Floating-block EC

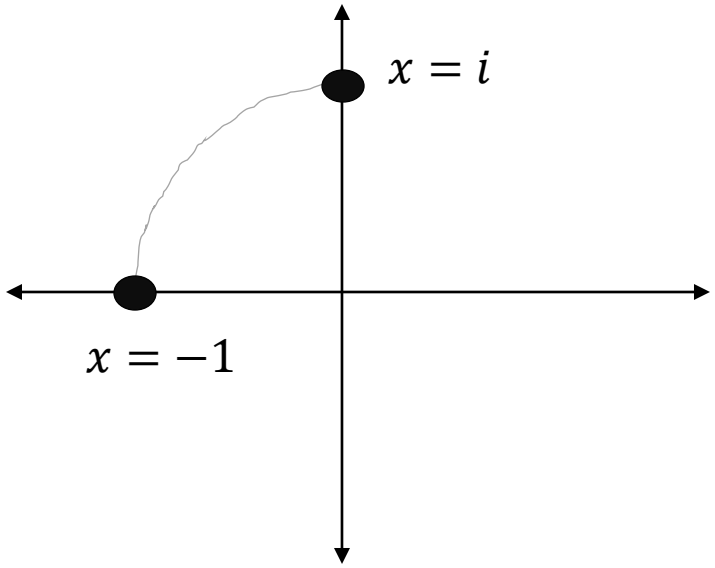
Avik Sarkar, Dean Lee, and Ulf-G. Meißner

Outline

- Eigenvector continuation (EC)
- Floating block algorithm for quantum Monte Carlo
- Results - EC Emulator with floating block
- Summary

Introduction

- Eigenvector continuation (EC) is a variational technique [1] to find the extremal eigenvalues and eigenvectors of a parameter dependent Hamiltonian matrix $H(c) = H_0 + cH_1$
- Key idea – dimensionality reduction.
- Roots of $x^2 + cx + 1 = 0$, when $c \in [0,2]$.
- Eigenvector $|\psi(c)\rangle$ trajectory approximated by a few dimensions.
- Smaller subspace -> faster calculations



[1] - Dillon Frame, Rongzheng He, Ilse Ipsen, Daniel Lee, Dean Lee, and Ermal Rrapaj. Eigenvector continuation with subspace learning. Phys. Rev. Lett., 121(3):032501, 2018.

Applications

- EC was designed to work in extremely large vector spaces, where we can calculate the inner products and matrix elements from Monte Carlo simulations, coupled cluster calculations, or other many-body methods.
- It has been used to extend quantum Monte Carlo methods to problems with strong sign oscillations [1], as a fast emulator for quantum many-body systems [2, 3] and scattering [4], and as a resummation method for perturbation theory [5]. It could be used to study geometric phases in the adiabatic evolution of a quantum Hamiltonian, or the quantum phase diagram of a many-body Hamiltonian with several tunable couplings.
- EC belongs to the family of Reduced Basis Methods (RBM) [6, 7], which can be applied to a broad set of problems.

[1] - D. K. Frame, Ph.D. thesis (2019), 1905.02782.
[2] - S. König, A. Ekström, K. Hebeler, D. Lee, and A. Schwenk (2019), 1909.08446
[3] - A. Ekström and G. Hagen, Phys. Rev. Lett.123, 252501 (2019),1910.02922
[4] - R. J. Furnstahl, A. J. Garcia, P. J. Millican, and X. Zhang, Phys. Lett. B 809, 135719 (2020), 2007.03635
[5] - P. Demol, T. Duguet, A. Ekström, M. Frosini, K. Hebeler, S. König, D. Lee, A. Schwenk, V. Somà, and A. Tichai, Phys.Rev.C101, 041302(R) (2020), 1911.12578
[6] - E. Bonilla, P. Giuliani, K. Godbey, and D. Lee (2022), 2203.05284
[7] - J. A. Melendez, C. Drischler, R. J. Furnstahl, A. J. Garcia, andX. Zhang (2022), 2203.05528.

Applying EC

- $H(c) = H_0 + cH_1$
- Notation: $H(c)|\psi(c)\rangle = E(c)|\psi(c)\rangle$, want $|\psi(c_t)\rangle$, and $E(c_t)$.
- Given snapshots $\{|\psi(c_1)\rangle, \ldots, |\psi(c_N)\rangle\}$ at training points $c = c_1, \ldots, c_N$.
- Project Hamiltonian onto smaller subspace,

$$\widetilde{H}_{i',i} = \langle\psi(c_{i'})|H(c_t)|\psi(c_i)\rangle$$

Applying EC

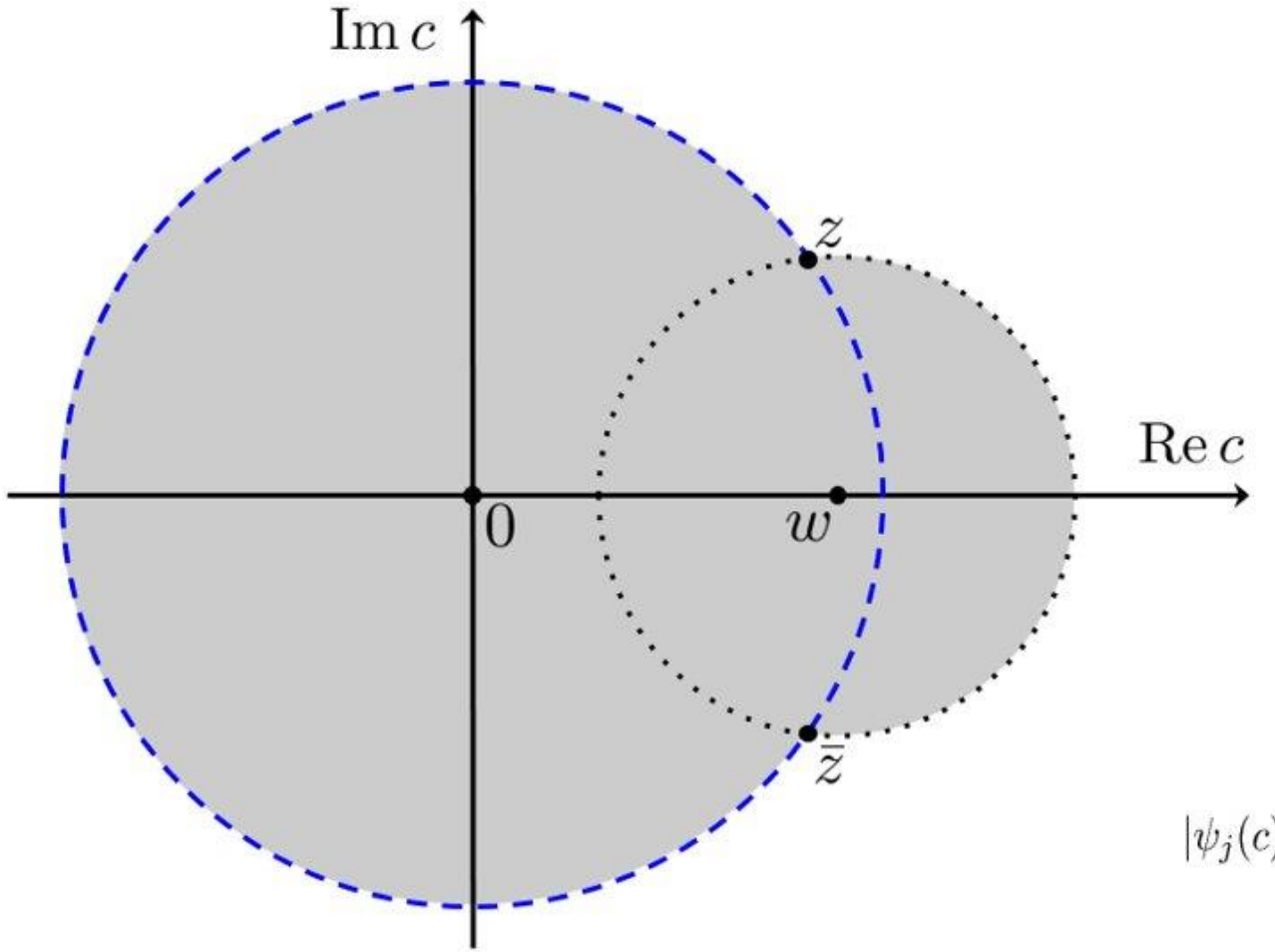
- Calculate norm matrix elements $N_{i',i} = \langle \psi(c_{i'}) | \psi(c_i) \rangle$.

- Solve the generalized eigenvalue problem

$$\tilde{H} | v(c_t) \rangle = \tilde{E}(c_t) N | v(c_t) \rangle$$

- Effectively, EC approximates $|\psi(c_t)\rangle$ by the best linear combination of $|\psi(c_1)\rangle, \ldots, |\psi\ (c_N)\rangle$ that minimizes error in energy $E(c)$.

Analytic Continuation



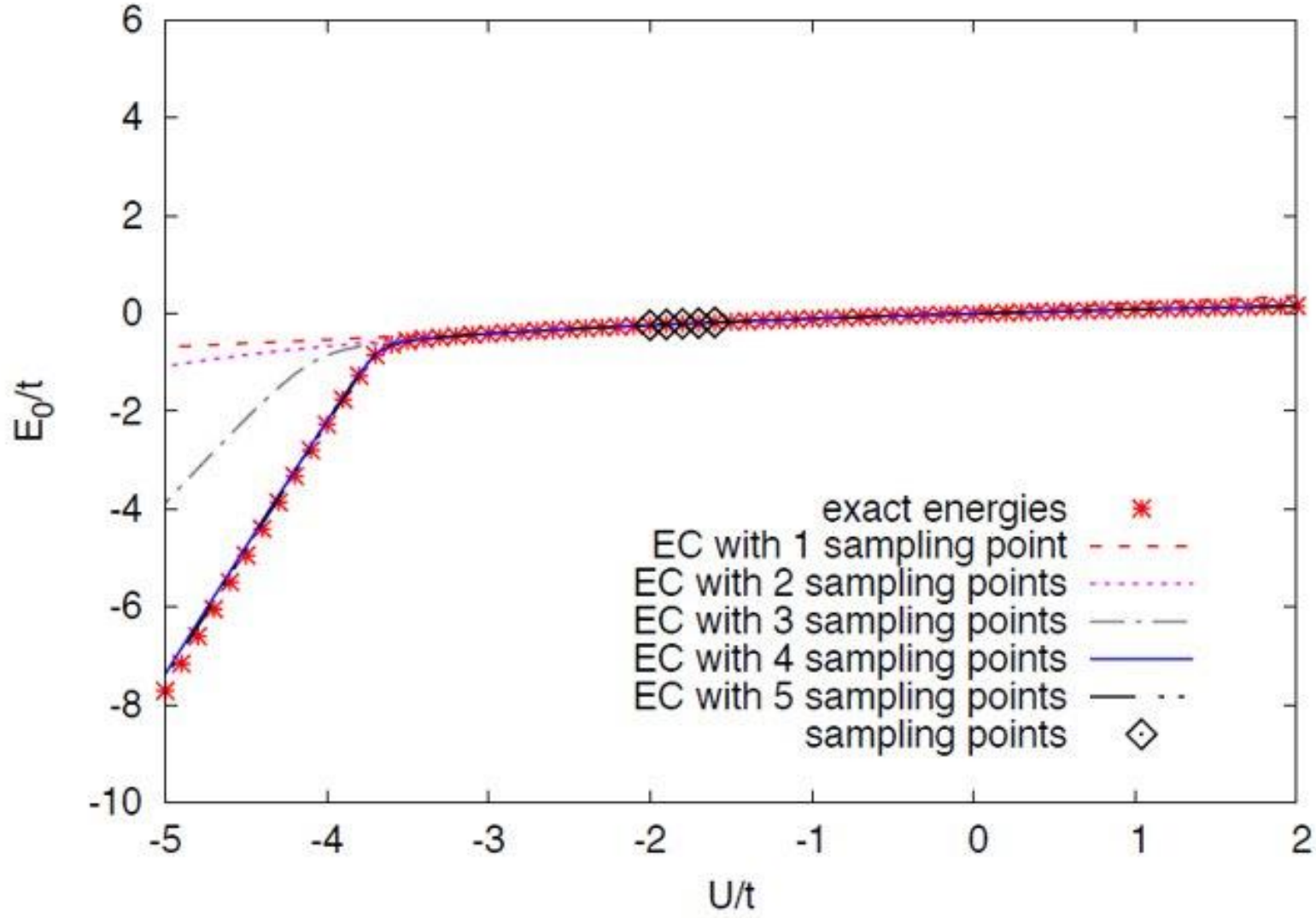
$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(0)\rangle c^n/n!$$

$$|\psi_j(c)\rangle = \sum_{n=0}^{\infty} |\psi_j^{(n)}(w)\rangle (c-w)^n/n!$$

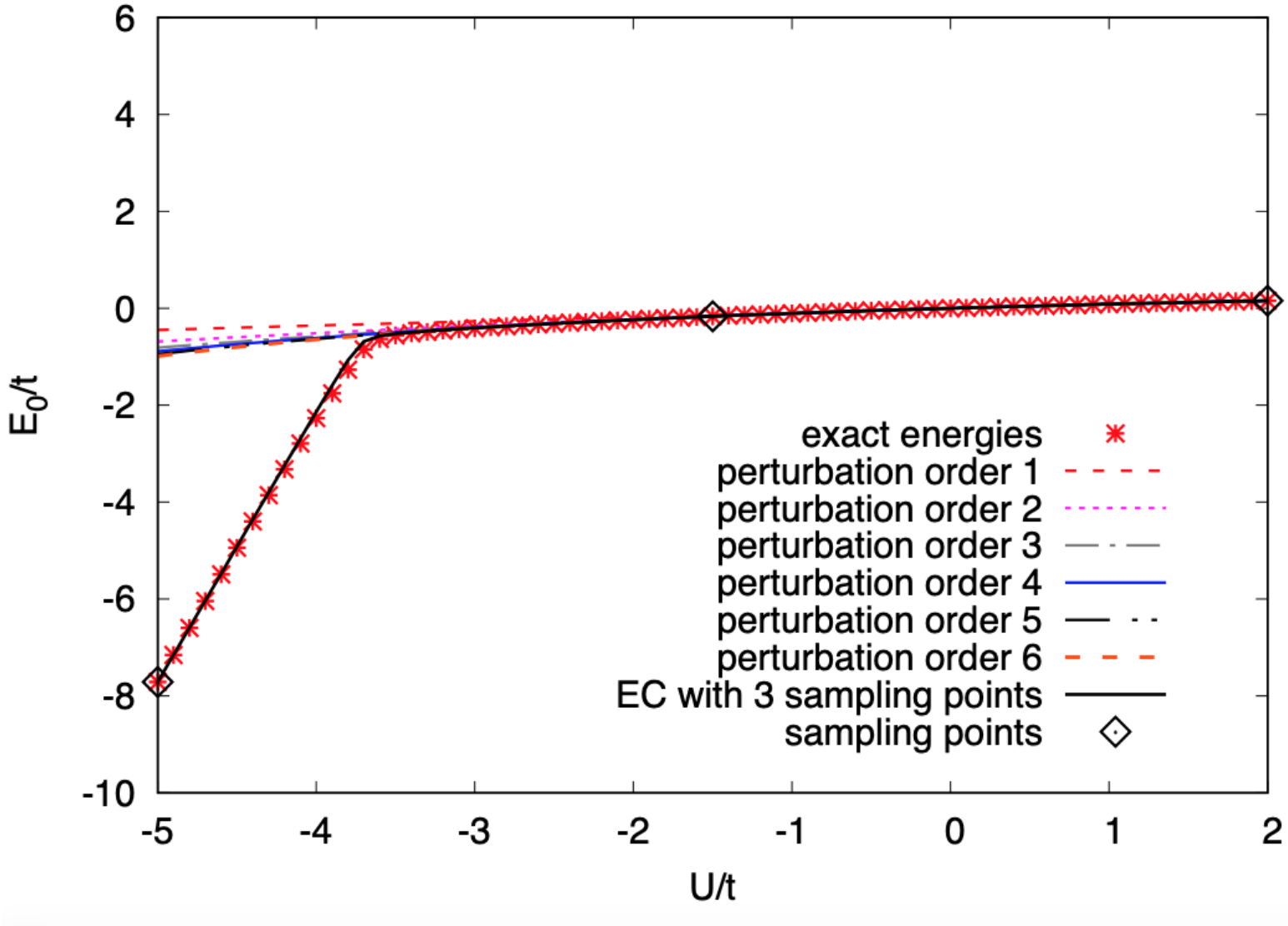
$$|\psi_j^{(n)}(w)\rangle = \sum_{m=0}^{\infty} |\psi_j^{(n+m)}(0)\rangle w^m/m!$$

$$|\psi_j(c)\rangle = \lim_{N,M\to\infty} \sum_{n=0}^{N}\sum_{m=0}^{M} |\psi_j^{(n+m)}(0)\rangle w^m (c-w)^n/(m!\,n!)$$

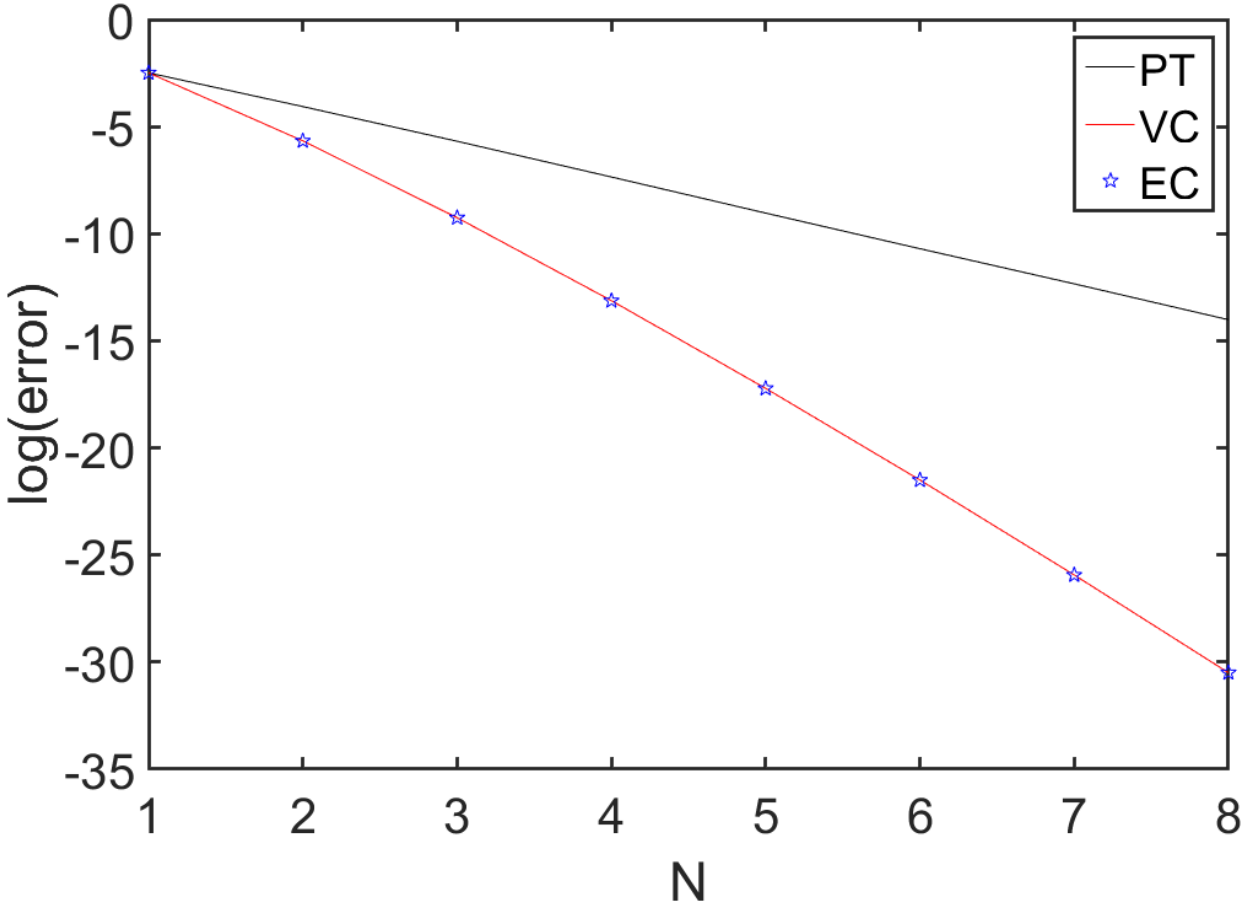
Extrapolation with EC



Interpolation with EC (emulators)



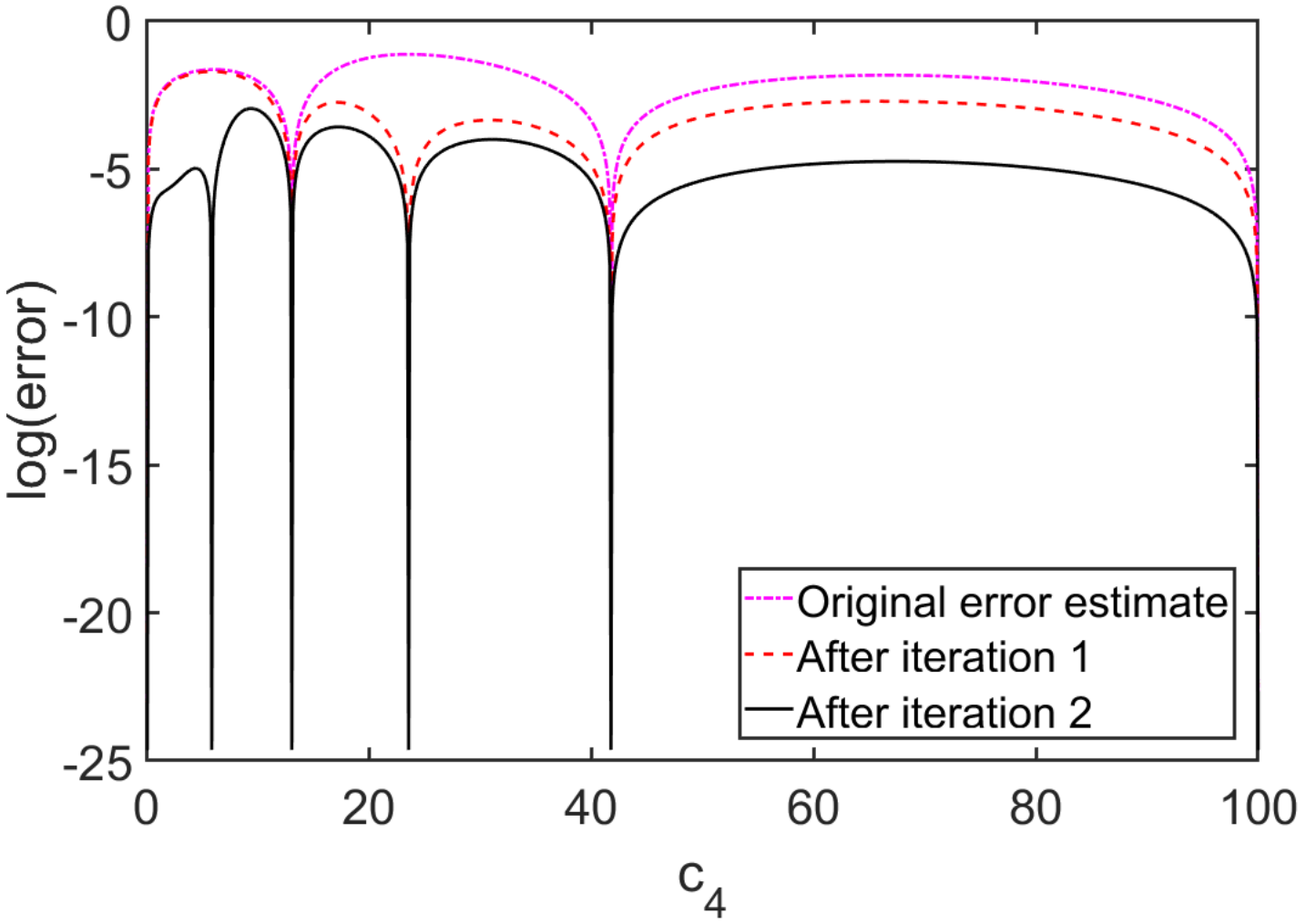
Convergence properties of EC



$$|\widetilde{v(c_t)}\rangle_{PT} = \sum_{n=0}^{N} |v^{(n)}(0)\rangle \frac{c_t^n}{n!}$$

[1] - A. Sarkar and D. Lee, Phys. Rev. Lett.126, 032501 (2021).

Self-learning process



[1] - A. Sarkar and D. Lee, PhysRevResearch.4.023214 (2022).

Quantum Monte Carlo

- Key idea: Euclidean time evolution

$$E_0 = \frac{\langle \psi_{trial} | e^{-H(c)\delta t} | \dots | H(c) | \dots | e^{-H(c)\delta t} | \psi_{trial} \rangle}{\langle \psi_{trial} | e^{-H(c)\delta t} | \dots | e^{-H(c)\delta t} | \psi_{trial} \rangle}$$

- Notation:

$$H_{ij}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | H(c_t) | c_j | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_i | \dots | c_i | c_j | \dots | c_j | \psi_{trial} \rangle}$$

- Problem: $N_{ij} = ??$

$$\frac{\langle \psi_{trial} | c_i | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_i | \dots | c_j | \psi_{trial} \rangle} = 1$$

Previous work - reweighting

$$H_{ij}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | H(c_t) | c_j | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_m | \dots | c_m | c_n | \dots | c_n | \psi_{trial} \rangle} \qquad N_{ij}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | c_j | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_m | \dots | c_m | c_n | \dots | c_n | \psi_{trial} \rangle}$$

- Extra factor drops out in generalized eigenvalue problem

[1] - D. K. Frame, Ph.D. thesis, Michigan State University (2019), 1905.02782.

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$$H_{ij}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | H(c_t) | c_j | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_m | \dots | c_m | c_n | \dots | c_n | \psi_{trial} \rangle} \qquad N_{ij}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | c_j | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_m | \dots | c_m | c_n | \dots | c_n | \psi_{trial} \rangle}$$

- Extra factor drops out in generalized eigenvalue problem

$$N'_{ij}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | c_j | \dots | c_j | \psi_{trial} \rangle}{\langle \psi_{trial} | c_j | \dots | c_j | c_j | \dots | c_j | \psi_{trial} \rangle} \qquad N'_{ii}(c_t) = \frac{\langle \psi_{trial} | c_i | \dots | c_i | c_i | \dots | c_i | \psi_{trial} \rangle}{\langle \psi_{trial} | c_j | \dots | c_j | c_j | \dots | c_j | \psi_{trial} \rangle}$$

$$\frac{|N'_{ii}(c_t)|^2}{N'_{ii}(c_t)} = \frac{|\langle \psi_{trial} | c_i | \dots | c_i | c_j | \dots | c_j | \psi_{trial} \rangle|^2}{\langle \psi_{trial} | c_j | \dots | c_j | c_j | \dots | c_j | \psi_{trial} \rangle \langle \psi_{trial} | c_i | \dots | c_i | c_i | \dots | c_i | \psi_{trial} \rangle}$$

[1] - D. K. Frame, Ph.D. thesis, Michigan State University (2019), 1905.02782.

Problems with old method

- Measured and sampled quantities are different -> stochastic noise.
  - Limits higher order EC and choice of training points

$$N_{ij}(c_t) = \frac{\langle \psi_{trial}|c_i|\dots|c_i|c_j|\dots|c_j|\psi_{trial}\rangle}{\langle \psi_{trial}|c_m|\dots|c_m|c_n|\dots|c_n|\psi_{trial}\rangle} \qquad N_{ik}(c_t) = \frac{\langle \psi_{trial}|c_i|\dots|c_i|c_k|\dots|c_k|\psi_{trial}\rangle}{\langle \psi_{trial}|c_m|\dots|c_m|c_n|\dots|c_n|\psi_{trial}\rangle}$$

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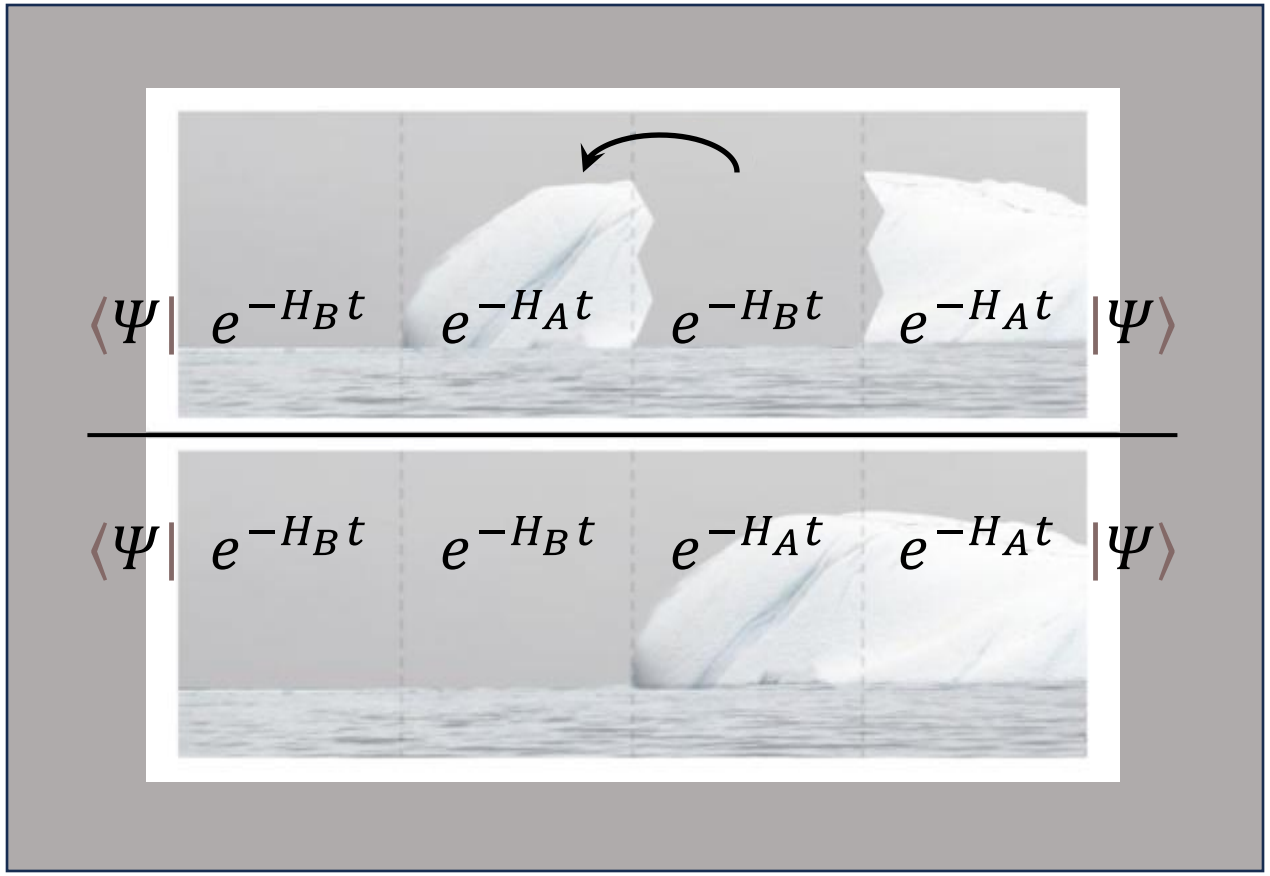
$$N_{ij}(c_t) = \frac{\langle \psi_{trial}|c_i|\dots|c_i|c_j|\dots|c_j|\psi_{trial}\rangle}{\langle \psi_{trial}|c_m|\dots|c_m|c_n|\dots|c_n|\psi_{trial}\rangle} \qquad N_{ik}(c_t) = \frac{\langle \psi_{trial}|c_i|\dots|c_i|c_k|\dots|c_k|\psi_{trial}\rangle}{\langle \psi_{trial}|c_m|\dots|c_m|c_n|\dots|c_n|\psi_{trial}\rangle}$$

- Extra energy factors

$$N_{ij}(c_t) = \frac{\left\langle \psi_{trial}\left|e^{-H(c_i)\delta t}\right|\dots\left|e^{-H(c_i)\delta t}\right|e^{-H(c_j)\delta t}\right|\dots|e^{-H(c_j)\delta t}\left|\psi_{trial}\right\rangle}{\left\langle \psi_{trial}\left|e^{-H(c_i)\delta t}\right|\dots\left|e^{-H(c_i)\delta t}\right|e^{-H(c_i)\delta t}\right|\dots|e^{-H(c_i)\delta t}\left|\psi_{trial}\right\rangle}$$

  - Norm matrix ill-conditioned

Floating block EC



[1] - Sarkar, Lee, and Meißner, arXiv:2306.11439, 2023

Floating-block details

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|c_j|\cdots|c_j|c_i|\cdots|c_i|c_j|\cdots|c_j|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|c_i|\cdots|c_i|c_j|\cdots|c_j|c_j|\cdots|c_j|\psi_{init}\rangle}$$

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|\sum_{k1}|\psi_{k1}\rangle\langle\psi_{k1}|c_j|\cdots|c_j|\sum_{k2}|\psi_{k2}\rangle\langle\psi_{k2}|c_i|\cdots|c_i|\sum_{k3}|\psi_{k3}\rangle\langle\psi_{k3}|c_j|\cdots|c_j|\sum_{k4}|\psi_{k4}\rangle\langle\psi_{k4}|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|\sum_{k5}|\psi_{k5}\rangle\langle\psi_{k5}|c_j|\cdots|c_j|\psi_{init}\rangle}$$

Floating-block details

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|c_j|\cdots|c_j|c_i|\cdots|c_i|c_j|\cdots|c_j|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|c_i|\cdots|c_i|c_j|\cdots|c_j|c_j|\cdots|c_j|\psi_{init}\rangle}$$

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|\sum_{k1}|\psi_{k1}\rangle\langle\psi_{k1}|c_j|\cdots|c_j|\sum_{k2}|\psi_{k2}\rangle\langle\psi_{k2}|c_i|\cdots|c_i|\sum_{k3}|\psi_{k3}\rangle\langle\psi_{k3}|c_j|\cdots|c_j|\sum_{k4}|\psi_{k4}\rangle\langle\psi_{k4}|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|\sum_{k5}|\psi_{k5}\rangle\langle\psi_{k5}|c_j|\cdots|c_j|\psi_{init}\rangle}$$

$$=\frac{\langle\psi_{init}|\psi(c_i)\rangle\langle\psi(c_i)|\psi(c_j)\rangle\langle\psi(c_j)|\psi(c_i)\rangle\langle\psi(c_i)|\psi(c_j)\rangle\langle\psi(c_j)|\psi_{init}\rangle}{\langle\psi_{init}|\psi(c_i)\rangle\langle\psi(c_i)|\psi(c_j)\rangle\langle\psi(c_j)|\psi_{init}\rangle}$$

Floating-block details

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|c_j|\cdots|c_j|c_i|\cdots|c_i|c_j|\cdots|c_j|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|c_i|\cdots|c_i|c_j|\cdots|c_j|c_j|\cdots|c_j|\psi_{init}\rangle}$$

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|\sum_{k1}|\psi_{k1}\rangle\langle\psi_{k1}|c_j|\cdots|c_j|\sum_{k2}|\psi_{k2}\rangle\langle\psi_{k2}|c_i|\cdots|c_i|\sum_{k3}|\psi_{k3}\rangle\langle\psi_{k3}|c_j|\cdots|c_j|\sum_{k4}|\psi_{k4}\rangle\langle\psi_{k4}|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|\sum_{k5}|\psi_{k5}\rangle\langle\psi_{k5}|c_j|\cdots|c_j|\psi_{init}\rangle}$$

$$=\frac{\langle\psi_{init}|\psi(c_i)\rangle\langle\psi(c_i)|\psi(c_j)\rangle\langle\psi(c_j)|\psi(c_i)\rangle\langle\psi(c_i)|\psi(c_j)\rangle\langle\psi(c_j)|\psi_{init}\rangle}{\langle\psi_{init}|\psi(c_i)\rangle\langle\psi(c_i)|\psi(c_j)\rangle\langle\psi(c_j)|\psi_{init}\rangle}$$

$$\frac{\langle\psi_{init}|c_i|\cdots|c_i|c_j|\cdots|c_j|c_i|\cdots|c_i|c_j|\cdots|c_j|\psi_{init}\rangle}{\langle\psi_{init}|c_i|\cdots|c_i|c_i|\cdots|c_i|c_j|\cdots|c_j|c_j|\cdots|c_j|\psi_{init}\rangle} = |\langle\psi(c_i)|\psi(c_j)\rangle|^2$$

Floating-block EC

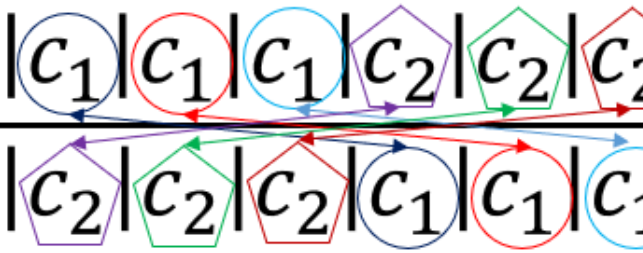
$$H_{ij}(c_t) = \frac{\langle \psi_{init}|c_i|\cdots|c_i|H(c_t)|c_j|\cdots|c_j|\psi_{init}\rangle}{\langle \psi_{init}|c_m|\cdots|c_m|c_n|\cdots|c_n|\psi_{init}\rangle}$$

$$N_{ij} = \left(\frac{\langle \psi_{init}|c_i|\cdots|c_i|c_j|\cdots|c_j|c_i|\cdots|c_i|c_j|\cdots|c_j|\psi_{init}\rangle}{\langle \psi_{init}|c_i|\cdots|c_i|c_i|\cdots|c_i|c_j|\cdots|c_j|c_j|\cdots|c_j|\psi_{init}\rangle}\right)^{\frac{1}{2}}$$

- Can now make fast EC emulators
- Two additional computational details

Shifting Auxiliary Fields

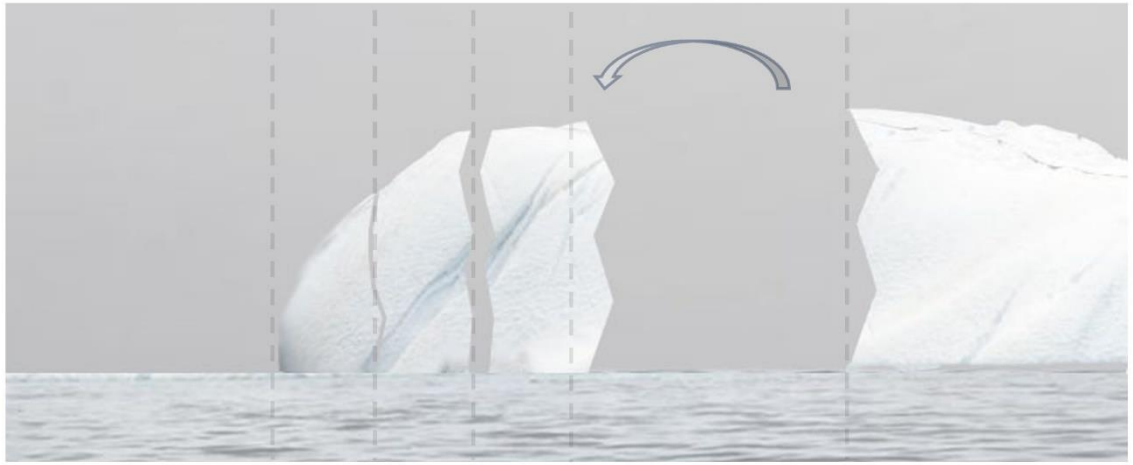
$$N^2 = \frac{|\langle \psi_{init}|c_2|c_2|c_2|c_1|c_1|c_1|c_2|c_2|c_2|c_1|c_1|c_1|\psi_{init}\rangle|}{|\langle \psi_{init}|c_2|c_2|c_2|c_2|c_2|c_2|c_1|c_1|c_1|c_1|c_1|c_1|\psi_{init}\rangle|}$$



- Improves stability of Monte Carlo. Effect of moving Auxiliary field depends on how different the two eigenvectors are.

Breaking down the steps

- If the number of time steps is too large, measured and sampled quantities differ by large amount.

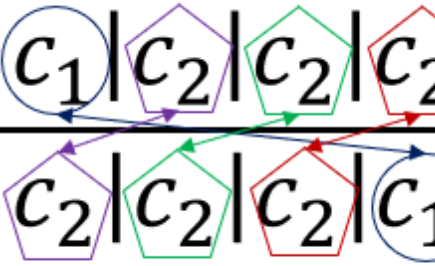


3-step Calculation

$$N_1 = \frac{|\langle\psi_{init}|c_2|c_2|c_2|c_1|c_2|c_2|c_2|c_1|c_1|c_1|c_1|c_1|\psi_{init}\rangle|}{|\langle\psi_{init}|c_2|c_2|c_2|c_2|c_2|c_2|c_1|c_1|c_1|c_1|c_1|c_1|\psi_{init}\rangle|}$$

$$N_2 = \frac{|\langle\psi_{init}|c_2|c_2|c_2|c_1|c_1|c_2|c_2|c_2|c_1|c_1|c_1|c_1|\psi_{init}\rangle|}{|\langle\psi_{init}|c_2|c_2|c_2|c_1|c_2|c_2|c_2|c_1|c_1|c_1|c_1|c_1|\psi_{init}\rangle|}$$

$$N_3 = \frac{|\langle\psi_{init}|c_2|c_2|c_2|c_1|c_1|c_1|c_2|c_2|c_2|c_1|c_1|c_1|\psi_{init}\rangle|}{|\langle\psi_{init}|c_2|c_2|c_2|c_1|c_1|c_2|c_2|c_2|c_1|c_1|c_1|c_1|\psi_{init}\rangle|}$$



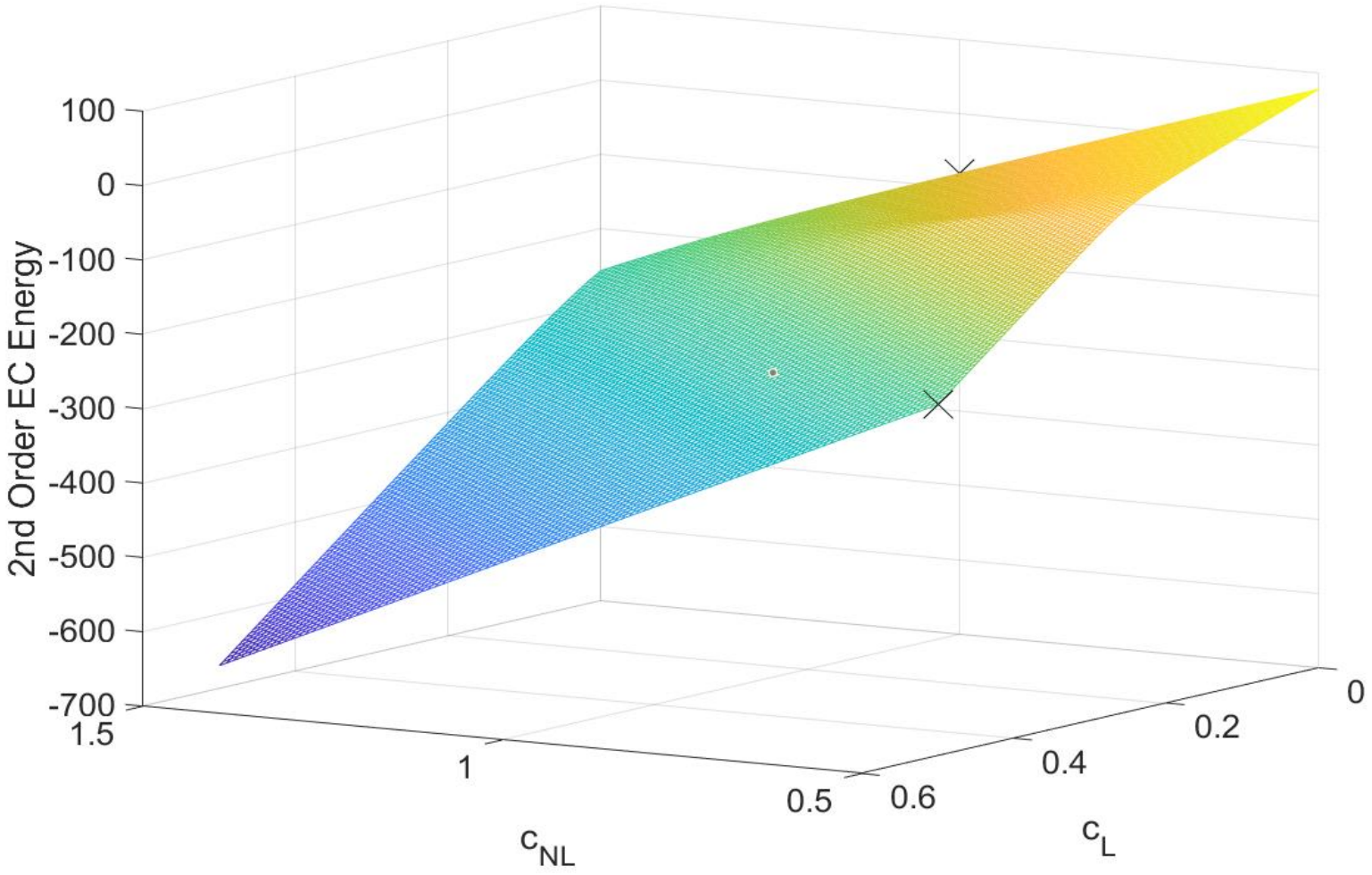
Results - EC emulator with floating block

- Study phase transition with two different interactions
- $H_a = K + V_L \ , \quad H_b = K + V_{NL}$
- Tune smearing parameters such that both interactions reproduce ^4He energy correctly.
- EC emulate: $H(c_L, c_{NL}) = K + c_L V_L + c_{NL} V_{NL}$ for ^8Be , ^{12}C , and ^{16}O
- V_L interaction produces tightly bound nuclear liquid, and V_{NL} interaction makes the system alpha gas.

Nuclear binding near a quantum phase transition

Serdar Elhatisari,[1] Ning Li,[2] Alexander Rokash,[3] Jose Manuel Alarcón,[1] Dechuan Du,[2] Nico Klein,[1] Bing-nan Lu,[2]
Ulf-G. Meißner,[1,2,4] Evgeny Epelbaum,[3] Hermann Krebs,[3] Timo A. Lähde,[2] Dean Lee,[5] and Gautam Rupak[6]

EC emulator for ^{12}C

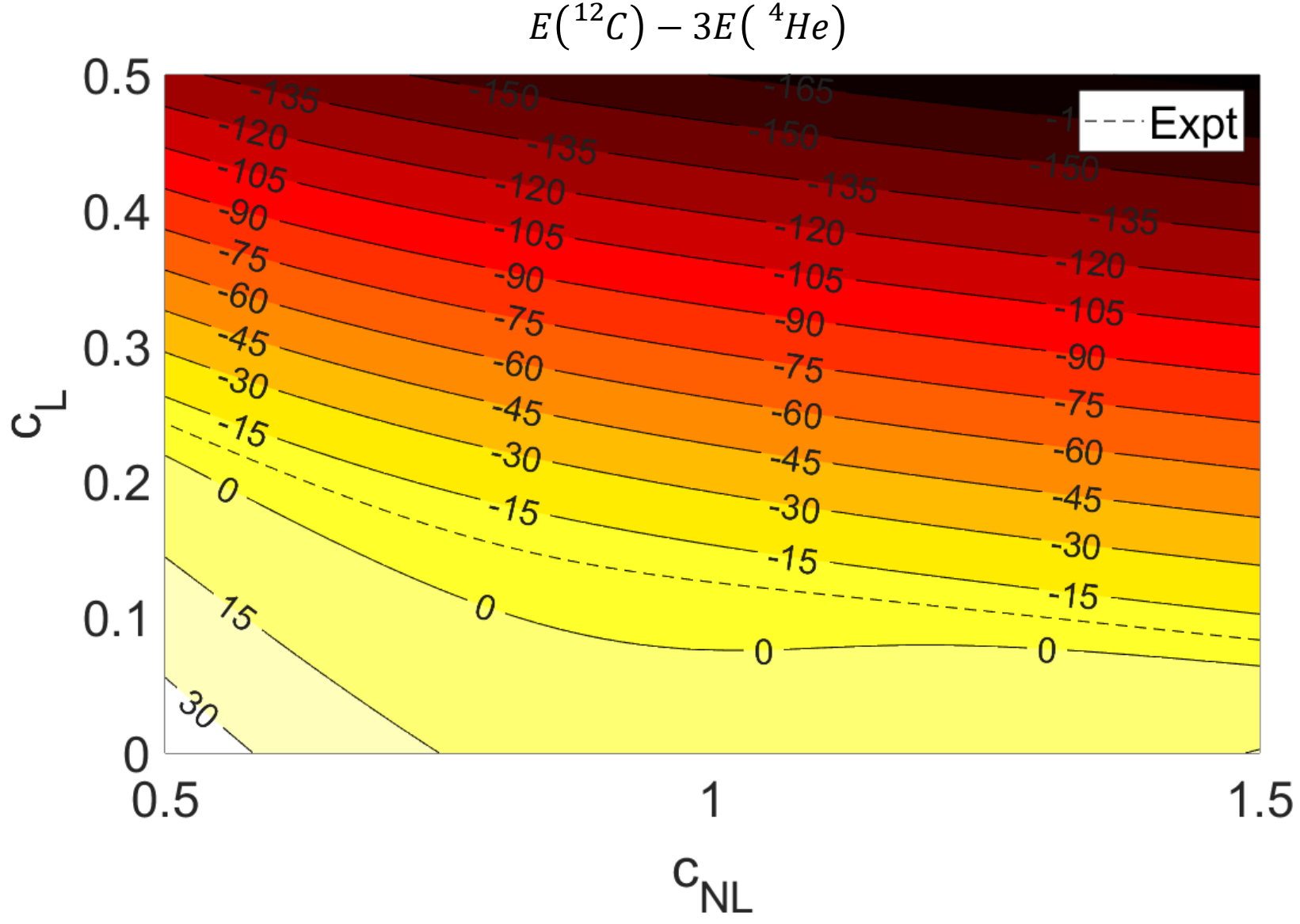


^{12}C Emulator error

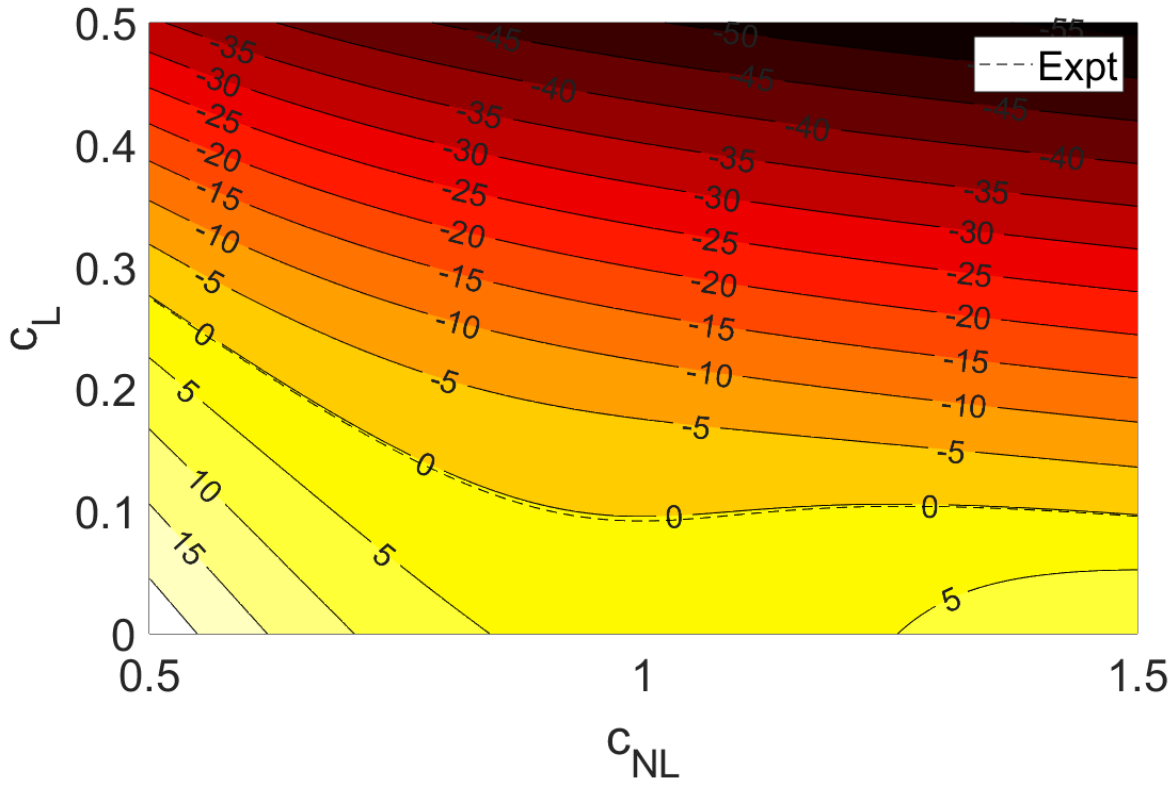
(c_L, c_{NL})	Full Simulation	2nd order EC	3rd order EC	4th order EC
(0.8,0.2)	-338.57 ± 0.03	-330.63 ± 0.26	-333.15 ± 1.85	-333.24 ± 1.14
(0.8,0.1)	-295.33 ± 0.02	-290.04 ± 0.24	-292.08 ± 1.51	-292.17 ± 1.03
(0.9,0.1)	-381.81 ± 0.02	-369.12 ± 0.28	-372.63 ± 2.24	-372.77 ± 1.83
(0.8,0.3)	-382.41 ± 0.03	-371.22 ± 0.27	-374.24 ± 2.25	-374.34 ± 1.42
(0.4,0.6)	-177.15 ± 0.05	-177.25 ± 0.19	-177.32 ± 0.46	-177.33 ± 0.24
(0.4,0.7)	-217.73 ± 0.04	-217.70 ± 0.19	-217.71 ± 0.38	-217.72 ± 0.21
(0.3,0.7)	-141.11 ± 0.05	-139.63 ± 0.19	-141.09 ± 0.71	-141.10 ± 0.35
(0.4,0.8)	-259.35 ± 0.06	-258.19 ± 0.20	-258.31 ± 0.30	-258.32 ± 0.28
(0.2,0.6)	-41.54 ± 0.05	-31.91 ± 0.15	-37.75 ± 0.50	-41.64 ± 0.14
(0.2,0.2)	31.26 ± 0.02	101.48 ± 0.17	99.18 ± 1.86	69.72 ± 1.77
(0.8,0.8)	-606.63 ± 0.05	-574.23 ± 0.37	-579.97 ± 4.02	-580.12 ± 2.70

- Training points: (0.5,0.5), (0.2,0.8), (0.0,1.0), (0.2,0.6)
- Error in each EC estimate can be calculated using trimmed sampling

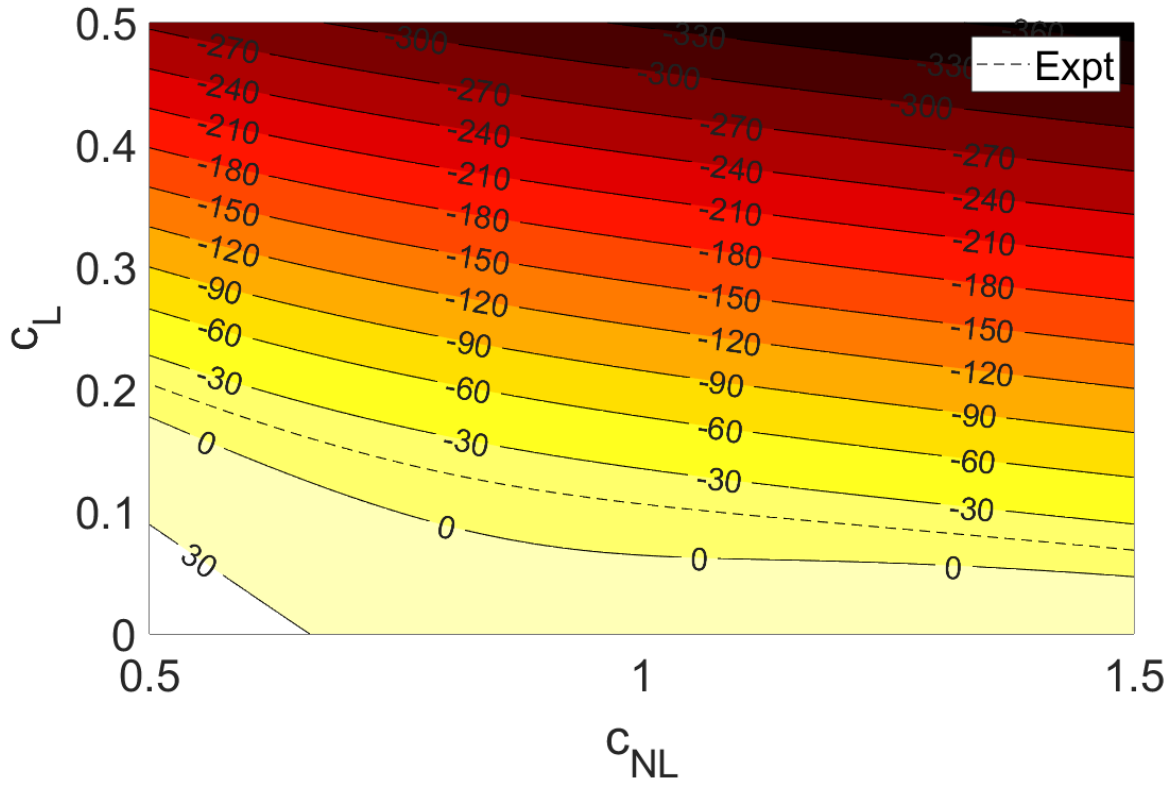
[1] – C. Hicks and D. Lee, Phys. Rev. Research **5**, L022001, 2023


$E(^{12}C) - 3E(^{4}He)$
Expt
c_L
c_{NL}
0.5
0.4
0.3
0.2
0.1
0
0.5
1
1.5
-135
-120
-105
-90
-75
-60
-45
-30
-15
0
15
30
-150
-165

$E(\,^{8}Be) - 2E(\,^{4}He)$



$E(^{16}O) - 4E(\,^{4}He)$



Summary and Outlook

- New algorithm to calculate inner products with quantum Monte Carlo by interleaving time blocks.
- Can use EC to interpolate and extrapolate
- Can be used to design time dependent Hamiltonian H(t) for efficient adiabatic quantum computing. Evolve wavefunction slowly, such that inner product between two steps remains large.
- Comparison with old reweighting – 8 orders of magnitude less error in norm.

Thank you for your attention