Eigenvector continuation for the anharmonic oscillator and the pairing Hamiltonian

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Eigenvector continuation (EC)

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- For Hamiltonians $\hat{H}(c)$ with continuous parametric dependence

$$\hat{H}(c) = \hat{H}_0 + c \cdot \hat{H}_1$$

- Based on **analytical continuation** of eigenvalues and eigenvectors outside original domain
  Frame *et al.*, PRL (2018)

- Predictions obtained by solving the generalized eigenvalue problem

$$HX = \epsilon NX$$

- With matrix elements

$$H_{pq} = \langle \Psi^{(p)} | \hat{H}(c) | \Psi^{(q)} \rangle$$

$$N_{pq} = \langle \Psi^{(p)} | \Psi^{(q)} \rangle$$

- For set of training vectors $|\Psi^{(p)}\rangle$

Eigenvector continuation

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This talk: Two different applications

- As a PT resummation tool
- State corrections as EC basis
  e.g. Demol *et al*. PRC (2020)
  Sakar and Lee PRL (2021)
- Here for the anharmonic oscillator (AHO) with high-order state corrections
- For the pairing Hamiltonian with low-order state corrections

- As an emulator tool
- Solution known for some c_i
- Exact solutions used as EC basis
  e.g. König *et al*. PLB (2020)
  Furnstahl *et al*. PLB (2020)
  Drischler *et al*. PLB (2021)
- For the pairing Hamiltonian with truncated training vectors

The anharmonic oscillator

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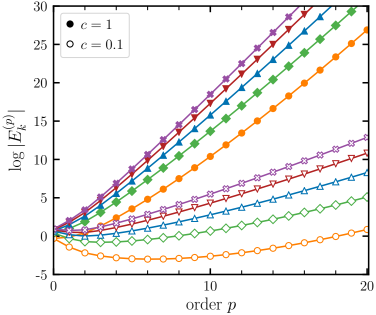
- Hamiltonian of a **harmonic** oscillator with a **quartic** perturbation (in natural units)

$$\hat{H}(c) = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + c\hat{x}^4$$

- Perturbation expansion is well known to **diverge** Bender, Wu, PR (1969) , PRD (1973)
- Expression in terms of ladder operators

$$\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2} + c\left(\frac{\hat{a}^\dagger + \hat{a}}{\sqrt{2}}\right)^4$$

- Pentadiagonal matrix



Companys Franzke et al., PLB (2022)

EC based on ground state

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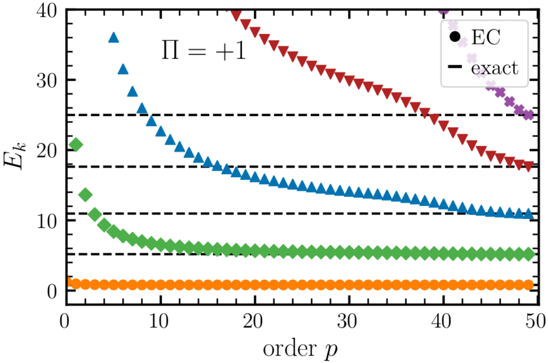
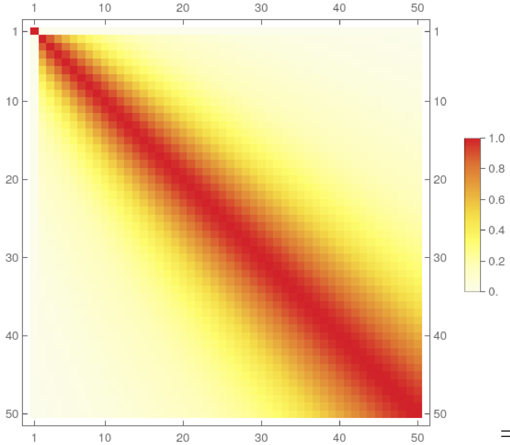
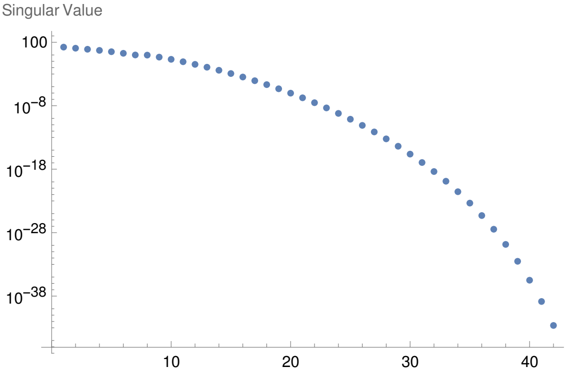
- EC basis generated by PT expansion
  - ▷ Reference state: ground state of HO
- Most rapid convergence for ground state
- Goal: Extend EC framework for excited states
- Also sequences for **excited states**
  - ▷ Solving the **same** generalized eigenvalue problem
  - ▷ Only eigenstates of the same symmetries can be accessed



Companys Franzke et al., PLB (2022)

Computational difficulties





$\Longrightarrow$ Norm matrix becomes singular for high orders

Orthogonalizing EC basis

- EC solves generalized eigenvalue problem $\mathbf{H}^V X = \epsilon \mathbf{N}^V X$ with EC basis V and

$$\mathbf{H}^V = V^T H V$$
$$\mathbf{N}^V = V^T V$$

- Equivalent to eigenvalue problem $(\mathbf{N}^V)^{-1}\mathbf{H}^V X = \epsilon X$

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Orthogonalizing EC basis

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$$\mathbf{H}^V = V^T H V$$
$$\mathbf{N}^V = V^T V$$

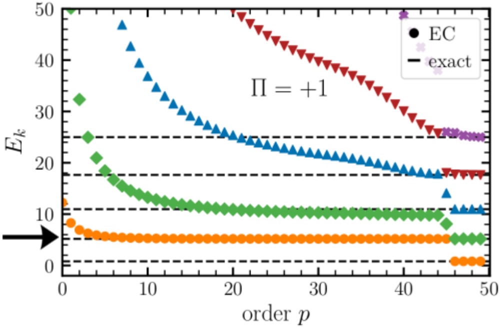
- Equivalent to eigenvalue problem $(\mathbf{N}^V)^{-1}\mathbf{H}^V X = \epsilon X$
- Can be shown to be equivalent to problem in orthogonal basis W
- Let T and T^{-1} be the transformation matrices, such that $V = W \cdot T$.

$$\Longrightarrow (\mathbf{N}^V)^{-1}\mathbf{H}^V = T^{-1}\mathbf{H}^W T$$

- Solve $\mathbf{H}^W Y = \epsilon Y$ for $Y = TX$ instead

EC based on an excited state

- EC basis generated by PT expansion
  - ▷ reference state: **excited** state of HO
- Reference state sequence converges quickly
- Other sequences do not converge to exact eigenvalues until high order
  - ▷ Jump at high orders
  - ▷ Variational principle



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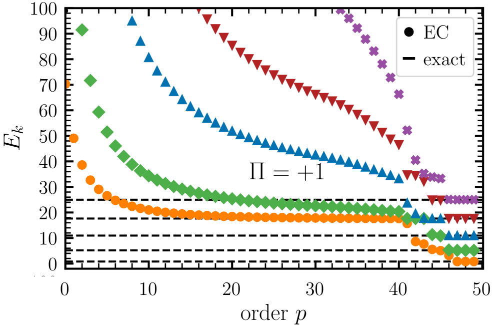
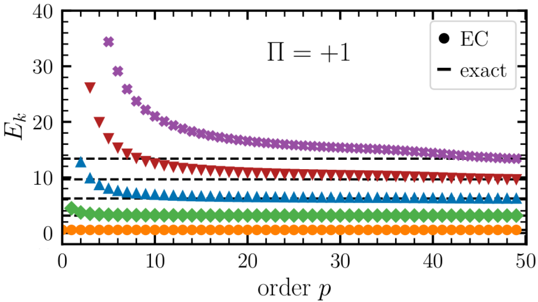
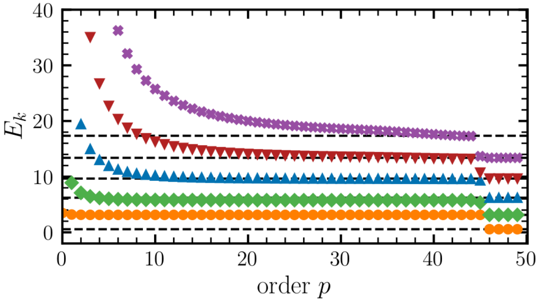


EC for coupling strength ($c = 0.1$)

Reference state: ground state



Reference state: first excited state



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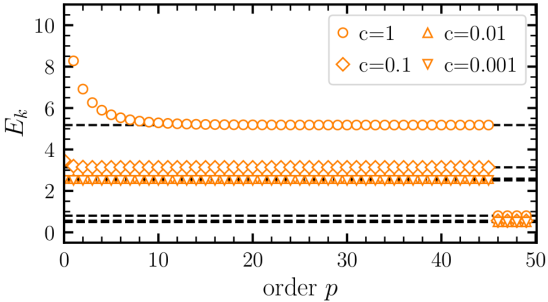
- ☐ Same general trend as for $c = 1$
- ☐ Converges faster

Variation of the coupling strength for EC

- EC basis from PT for first excited state for different c
  - Only lowest sequence shown
- Jump **independent of** *c*
  - EC spans the same subspace



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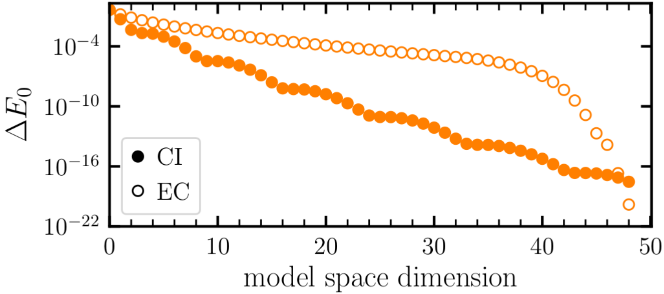
EC compared to configuration interaction

- Configuration interaction (CI) basis consists of the eigenstates of the HO
- Diagonalization in truncated HO basis
- PT strongly divergent
  - EC performs worse than CI
  - EC still converges

$\Longrightarrow$ PT chooses poor basis



Companys Franzke et al., PLB (2022)

Summary AHO

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- ☐ EC sequence converges quickly for the reference state
- ☐ EC for the ground-state reference state also produces sequences converging to exited states
- ☐ Reference state EC sequence converges faster than same state in ground-state EC
  - ▷ Simultaneous assessment of multiple excited states challenging
- ☐ The EC order where the jump occurs is independent of c

$\Longrightarrow$ EC provides a robust framework to extract ground and excited states

Pairing Hamiltonian

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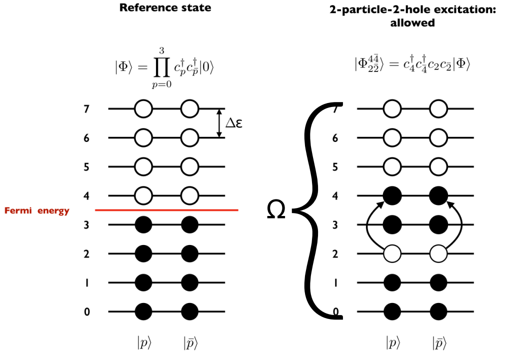
- ☐ Pairing Hamiltonian for model-space size Ω and pair states p and $\bar{p}$

$$\hat{H}_{\text{pairing}} \equiv \sum_{p}^{\Omega} \epsilon_p \left(c_p^\dagger c_p + c_{\bar{p}}^\dagger c_{\bar{p}}\right) - g \sum_{pq}^{\Omega} c_p^\dagger c_{\bar{p}}^\dagger c_{\bar{q}} c_q \,,$$

$\Longrightarrow$ exactly solvable due to Richardson without large-scale diagonalization
e.g. Richardson *et al.* PL (1964)



Courtesy of Alexander Tichai

Pairing Hamiltonian

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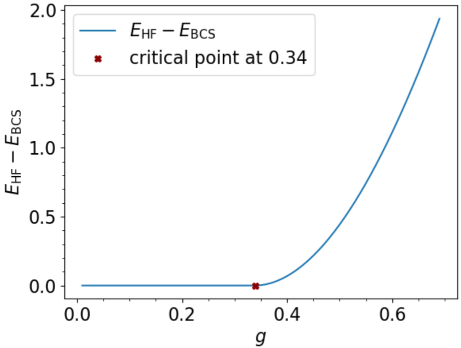
- Phase transition to superfluid state for $g > g_{crit}$



EC as a resummation method of PT (1/2)

- PT: $\hat{H}_0 = \hat{H}^{(0)} + \hat{H}^{(1)}$ and $\hat{H}_1 = \hat{H}^{(2)}$
- $\hat{H}^{(k)}$ normal ordered k-body part of the Hamiltonian

$$E^{(0)}|\Phi\rangle = H_0|\Phi\rangle = (2\sum_i \epsilon_i - gN_{\mathrm{occ}})|\Phi\rangle$$

$$|\Psi^{(1)}\rangle = \frac{1}{2}\sum_{ai} \frac{g}{f_i - f_a}|\Phi_{i\bar{i}}^{a\bar{a}}\rangle$$

$$E^{(2)} = -\frac{1}{2}\sum_{ai} \frac{g^2}{f_i - f_a}$$

- Where $f_p = \epsilon_p - n_p g$

- Reference state:

$$|\Phi\rangle \equiv \prod_{i=1}^{N_{\mathrm{occ}}} c_i^\dagger c_{\bar{i}}^\dagger |0\rangle .$$

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- Reference state:

$$|\Phi\rangle \equiv \prod_{i=1}^{N_{\text{occ}}} c_i^\dagger c_{\bar{i}}^\dagger |0\rangle\,.$$

- EC:

$$\mathbf{H} = \begin{pmatrix} \langle\Psi^{(0)}|\hat{H}|\Psi^{(0)}\rangle & \langle\Psi^{(0)}|\hat{H}|\Psi^{(1)}\rangle \\ \langle\Psi^{(1)}|\hat{H}|\Psi^{(0)}\rangle & \langle\Psi^{(1)}|\hat{H}|\Psi^{(1)}\rangle \end{pmatrix} = \begin{pmatrix} E^{(0)} & E^{(2)} \\ E^{(2)} & \mathbf{H}_{11} \end{pmatrix}$$

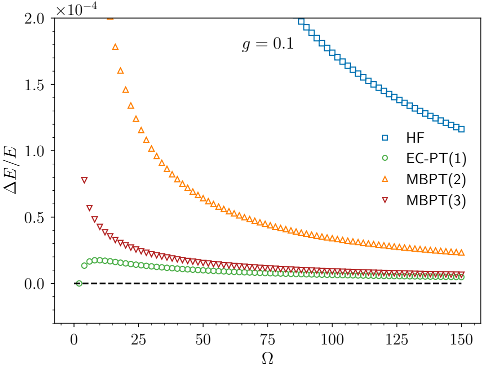
$$\mathbf{N} = \begin{pmatrix} \langle\Psi^{(0)}|\Psi^{(0)}\rangle & \langle\Psi^{(0)}|\Psi^{(1)}\rangle \\ \langle\Psi^{(1)}|\Psi^{(0)}\rangle & \langle\Psi^{(1)}|\Psi^{(1)}\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \mathbf{N}_{11} \end{pmatrix}\,.$$

EC as a resummation method of PT (2/2)

$$\mathbf{N}_{11} = \frac{1}{4}\sum_{abij} \frac{g^2 \langle \Phi_{i\bar{i}}^{a\bar{a}} | \Phi_{i\bar{i}}^{a\bar{a}} \rangle}{(f_i - f_a)(f_j - f_b)} = \frac{1}{4}\sum_{ai} \frac{g^2}{(f_i - f_a)^2}$$

$$\mathbf{H}_{11} = \frac{1}{4}\sum_{ai} \frac{g^2(2\sum_k \epsilon_k - gN_{\mathrm{occ}})}{(f_i - f_a)^2} - \frac{1}{2}\sum_{ai}\frac{g^2}{f_i - f_a} - \frac{1}{4}\left(\sum_{abi}\frac{g^3}{(f_i - f_a)(f_i - f_b)} + \sum_{aij}\frac{g^3}{(f_i - f_a)(f_j - f_a)}\right)$$

- ☐ Scales polynomially with system size
- ☐ Similar in spirit to Ekström and Hagen PRL (2019)



Companys Franzke, M.Sc. thesis (2023)

EC as a resummation method of PT (2/2)

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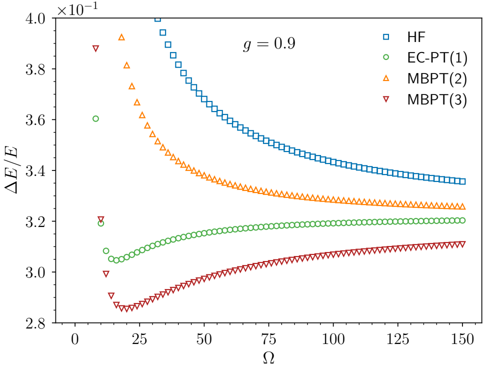
- Scales polynomially with system size
- Similar in spirit to Ekström and Hagen PRL (2019)
- Superfluidity cannot be captured by MBPT around normal state



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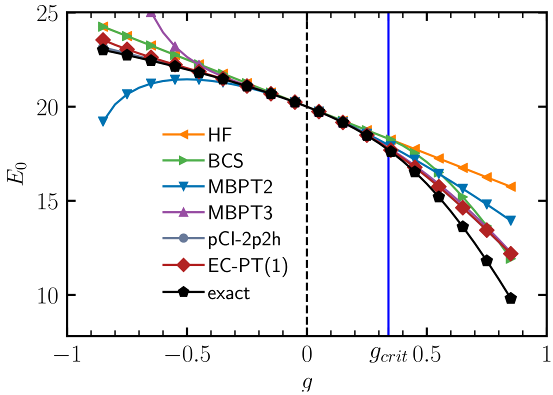
EC compared to other methods



Companys Franzke et al., arXiv:2302.08373

$$E^{(2)} = -\frac{1}{2}\sum_{ai}\frac{g^2}{f_i - f_a} \text{ with } f_p = \epsilon_p - n_p g$$

- Singularity at $g = -\Delta\epsilon = -1$
- pCI-2p2h and EC-PT(1) both are diagonalizations on 2p2h-spaces

EC compared to other methods

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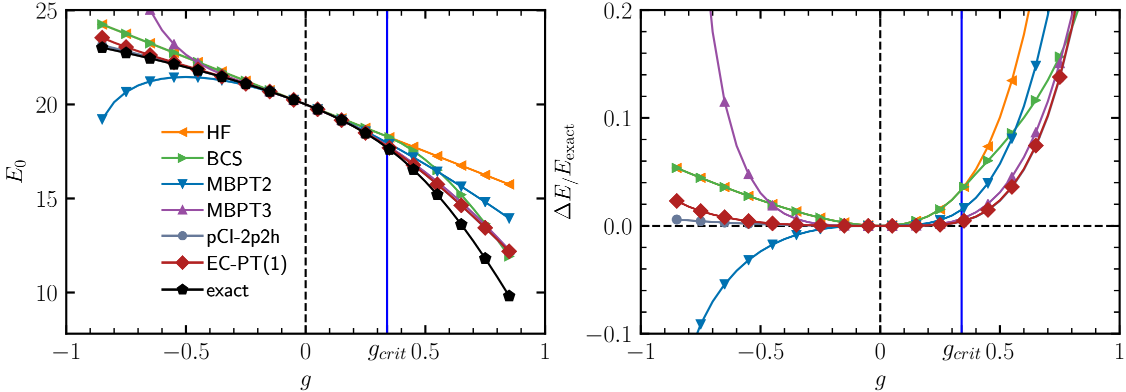

Companys Franzke et al., arXiv:2302.08373

$\Longrightarrow$ EC gives good approximations for large coupling range, although HF and MBPT(2) do not

EC as an emulation tool

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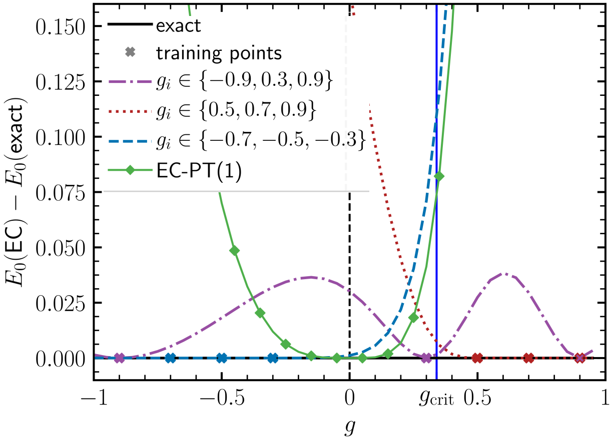
- EC can be used to emulate Hamiltonians from training data
  e.g. Frame *et al.* PRL (2018)
  Baran and Nichita PRB (2023)
- Can be used to
  - Interpolate with training points from both sides of g_{crit}
  - Extrapolate from only normal or superfluid training points
- Either exact or approximated training data can be used
  - Here the CI truncation of the training states is varied

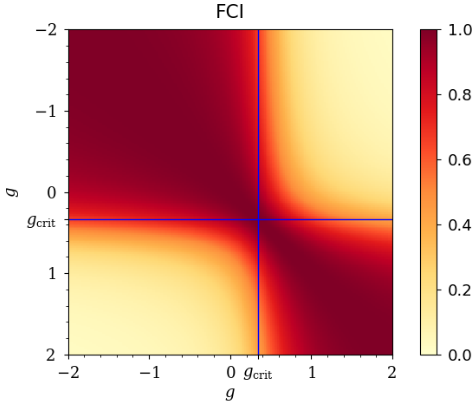
Different EC applications for the pairing Hamiltonian

- ☐ EC from PT state corrections only good around $g = 0$
- ☐ One-sided training points only approximate the same side well
- ☐ Training points from both sides of the interval give good results



Companys Franzke et al., arXiv:2302.08373 (2023)

Norm matrix for the pairing Hamiltonian



Companys Franzke et al., arXiv:2302.08373

- ☐ Block matrix structure
- ☐ Dependent on critical g
- ☐ Strongly suppressed overlap between normal and superfluid ground state

Norm matrix for the pairing Hamiltonian

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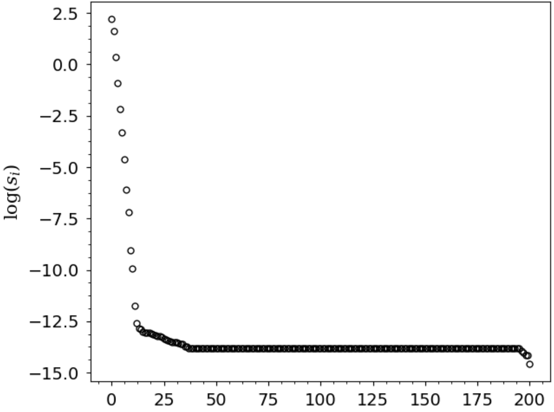

Companys Franzke, M.Sc. thesis (2023)

- ☐ Block matrix structure
- ☐ Dependent on critical g
- ☐ Strongly suppressed overlap between normal and superfluid ground state
- ☐ Most singular values zero

Variation of the CI truncation of the EC training points

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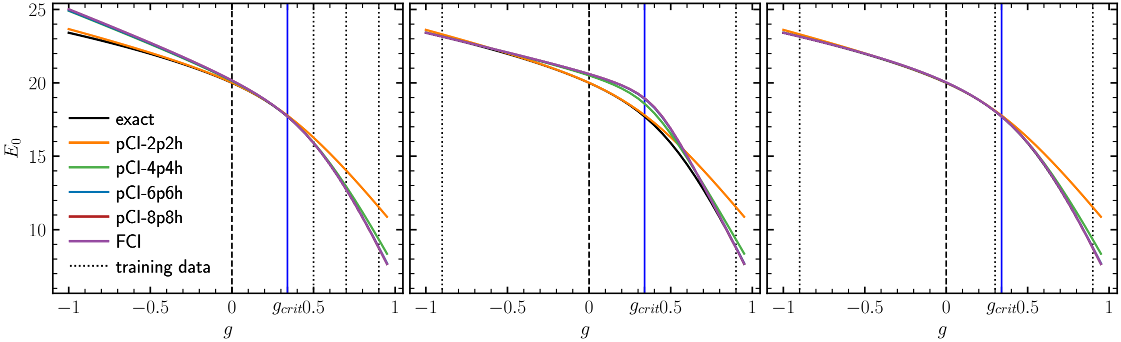

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$\Longrightarrow$ 6p6h truncated CI gives basically the same results as full CI

Eigenvector continuation compared to configuration interaction

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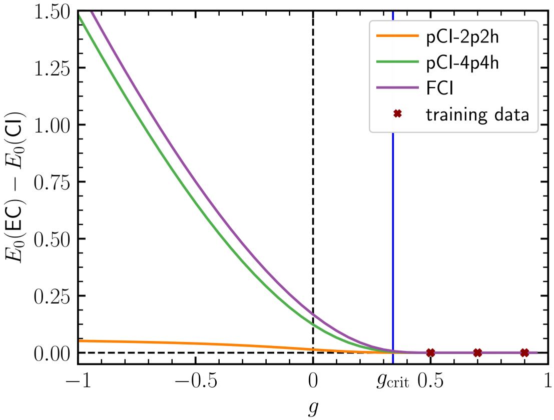
- ☐ EC approximates CI with lower truncation better



Companys Franzke et al., arXiv:2302.08373 (2023)

Eigenvector continuation compared to configuration interaction

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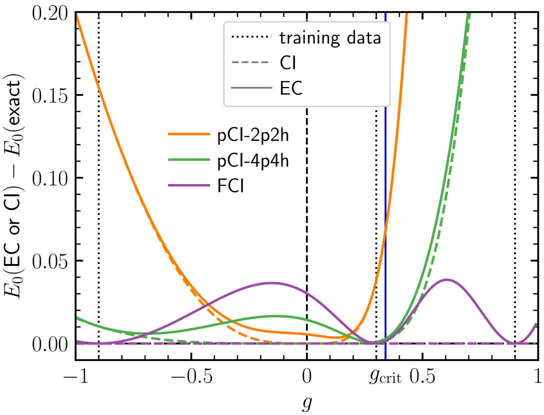
- ☐ EC approximates CI with lower truncation better
- ☐ Higher CI truncations give more accurate training vectors



Companys Franzke et al., arXiv:2302.08373

Summary Pairing Hamiltonian

arXiv:2302.08373

- ☐ Pairing Hamiltonian changes from normal to superfluid ground state with increasing coupling
- ☐ Eigenvector continuation with MBPT state correction only approximates solutions around $g = 0$ well
- ☐ One-sided training points can only approximate coupling values from the same side well
- ☐ Overlap between eigenvectors from superfluid couplings with eigenvectors from normal couplings is small
- ☐ Eigenvector continuation approximates lower CI truncations better

Outlook

- ☐ Design of many-body emulator for chiral Hamiltonians following the work of Ekström and Hagen PRL (2019)

- ☐ Hartree-Fock states as EC basis

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Thank you for your attention!