Optimization of generator coordinate method with machine-learning techniques for nuclear spectra and neutrinoless double-beta decay

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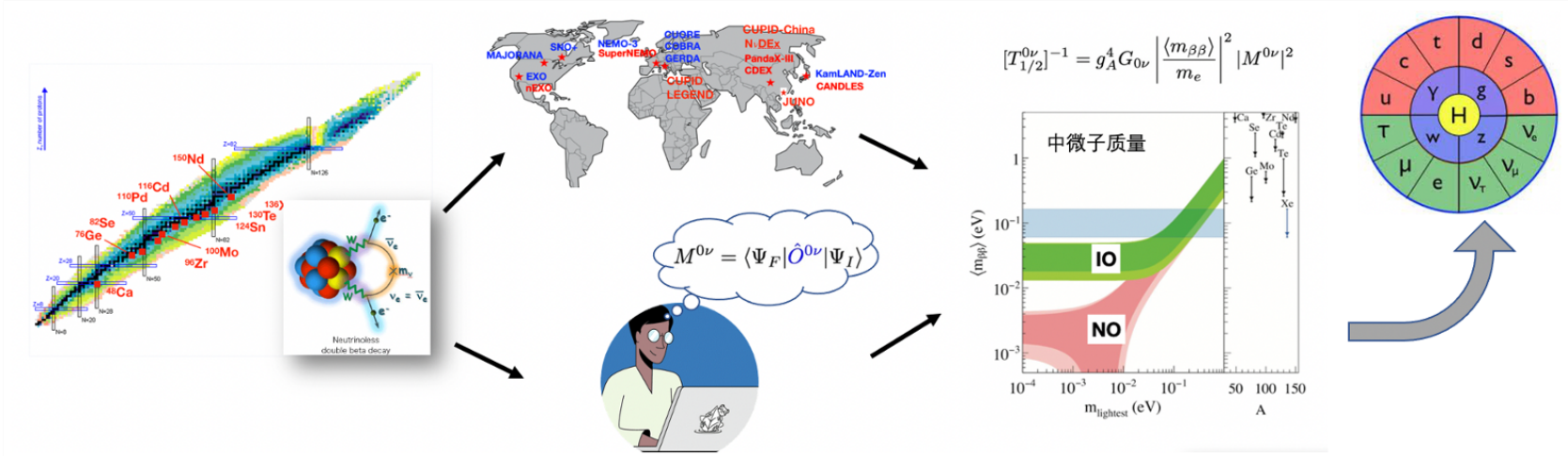
无中微子双贝塔衰变研讨会　2023年5月22日

The neutrinoless double beta decay



Generator coordinate method (GCM) : one of nuclear models for nuclear matrix element

- Energy density functionals

  Rodríguez2010PRL; Vaquero2013PRL; Song2014PRC; Yao2015PRC
- Shell-model Hamiltonian

  Jiao2017PRC; Yao2018PRC; Jiao2019PRC
- Interaction from chiral EFT

  Yao2020PRL

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

$$|\Psi_{\alpha}^{JNZ}\rangle = \sum_{K=-J}^{J} \sum_{n=1}^{N_a} f_{K,\boldsymbol{a}}^{J\alpha} |JMK, \boldsymbol{a}\rangle$$

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

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

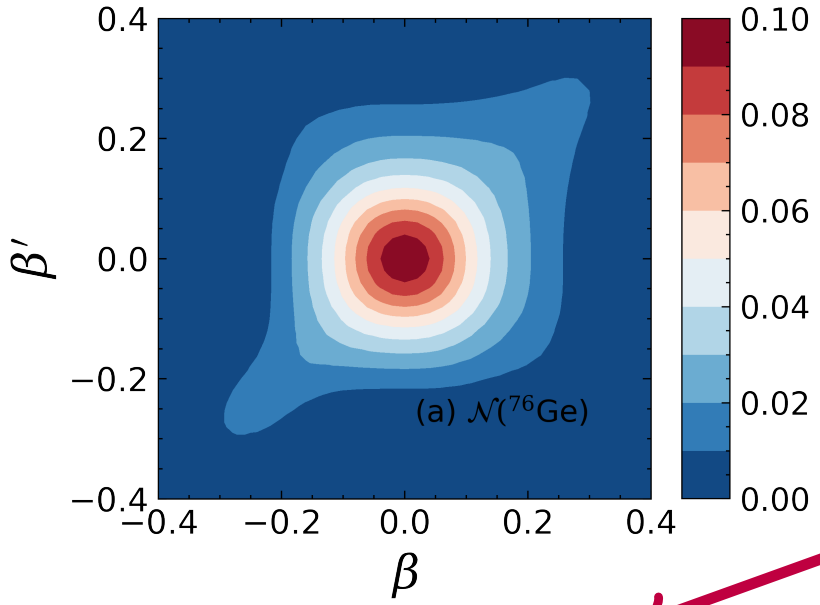
$$\sum_{K',\boldsymbol{a}'} \left[\mathcal{H}_{KK'}^{J}(\boldsymbol{a}, \boldsymbol{a}') - E_{\alpha}^{J} \mathcal{N}_{KK'}^{J}(\boldsymbol{a}, \boldsymbol{a}')\right] f_{K',\boldsymbol{a}'}^{J\alpha} = 0$$

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

$$\mathcal{N}_{KK'}^{J}(\boldsymbol{a}, \boldsymbol{a}') = \langle JMK, \boldsymbol{a} \mid JMK', \boldsymbol{a}'\rangle$$

$$\mathcal{H}_{KK'}^{J}(\boldsymbol{a}, \boldsymbol{a}') = \langle JMK, \boldsymbol{a}|\hat{H}|JMK', \boldsymbol{a}'\rangle$$

P. Ring and P. Schuck, The nuclear many-body problem (1980)



Gaussian overlap approximation:

$$\mathcal{N}\left(\beta,\beta'\right) \simeq \exp\left[-\frac{\gamma(q)}{2}(\beta-\beta')^2\right]$$

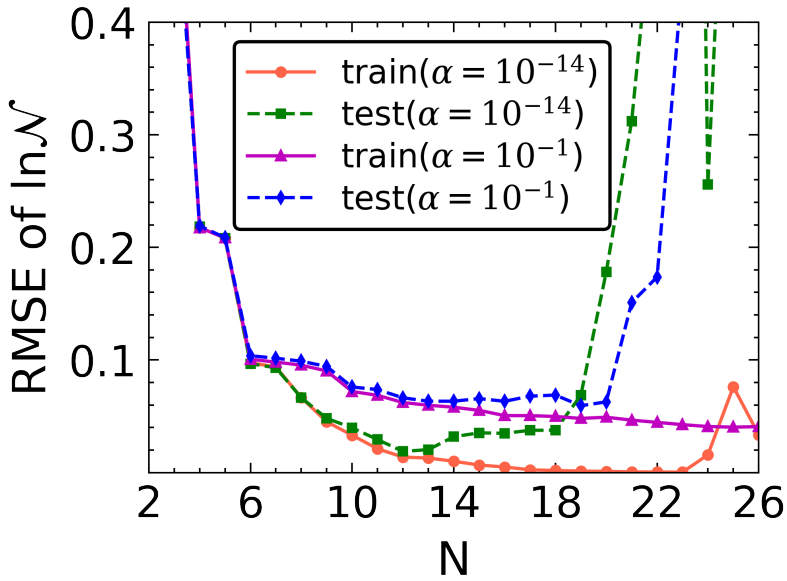
$$\frac{\mathcal{H}\left(\beta,\beta'\right)}{\mathcal{N}\left(\beta,\beta'\right)} \simeq P\left[(\beta-\beta')^2,(\beta+\beta')^2\right]$$

J. J. Griffin, J. A. Wheeler, Phys. Rev. 108, 311 (1957)

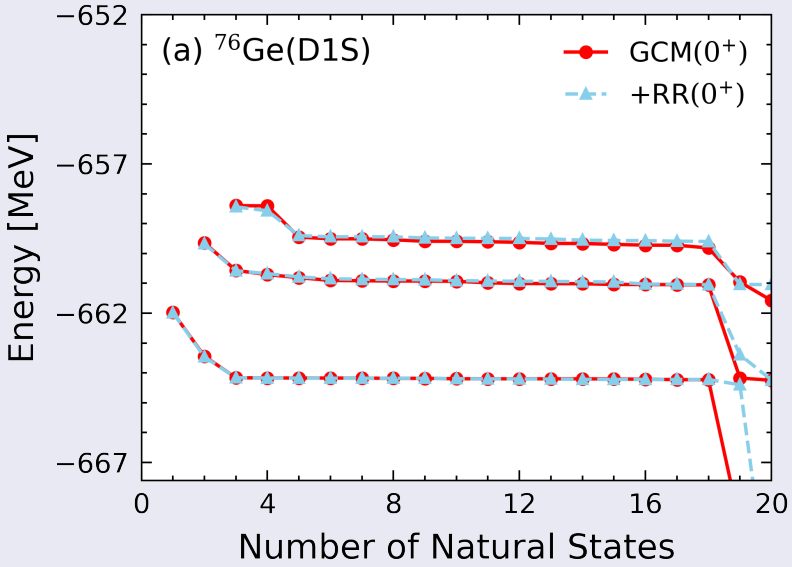
Polynomial ridge regression:

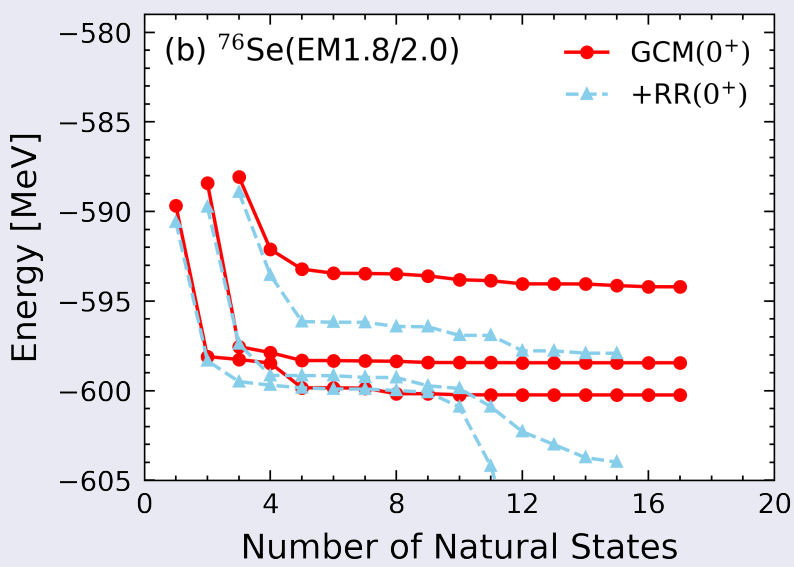
$$\hat{y}_N = \boldsymbol{\theta}\cdot P_N(\beta,\beta')$$

$$\mathcal{L}(\boldsymbol{N},\boldsymbol{\alpha}) = \sum_{i=1}^{M_{\mathrm{train}}}\left[\hat{y}_N^{(i)} - y^{(i)}\right]^2 + \alpha\boldsymbol{\theta}^T\boldsymbol{\theta}$$



The solution to HWG equations



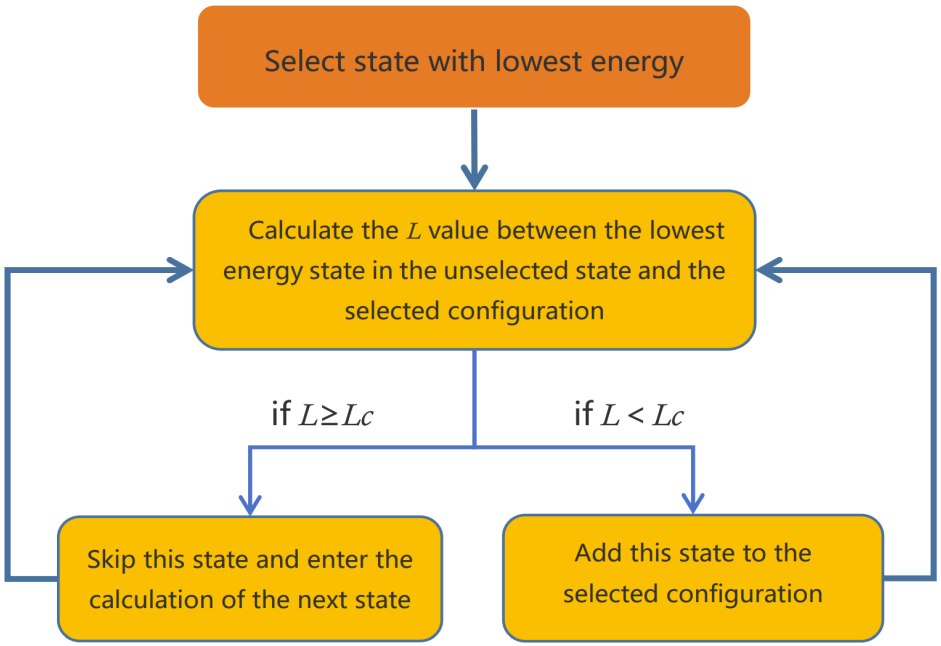


Challenge

- The solutions of GCM are sensitive to the accuracy of the kernels.
- The description of excited state by machine learning directly is poor.
- The calculation of the Hamiltonian kernel for training set is still time-consuming.

OC

Orthogonality condition (OC) method can determine the subspace in which the wave functions of nuclear low-lying states can be well represented.



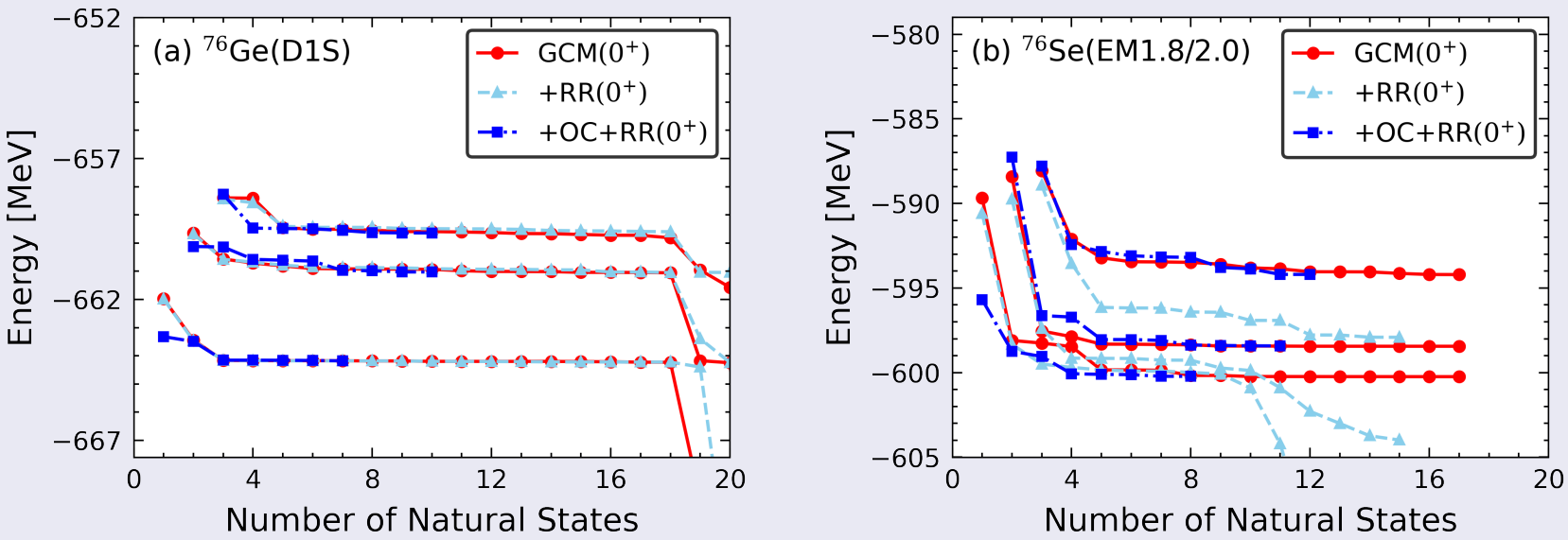
Here the value L is defined by:

$$L(n, n+1) = \frac{\left\langle n+1 \left| P^{(n)} \right| n+1 \right\rangle}{\langle n+1 \mid n+1 \rangle} = \frac{\beta^{(n)\dagger} \left(\boldsymbol{S}^{(n)} \right)^{-1} \beta^{(n)}}{\langle n+1 \mid n+1 \rangle}$$

$S_{ij}^{(n)} = \langle i \mid j \rangle$ and $\beta_i^{(n)} = \langle i \mid n+1 \rangle$ are nothing but the matrix elements of the norm kernel

A. M. Romero, J. M. Yao, B. Bally, T. R. Rodríguez, J. Engel, Phys. Rev. C 104, 054317 (2021)

The resolution to HWG equations



- OC method can help to select less configurations.
- OC method is not sensitive to the accuracy of norm and Hamiltonian kernels.
- When using OC to select subspaces for excited states, there are more subspaces than the ground state.

Energy spectrum (GCM+OC+ML)

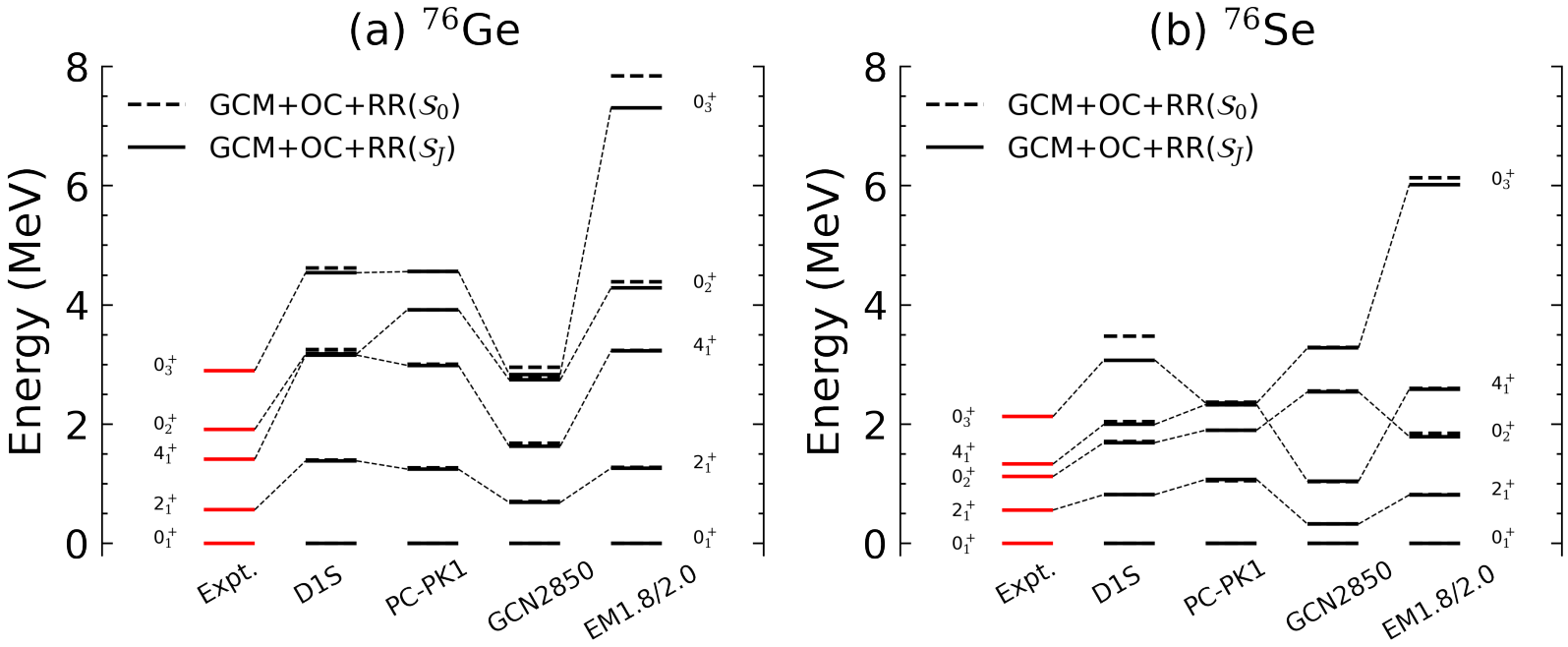


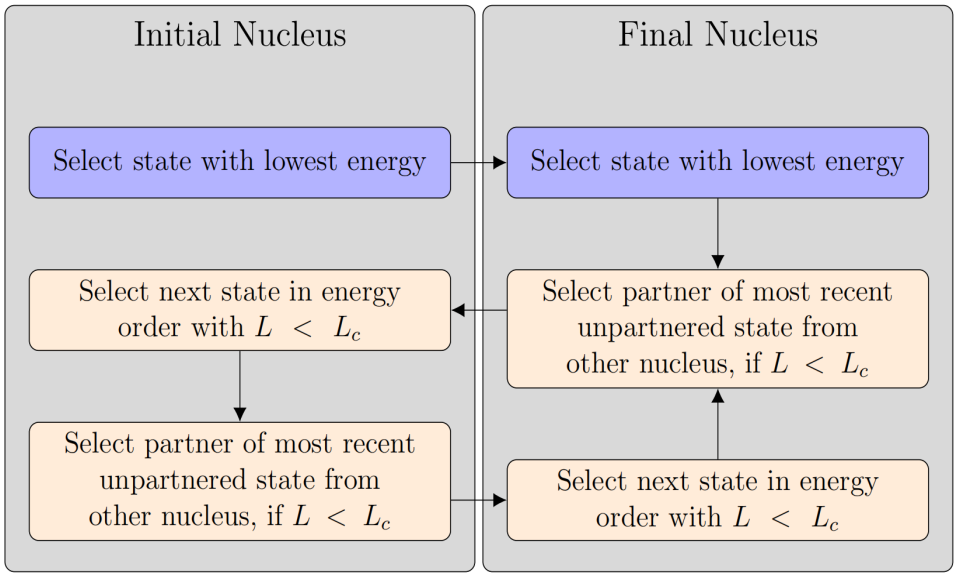
Figure: (Color online) The low-lying energy spectra of (a) ^{76}Ge and (b) ^{76}Se from GCM+OC+RR calculations based on two different nuclear Hamiltonian and two EDFs.

Using OC+RR method can screen out one-third of the original configurations and save at least 90% of the time!

X. Zhang, W. Lin, J. M. Yao, C. F. Jiao, A. M. Romero, T. R. Rodríguez, H. Hergert, Phys. Rev. C 107, 024304(2023)

ENTROP

Using energy-transition-orthogonality procedure (ENTROP) can determine the subspace of both initial nucleus and final nucleus.



- States with lower expectation values for the Hamiltonian are in general more important than those with higher expectation values.
- The largest contributions to NMEs often come from transitions between basis states with the same values for the collective coordinates $\boldsymbol{a}$.

A. M. Romero, J. M. Yao, B. Bally, T. R. Rodríguez, J. Engel, Phys. Rev. C 104, 054317 (2021)

NME (GCM+OC/ENTROP+ML)

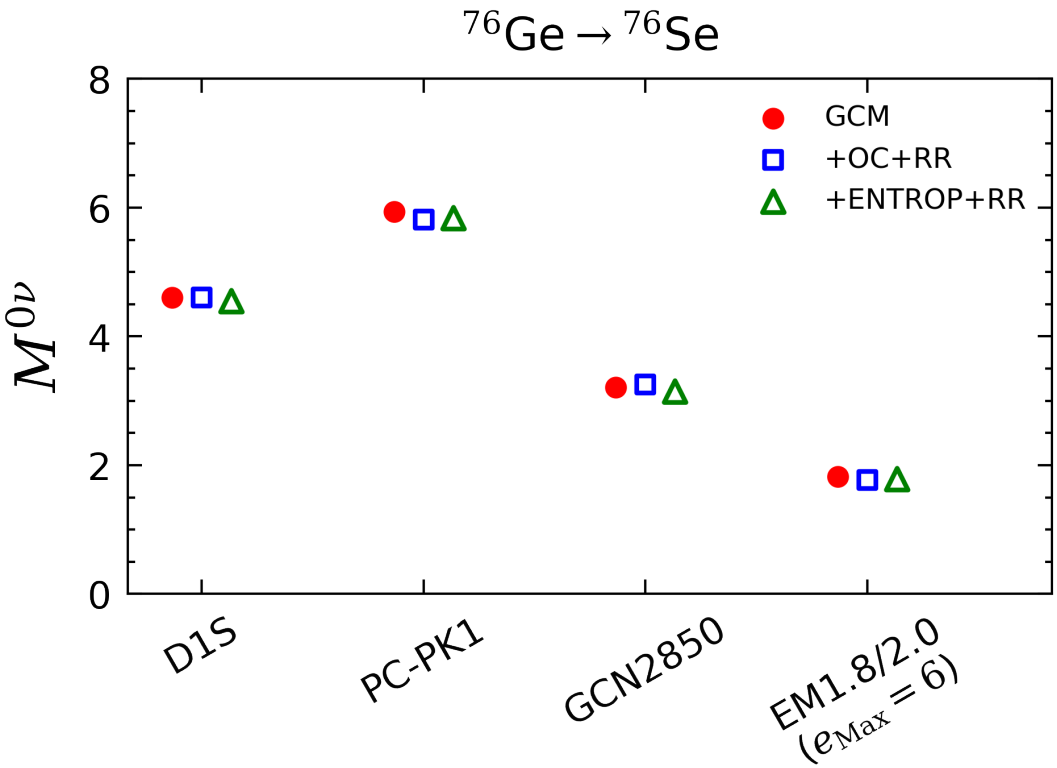


Figure: (Color online) Comparison of NMEs for the $0\nu\beta\beta$ decay of ^{76}Ge from the GCM, GCM+OL+RR and GCM+ENTROP+RR calculations.

- Using both method can screen out one-third of the original configurations in two nucleus and save at least 90% of the time!

Summary and outlook

Summary

- We have developed a machine learning algorithm in order to speed up the GCM calculations and test the RMSE and final result of the algorithm.
- The results have shown that the noise introduced by the optimized ML model can spoil the description of GCM for nuclear spectra, but this issue can be overcome by applying subspace reduction algorithms based on the OC or ENTROP method for the basis functions.

Outlook

- One can anticipate that this factor will be significantly larger in GCM calculations with multiple generator coordinates. Extensions of our approach in this direction are in progress.

Thank you for your attention!

Point taking method for ML

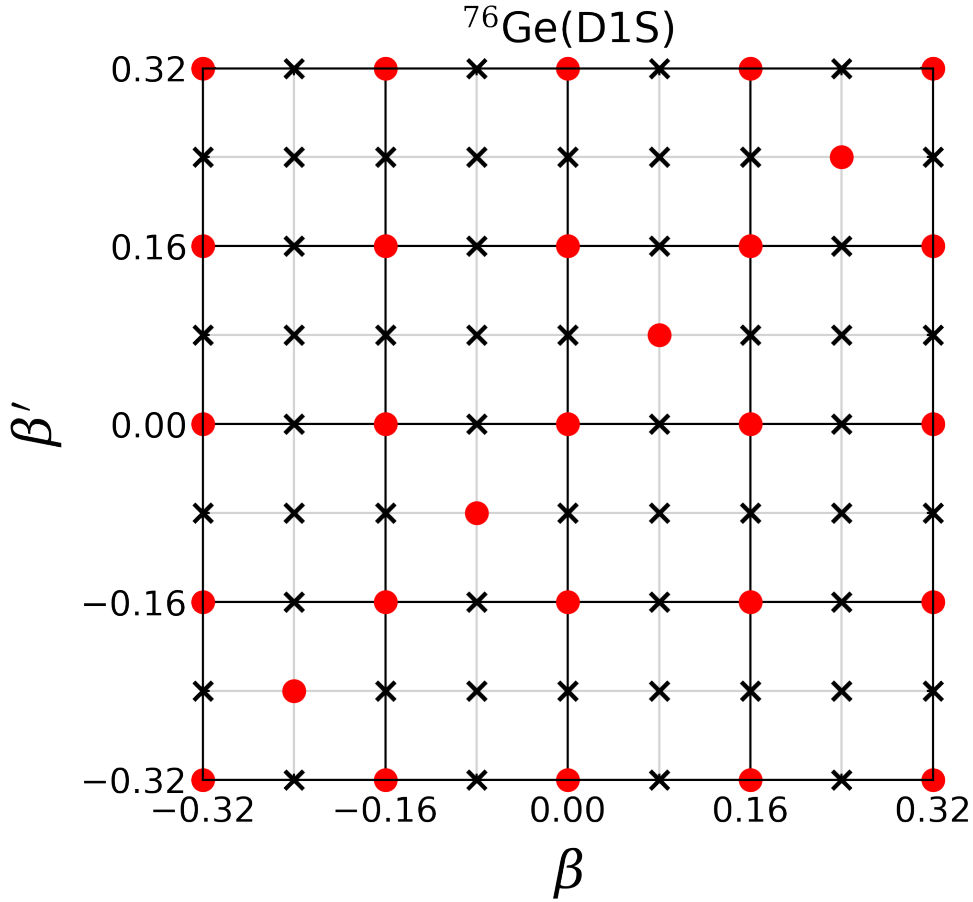


Figure: Point taking method. The red dots are for training set and the black crosses are for testing set. The step of lattice in the diagram is $|\Delta\beta|$=0.08

Flow chart

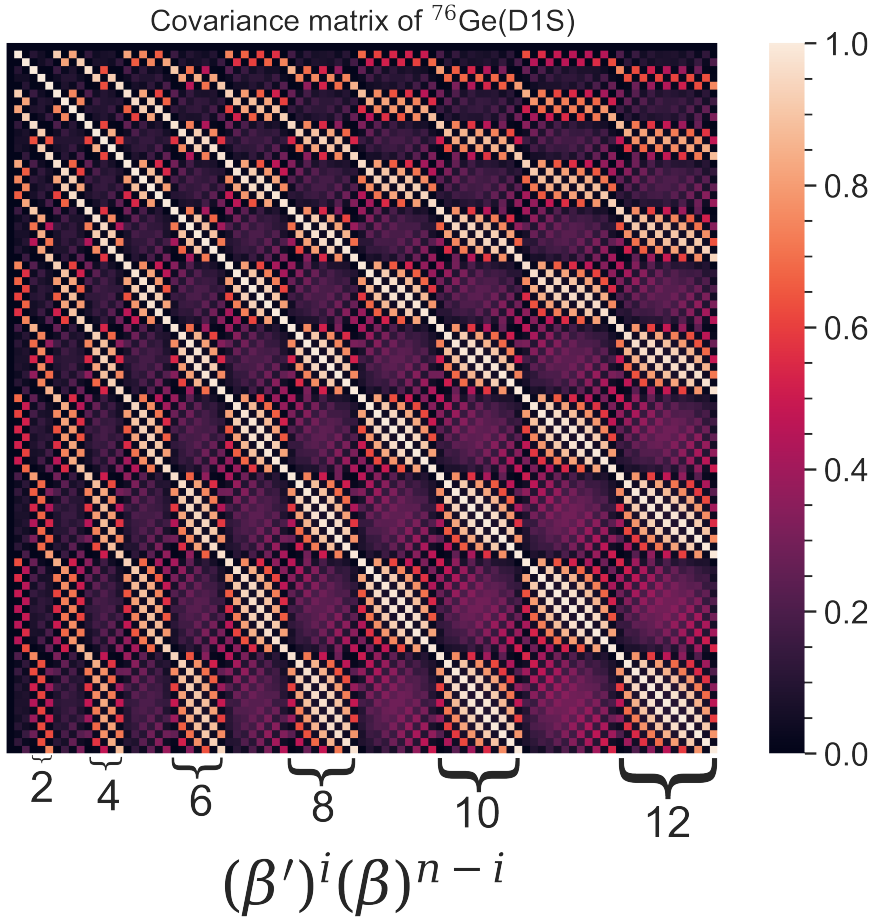


Figure: The covariance matrix of the RR model for the norm kernels of ^{76}Ge with $J = 0$ by the Gogny D1S force, where the degree parameter $N = 12$ and ridge parameter $\alpha = 10^{-14}$. The number of features $(\beta')^i(\beta)^{n-i}$ is $(N+2)(N+1)/2$, where the integer number $n \in [0, N]$ is shown in the bottom of the figure with the integer number i varying from 0 to n.

Flow chart

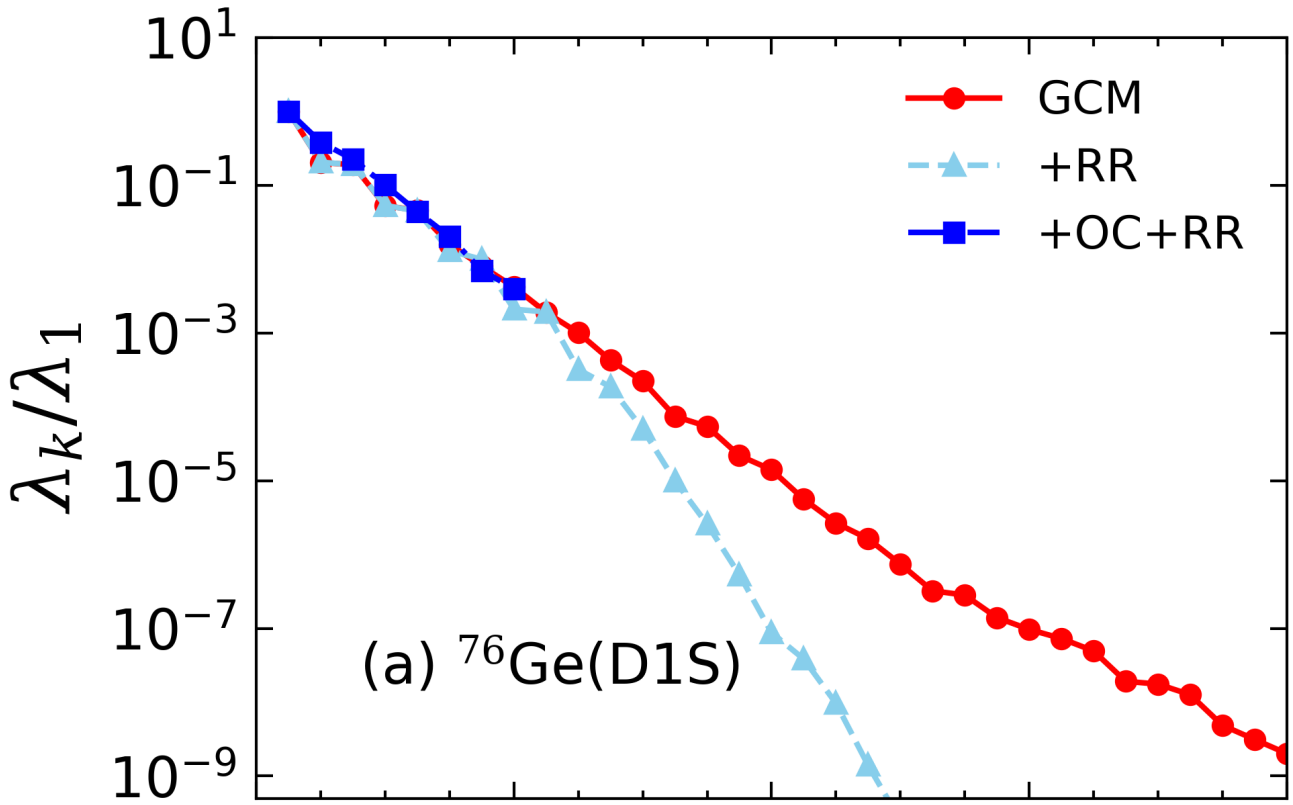


Figure: (Color online) The ratio of n-th eigenvalue to the first eigenvalue, using GCM, GCM+RR and GCM+OC+RR, respectively.

Details for OC method

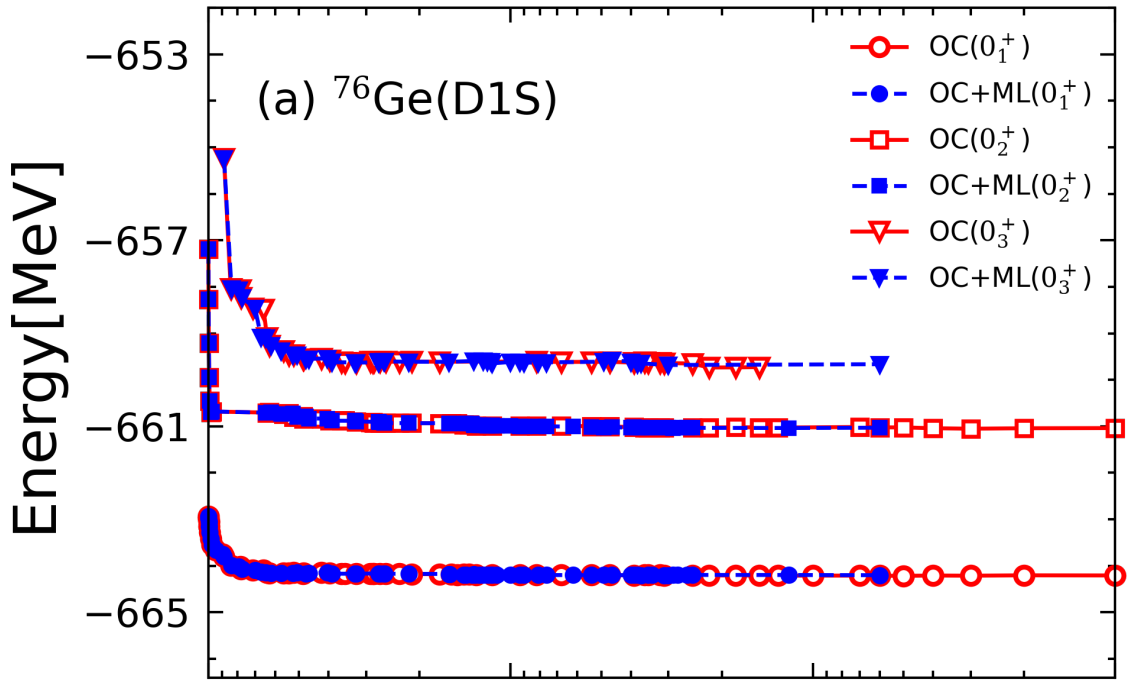
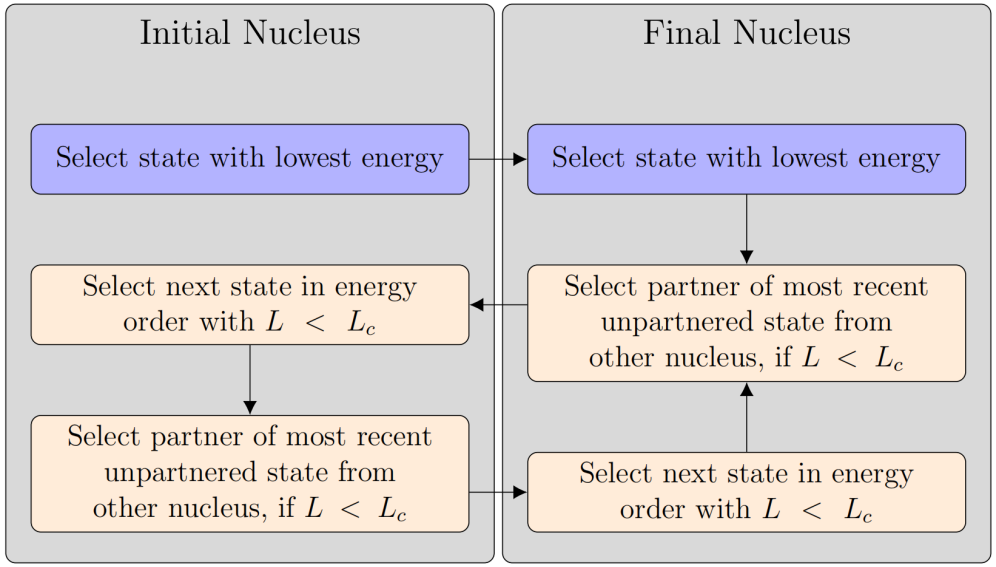


Figure: the convergence of the energies of the first three 0^+ states as a function of the cutoff parameter L_c

Details for ENTROP method



1. Sort the projected states by their diagonal energies.
2. Consider the first N states in each nucleus for several values of N.
3. Find the smallest value of L_c that, when the selection scheme in above diagram is applied, leads to subsets of the first N states (for all the values of N) that succeed in reproducing the corresponding NME.
4. Use that value of L_c to create a subspace pair in the full GCM spaces, solve the corresponding HWG equations, and compute the NME.