Emulating the generator coordinate method with extended eigenvector continuation for the Lipkin-Meshkov-Glick model

Qingyang Luo

School of Physics and Astronomy, Sun Yat-Sen University

Q.Y.Luo, X.Zhang, L.H.Chen, J.M.Yao, PRC 110, 014309(2024)

第三届“粤港澳”核物理会议， 深圳， 2024.11.18

Introduction: GCM for nuclear physics

- The generator coordinate method (GCM) is an important tool for modeling large-amplitude collective motions in atomic nuclei.

☐ Nucleus collective excitations	E.F.Zhou et al., Int.J.Mod.Phys.E 32, 2340011(2023) J. A. Sheikh et al., J.Phys.G 48,123001(2021)
☐ Dynamics of nucleus clusters	M. Freer et al., Rev.Mod.Phys. 90, 035004(2018) B. Zhou et al., Fronti. Phys.15, 14401(2019)
☐ *Ab initio* methods	J.M.Yao et al., PRL 124, 232501(2020) M. Frosini et al., Eur. Phys. J. A 58,64 (2022)
☐ Neutrinoless double-beta decay	J.M.Yao et al., Prog. Part. Nucl. Phys. 126, 103965 (2022) A.Belly et al., PRL 132, 182502 (2024)

- Uncertainty quantification is important but challenging in the modeling of nuclear collective-excitation states and the nuclear matrix elements of neutrinoless double-beta decay.

Introduction: challenges of uncertainty quantification

- Quantification of statistical uncertainty requires us to perform large-scale calculations with different parameters of the Hamiltonian or energy density functionals.

- The GCM becomes an exact method as long as the number of generator coordinates is sufficient. However, the complexity and computation time of the GCM grows rapidly with the number of generator coordinates.

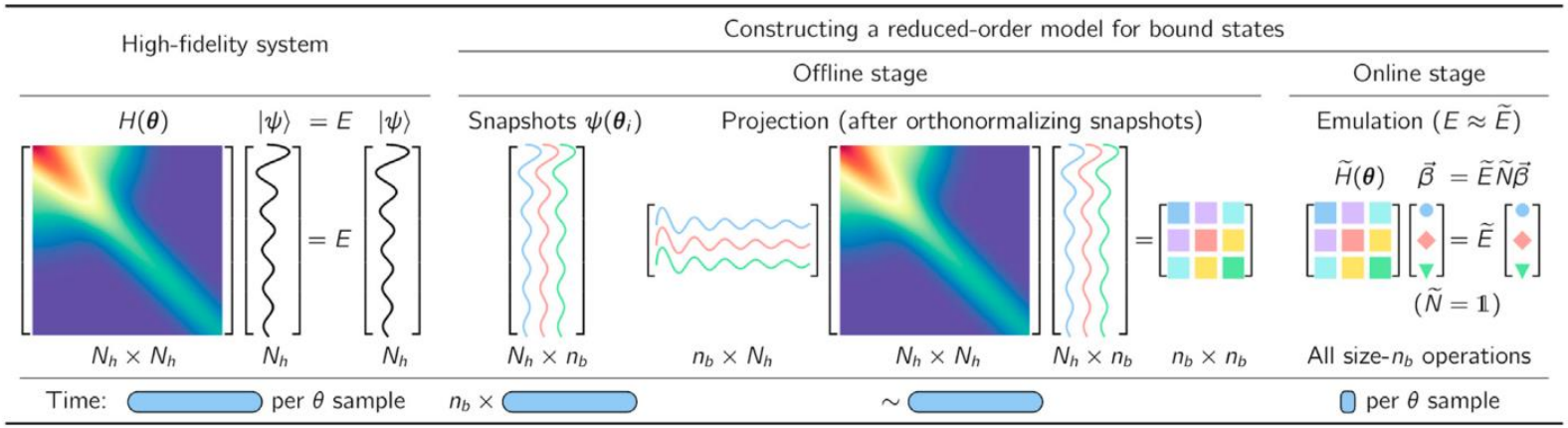
- Therefore, it is highly interesting to optimize or emulate the GCM calculations.

Introduction: Idea of EC method

- In recent years, the eigenvector continuation (EC) method has been proposed and extensively applied to optimize or emulate nuclear many-body calculations.

  D. Frame et al., PRL121, 032501(2018)

- In the EC, the complicated many-body wave function (original dimension N_h) of a Hamiltonian is expanded in a set of limited number (n_b) of basis given by the wave functions of the same Hamiltonian/EDF but with different parameters.



$$|\Psi(\theta_\odot)\rangle = \sum_{i=1}^{N_h} d_i |\Phi_i\rangle \qquad |\Psi(\theta_b)\rangle = \sum_{i}^{N_h} d'_i |\Phi_i\rangle \qquad |\Psi(\theta_\odot)\rangle = \sum_{b=1}^{n_b} d_b |\Psi(\theta_b)\rangle$$

C. Drischler , 10.3389/fphy.2022.1092931 .

This work

- We implement the EC method to emulate GCM calculation.
- The Lipkin model is an exactly solvable model which has been widely used for testing various many-body approaches.
- We examine the efficiency and accuracy of the EC+GCM for nuclear low-lying states based on the Lipkin model.

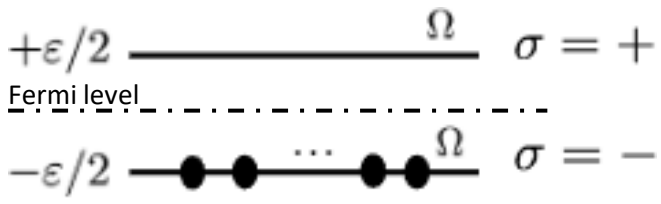
The Lipkin model

- The Hamiltonian:

$$\hat{H} = \varepsilon \hat{K}_0 - \frac{1}{2} V(\hat{K}_+ \hat{K}_+ + \hat{K}_- \hat{K}_-)$$

$$\hat{K}_0 = \frac{1}{2} \sum_{m=1}^{\Omega} (c^\dagger_{+m} c_{+m} - c^\dagger_{-m} c_{-m})$$

$$\hat{K}_+ = \sum_{m=1}^{\Omega} c^\dagger_{+m} c_{-m} \quad \hat{K}_- = (\hat{K}_+)^\dagger$$



P. Ring et al., *The nuclear many-body problem*, 1980.

- The parameter of the Hamiltonian

$$\chi = \frac{V}{\varepsilon}(\Omega - 1)$$

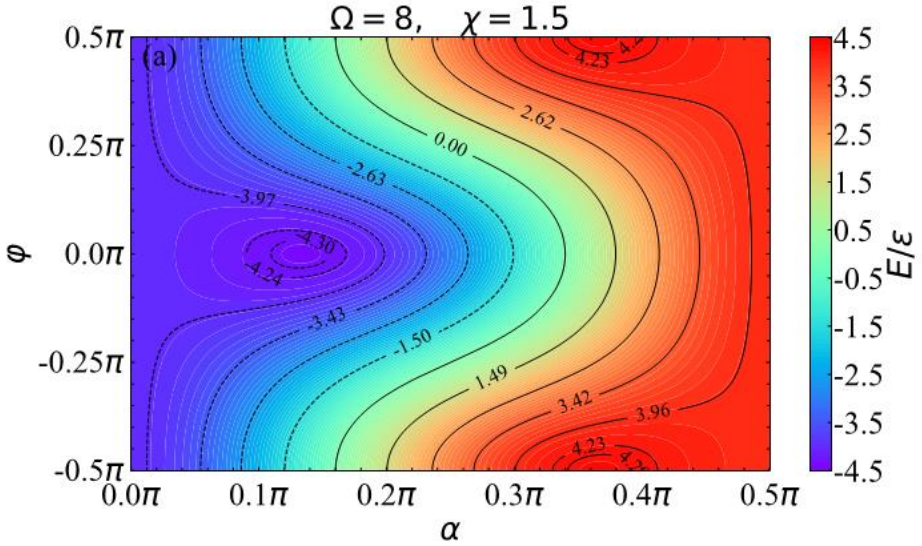
Which describes many-body correlations in the system.

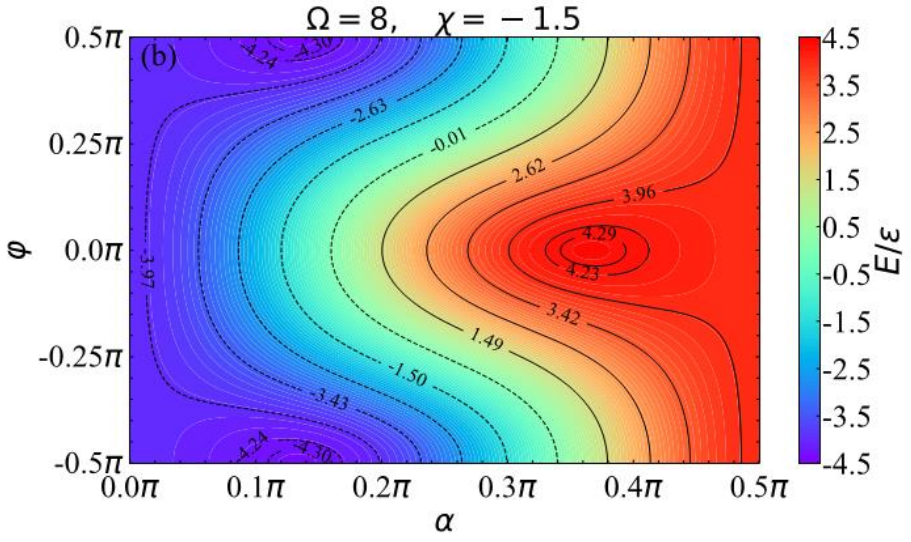
HF solution

- For a given interaction parameter, the wave function In the Hartree-Fock(HF) approximation is given by,

$$|\Phi\rangle = \prod_{m=1}^{\Omega} a_{0m}^{\dagger}|-\rangle \qquad |\Phi_0\rangle = \prod_{m=1}^{\Omega} c_{-m}^{\dagger}|-\rangle \qquad \begin{pmatrix} a_{0m}^{\dagger} \\ a_{1m}^{\dagger} \end{pmatrix} = \begin{pmatrix} \cos\alpha_1 & \sin\alpha_1 e^{-i\varphi_1} \\ -\sin\alpha_1 e^{i\varphi_1} & \cos\alpha_1 \end{pmatrix} \begin{pmatrix} c_{-m}^{\dagger} \\ c_{+m}^{\dagger} \end{pmatrix}$$

$$E_0^{HF} = -\frac{\varepsilon}{2}\Omega\left(\cos 2\alpha + \frac{1}{2}\chi \sin^2 2\alpha \cdot \cos 2\varphi\right)$$





GCM solution

- In the GCM, the wave functions is written as a linear combination of the constrained HF states $|\Phi(\alpha,\varphi)\rangle$

$$|\Psi^k\rangle = \int_{-\pi/2}^{+\pi/2} d\alpha \int_{-\pi/2}^{+\pi/2} d\varphi\ f^k(\alpha,\varphi)|\Phi(\alpha,\varphi)\rangle$$

- The unknown weight function $f^k(\alpha,\varphi)$ is determined by the Hill-Wheeler equation

$$\int_{-\pi/2}^{+\pi/2} d\alpha \int_{-\pi/2}^{+\pi/2} d\varphi \left(\langle\Phi(\alpha,\varphi)|\hat{H}|\Phi(\alpha',\varphi')\rangle - E^k\langle\Phi(\alpha,\varphi)|\Phi(\alpha',\varphi')\rangle\right) f^k(\alpha,\varphi) = 0$$

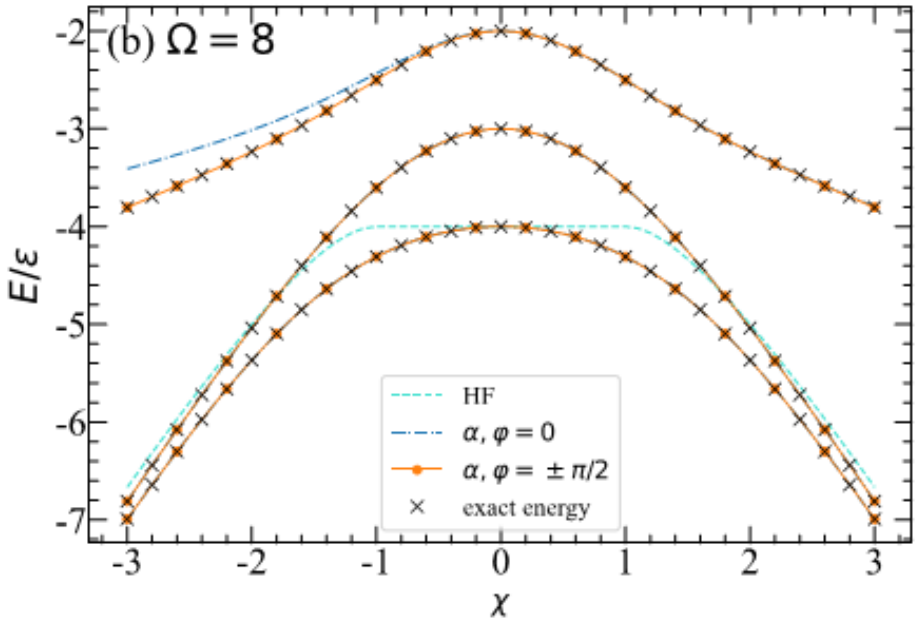
- In practical calculations, the generator coordinates are discretized, and the norm and Hamiltonian kernels are given by

$$\langle\Phi(\alpha_1,\varphi_1)|\Phi(\alpha_2,\varphi_2)\rangle = \left[\cos\alpha_1\cos\alpha_2 + \sin\alpha_1\sin\alpha_2 e^{i(\varphi_1-\varphi_2)}\right]^{\Omega} \equiv \mathcal{N}^{\Omega}$$

$$\langle\Phi(\alpha_1,\varphi_1)|\hat{H}|\Phi(\alpha_2,\varphi_2)\rangle = -\frac{\varepsilon\Omega}{2}\Big\{\cos^2\alpha_1\cos^2\alpha_2 - \sin^2\alpha_1\sin^2\alpha_2 e^{2i(\varphi_1-\varphi_2)} + \chi\left[\sin^2(\alpha_1)\cos^2(\alpha_2)e^{2i\varphi_1} + \sin^2(\alpha_2)\cos^2(\alpha_1)e^{-2i\varphi_2}\right]\Big\}\mathcal{N}^{\Omega-2}$$

A. P. Severyukhin et al., PRC74,024311(2006)

GCM solutions



- The energy of the states in the Lipkin model as the function of interaction parameter from different calculations.
- The low-lying states can be excellently reproduced by the GCM method.

Implementation of EC into GCM

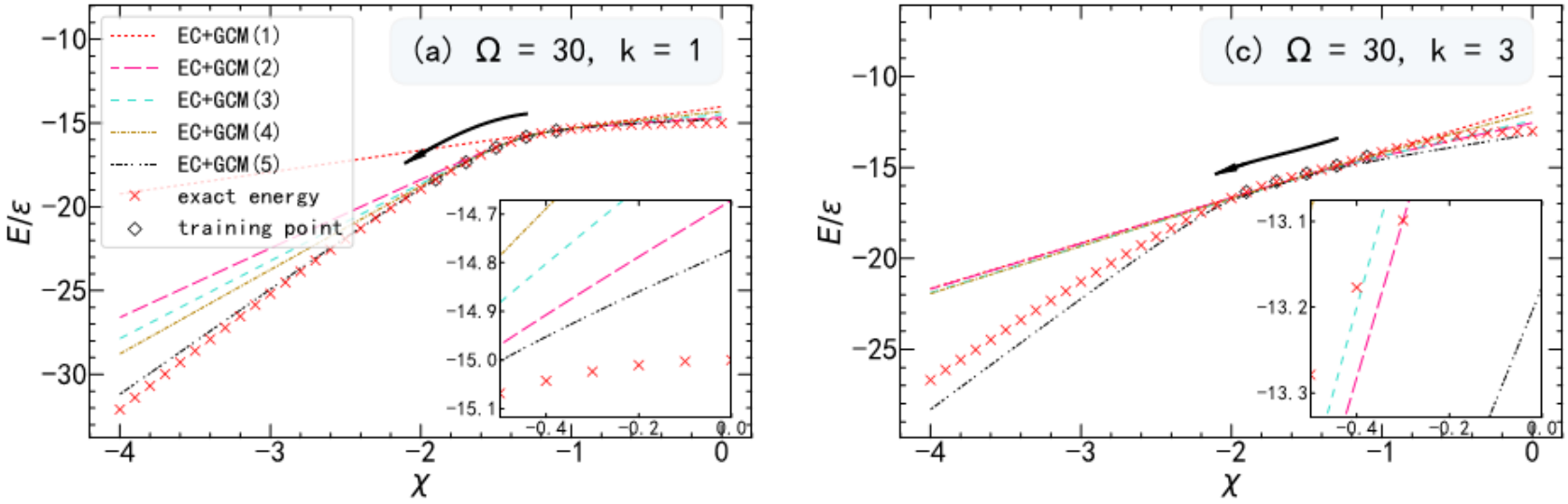
- **The wave function in the EC+GCM**

$$|\Psi^k_{\mathrm{EC}}(\chi)\rangle = \sum_{t=1}^{N_t} g^k(\chi_t)\,|\Psi^k_{\mathrm{GCM}}(\chi_t)\rangle\,,$$

Target interaction para.

Training interaction paras

This is referred to EC_1+GCM (N_t) scheme.



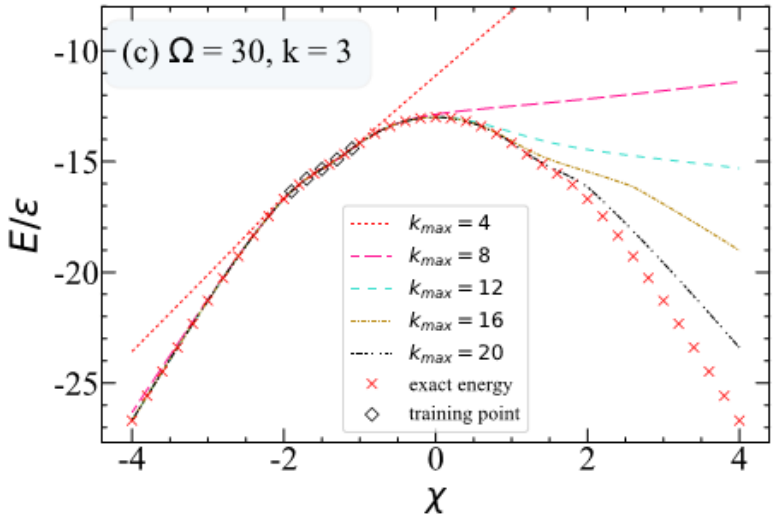
The EC_1 +GCM(N_t) scheme works well for ground state, but not for excited states.

Implementation of EC into GCM

- **The wave function in the EC_{kmax}+GCM scheme**

$$|\Psi^{k}_{EC}(\chi_{\odot})\rangle = \sum_{\kappa=1}^{k_{max}\geq k} \sum_{t=1}^{N_t} g^{k}(\kappa,\chi_t)|\Psi^{\kappa}_{\mathrm{GCM}}(\chi_t)\rangle$$

Including the first kmax states additionally



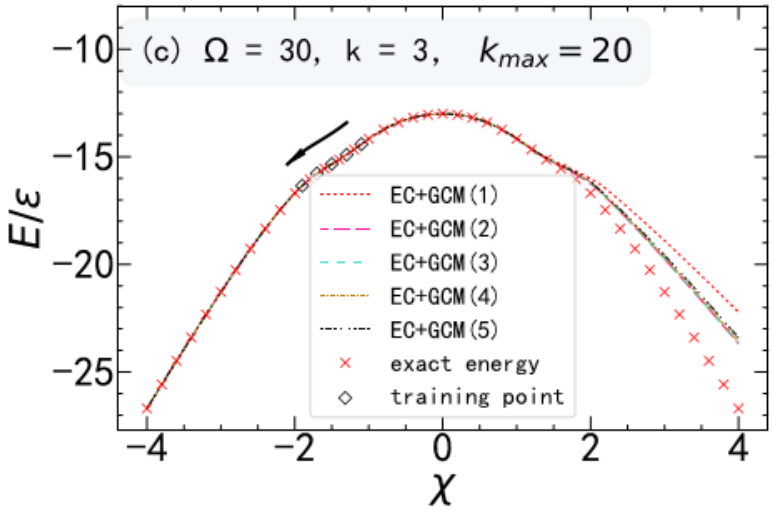
- **With a proper choice of kmax value, the EC_{kmax} +GCM(N_t) scheme works well for both ground state and excited states.**

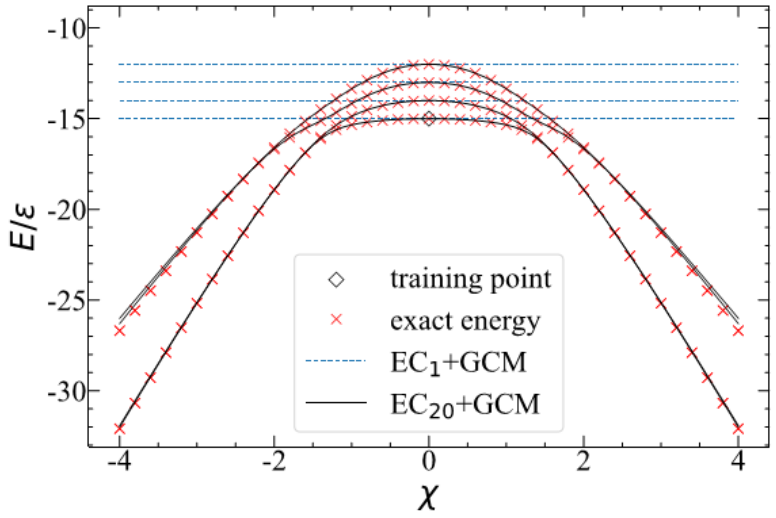
Implementation of EC into GCM

- **The wave function in the EC_{kmax}+GCM scheme**

$$|\Psi^{k}_{EC}(\chi_{\odot})\rangle = \sum_{\kappa=1}^{k_{max}\geq k} \sum_{t=1}^{N_t} g^{k}(\kappa,\chi_t)|\Psi^{\kappa}_{\mathrm{GCM}}(\chi_t)\rangle$$

Including the first kmax states additionally





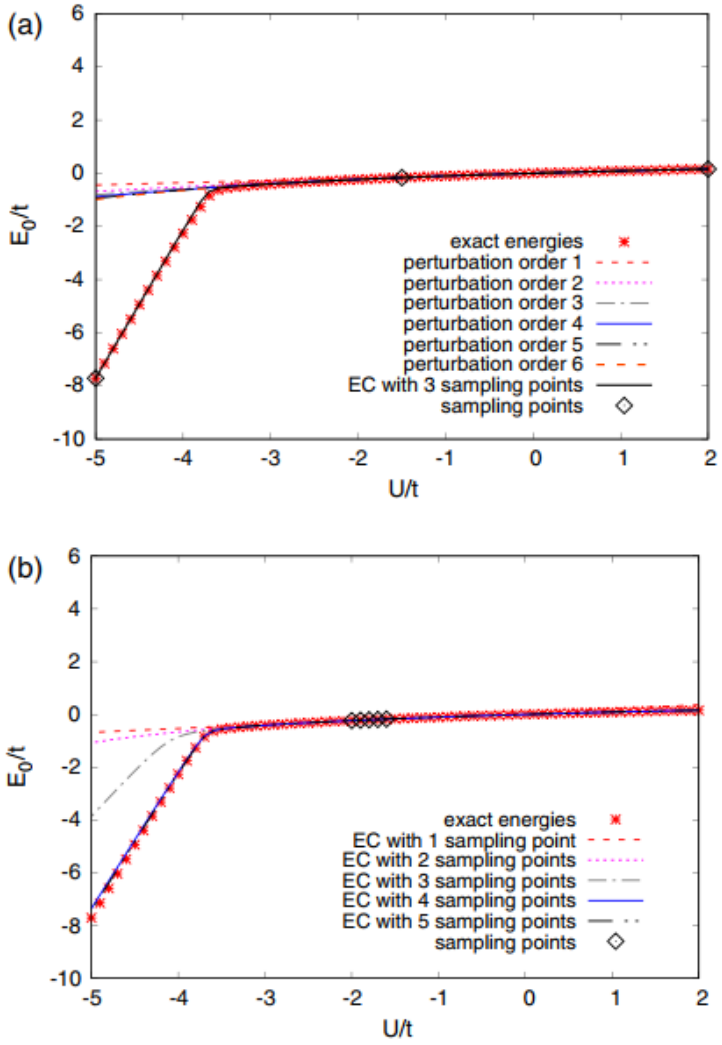
- **With a proper choice of kmax, the Nt can be significantly reduced.**

Summary

- We have implemented EC method into GCM for the low-lying states of Lipkin model.
- We found that compared to EC_1 +GCM scheme, the EC_{kmax} +GCM scheme performs well not only for ground state, but also for excited states.
- Next: application of the EC_{kmax}+GCM for nuclear low-lying states and neutrinoless double beta decay starting from chiral nuclear forces or nuclear energy density functionals.

Thanks for your attention

Eigenvector continuation

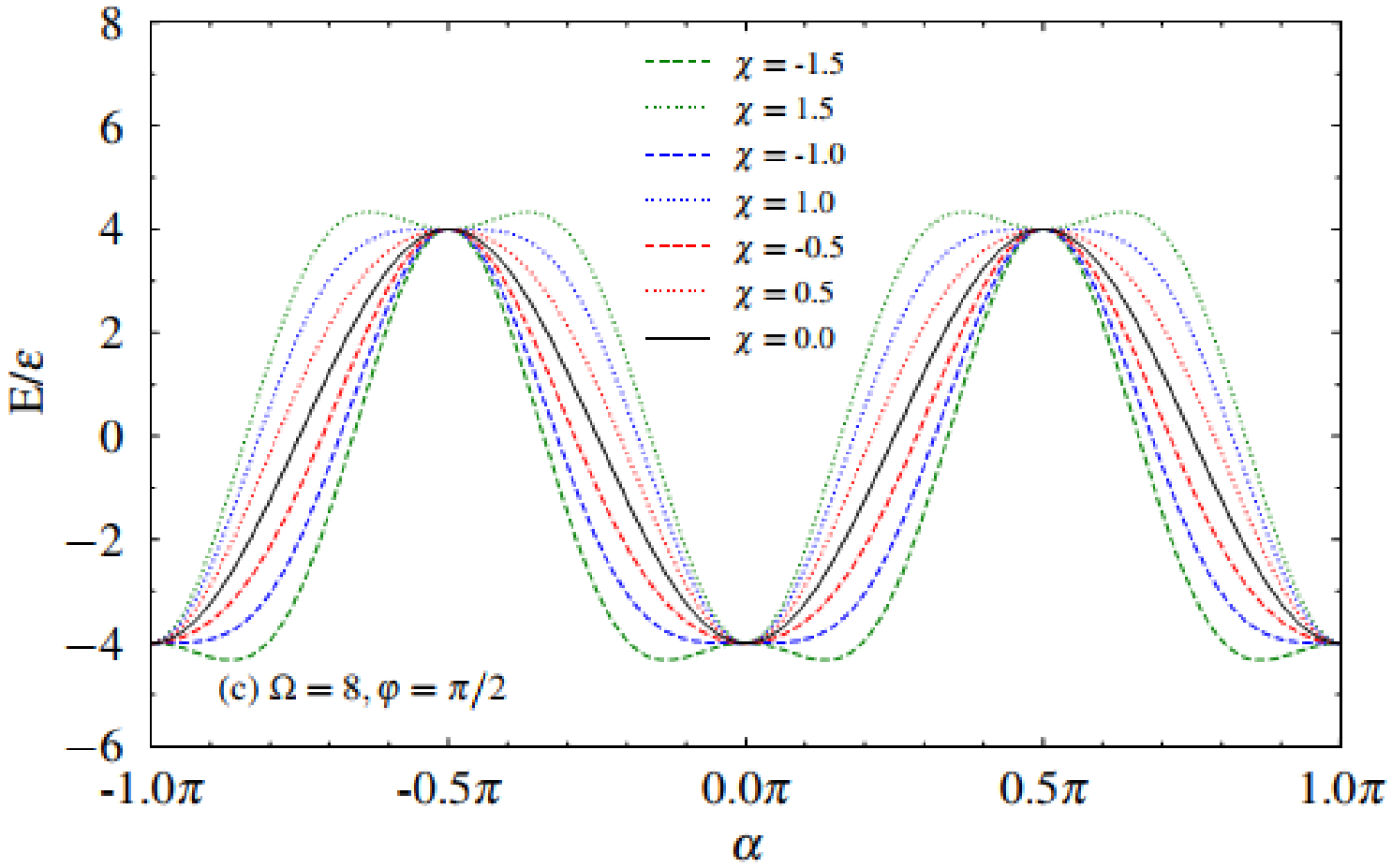


D. Frame et al., PRL121, 032501(2018)

- The development of EC in was inspired by the quantum many-body problem and the desire to find the extremal eigenvalues and eigenvectors of a Hamiltonian matrix too large to store in computer memory.

$$\tilde{H}(\boldsymbol{\theta})\vec{\beta}(\boldsymbol{\theta}) = \tilde{E}(\boldsymbol{\theta})\tilde{N}(\boldsymbol{\theta})\vec{\beta}(\boldsymbol{\theta}),$$
$$\tilde{H}_{ij}(\boldsymbol{\theta}) = \langle\psi_i|H(\boldsymbol{\theta})|\psi_j\rangle\,,$$
$$\tilde{N}_{ij}(\boldsymbol{\theta}) = \langle\psi_i|\psi_j\rangle\,.$$

- The core of the EC method is to interact with the eigenvector and the target Hamiltonian under different interactions, and use the variational idea to solve this generalized eigenvalue problem.


8
6
4
2
0
−2
−4
−6
E/ε
-1.0π
-0.5π
0.0π
0.5π
1.0π
α
χ = -1.5
χ = 1.5
χ = -1.0
χ = 1.0
χ = -0.5
χ = 0.5
χ = 0.0
(c) Ω = 8, φ = π/2