Optimization of the number of intrinsic states included in the discrete Generator Coordinate Method

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Outline

1 What's the research topic of the paper?

2 What's the research status of the topic?
- GCM in a nutshell

3 What has been done in this paper?

4 What's the conclusion?

5 What's the novelty?

What's the research topic of the paper?

Optimization of the the number of intrinsic states in GCM

GCM

(i) The purpose of GCM: provides a general framework to give variational solutions to the many-body problem.

(ii) The realizations of the GCM: the mixing of symmetry-restored (particle-number, parity and angular momentum projected) intrinsic quasiparticle states obtained from self-consistent mean-field calculations.

(iii) The different method context mixed with GCM: EDF, MR-EDF, SCCM, PGCM, DNO-SM, MCSM, ...

(iv) The detail of GCM: ...

Optimization

Optimal number of intrinsic states$\rightarrow$ Hamiltonian matrix elements $\rightarrow$ HWG equation $\rightarrow$ Energy,wave functions,...

What's the research status of the topic?

PGCM

- Nuclear wave function $|\Psi_{I/F}\rangle$ is expanded on a set of non-orthogonal basis:

$$\left|\Psi_{\alpha}^{JNZ}\right\rangle = \sum_{K=-J}^{J} \sum_{n=1}^{N_q} f_{K,\boldsymbol{q}_n}^{J\alpha} \left|JMK, \boldsymbol{q}_n\right\rangle$$

  where $|JMK, \boldsymbol{q}_n\rangle$ are symmetry-projected quasiparticle vacua,

$$|JMK, \boldsymbol{q}_n\rangle = \hat{P}_{MK}^{J} \hat{P}^{N} \hat{P}^{Z} |\Phi(\boldsymbol{q}_n)\rangle$$

- The Hill-Wheeler-Griffin (HWG) equations:

$$\sum_{K', \boldsymbol{q}'} \left[\mathcal{H}_{KK'}^{J}(\boldsymbol{q}, \boldsymbol{q}') - E_{\alpha}^{J} \mathcal{N}_{KK'}^{J}(\boldsymbol{q}, \boldsymbol{q}')\right] f_{K', \boldsymbol{q}'}^{J\alpha} = 0$$

- The Hamiltonian and norm kernels $\mathcal{H}$ and $\mathcal{N}$ are given by:

$$\mathcal{H}_{KK'}^{J}(\boldsymbol{q}, \boldsymbol{q}') = \left\langle JMK, \boldsymbol{q} | \hat{H} | JMK', \boldsymbol{q}' \right\rangle$$
$$\mathcal{N}_{KK'}^{J}(\boldsymbol{q}, \boldsymbol{q}') = \langle JMK, \boldsymbol{q} \mid JMK', \boldsymbol{q}' \rangle$$

Solution of the HWG equation

- For non diagonal matrix $\mathcal{N}$ (the norm kernels) , general method is constructing natural states $|\Lambda_j\rangle$:

$$\sum_{K',\boldsymbol{q}'} \mathcal{N}^J_{KK'}\left(\boldsymbol{q},\boldsymbol{q}'\right) u^J_{K',j}\left(\boldsymbol{q}'\right) = n^J_j u^J_{K',j}(\boldsymbol{q})$$

$$|\Lambda^J_{K,j}\rangle = \frac{1}{\sqrt{n^J_j}} \sum_{\boldsymbol{q}} u^J_{K,j}(\boldsymbol{q})|JMK,\boldsymbol{q}\rangle \tag{1}$$

$$g^J_\alpha(K,\boldsymbol{q}) = \sum_{K',\boldsymbol{q}'} \left[\mathcal{N}^J_{KK'}\left(\boldsymbol{q},\boldsymbol{q}'\right)\right]^{1/2} f^{J\alpha}_{K',\boldsymbol{q}'}$$

- under the natural states, the HWG equations are:

$$\sum_{j'} \langle\Lambda_j|\hat{H}|\Lambda_{j'}\rangle g^J_{\alpha,j'} = E^J_\alpha g^J_{\alpha,j'} \tag{2}$$

- This work they use the axial quadrupole deformation, which means K=0 and $\boldsymbol{q}$ only contains β_2 as the generating coordinate.

Solution of the HWG equation

Let us back to the first step which construct the natural states!

Since the norm overlap matrix is positive semi-definite, the eigenvalues of the norm kernel $\{n_j^J \geq 0\}$

Three cases

1. if $n_j^J \gg 0$: $|\Lambda_{K,j}^J\rangle = \frac{1}{\sqrt{n_j^J}} \sum_{\boldsymbol{q}} u_{K,j}^J(\boldsymbol{q})|\Phi(\boldsymbol{q})\rangle$
2. if $n_j^J = 0$: It indicates that a state is strictly linear dependence of the intrinsic set of states. . If there are L_{exa} intrinsic states such that $|\Phi_{q_m}\rangle = \sum_{i=1}^{N_{\rm int}-L_{\rm exa}} a_i \left|\Phi_{q_i}\right\rangle$, then there will be $L_{\rm exa}$ eigenvalues with λ_m exactly zero and the natural basis states coming from these eigenvalues/eigenvectors must not be taken into account ($m = N_{\rm int} - L_{\rm exa} + 1, \ldots, N_{\rm int}$)
3. if $n_j^J \to 0$: small and different from zero eigenvalues may naturally appear in large positive definite matrices, this approximate linear dependence(LD) may cause a numerically meaningless definition of several natural basis states

$\rightarrow$we have to remove additionally L_{app} states that correspond to $n_j^J < \varepsilon_n$, and get faithful truncated natural basis $\{|\Lambda_j\rangle\}_{j=1}^{N_{nat}}$ with $N_{nat} = N_{int} - L_{exa} - L_{app}$

What has been done in this paper?

How to define ε

Instead of using ε_n, they propose in the present work to use the deviation of the natural basis from its orthonormality as a more restricted and numerically stable method to determine the number of elements of the natural basis:

$$\left\langle \Lambda_j \mid \Lambda_{j'} \right\rangle - \delta_{jj'} < \varepsilon_{\text{nat}}; \forall j, j' \tag{3}$$

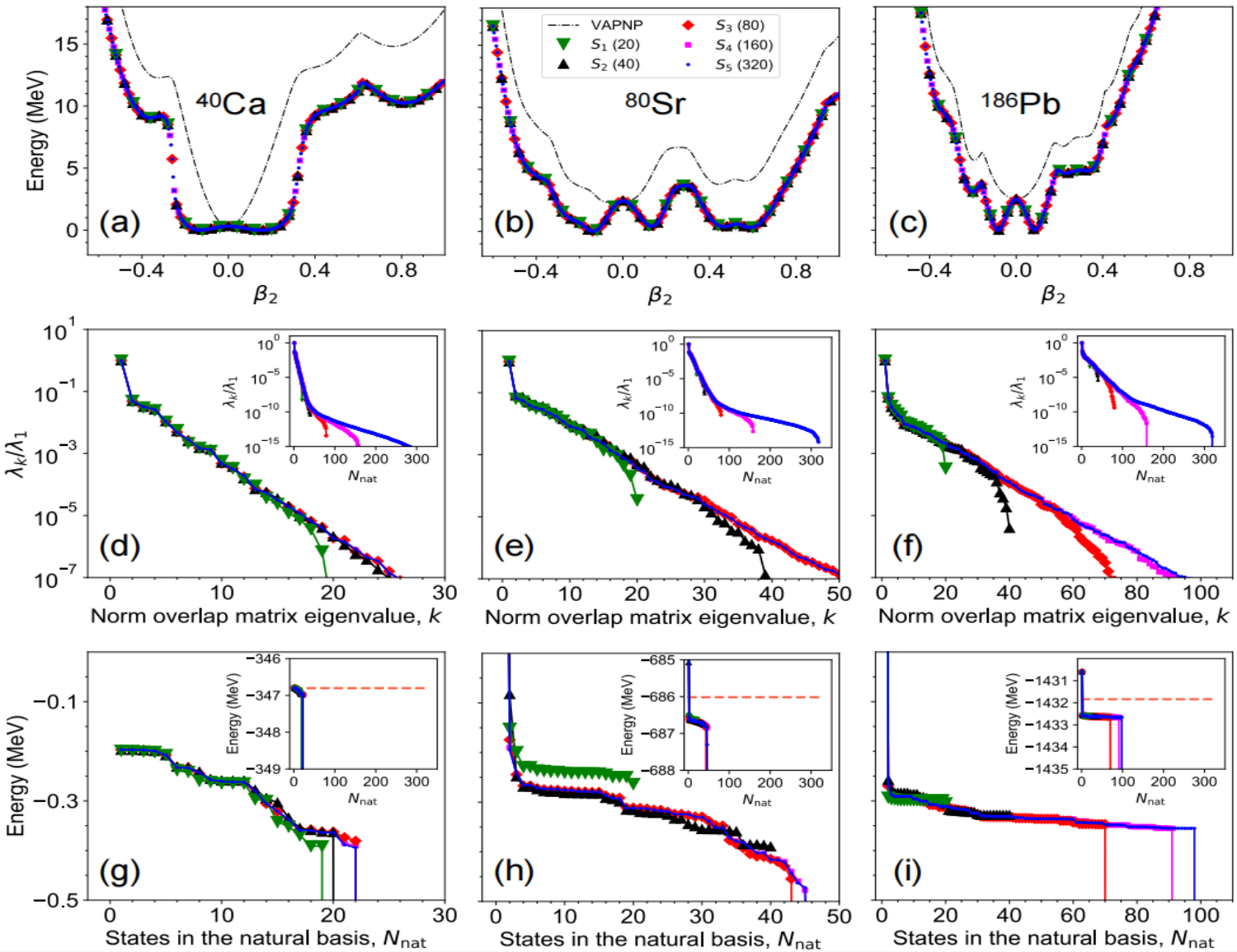
Two cases

1. if $j = j'$: $\left\langle \Lambda_j \mid \Lambda_{j'} \right\rangle = \frac{1}{n_j} \sum_{q,q'} u_j(\boldsymbol{q}) u_j(\boldsymbol{q'}) \left\langle JMK, \boldsymbol{q} \mid JMK', \boldsymbol{q'} \right\rangle = 1$
2. if $j \neq j'$: $\left\langle \Lambda_j \mid \Lambda_{j'} \right\rangle = \frac{1}{\sqrt{n_j n_{j'}}} \sum_{q,q'} u_j(\boldsymbol{q}) u_{j'}(\boldsymbol{q'}) \left\langle JMK, \boldsymbol{q} \mid JMK', \boldsymbol{q'} \right\rangle =$
   $\frac{\sqrt{n_{j'}}}{\sqrt{n_j}} \sum_q u_j(\boldsymbol{q}) u_{j'}(\boldsymbol{q})$=0 ; $\forall j, j'$?

GCM method under harmonic oscillator model

- Find a sparse set of intrinsic wave functions in the interval $q_i \in [q_{\min}, q_{\max}]$, $S = \left\{ \left| \Phi_{q_i} \right\rangle \right\}_{i=1,\ldots,N_{\text{int}}}$
- Solve Eq.(1) and build the natural basis states, $\left\{ \left| \Lambda_j \right\rangle \right\}_{j=1,\ldots,N_{\text{int}}}$
- Build the $N_{int} \times N_{int}$ natural basis norm overlap matrix and keep only the Nnat states that fulfill the orthonormalization condition for a chosen ε_{nat}
- If $N_{nat} \simeq N_{int}$, repeat the process but increasing the density of states in the set S in order to reach the saturation point. Otherwise, solve the HWG equation (Eq. (2)) by diagonalizing (without truncations related with ε_{nat}) the corresponding $N_{nat} \times N_{nat}$ Hamiltonian matrix.

Result


VAPNP
S_1 (20)
S_2 (40)
S_3 (80)
S_4 (160)
S_5 (320)
^{40}Ca
^{80}Sr
^{186}Pb
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
Energy (MeV)
β_2
λ_k/λ_1
N_{nat}
Norm overlap matrix eigenvalue, k
States in the natural basis, N_{nat}

Result

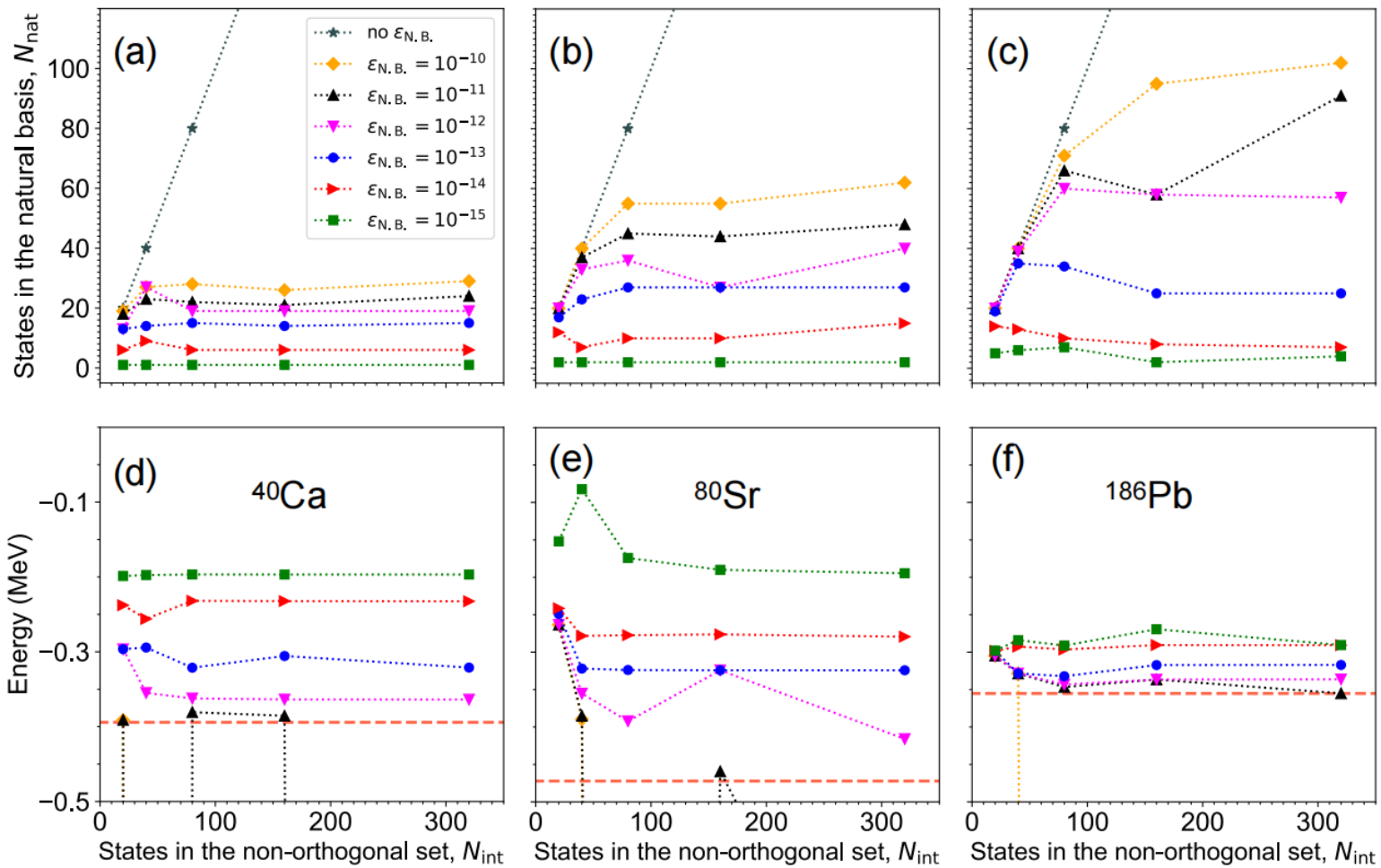
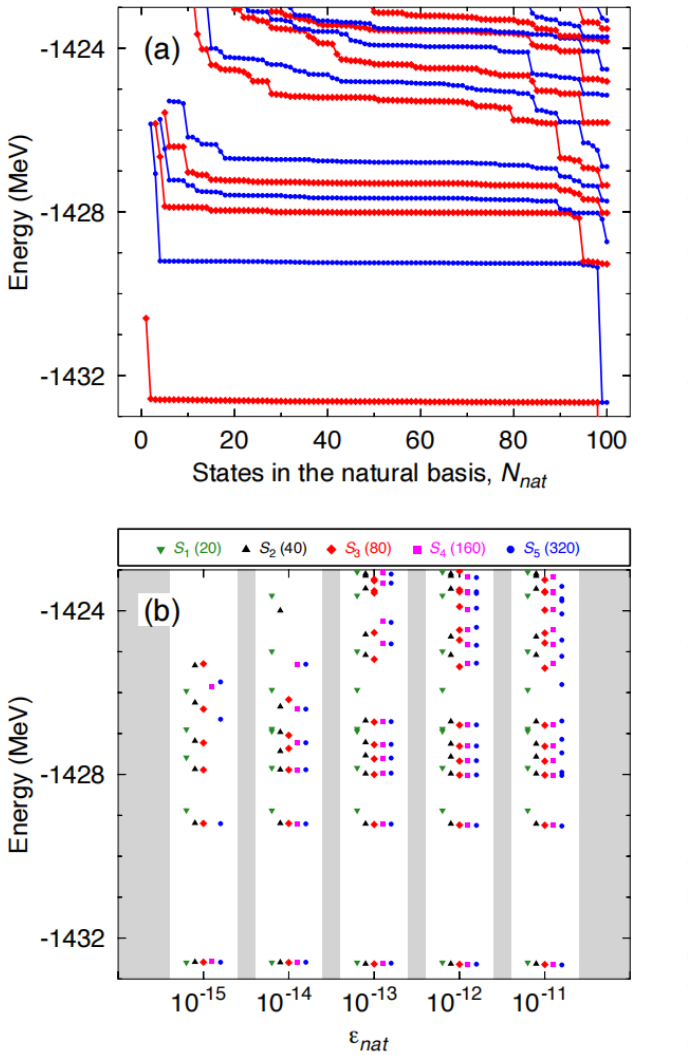


Figure: the value of ε nat should be small enough to ensure a numerically sound natural basis but not too small to leavenatural bases made of too few states.

Result

Convergence of the GCM excited states



analysis

- Some of these discontinuities fall down to the next lower plateau due to the appearance of one state with lower energy that makes that such a state
- For the rest of values of ε_{nat} we observe that the set with a smaller number of intrinsic states, S1, is the one that deviates most from the rest, even for small values of σ.
- The results show an excellent agreement for the different initial sets $S_{j=2-5}$ in the states with $\sigma = 2 - 6$ for values of $\varepsilon_{\text{nat}} = 10^{-13} - 10^{-12}$. For larger σ , the energies are rather dependent both on ε_{nat} and S_j and some degenerated states are also observed, e.g.

What's the conclusion?

Conclusion

1. They have observed that the largest normalized eigenvalues of the norm overlap matrices are very similar for all the sets although the sets with more intrinsic states accumulate more small eigenvalues. They also see similar energy plateaux for the different sets suggesting that a lot of redundancies (or approximate linear dependencies) are contained in the sets with a larger number of intrinsic states.
2. They have proposed a way of determining a priori (without evaluating Hamiltonian overlaps) natural bases with much less approximate linear dependencies based on their orthonormality conditions. They have clearly seen the saturation of the number of states in the natural basis with the number of initial states
3. They have also analyzed the excited states ($J \neq 1$) and they have seen the difficulties of using the plateau criterium to determine the excitation energies reliably.

What's the novelty?

novelty

EC

From the perspective of natural states $\{|\Lambda_j\rangle\}_{j=1,\ldots,N_{\mathrm{int}}}$

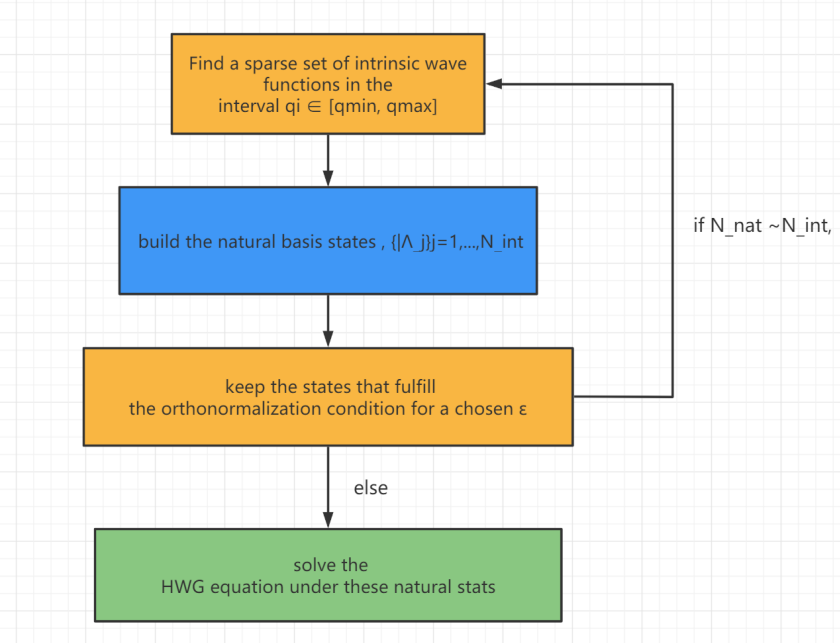


Figure: OC method

OC

From the perspective of HFB wave function $|JMK, \boldsymbol{q}\rangle$

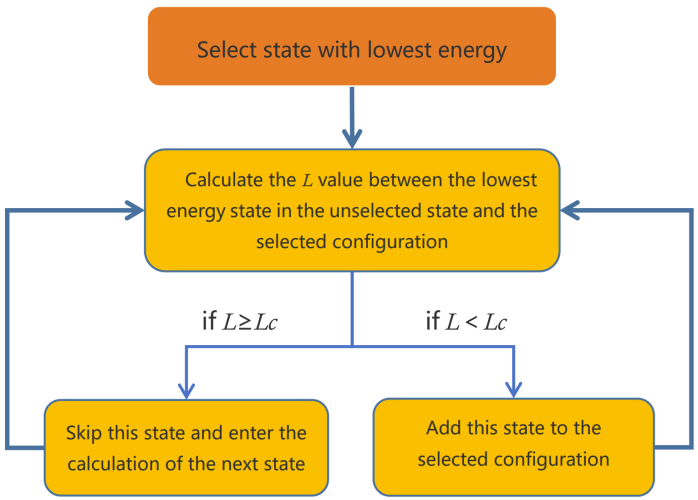


Figure: OC method

Thank you for your attention!