An extension of the generator coordinate method with basis optimization

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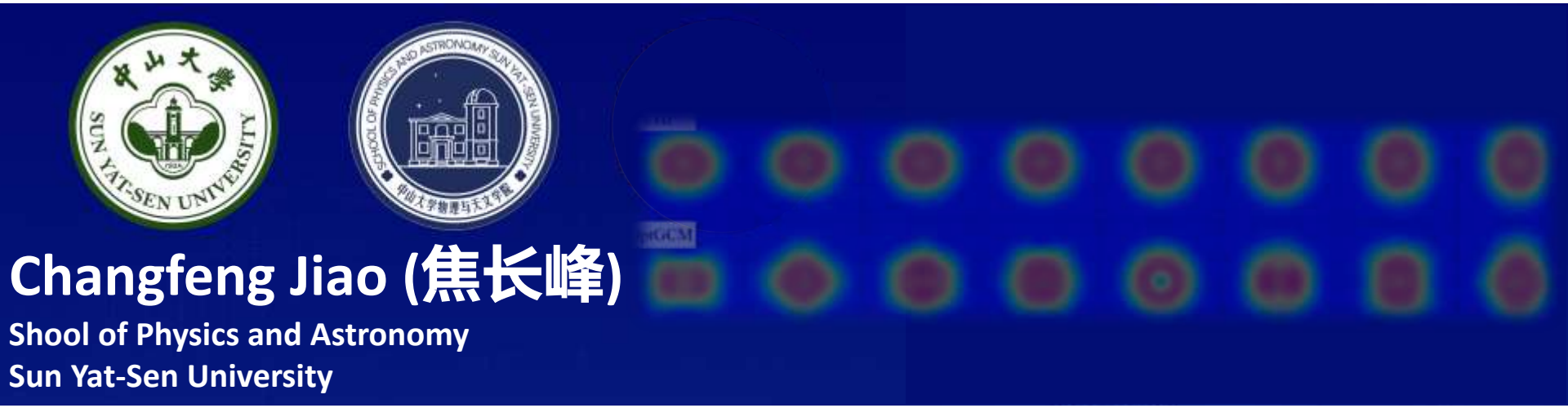

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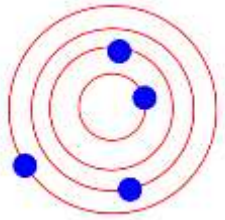
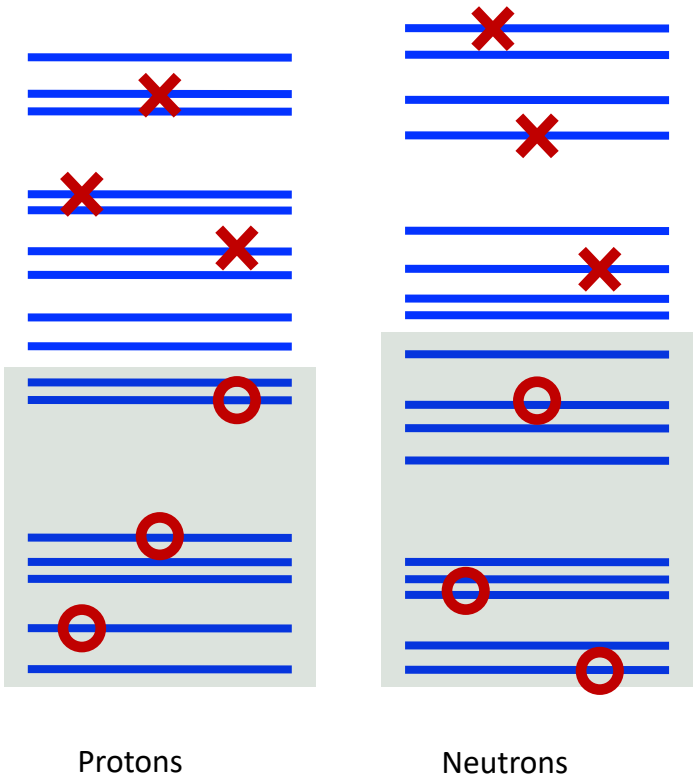
Motivation

Some models are built on single independent-particle state.





Protons

Neutrons

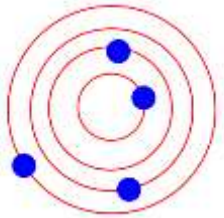
Starting from one Slater determinant, e.g., the HF state $|\psi_0\rangle$, the ground state

$$|0\rangle = |\psi_0\rangle + \sum C^0_{mi} a^\dagger_m a_i |\psi_0\rangle + \frac{1}{4} \sum_{mnij}^{mi} C^0_{mn,ij} a^\dagger_m a^\dagger_n a_i a_j |\psi_0\rangle + \cdots$$

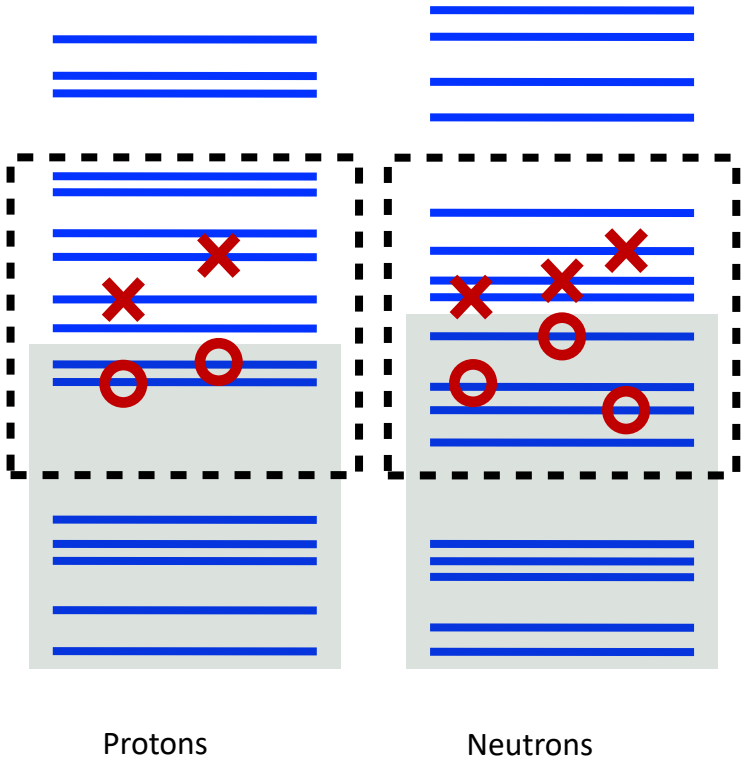
But exact diagonalization in complete Hilbert space is not solvable.

Motivation

Some models are built on single independent-particle state.



Interacting shell model (ISM)



- Same starting point . $|0\rangle$
- Instead of solving Schrödinger equation in complete Hilbert space, one restricts the dynamics in a configuration space.

$$H|\Phi_i\rangle = E_i|\Phi_i\rangle \rightarrow H_{\text{eff}}|\bar{\Phi}_i\rangle = E_i|\bar{\Phi}_i\rangle$$

Configuration interaction of orthonormal Slater determinants:

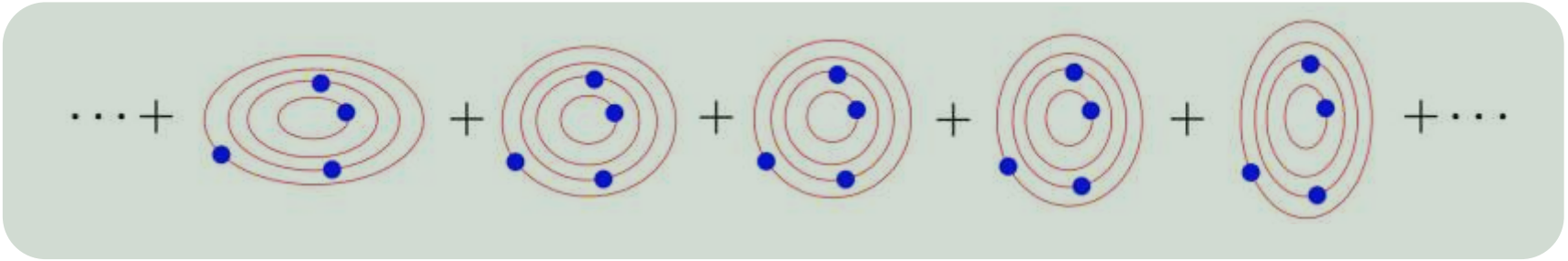
$$|\bar{\Phi}_i\rangle = \sum_j c_{ij}|\psi_j\rangle, \quad \langle\psi_j|\psi_k\rangle = \delta_{jk}$$

Diagonalizing the H_{eff} in the orthonormal basis.

Motivation

Another way to build many-body states:

Instead of configuration interaction with orthogonal states, one can diagonalize the Hamiltonian in a set of ***non-orthogonal*** basis.



$$|\Phi\rangle = \sum_j c_j |\psi_j\rangle, H_{jk} = \langle j|H|k\rangle$$

$$\sum_k H_{jk}c_k = E\sum_k N_{jk}c_k, N_{jk} = \langle j|k\rangle$$

The non-orthogonal states can be ***highly optimized***, and hence reduce the dimension of basis states.

→ *Generator-coordinate method*

Motivation

"One of the unique features in nuclear systems is that large-amplitude collective motions often play essential roles in phenomena such as nuclear fission and shape coexistence. To describe such collective motions in a microscopic way is one of the major goals of quantum many-body problems. "

The generator coordinate method (GCM) is essential for treating large-amplitude motions, however...

How to pin down all the correlations that are relevant?

This Letter proposes a new method **without** pre-fixed collective coordinates based on multi-reference DFT. In this new method, the trial many-body state is given by a superposition of Slater Determinants as in GCM, but both the weights **and the basis SDs** are determined by variation, referred as **Optimized-basis GCM (OptGCM).**

An idea: QTDA-driven GCM

How to pin down all the correlations that are relevant?

A novel idea to incorporate important correlations in GCM.

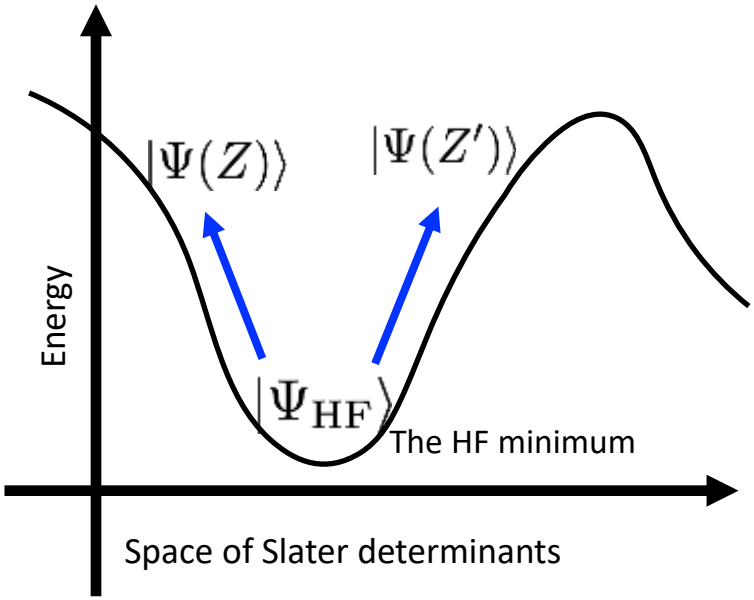
Starts from the HF minimum.

Apply Thouless evolution to explore the energy landscape

Thouless theorem:

$$\exp(\hat{Z})|\Psi\rangle = |\Psi'\rangle \equiv |\Psi(Z)\rangle$$

$$\Rightarrow \quad |\Psi(Z)\rangle = \exp(\hat{Z})|\Psi_{\mathrm{HF}}\rangle$$



Define an energy landscape $E(Z) = \langle\Psi(Z)|\hat{H}|\Psi(Z)\rangle$ which can be expanded in Z. Note that the curvature around HF minimum approximates the landscape as a quadratic in Z and thus a multi-dimensional harmonic oscillator, leading to TDA/RPA and their quasiparticle extension.

An idea: QTDA-driven GCM

Here we generate non-orthogonal states by applying Thouless evolution with QTDA operators.

Low-lying excited states are approximated as linear combinations of two-quasiparticle excitations, represented by QTDA operator:

$$\hat{Z}_r = \frac{1}{2}\sum_{\alpha\alpha'} Z^r_{\alpha\alpha'}\hat{c}^\dagger_\alpha(0)\hat{c}^\dagger_{\alpha'}(0) \qquad \text{where} \quad \hat{c}_\alpha(0) = \sum_\beta \hat{a}_\beta U^*_{\beta\alpha}(0) + \hat{a}^\dagger_\beta V^*_{\beta\alpha}(0)$$

One computes the matrix elements of the Hamiltonian in a basis of two-quasiparticle excited states

$$A_{\alpha\alpha',\beta\beta'} = \langle\Phi_0|[\hat{c}_{\alpha'}(0)\hat{c}_\alpha(0), [\hat{H}, \hat{c}^\dagger_\beta(0)\hat{c}^\dagger_{\beta'}(0)]]|\Phi_0\rangle$$

We then solve $\sum_{\beta\beta'} A_{\alpha\alpha',\beta\beta'} Z^r_{\beta\beta'} = E^{\mathrm{QTDA}}_r Z^r_{\alpha\alpha'}.$

to find the coefficients $Z^r_{\alpha\alpha'}$ of QTDA operator, and apply Thouless theorem to get a new state

$$|\Phi_r\rangle = \exp\left(\lambda\hat{Z}_r\right)|\Phi_0\rangle$$

An idea: QTDA-driven GCM

We approximate the QTDA states by applying Thouless's theorem

$$|\Phi_r\rangle = \exp(\lambda \hat{Z}_r)|\Phi_0\rangle \approx |\Phi_0\rangle + \lambda \hat{Z}_r|\Phi_0\rangle$$

$$= \exp\left\{\lambda \frac{1}{2} \sum_{\alpha\alpha'} Z^r_{\alpha\alpha'} \hat{c}^\dagger_\alpha(0)\hat{c}^\dagger_{\alpha'}(0)\right\}|\Phi_0\rangle$$

With application of Thouless's theorem we have a new quasiparticle vacuum $|\Phi_r\rangle$, and we need to file new quasiparticle operators that annihilate it. First we define that

$$\tilde{c}_\alpha(r) = \hat{c}_\alpha(0) + \lambda \sum_\mu \hat{c}^\dagger_\beta(0) Z^r_{\beta\alpha} \quad \text{Apparently,} \quad \tilde{c}_\alpha(r)|\Phi_r\rangle = 0$$

However, they do ***not*** satisfy fermion anticommutation relations:

$$\{\tilde{c}_\alpha(r), \tilde{c}^\dagger_{\alpha'}(r)\} = \delta_{\alpha\alpha'} + \lambda^2 \sum_\mu Z^r_{\mu\alpha} Z^{r*}_{\mu\alpha'}.$$

We define $\mathbf{L}\mathbf{L}^\dagger = \mathbf{I} + \lambda^2 \mathbf{Z}^T \mathbf{Z}^*$

where $\mathbf{I}$ is the unit matrix, and $\mathbf{L}$ is a lower triangular matrix.

An idea: QTDA-driven GCM

Now we define

$$\hat{c}_\alpha(r) = \sum_{\alpha'} L^{-1}_{\alpha\alpha'} \tilde{\mathrm{c}}_\alpha(r),$$

which satisfy the anticommutation relations,

$$\{\hat{c}_\alpha(r), \hat{c}^\dagger_{\alpha'}(r)\} = \sum_{\mu\mu'} L^{-1}_{\alpha\mu} \left[L^{-1}_{\alpha'\mu'}\right]^* \{\tilde{\mathrm{c}}_\mu(r), \tilde{\mathrm{c}}^\dagger_{\mu'}(r)\}$$
$$= (\mathbf{L}^{-1}(\mathbf{I} + \lambda^2 \mathbf{Z}^T \mathbf{Z}^*)[\mathbf{L}^{-1}]^\dagger)_{\alpha\alpha'} = \delta_{\alpha\alpha'}.$$

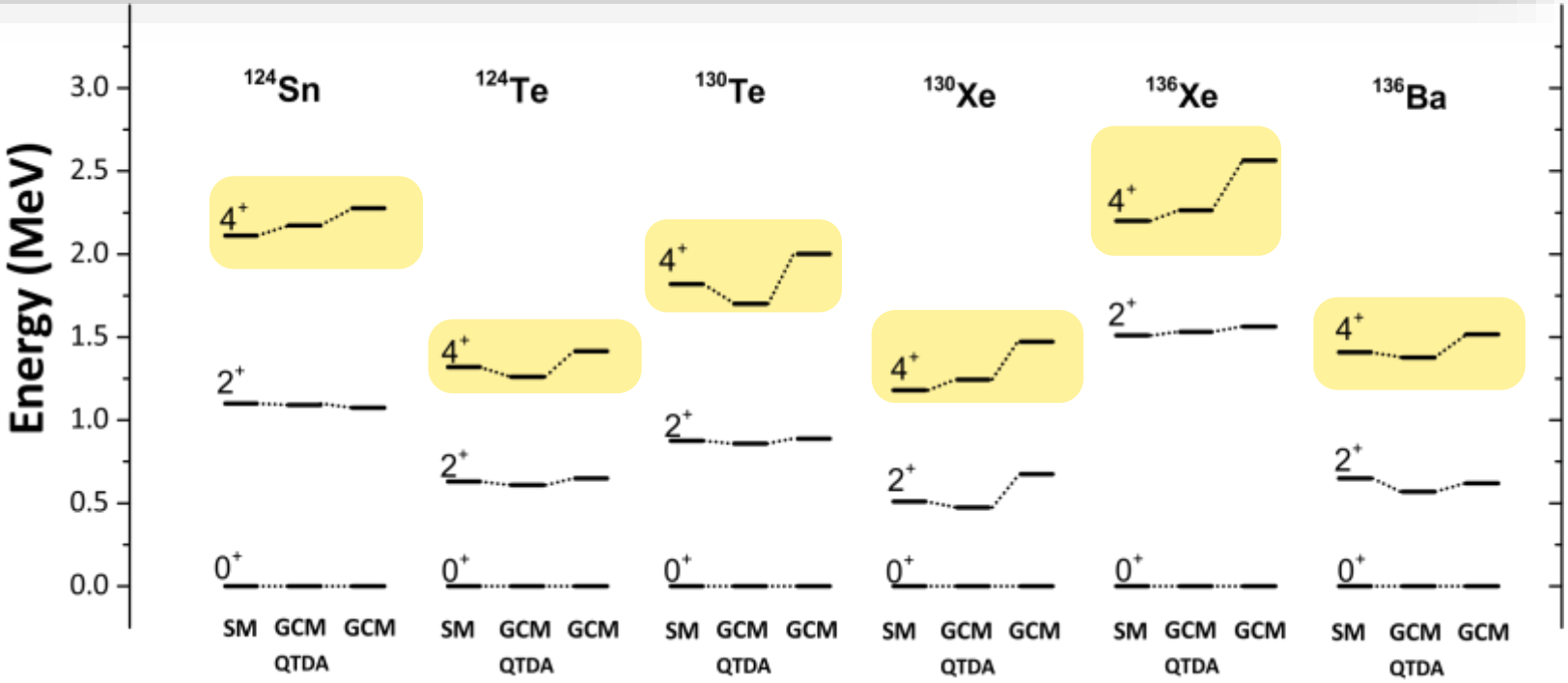
The resultant Bogoliubov transformation matrix of the transformed state is given by

$$\begin{pmatrix} \hat{c}^\dagger(r) \\ \hat{c}(r) \end{pmatrix} = \begin{pmatrix} [\mathbf{L}^{-1}]^* & \lambda[\mathbf{L}^{-1}\mathbf{Z}^T]^* \\ \lambda\mathbf{L}^{-1}\mathbf{Z}^T & \mathbf{L}^{-1} \end{pmatrix} \times \begin{pmatrix} \mathbf{U}(0)^T & \mathbf{V}(0)^T \\ \mathbf{V}(0)^\dagger & \mathbf{U}(0)^\dagger \end{pmatrix} \begin{pmatrix} \hat{a}^\dagger \\ \hat{a} \end{pmatrix}$$
$$= \begin{pmatrix} \mathbf{U}(r)^T & \mathbf{V}(r)^T \\ \mathbf{V}(r)^\dagger & \mathbf{U}(r)^\dagger \end{pmatrix} \begin{pmatrix} \hat{a}^\dagger \\ \hat{a} \end{pmatrix}$$

Where

$$\mathbf{U}(r) = (\mathbf{U}(0) + \lambda \mathbf{V}(0)^* \mathbf{Z}^*)[\mathbf{L}^{-1}]^\dagger$$
$$\mathbf{V}(r) = (\mathbf{V}(0) + \lambda \mathbf{U}(0)^* \mathbf{Z}^*)[\mathbf{L}^{-1}]^\dagger$$

An idea: QTDA-driven GCM



		$M^{0\nu}_{GT}$	$M^{0\nu}_{F}$	$M^{0\nu}_{T}$	$M^{0\nu}$
^{124}Sn	CHFB-GCM	2.48	−0.51	−0.03	2.76
	QTDA-GCM	2.08	−0.73	−0.01	2.53
	SM	1.85	−0.47	−0.01	2.15
^{130}Te	CHFB-GCM	2.25	−0.47	−0.02	2.52
	QTDA-GCM	1.97	−0.69	−0.01	2.39
	SM	1.66	−0.44	−0.01	1.94
^{136}Xe	CHFB-GCM	2.17	−0.32	−0.02	2.35
	QTDA-GCM	1.65	−0.50	−0.01	1.96
	SM	1.50	−0.40	−0.01	1.76

Nuclei	CHFB-GCM	QTDA-GCM	SM
^{124}Sn	−15.733	−15.684	−16.052
^{124}Te	−23.082	−22.641	−24.446
^{130}Te	−25.705	−25.563	−26.039
^{130}Xe	−32.583	−32.220	−33.313
^{136}Xe	−34.931	−34.912	−34.971
^{136}Ba	−40.341	−40.176	−40.745

CFJ and C.W. Johnson, PRC 100, 031303(R) (2019)

The models

Back to this paper. Assume that the g.s. wave function is given by

$$|\Psi\rangle = \sum_{a=1}^{M} f_a \, |\Phi_a\rangle$$

where $|\Phi_a\rangle$ are the basis SDs with the antisymmetrized product of *N* orthonormal single-particle orbitals $\varphi_i^{(a)} \; (i = 1, 2, ..., N)$

Minimize the total energy for a given Hamiltonian *H*,

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

where N_{ab} and H_{ab} are the norm and Hamiltonian kernels,

$$N_{ab} = \langle \Phi_a \mid \Phi_b \rangle$$
$$H_{ab} = \langle \Phi_a | H | \Phi_b \rangle$$

The models

The transition density matrix

$$\rho_{\beta\alpha}^{(ab)} = \frac{\left\langle \Phi_a \left| a_\alpha^\dagger a_\beta \right| \Phi_b \right\rangle}{\left\langle \Phi_a \mid \Phi_b \right\rangle},$$

The energy density functional

$$E^{(ab)} = E\left[\rho^{(ab)}\right] = H_{ab}/N_{ab}$$

The Hartree-Fock (HF) Hamiltonian

$$h_{\alpha\beta}^{(ab)} = \frac{\delta E\left[\rho^{(ab)}\right]}{\delta \rho_{\beta\alpha}^{(ab)}}$$

with the particle creation (annihilation) operator $a_\alpha^\dagger$ (a_α) of the single-particle state $\boldsymbol{\alpha}$.

The models

The total energy *E* should be stationary under an arbitrary variation of the variational parameters f_a and $\varphi_i^{(a)}$

$$\frac{\delta E}{\delta f_a^*} = \frac{1}{\langle \Psi \mid \Psi \rangle} \sum_b \left(H_{ab} - E N_{ab} \right) f_b .$$

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

Key feature

The ground state corresponds to

$$\frac{\delta E}{\delta \left\langle \varphi_i^{(a)} \right|_{ph}} = 0 \quad \text{and} \quad \boxed{\frac{\delta E}{\delta f_a^*} = 0}$$

Hill-Wheeler equation

The models

It is discussed in **N. Shimizu et. al., Prog. Theor. Exp. Phys. 2012 (2012), 01A205,** as

$$\frac{\partial E_N}{\partial D^{m*}} = (1 - D^m D^{m\dagger}) \sum_{M,n,K,\lambda} f^*_{mM} f_{nK} W^{I\pi(\lambda)}_{MK} \langle \phi_m | \phi^{(\lambda)}_n \rangle$$

$$\times \left((1 - \rho^{(\lambda)})(t + \Gamma^{(\lambda)}) + \left(\mathrm{Tr} \left(\left(t + \frac{1}{2}\Gamma^{(\lambda)} \right) \rho^{(\lambda)} \right) - E_N \right) \right) \rho^{(\lambda)} D^m$$

where a matrix D^m represents the single SD $\quad |\varphi^m\rangle = \prod_{k=1}^{N_\mathrm{f}} \left(\sum_{l=1}^{N_\mathrm{sp}} D^m_{lk} c^\dagger_l \right) |-\rangle$

$$\frac{\delta E}{\delta \left\langle \varphi^{(a)}_i \right|_{ph}} = \sum_b \frac{f^*_a N_{ab} f_b}{\langle \Psi \mid \Psi \rangle} \left(1 - \rho^{(ab)} \right)$$

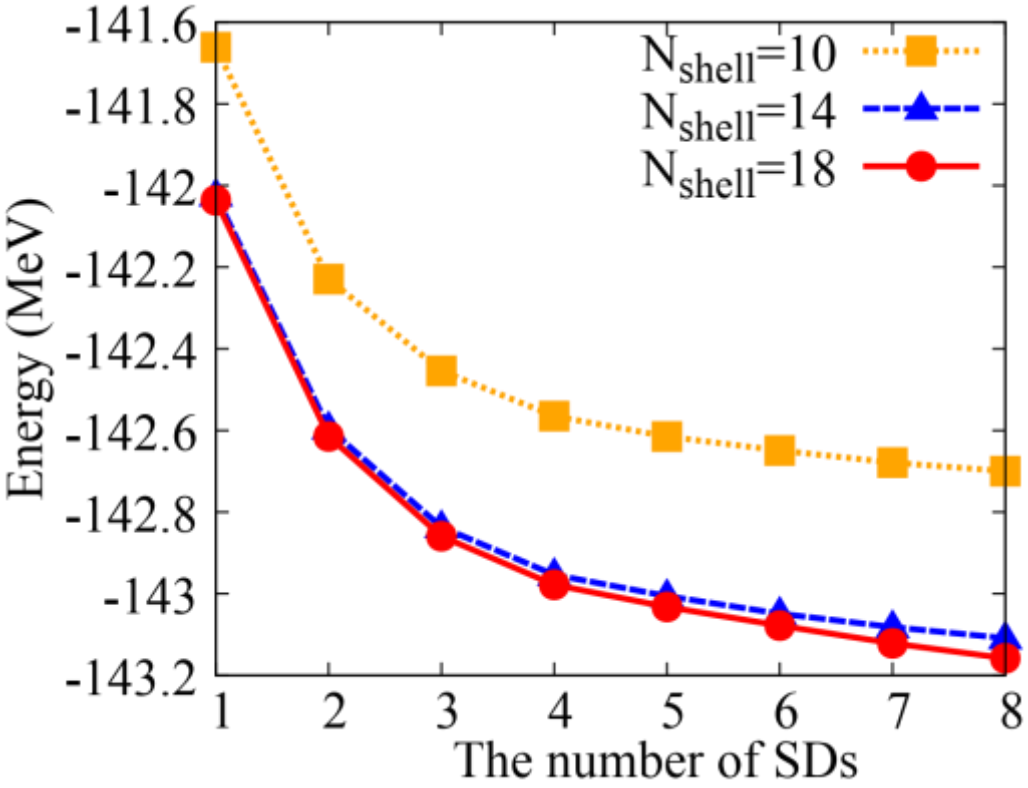
$$\times \left[E - E^{(ab)} + h^{(ab)} \rho^{(ab)} \right] \left| \varphi^{(a)}_i \right\rangle$$

Key feature

Application of this method to the g.s. of the ^{16}O

The initial set of SDs are given by Woods-Saxon potentials with different deformations, and the initial values of the weight factors are set as f_a = 1 for all a.

The results are independent of the choice of the initial SDs and f_a.



The g.s. energy against the number of SDs. The energies are calculated for 10, 14, and 18 of HO major shells for the basis set.

Converge as the number of SDs increases, and converge for the number of major shells.

Application of this method to the g.s. of the ^{16}O

- Compares OptGCM results with those of the conventional GCM.

  Take the OptGCM results for 8 SDs with 14-major-shell HO basis.

  For conventional GCM (referred as GCM afterwards),

$$|\Psi_{\mathrm{GCM}}\rangle = \sum_{a=1}^{8} f_a \left|\Phi\left(Q_2^{(a)}\right)\right\rangle$$

$|\Phi(Q_2^{(a)})\rangle$ are the HF states constrained with

$$\left\langle \Phi_a\left(Q_2^{(a)}\right)\left|\hat{Q}_2\right|\Phi_a\left(Q_2^{(a)}\right)\right\rangle = Q_2^{(a)}$$

Here $\hat{Q}_\lambda$ is the multipole moment operator,

$$\hat{Q}_\lambda = \int d^3r r^\lambda Y_{\lambda 0}(\hat{\boldsymbol{r}})\hat{\rho}(\boldsymbol{r})$$

Also 8 SDs with -7.73 ≤ $Q_2^{(a)}$ ≤8.36 fm^2

Application of this method to the g.s. of the ^{16}O

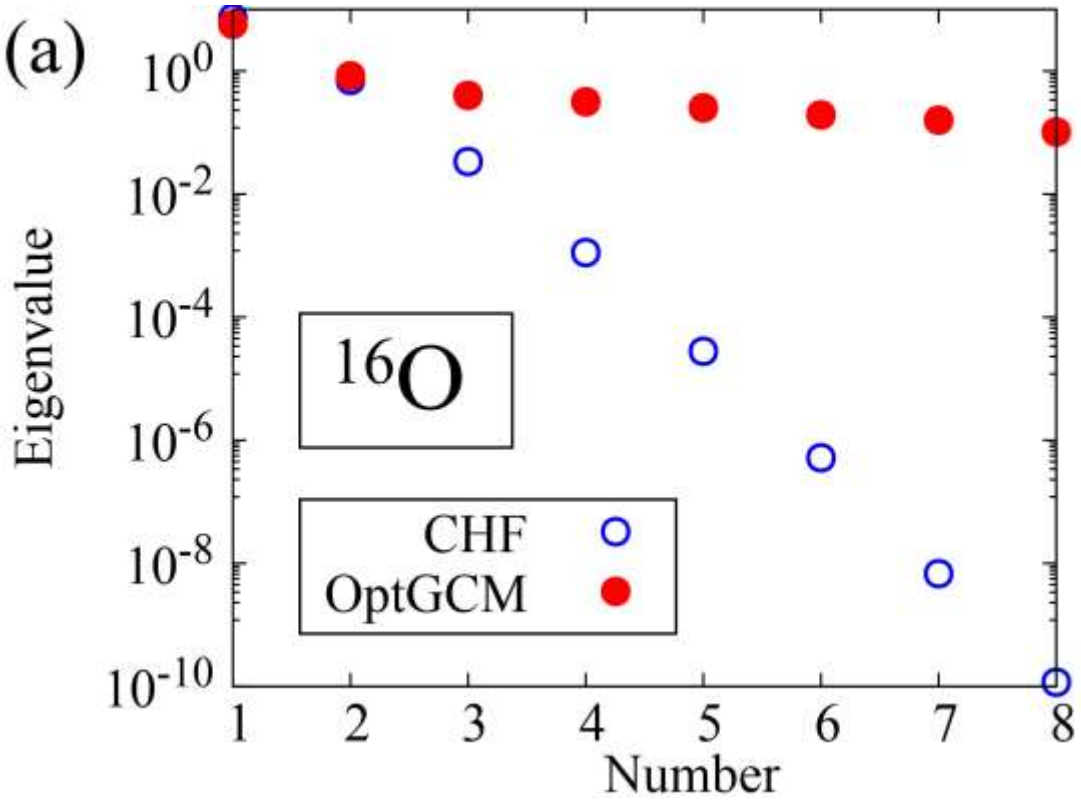
TABLE I. The ground state energies, the quadrupole moments, Q_2, and the hexadecupole moments, Q_4, obtained with the HF, GCM and OptGCM methods.

Method	Energy (MeV)	Q_2 (fm^2)	Q_4 (fm^4)
HF	-142.024	0.000	0.000
GCM	-142.407	0.179	9.324
OptGCM	-143.109	0.165	1.127

This implies that the optimized basis states gain more correlations than the Q_2-CHF basis states.

Application of this method to the g.s. of the ^{16}O

Understanding the difference between the OptGCM and the conventional GCM

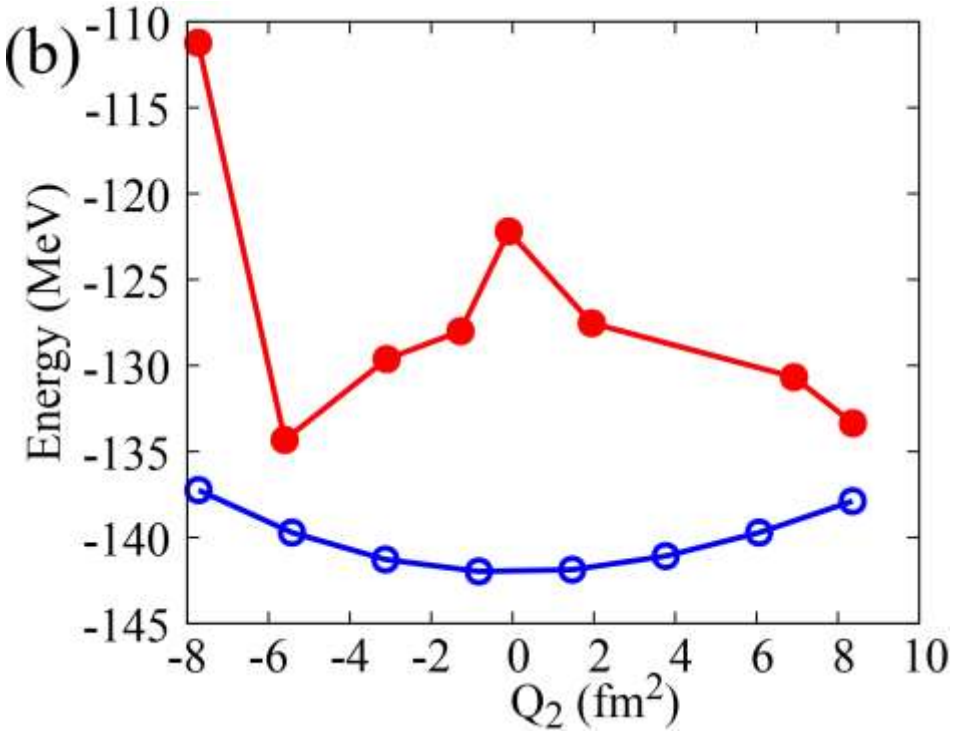


The eigenvalues of the norm kernel

- **CHF:** the basis are not fully linearly independent.
- **OptGCM:** the optimized basis spans in a larger subspace.

Application of this method to the g.s. of the ^{16}O

Understanding the difference between the OptGCM and the conventional GCM



The energies of each SD

The optimized bases have higher energies.

- ***The optimized bases correspond to excited states on top of the PEC.***

- ***The optimized bases gain more correlations***

Application of this method to the g.s. of the ^{16}O

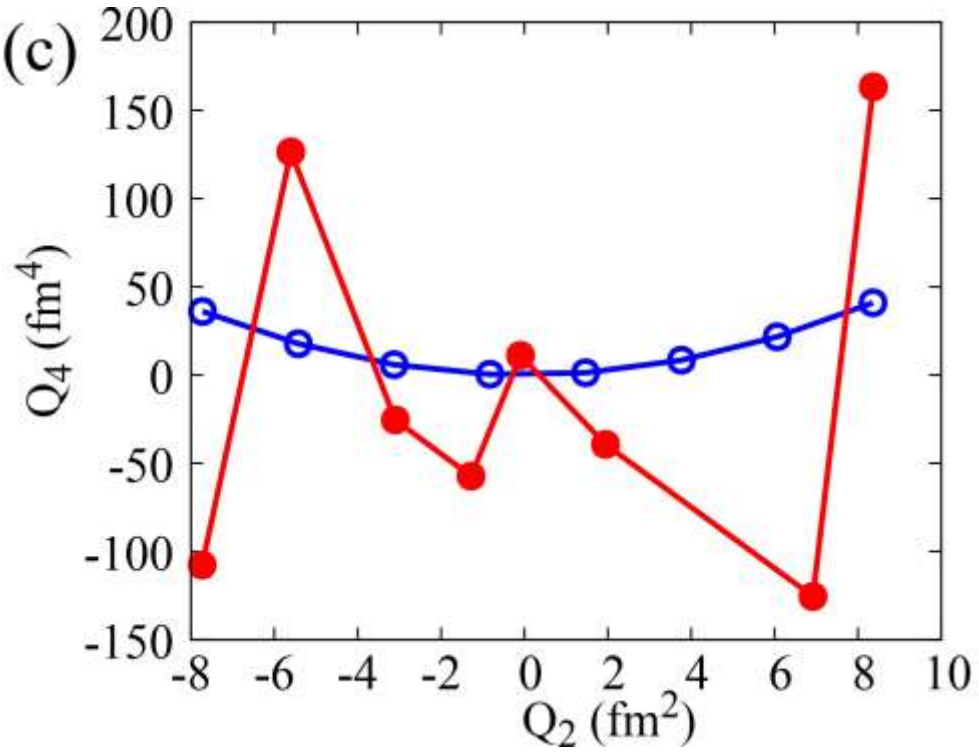
Understanding the difference between the OptGCM and the conventional GCM

The quadrupole and the hexadecupole moment.

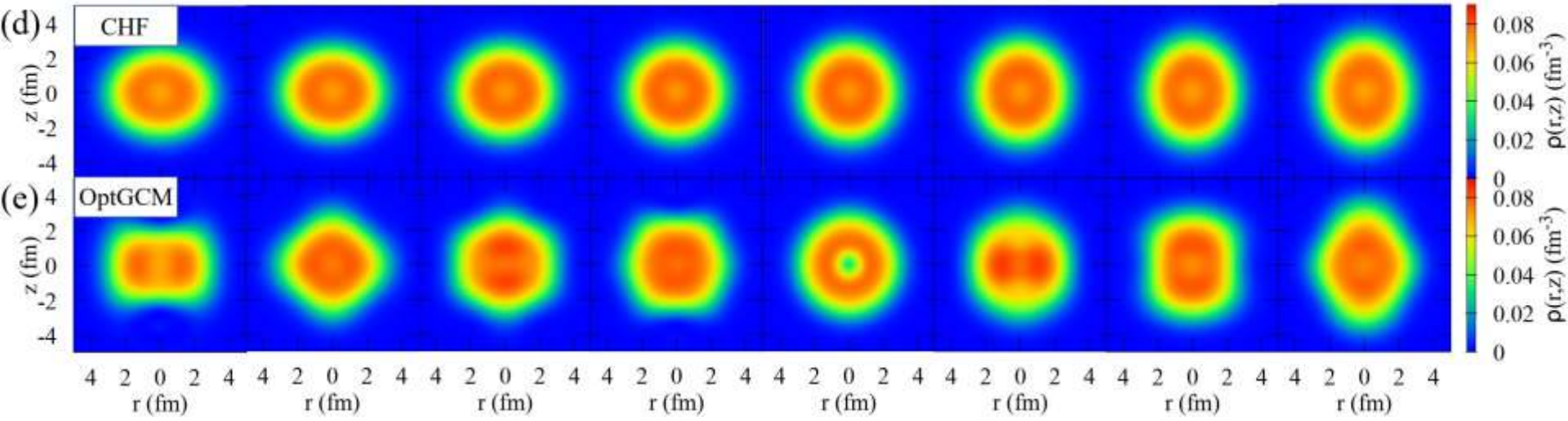
$$Q_2 = \frac{\langle \Psi | \hat{Q}_2 | \Psi \rangle}{\langle \Psi | \Psi \rangle}, Q_4 = \frac{\langle \Psi | \hat{Q}_4 | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Large fluctuation of Q_4 in the OptGCM, indicates:

- The fluctuation of Q_4 is important for g.s.
- The excitations of nuclei should be included as a collective coordinate.



Application of this method to the g.s. of the ^{16}O

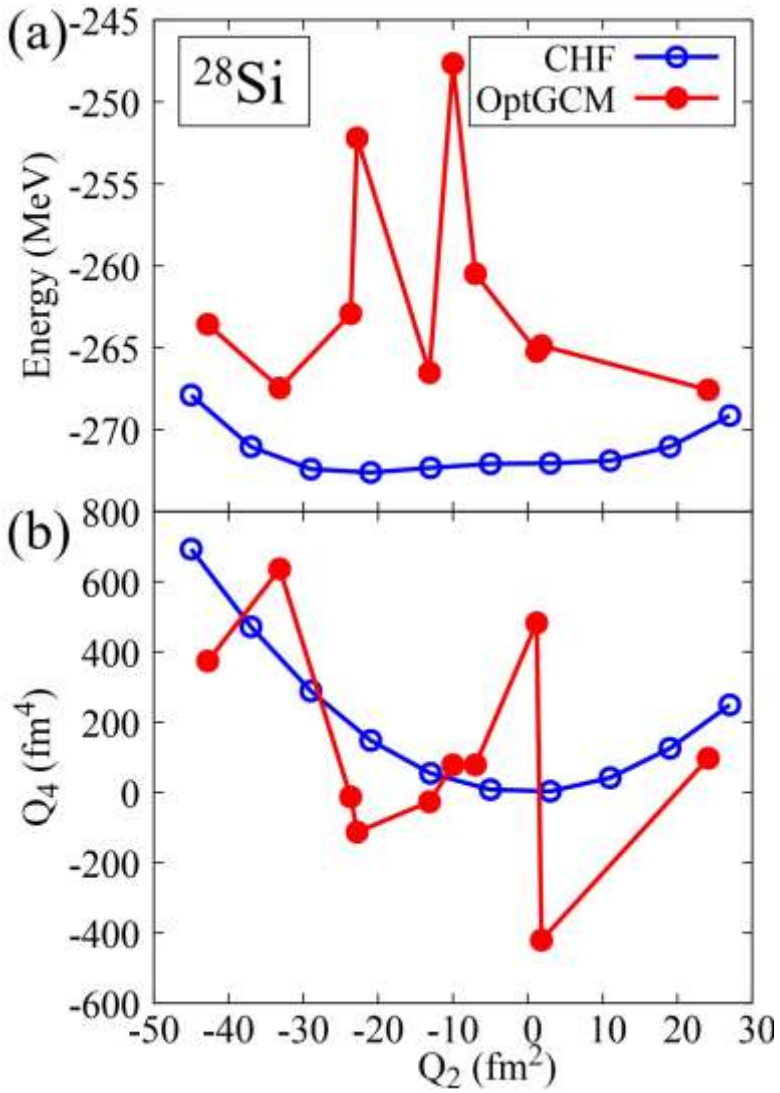


The neutron density distributions of each SD

A variety of shapes are obtained for the bases with the OptGCM.

It suggests that the OptGCM is capable of automatically describing multiple collective modes.

Application of this method to the g.s. of the ^{28}Si



The g.s. energies

HF: -272.63 MeV

GCM: -273.95 MeV

OptGCM: -275.00 MeV

Similarly, the bases with the OptGCM correspond to excited states and the Q_4 are largely fluctuated.

Summary

- A novel extension of the GCM in which both the basis SDs and the weight factors are optimized according to the variational principle.
- The optimized SDs correspond to excited states rather than the local ground states.
- Q_2 is not enough. we ask for more (at least Q_2 and Q_4).

Perspectives:

- A Systematic investigation in many nuclei with this method, compared with other method.
- Not only g.s., but also the excited states.