Non-empirical description of nuclear collective motion with optimized basis for multi-reference DFT

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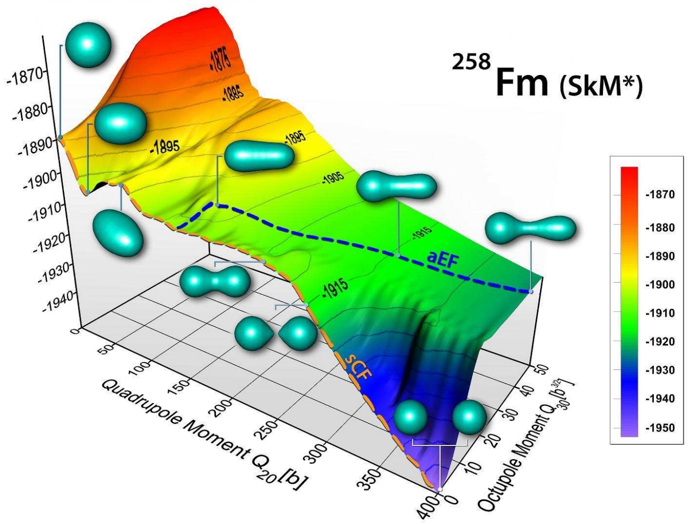
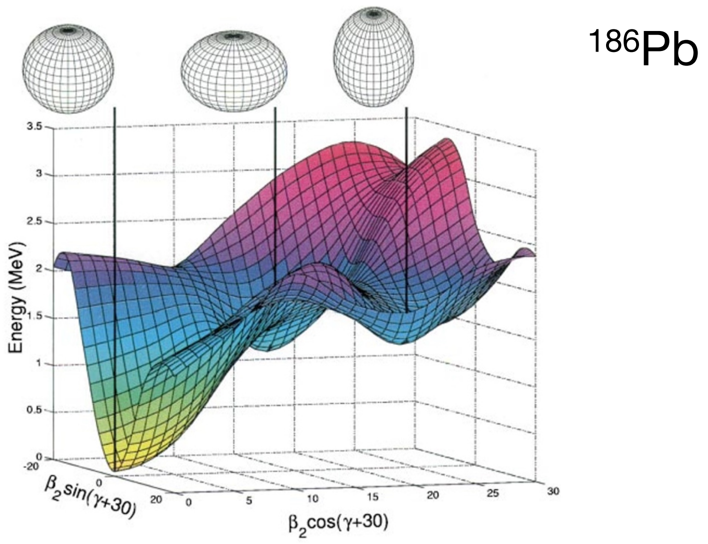
Nuclear collective motion

"**Collective**" aspects in nuclei by **microscopic** theory: essential problem

Especially, large amplitude collective motion is very important



Nuclear fission



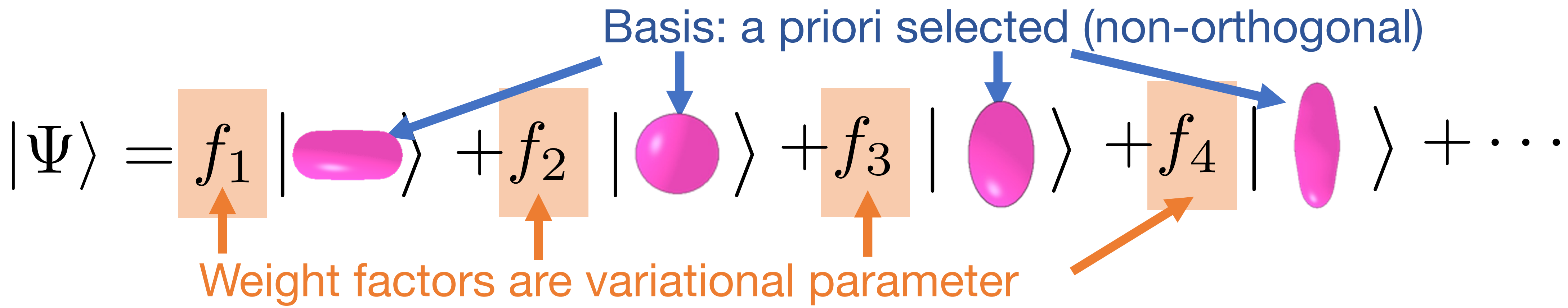
Shape coexistence

Non-empirical description of collective motion based on DFT

J. Dobaczewski, J. Phys.: Conf. Ser. **312** 092002 (2011). / A. N. Andreyev. *et al.* Nature **405**, 430 (2000).

Many-body states for collective motions

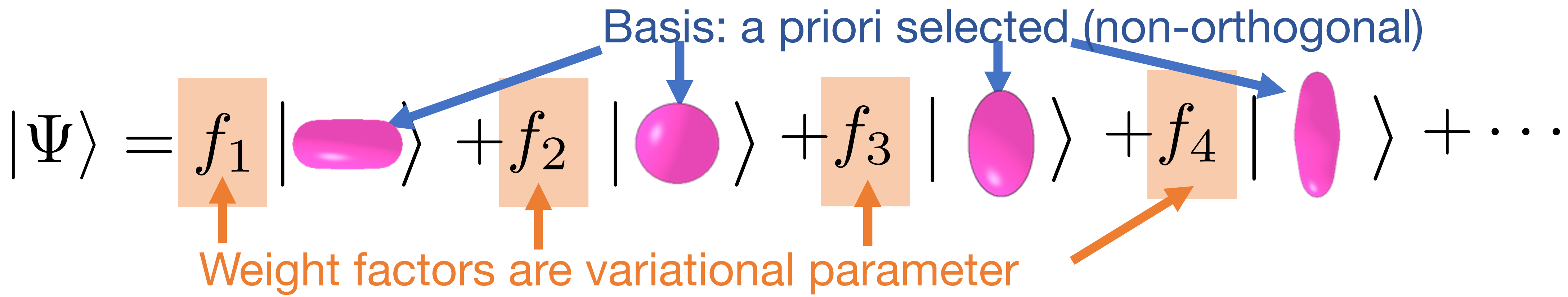
Generator coordinate method



Relying on empirical / phenomenological theory !

Many-body states for collective motions

Generator coordinate method



Relying on empirical / phenomenological theory !

Our method Optimize both weight and basis at same time

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

✓ Does not need pre-fixed effective DOFs

Non-empirical description of collective motion

Optimized-GCM

Trial function:

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

Slater determinant (↑ Φ_a) Single-particle states (orthonormal set) (↑ $\varphi_1^{(a)} \varphi_2^{(a)} \dots \varphi_N^{(a)}$)

Total energy to be minimized:

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

$$H_{ab} = \langle\Phi_a|H|\Phi_b\rangle$$: Hamiltonian kernel

$$N_{ab} = \langle\Phi_a|\Phi_b\rangle$$: Norm kernel

$$\rho_{\beta\alpha}^{(ab)} = \frac{\langle\Phi_a|\, a_\alpha^\dagger a_\beta \,|\Phi_b\rangle}{\langle\Phi_a|\Phi_b\rangle}$$: Transition DM

$$E^{(ab)} = E[\rho^{(ab)}]$$: EDF

$$h_{\alpha\beta}^{(ab)} = \frac{\delta E[\rho^{(ab)}]}{\delta\rho_{\beta\alpha}^{(ab)}}$$: HF Hamiltonian

Optimized-GCM

Calculate gradient of Energy

- Single particle states

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

- Weight function

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

Minimum search with CG method

$$H_{ab} = \langle \Phi_a | H | \Phi_b \rangle$$: Hamiltonian kernel

$$N_{ab} = \langle \Phi_a | \Phi_b \rangle$$: Norm kernel

$$\rho_{\beta\alpha}^{(ab)} = \frac{\langle \Phi_a | a_\alpha^\dagger a_\beta | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle}$$: Transition DM

$$E^{(ab)} = E[\rho^{(ab)}]$$: EDF

$$h_{\alpha\beta}^{(ab)} = \frac{\delta E[\rho^{(ab)}]}{\delta \rho_{\beta\alpha}^{(ab)}}$$: HF Hamiltonian

Set up

^{16}O Ground state

Axial / reflection / time-reversal symmetry
basis expansion with axial harmonic oscillator

- Skyrme (w/o time-odd components)

  SIII M. Beiner et al., Nucl. Phys. A 238, 29 (1975).

- No coulomb interaction

Initial states: WS potentials with different deformation

Results ^{16}O

Hartree-Fock $|\Psi\rangle = |\Phi\rangle$ –142.02 MeV

-0.4 MeV

GCM $|\Psi\rangle = \sum_a f_a |\Phi_a(Q_2^{(a)})\rangle$ –142.40 MeV

Bases are local ground states
obtained by constrained HF (next slide)

-0.7 MeV

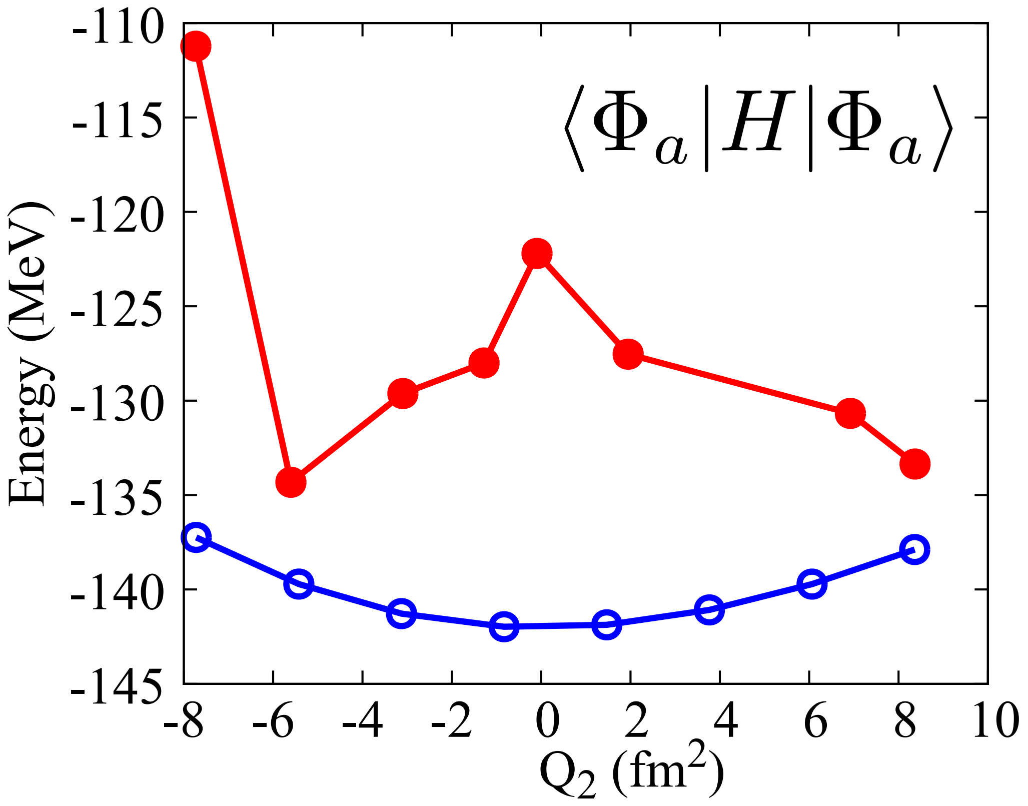
Optimized-GCM $|\Psi\rangle = \sum_a f_a |\Phi_a\rangle$ –143.10 MeV

Not enough in conventional method !

Results ^{16}O

"Usual" selection of the bases in GCM:

The ground states that minimize the energy for given values of deformation



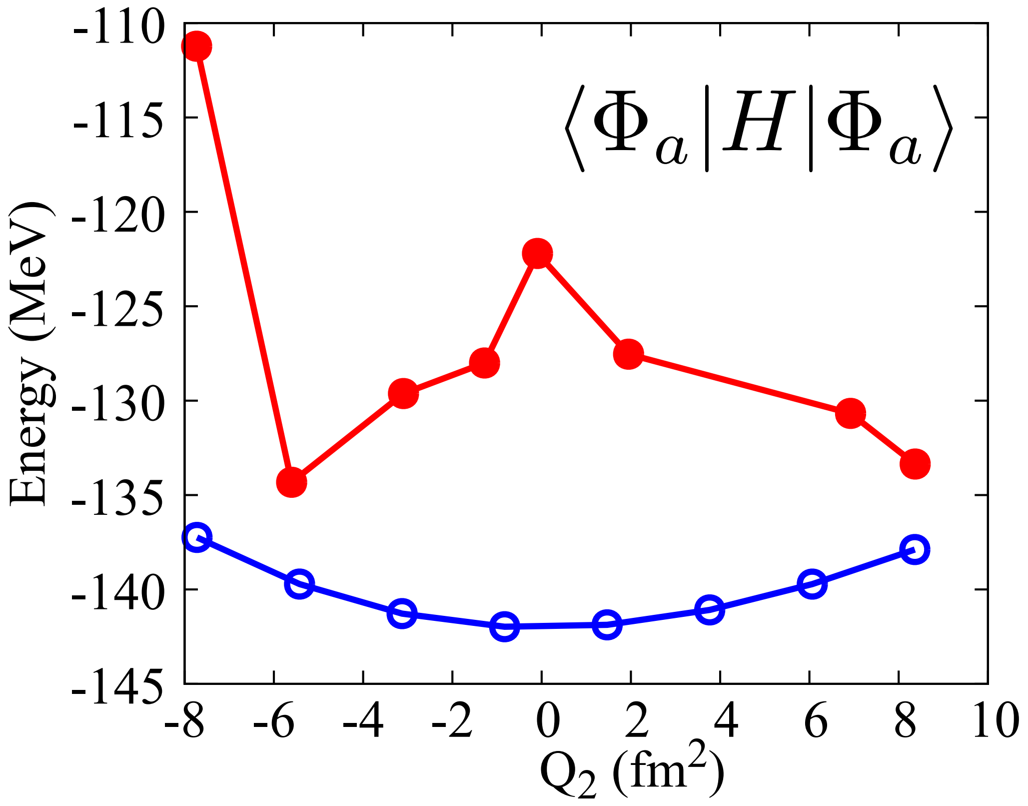
Blue: Constrained HF
Red: Optimized-GCM

Optimal bases are NOT the ground states of the each deformations

Results ^{16}O

"Usual" selection of the bases in GCM:

The ground states that minimize the energy for given values of deformation

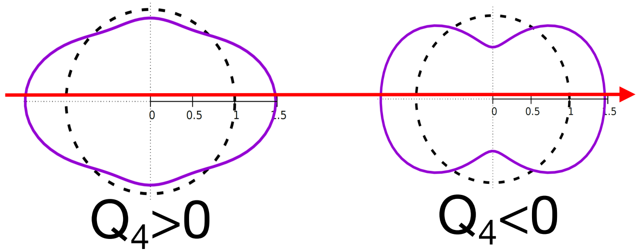


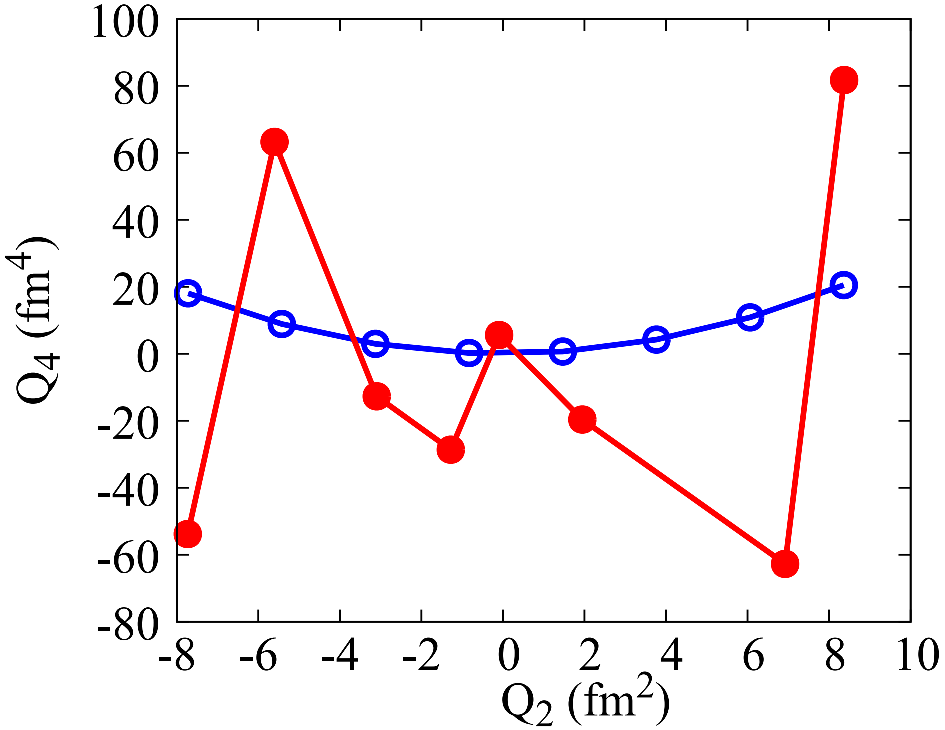
Blue: Constrained HF
Red: Optimized-GCM

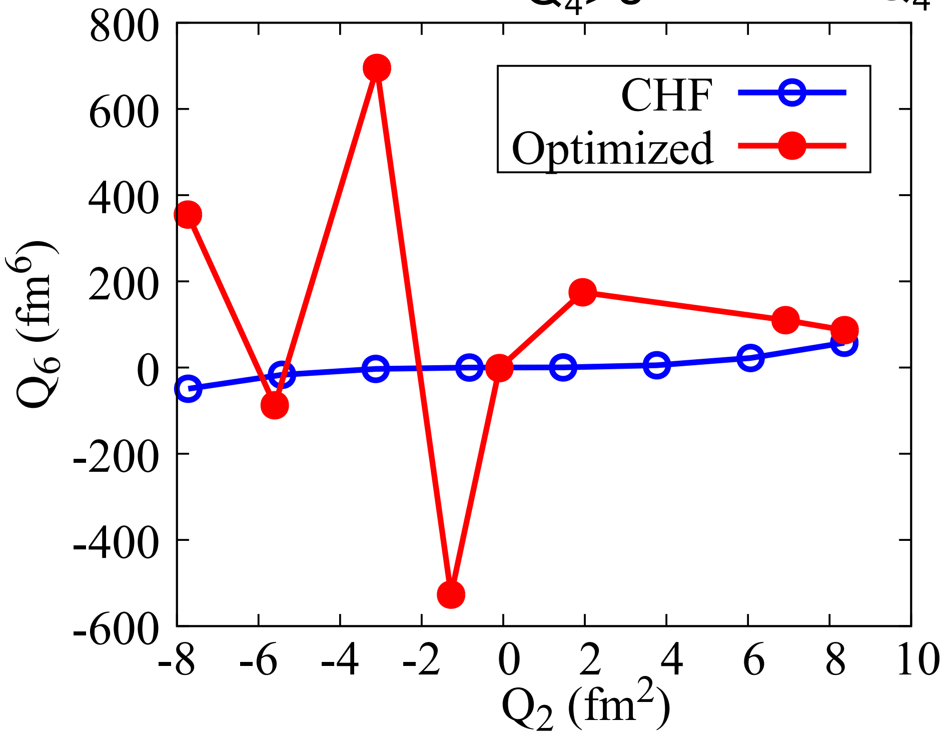
One needs to take into account excitations of nuclei in determining a collective coordinate

Results ^{16}O

Q_4 / Q_6 of optimal bases (the next higher moment)





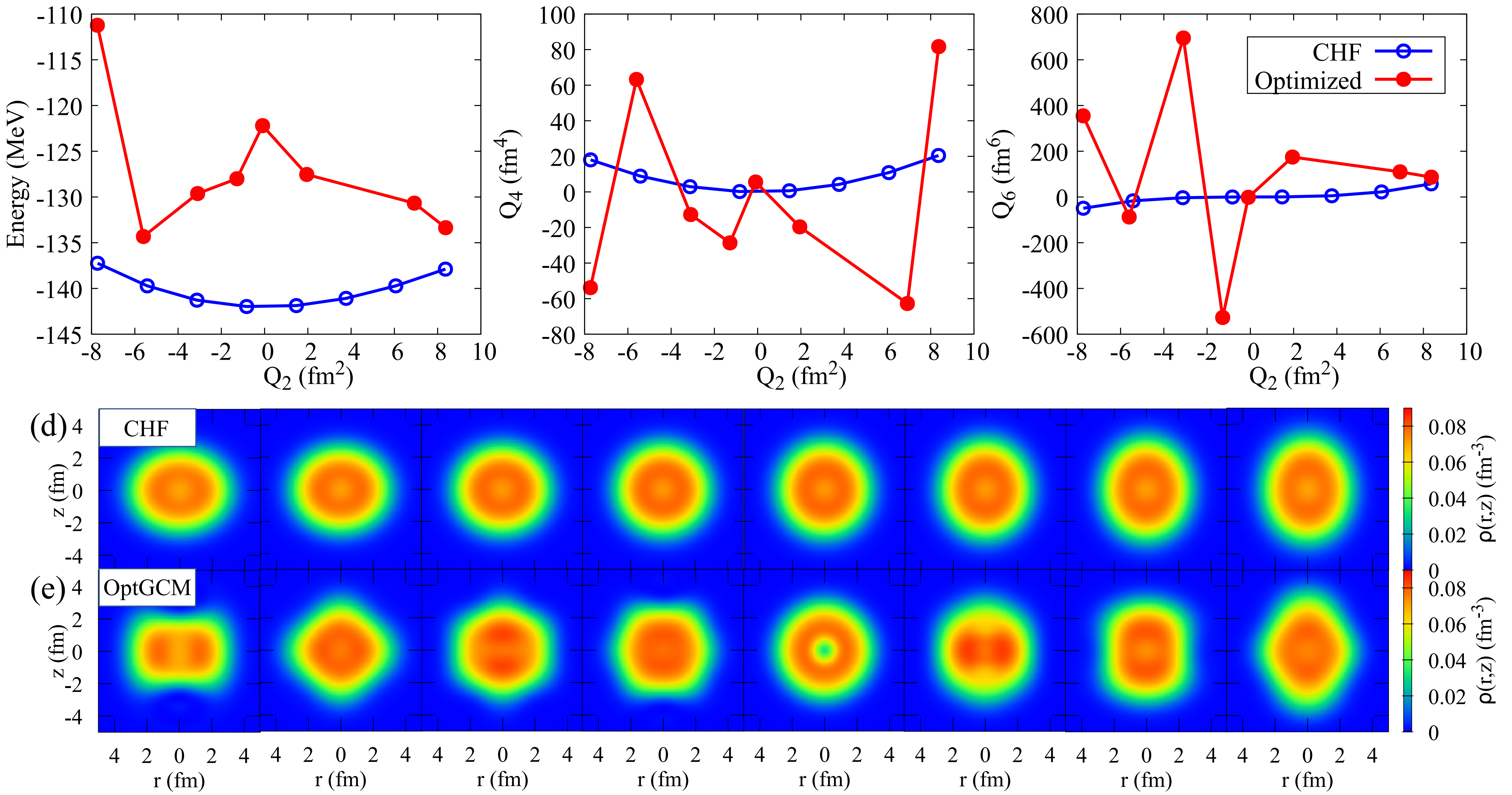


There are large fluctuations in higher moments

→ Q_2 alone does not make a good collective coordinate

at least both Q_2 and Q_4 are needed cf.) C. V. N. Kumar and L. M. Robledo, PRC 108, 034312 (2023).
N. Hizawa, and K. Hagino, PRC 109, 014312 (2024).

Results ^{16}O



Energy (MeV)
Q_2 (fm^2)
Q_4 (fm^4)
Q_6 (fm^6)
CHF
Optimized
(d)
CHF
(e)
OptGCM
z (fm)
r (fm)
ρ(r,z) (fm^{-3})

Summary

✓ Generator coordinate method with variational basis optimization

→ This method can describe collective motion

without pre-fixed collective degree of freedom

✓ ^{16}O: bases with high excitation energy were obtained Similar results for ^{28}Si

✓ One needs to take into account excitations of nuclei

in determining a collective coordinate

Future Work

* Analysis of collective motions in excited states

(angular momentum projection)

* Connection to existing collective model