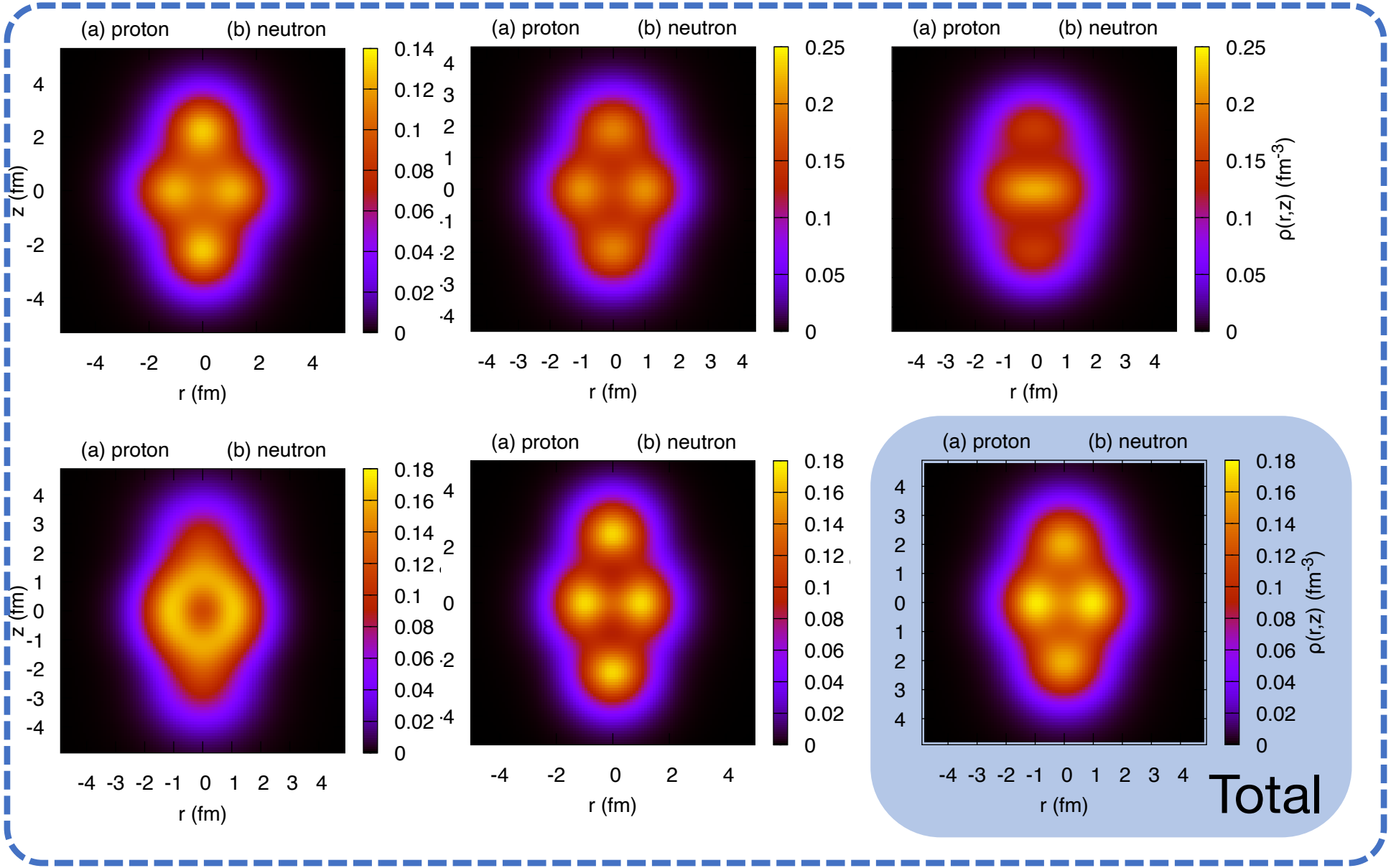
- ✓ Fluctuation in collective space is automatically optimized



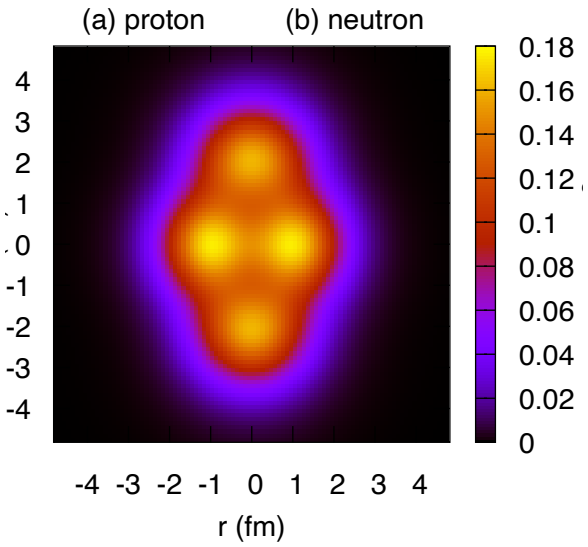




Results



HF



✓ Consistent

Summary / Perspectives

- ✓ We have developed Multi-reference energy density functional method with basis optimization
- ✓ We have applied the method to Volkov interaction

Future work:

- Extension to Gogny EDF
  (including density dependent, LS & Coulomb terms)
- Lift symmetry restrictions; symmetry restoration before variation
- Discussion of optimized collective space

Problems

How to construct EDF
suitable for Multi-reference EDF with full variation?

In fact, we have tested on Skyrme EDF (zero-range), but it failed

✓ Used 2-body Hamiltonian with Gaussian shape (Volkov int.)

→ Gogny EDF (Gaussian shape)

Finite-range is better

However, **we cannot use EDF fitted to single SD** to obtain reasonable solution

- How to construct?
- Is there a global EDF such that we can use as many SDs as we want?