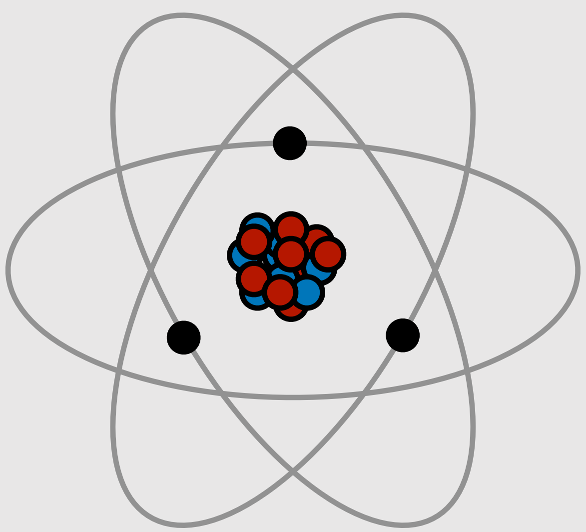
Nuclear superfluidity

The Pairing Hamiltonian as a many-body testbed

MSQM 2024

Workshop on model systems in quantum mechanics

January 12th, 2024



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TECHNISCHE UNIVERSITÄT DARMSTADT

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Outline

Nuclear superfluidity

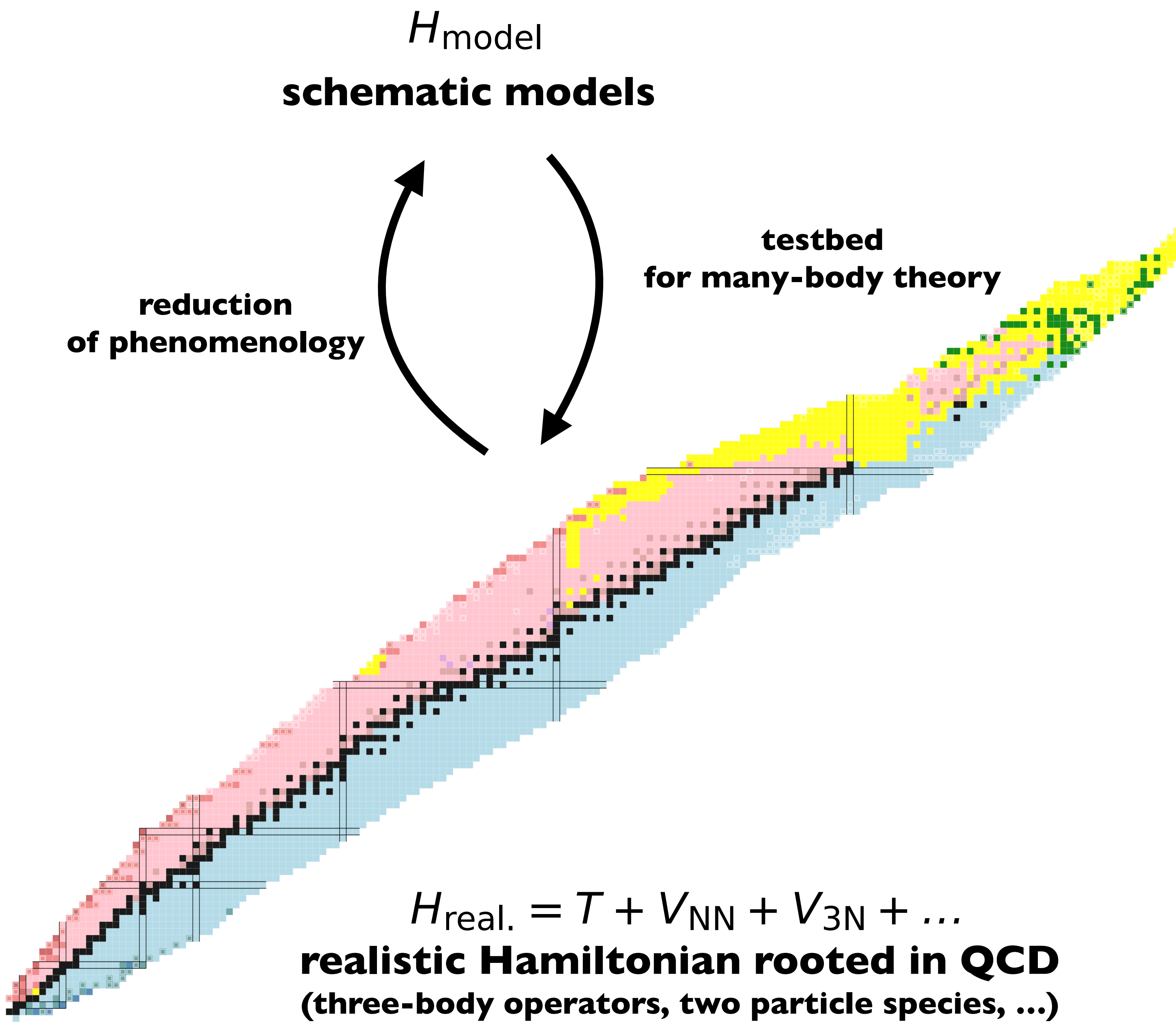
The pairing Hamiltonian

Richardson solution

Mean-field approach

Many-body expansions

Emulators



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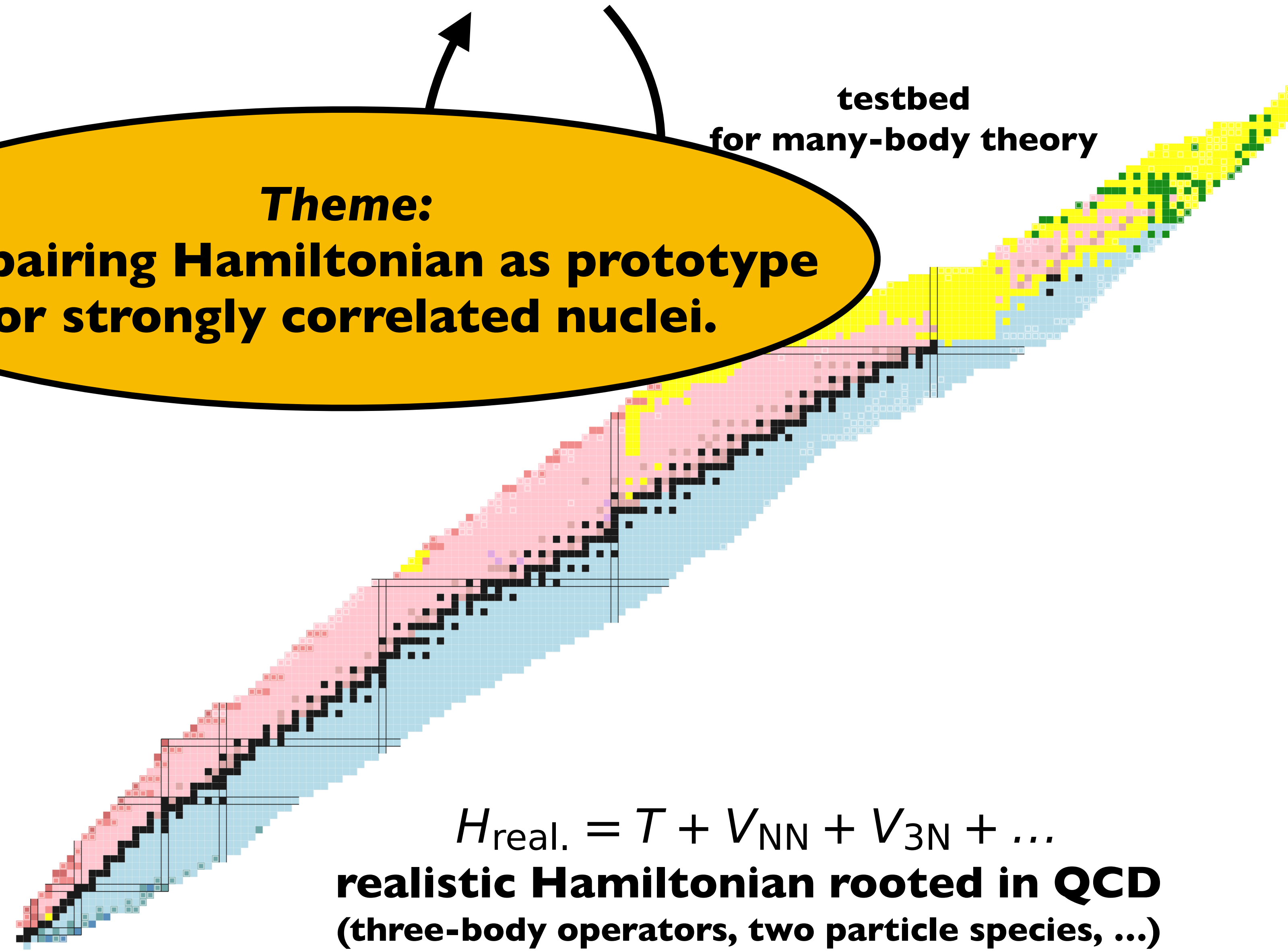
H_{model}

schematic models



Theme:
The pairing Hamiltonian as prototype for strongly correlated nuclei.

$H_{\text{real.}} = T + V_{\text{NN}} + V_{\text{3N}} + \ldots$

realistic Hamiltonian rooted in QCD

(three-body operators, two particle species, ...)

Nuclear phenomenology

- Odd-even staggering of experimental binding energies along isotopic chains

- Three-point mass differences give estimate for the (neutron) pairing gap

$$\Delta_N^{(3)} = \frac{(-1)^N}{2}\left(E_{N+1} - 2E_N + E_{N-1}\right)$$

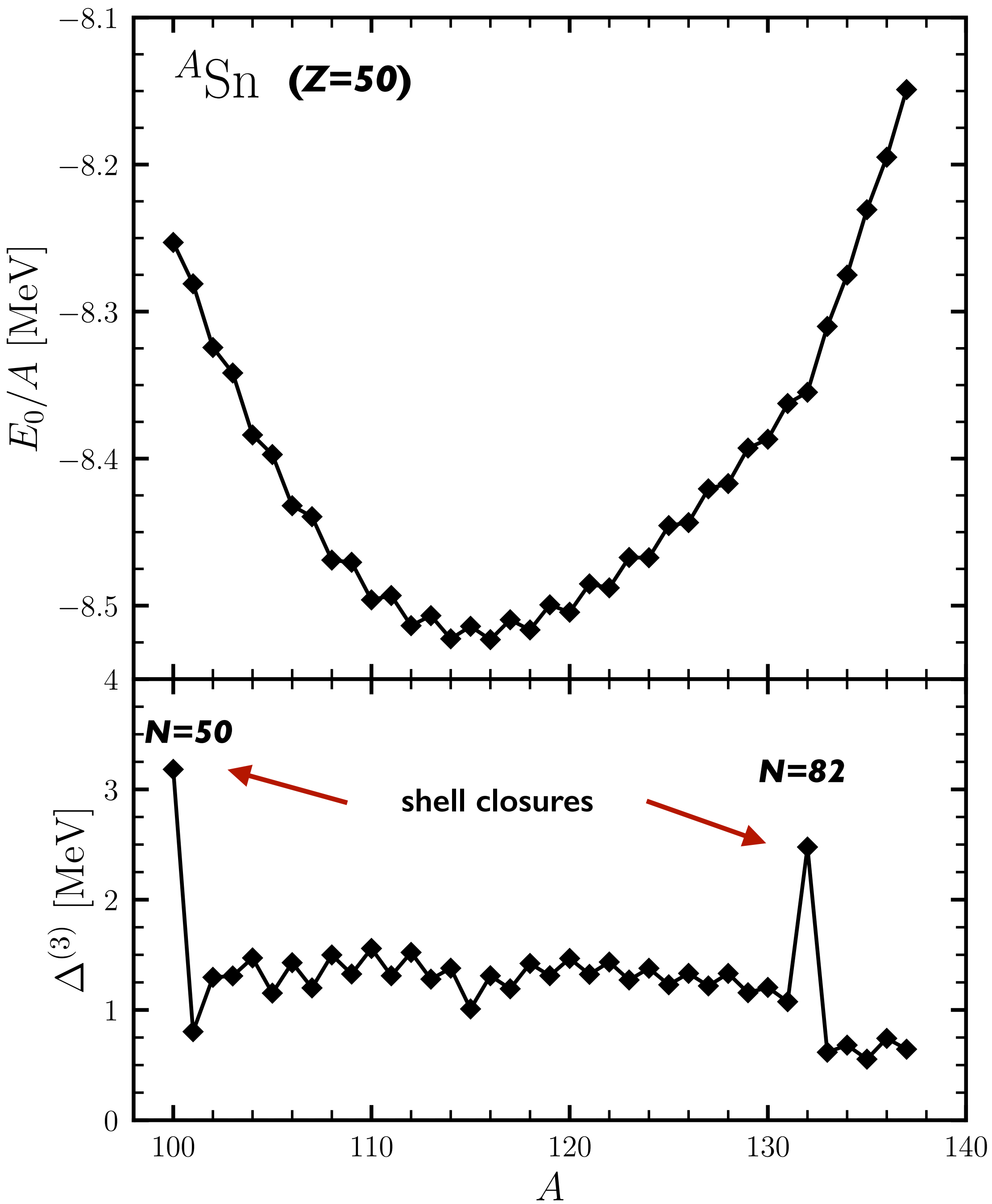
- Experimental evidence of formation of Cooper pairs in atomic nuclei

short-range attractive two-body interaction

- Nuclear phenomenology emerges from interplay of pairing and deformation

→ **see also talk by D. Lacroix**

Nuclear masses of tin isotopes (AME2020)



The Pairing Hamiltonian

- **One-parameter interaction describing superfluidity**

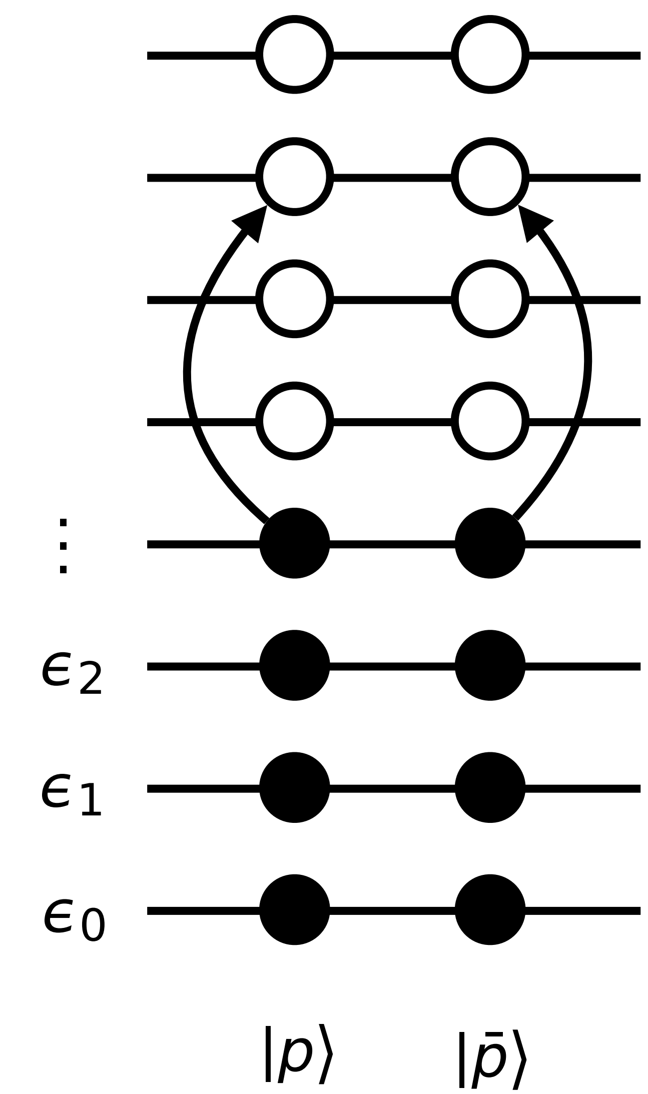
$$H_{\text{pairing}} = \sum_p \epsilon_p \left(c_p^\dagger c_p + c_{\bar{p}}^\dagger c_{\bar{p}}\right) + g \sum_{pq} c_p^\dagger c_{\bar{p}}^\dagger c_{\bar{q}} c_q$$

- **Generation of a pair of time-reversed states**

$$|p\rangle = |n_p l_p j_p m_p\rangle \quad \rightarrow \quad |\bar{p}\rangle = |n_p l_p j_p - m_p\rangle$$

Number of levels $\Omega = 8$

Occupied levels $N_{\text{occ}} = 4$



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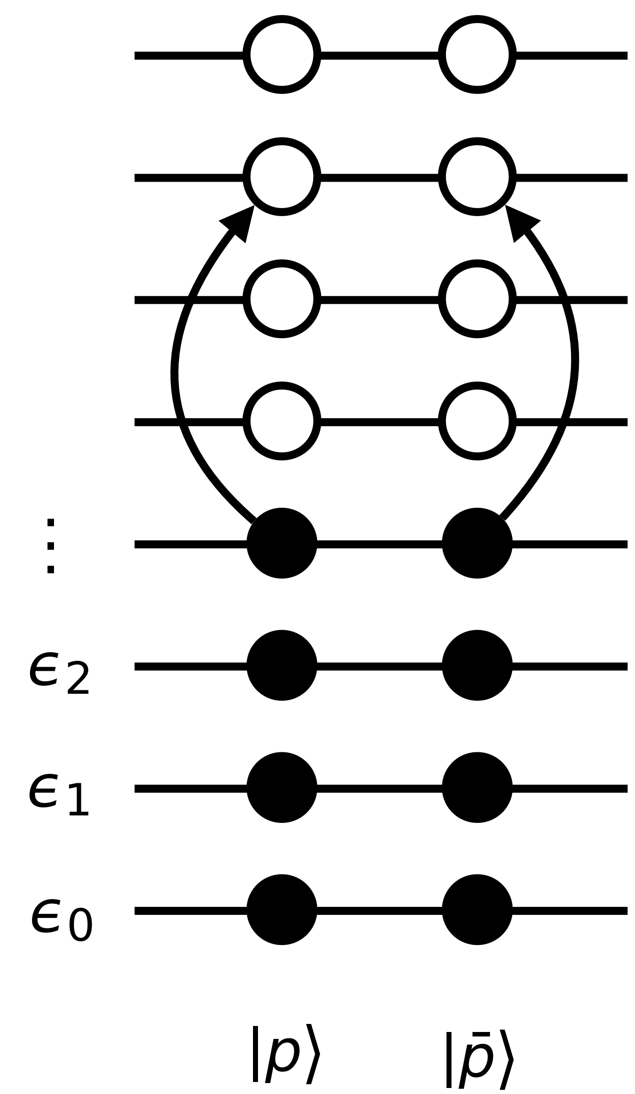

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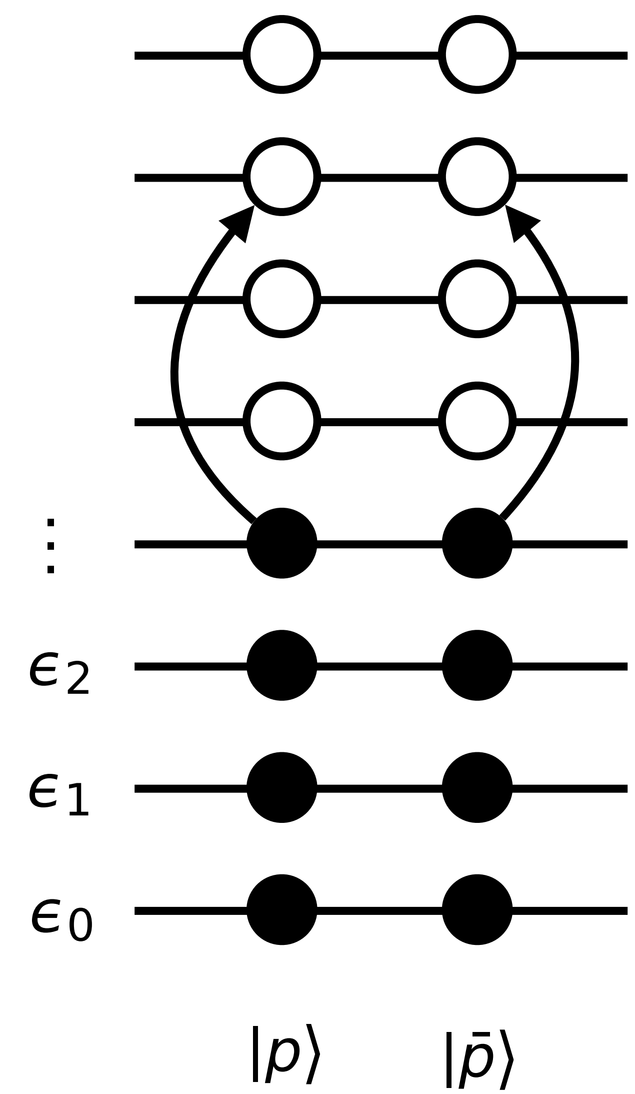

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- **Admits for a transition to superfluid regime at critical coupling strength**

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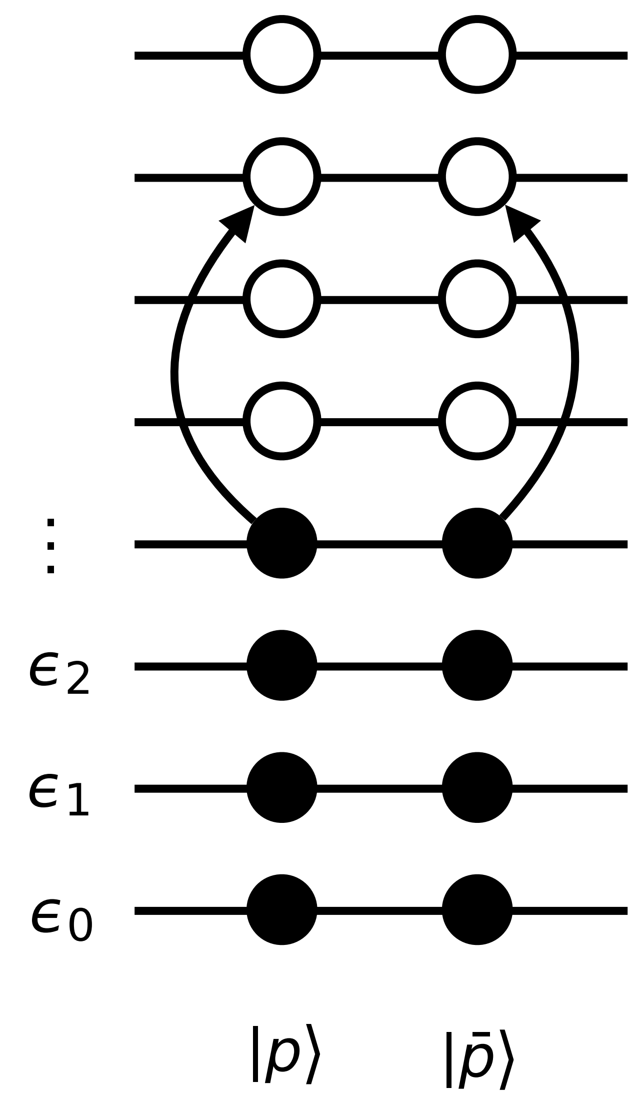

The pairing Hamiltonian

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H_{pairing}

- Introduction of

$N_p = c_p^\dagger c_p + c_{\bar{p}}^\dagger$

- Re-writing in SU

H_p

- Admits for a ph
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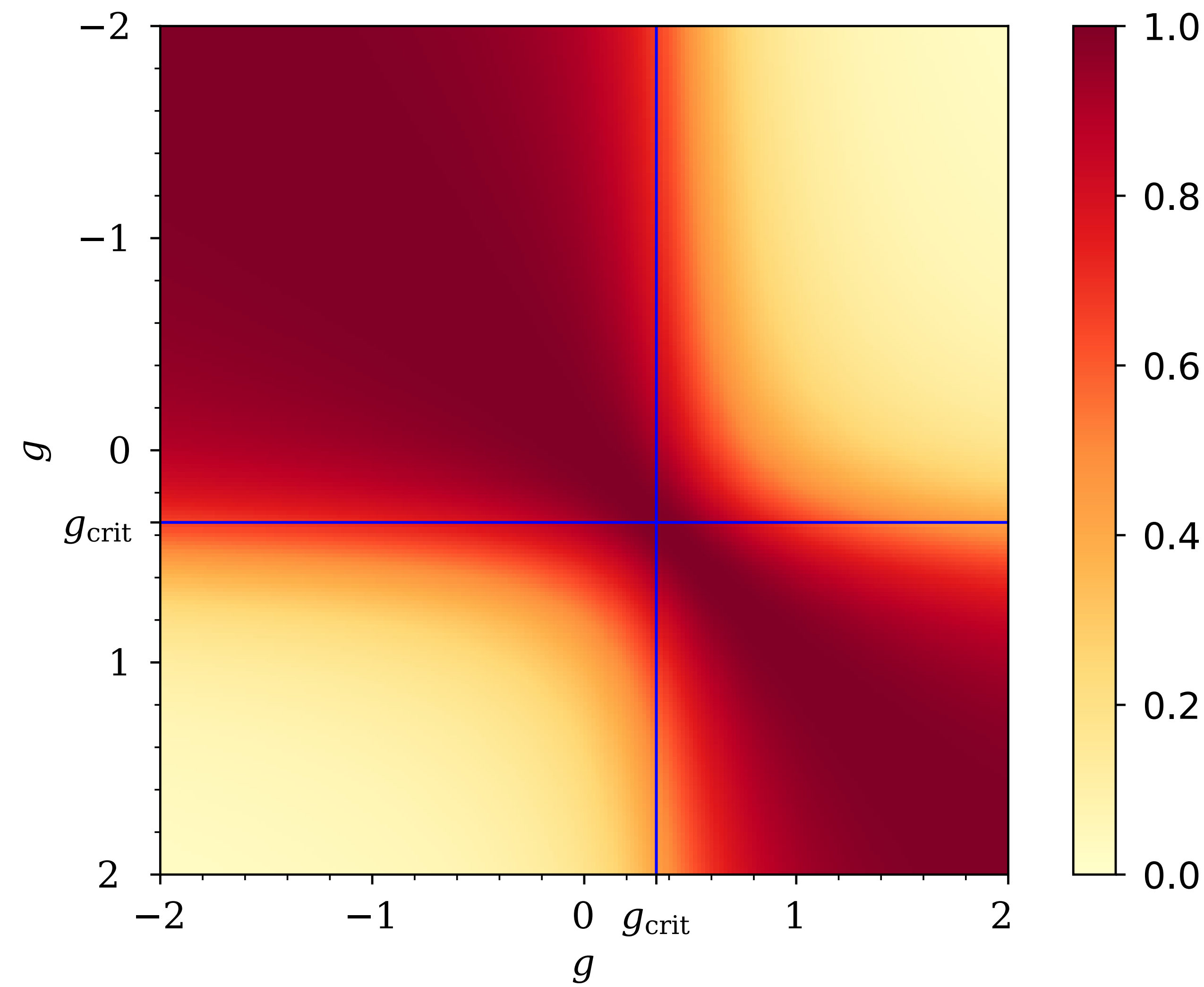
Overlap between eigenstates at different coupling strengths



Companys Franzke, Tichai, Hebeler, Schwenk, PRC (2024)

Richardson solution

- **Richardson solution: exact wave function is written from pair creation operators**

Richardson, PL (1965), PR (1966)

$$|\Psi\rangle = B_1^\dagger \cdot \ldots \cdot B_\Omega^\dagger |0\rangle \qquad B_\alpha^\dagger = \sum_{p=1}^{\Omega} \frac{1}{2\epsilon_p - E_\alpha} P_p^\dagger$$

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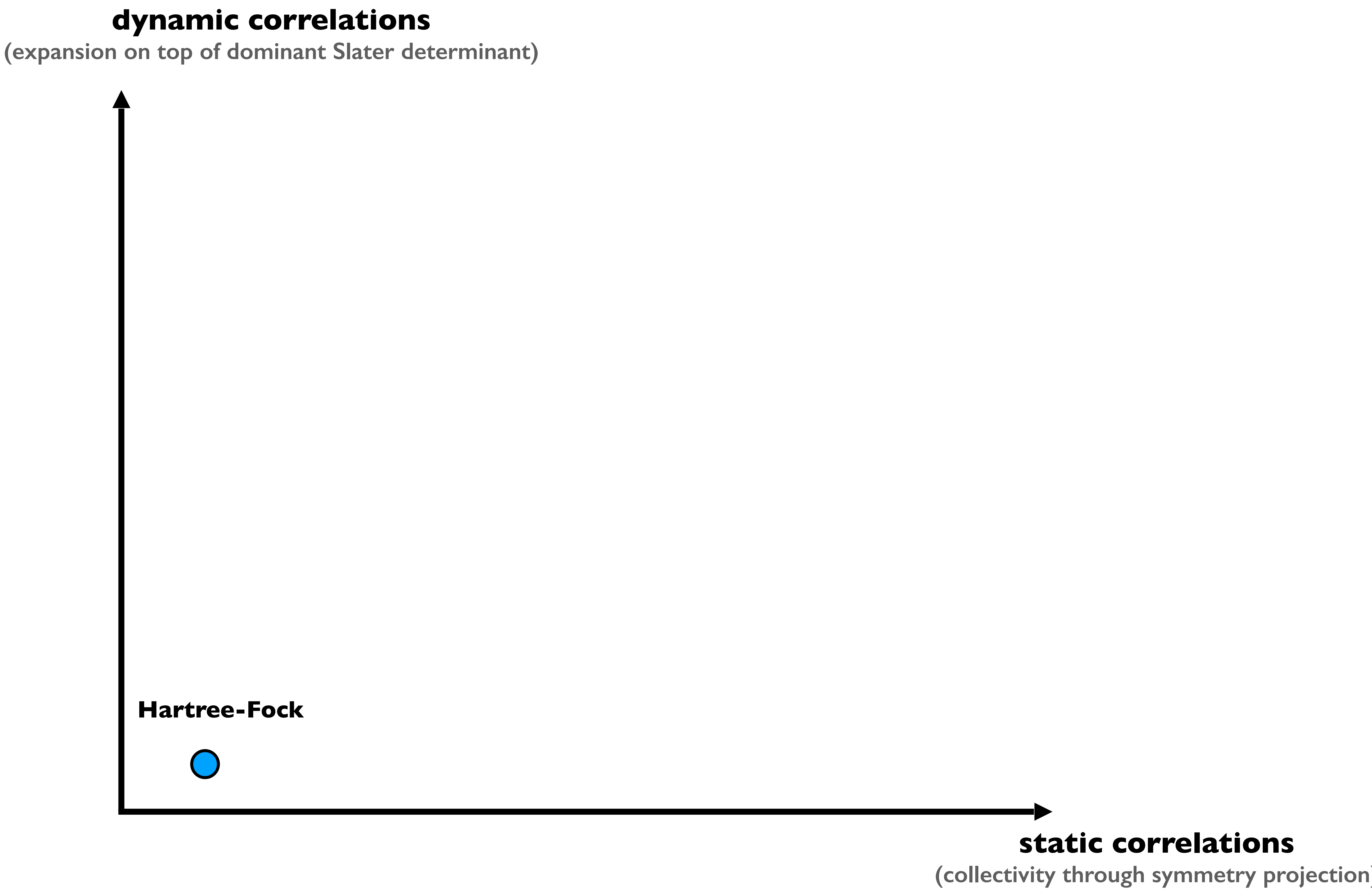
- **Extend full configuration interaction (FCI) capacities: limited to ~20 levels**

Many-body correlations



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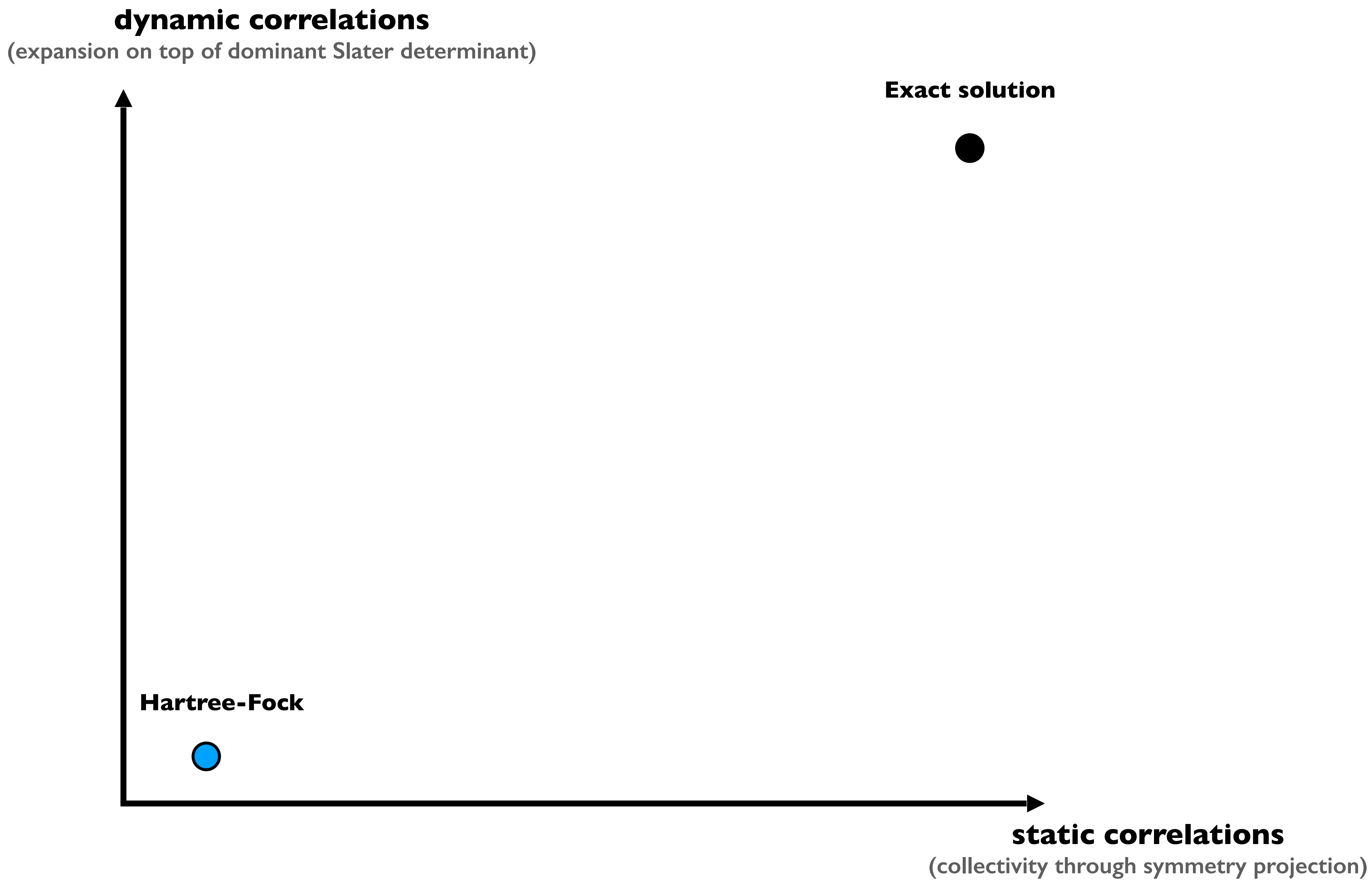

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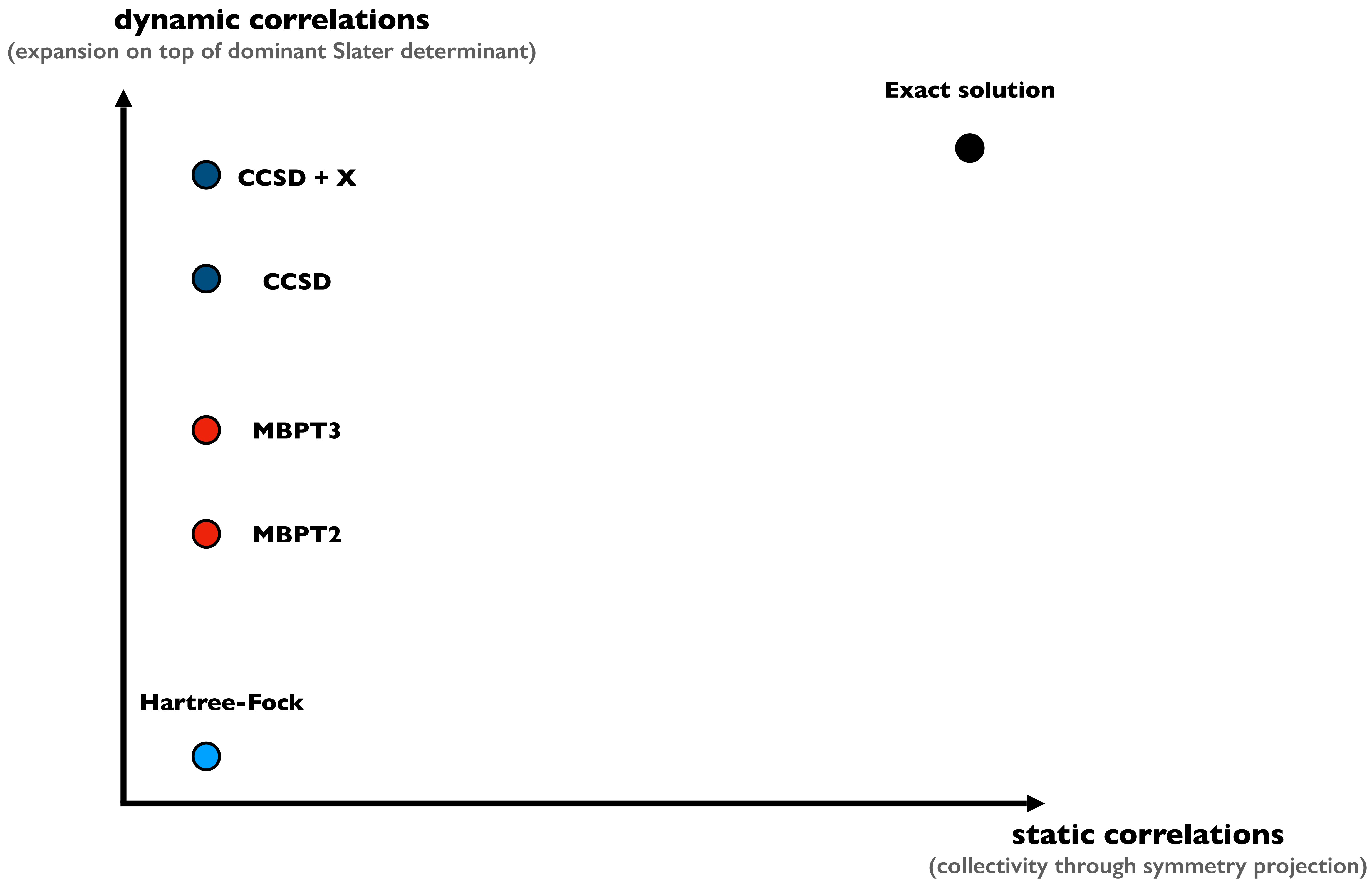

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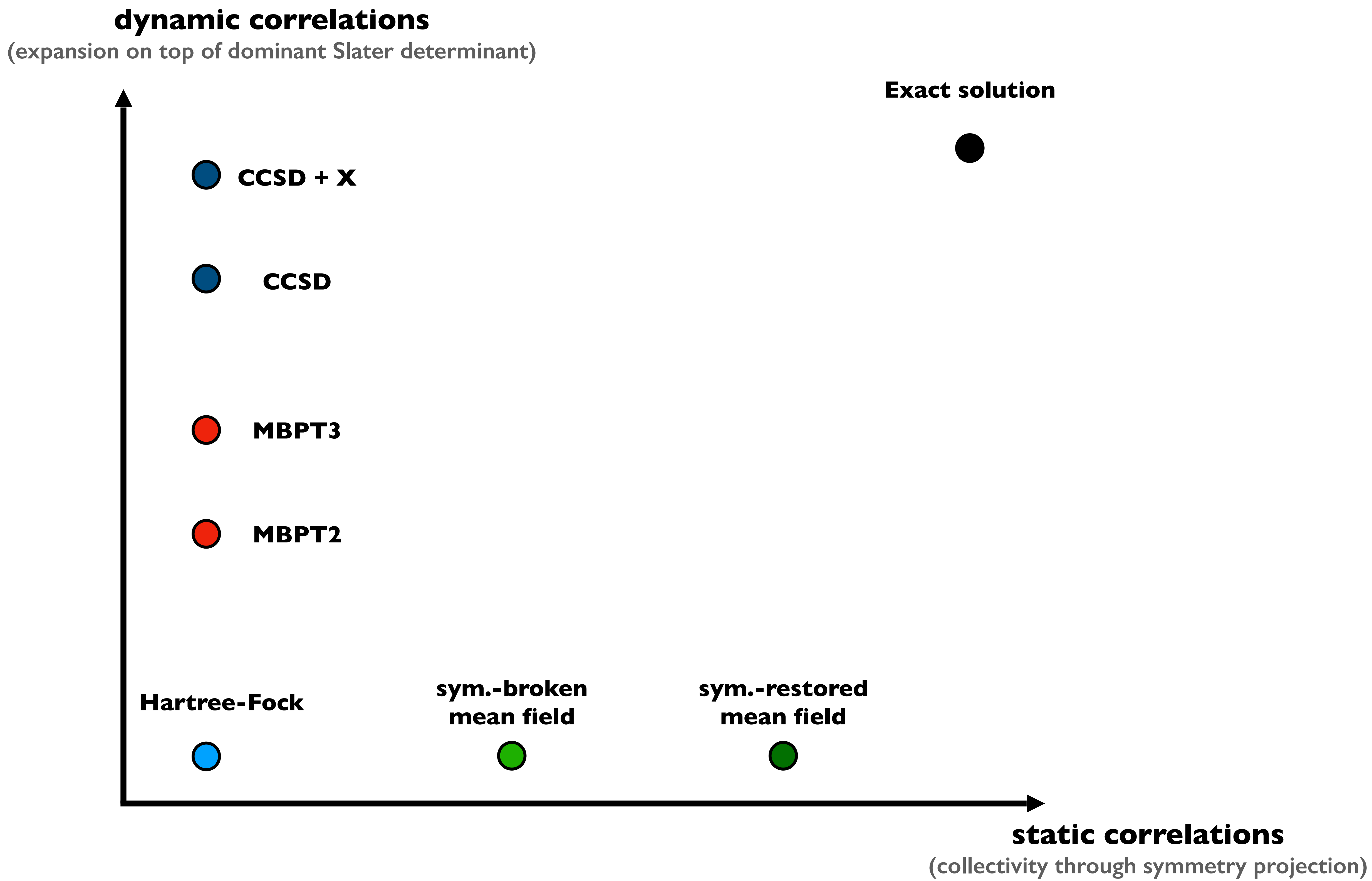

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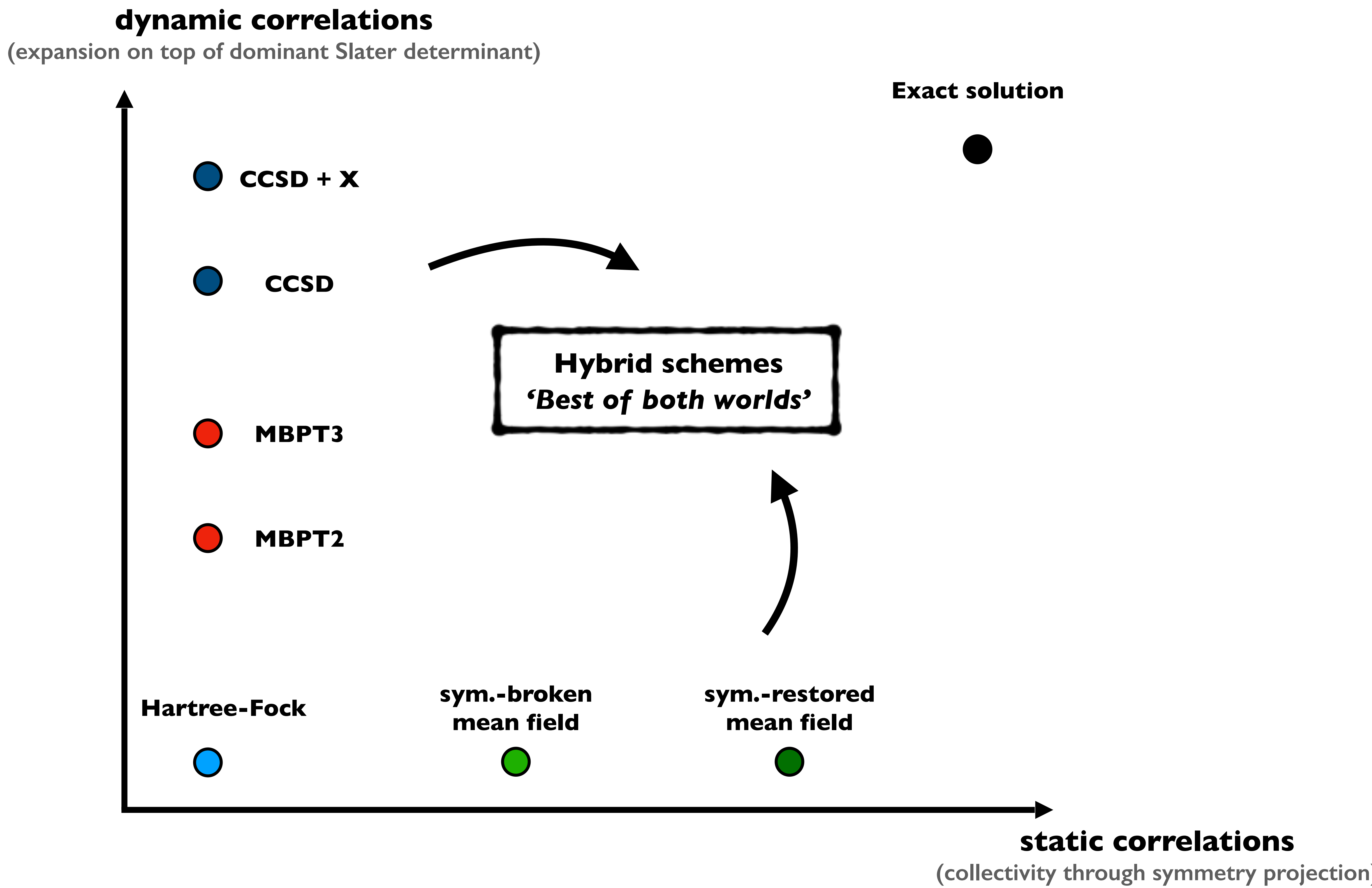

Particle-number-broken mean field

- **BCS wave-function ansatz for superfluid system**

(Bardeen-Cooper-Schrieffer)

$$|\Phi_{\mathrm{BCS}}\rangle = \prod_{p>0} (u_p + v_p \, c^\dagger_p c^\dagger_{\bar{p}}) \, |0\rangle$$

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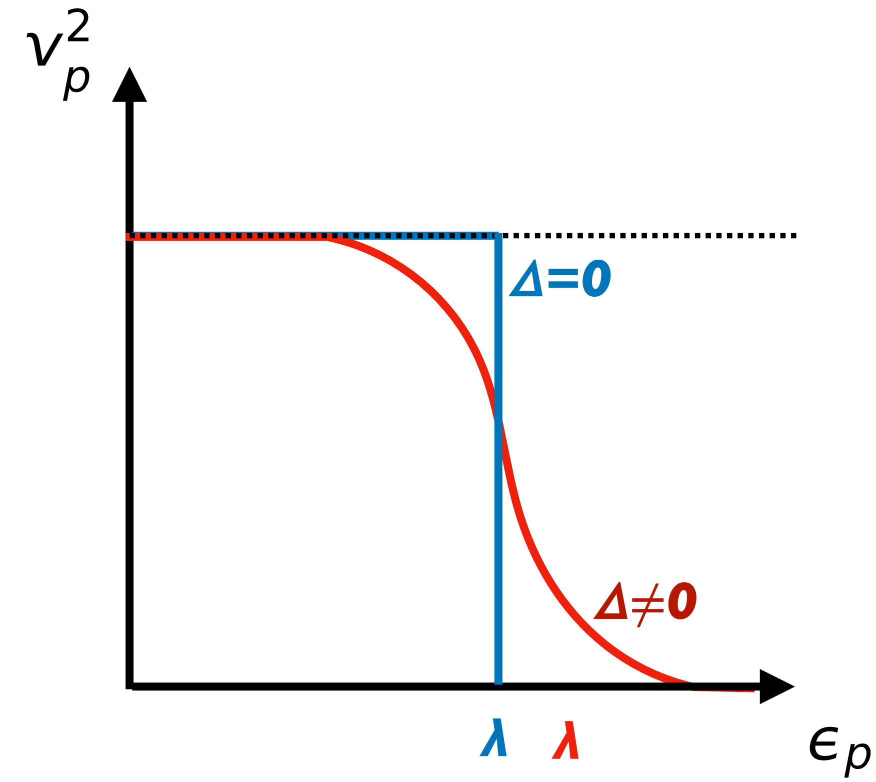
BCS occupation profile

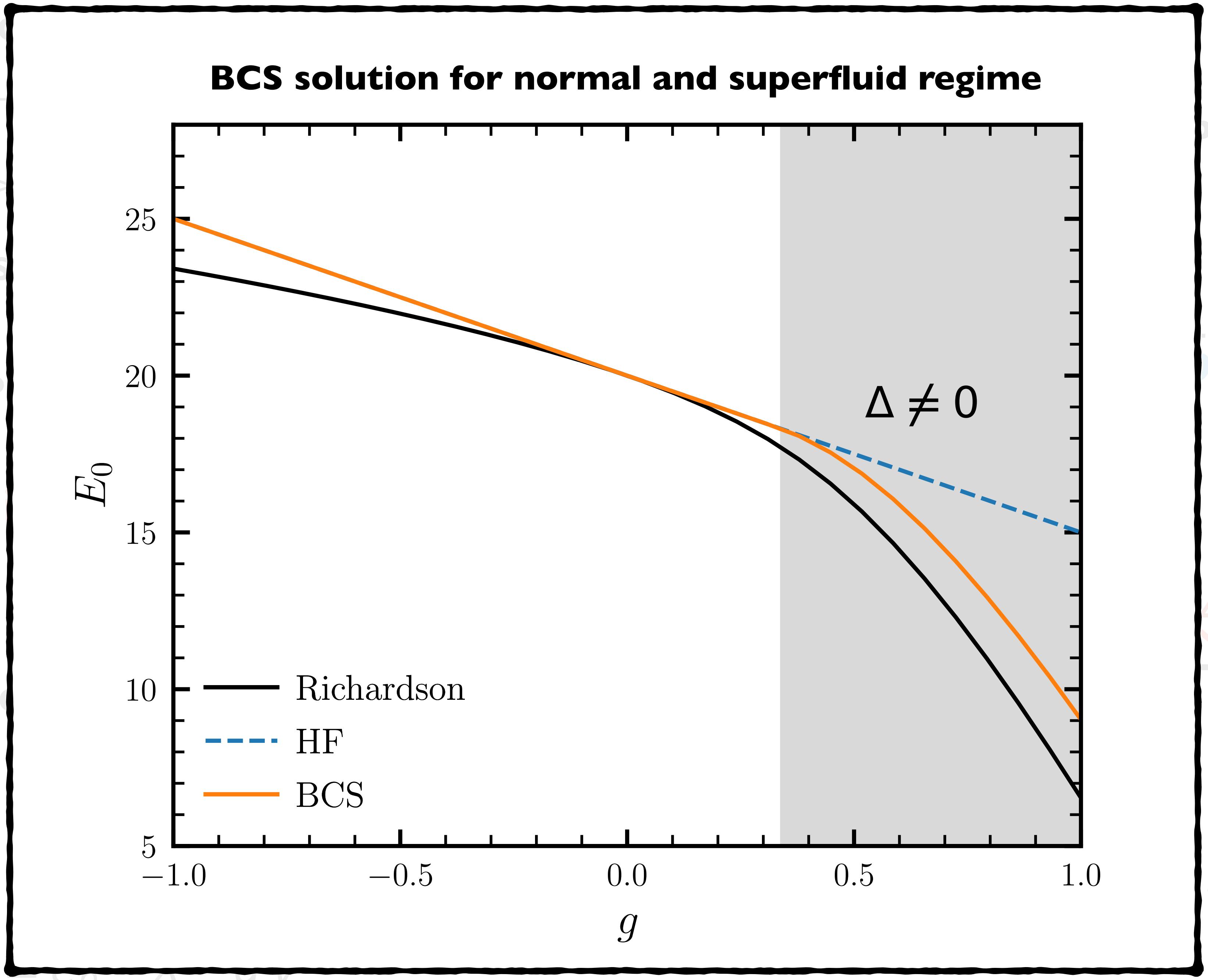


$$\Delta = \langle \Phi_{\rm BCS}| c^\dagger_p c^\dagger_{\bar{p}} |\Phi_{\rm BCS}\rangle = g \sum_{p>0} u_p v_p$$

BCS gap parameter

Particle-number-broken mean field

- BCS wave-functi
- BCS state breaks
- Constrained min
- Solution obtaine



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Symmetry projection

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- Similar expressions hold for other symmetries, e.g., rotational invariance SU(2)

Perturbation theory

Lacroix, Gambacurta, PRC (2012)

- **Partitioning of full Hamiltonian into unperturbed part and perturbation**

$$H = H_0 + H_1$$

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$E_p > 0$: quasi-particle energies

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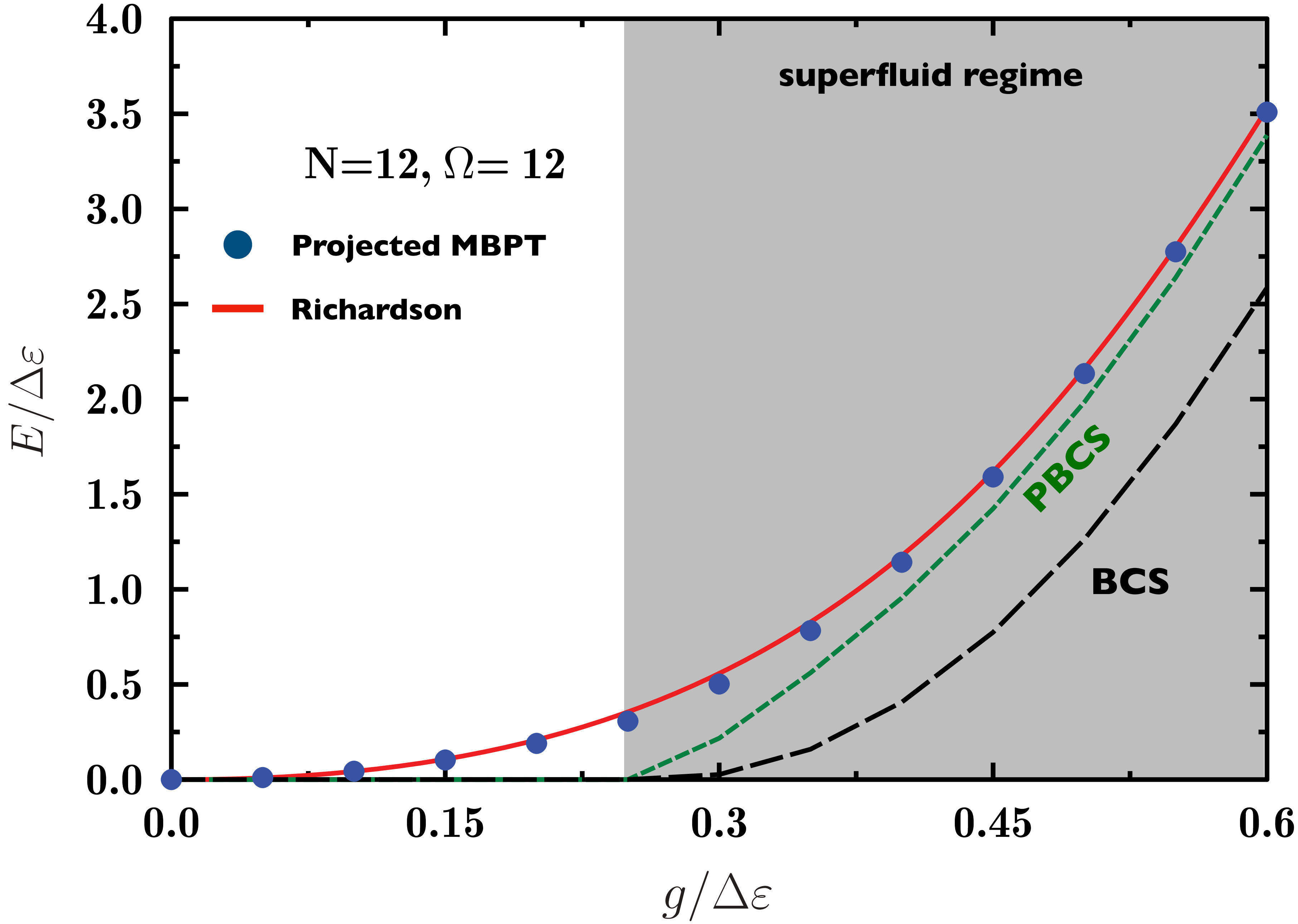
- **Standard HF-MBPT is recovered in limiting case of vanishing pairing gap**

Results of perturbation theory

Lacroix, Gambacurta, PRC (2012)

Correlation energy as a function of coupling strength



Coupled-cluster theory for BCS states

Henderson *et al.*, PRC (2014)

- **Bogoliubov coupled-cluster (BCC) theory:** CC extension for BCS reference states

$$|\Psi_{\text{BCC}}\rangle = e^{T} |\Phi_{\text{BCS}}\rangle$$

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- **Evaluate amplitude equations using Wick theorem for SU(2) algebra**

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Coupled-cluster theory for BCS states

Henderson *et al.*, PRC (2014)

- **Bogoliubov coupled-cluster (BCC) theory:** CC extension for BCS reference states

$$|\Psi_{\text{BCC}}\rangle = e^{T}|\Phi_{\text{BCS}}\rangle$$

- **Many-body operators are transformed to quasiparticle basis using *u*/*v* coefficients**

$$\beta_p^\dagger = u_p c_p^\dagger + v_p c_{\bar{p}} \qquad \beta_{\bar{p}}^\dagger = u_p c_{\bar{p}}^\dagger - v_p c_p$$

- **Cluster operator is expressed in SU(2) algebra (but now with quasiparticles!)**

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Coupled-cluster theory for BCS states

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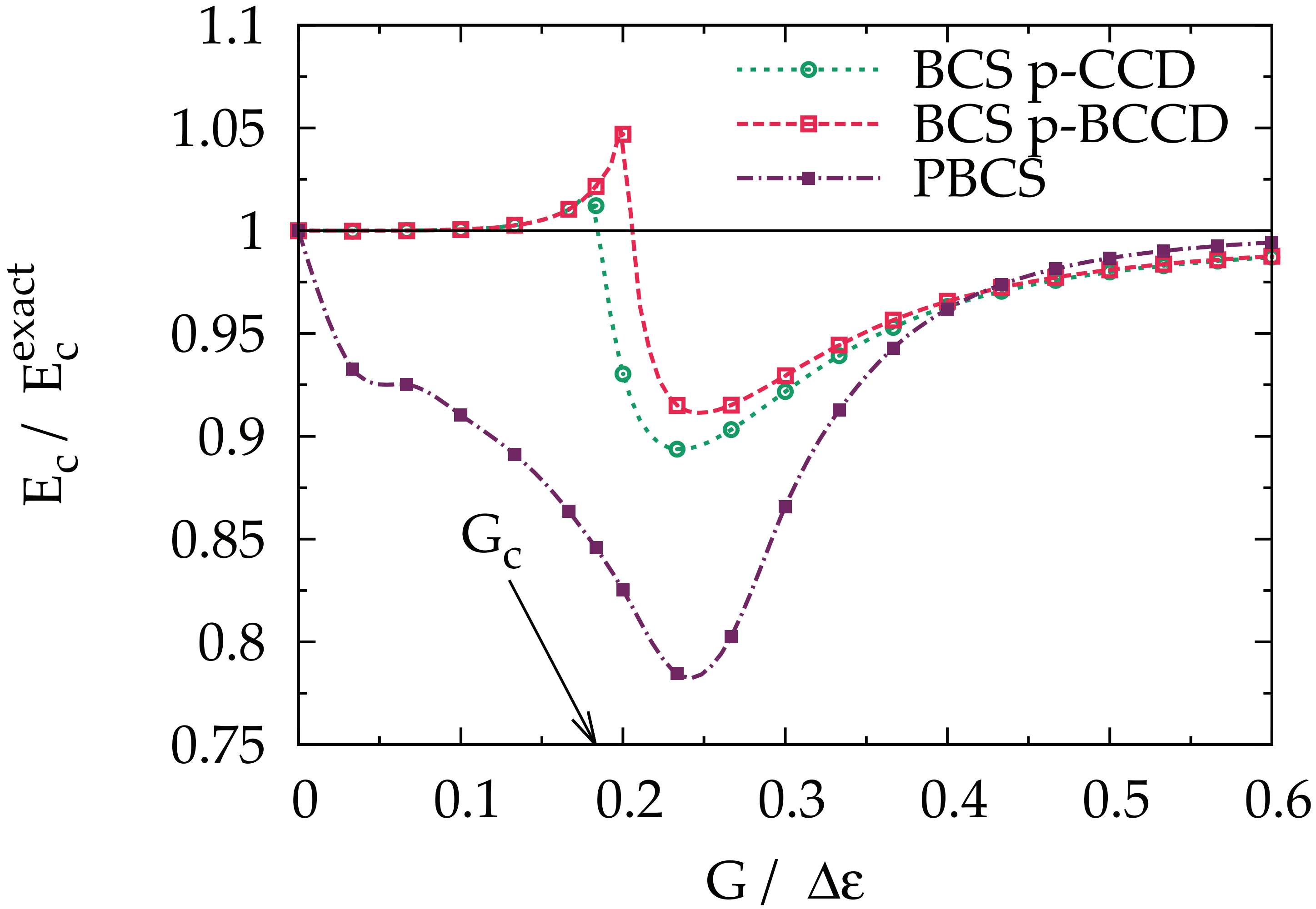
- Bogoliubov coup… …ce states
- Many-body opera… …efficients
- Cluster operator…
- Evaluate amplitu…

BCC performance in superfluid phase



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Projected coupled-cluster theory

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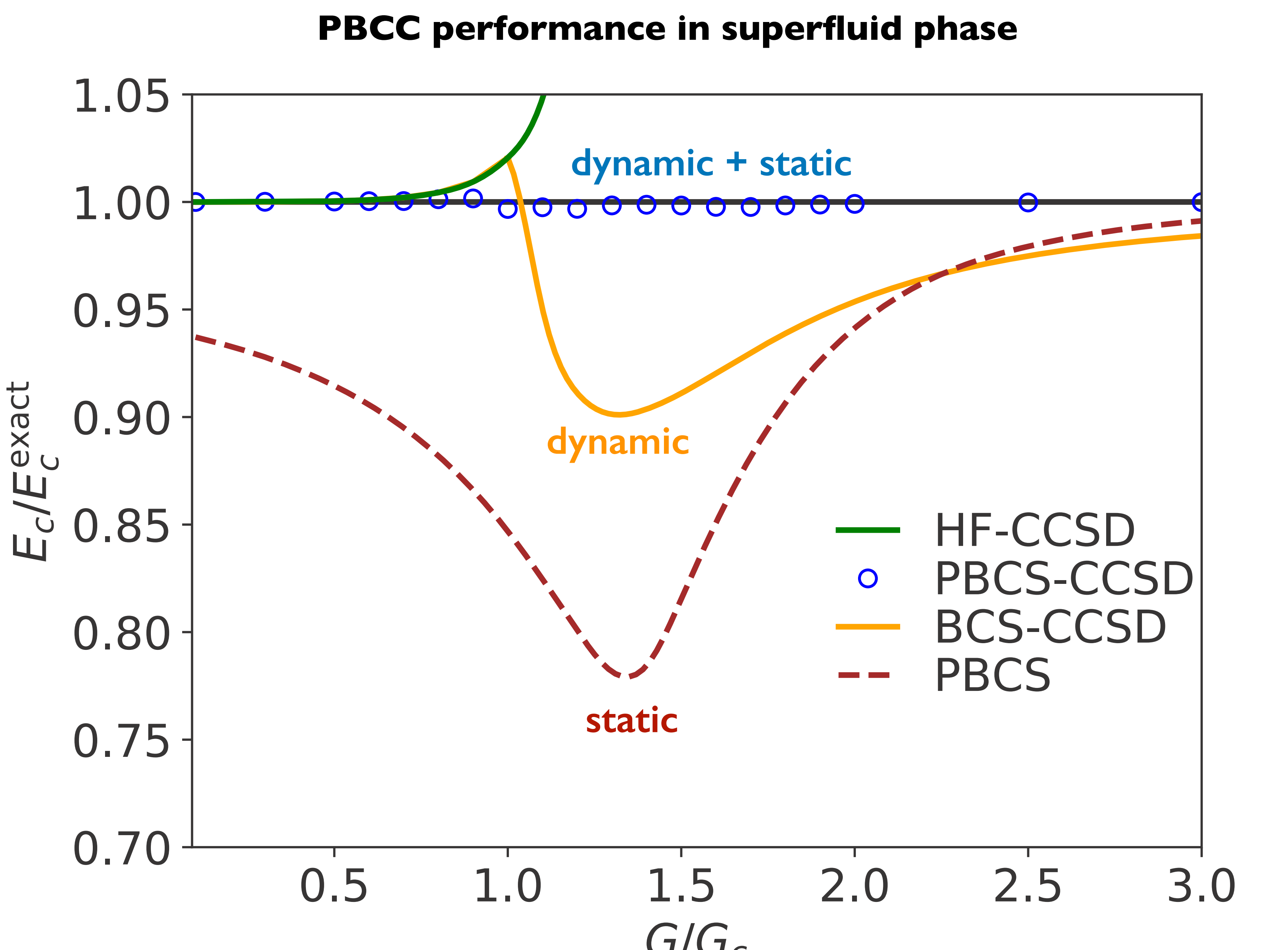
- Numerical implementation is computationally very demanding in practice

Projected coupled-cluster theory



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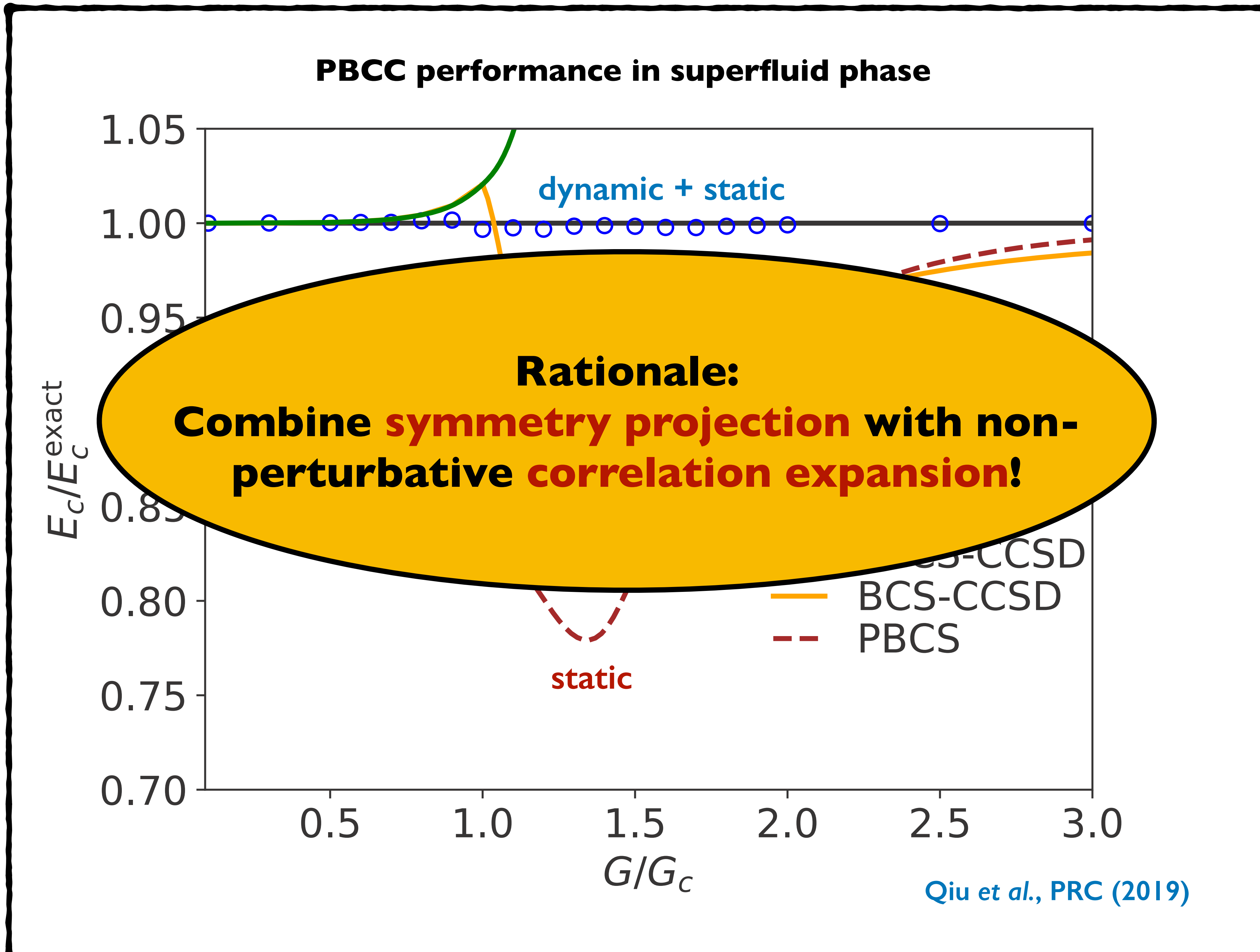
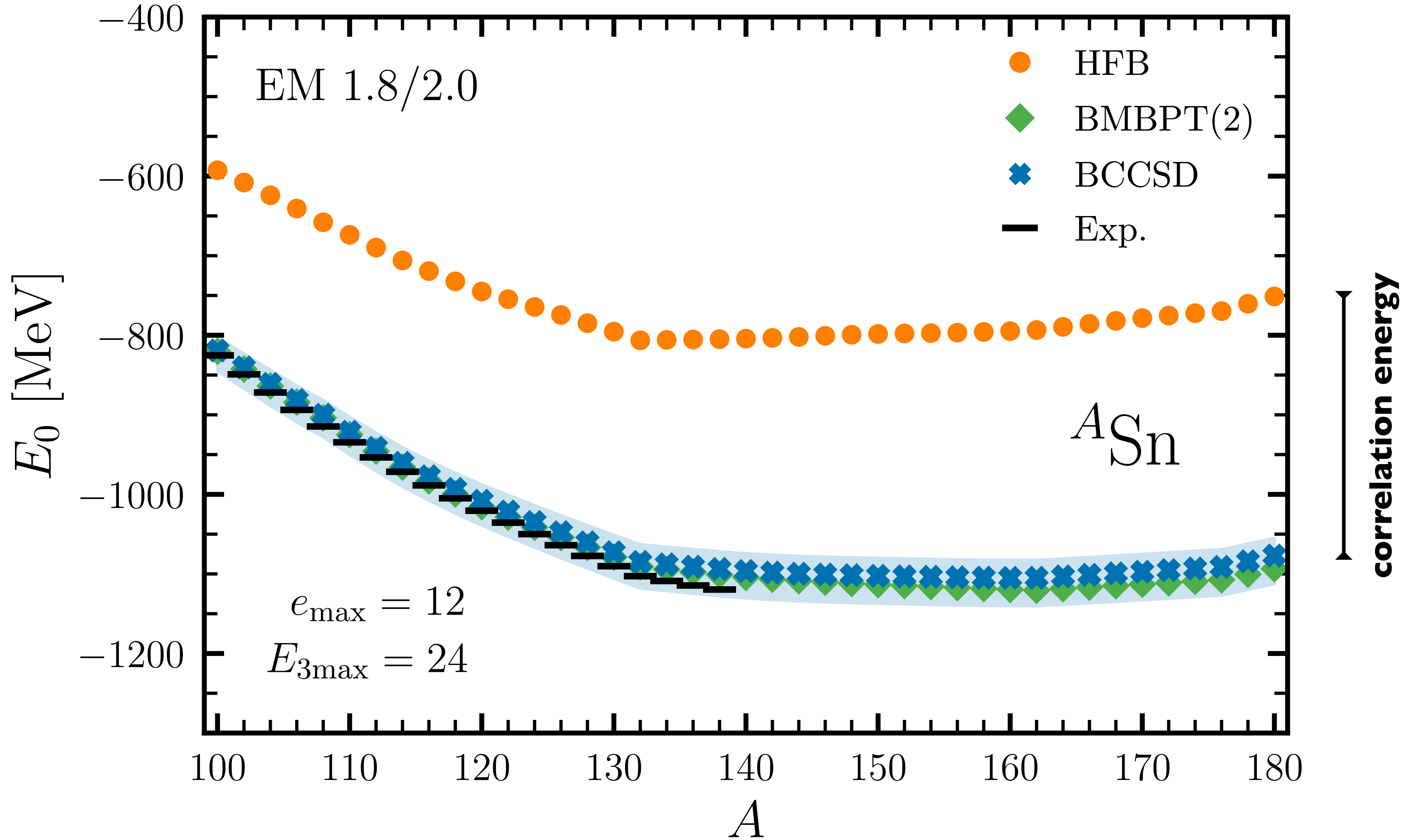


Rationale:
Combine symmetry projection with non-perturbative correlation expansion!

Large-scale *ab initio* applications

Particle-number-broken many-body frameworks for open-shell nuclei



Tichai, Demol, Duguet, arXiv:2307.15619 (2023)

No full projection yet!

Many-body emulators

- **Question**: can we emulate the many-body solution based on training data?

$\{g_1, ..., g_N\}$	$\{\|\Psi(g_1)\rangle, ..., \|\Psi(g_N)\rangle\}$	$\longrightarrow$	$g_\odot$ $\|\Psi(g_\odot)\rangle$
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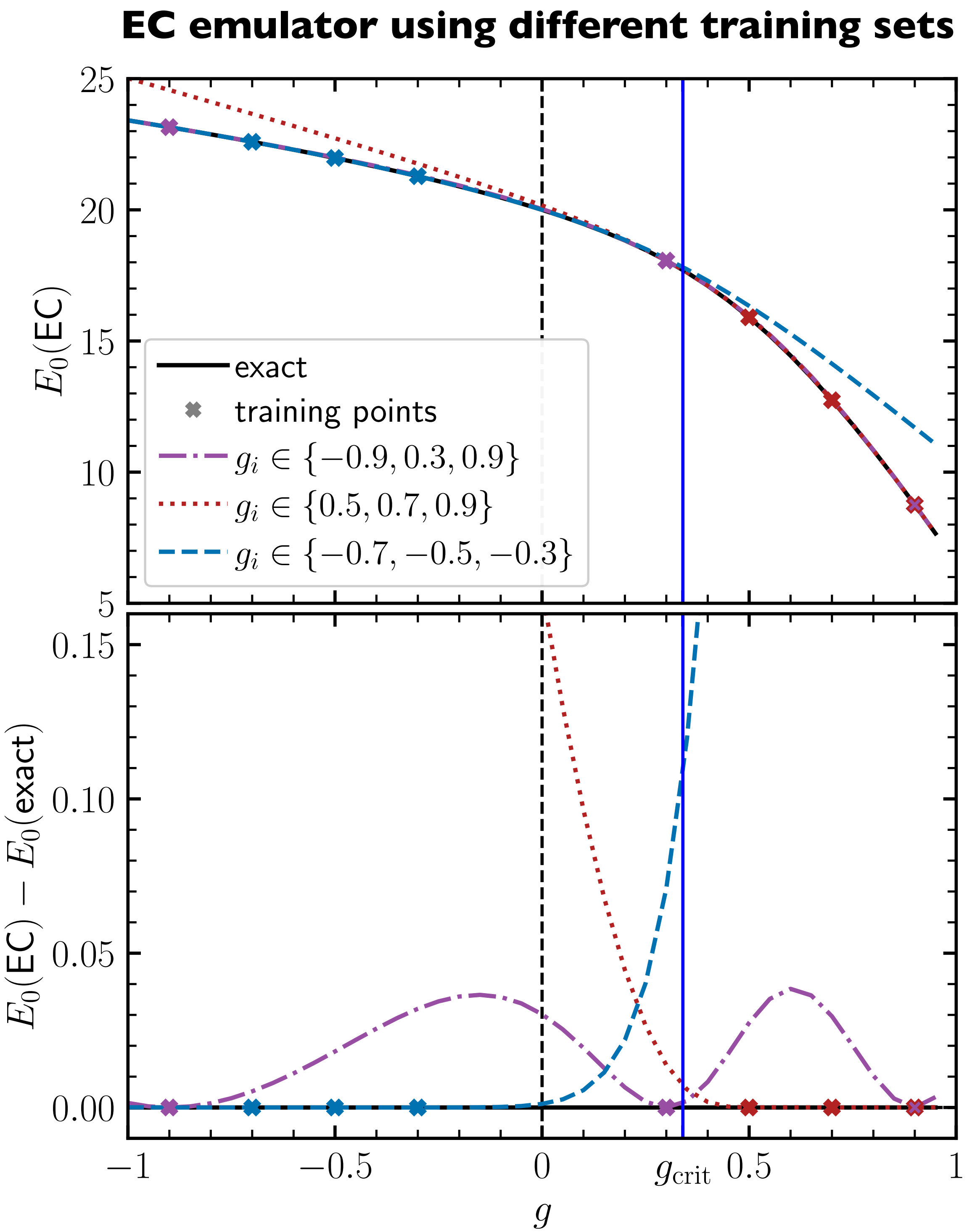
- Hot topic: **emerging field in nuclear physics** with numerous applications

Duguet *et al.*, arXiv:2310.19419 (2023)

Performance of the EC emulator



Companys Franzke, Tichai, Hebeler, Schwenk, PRC (2024)

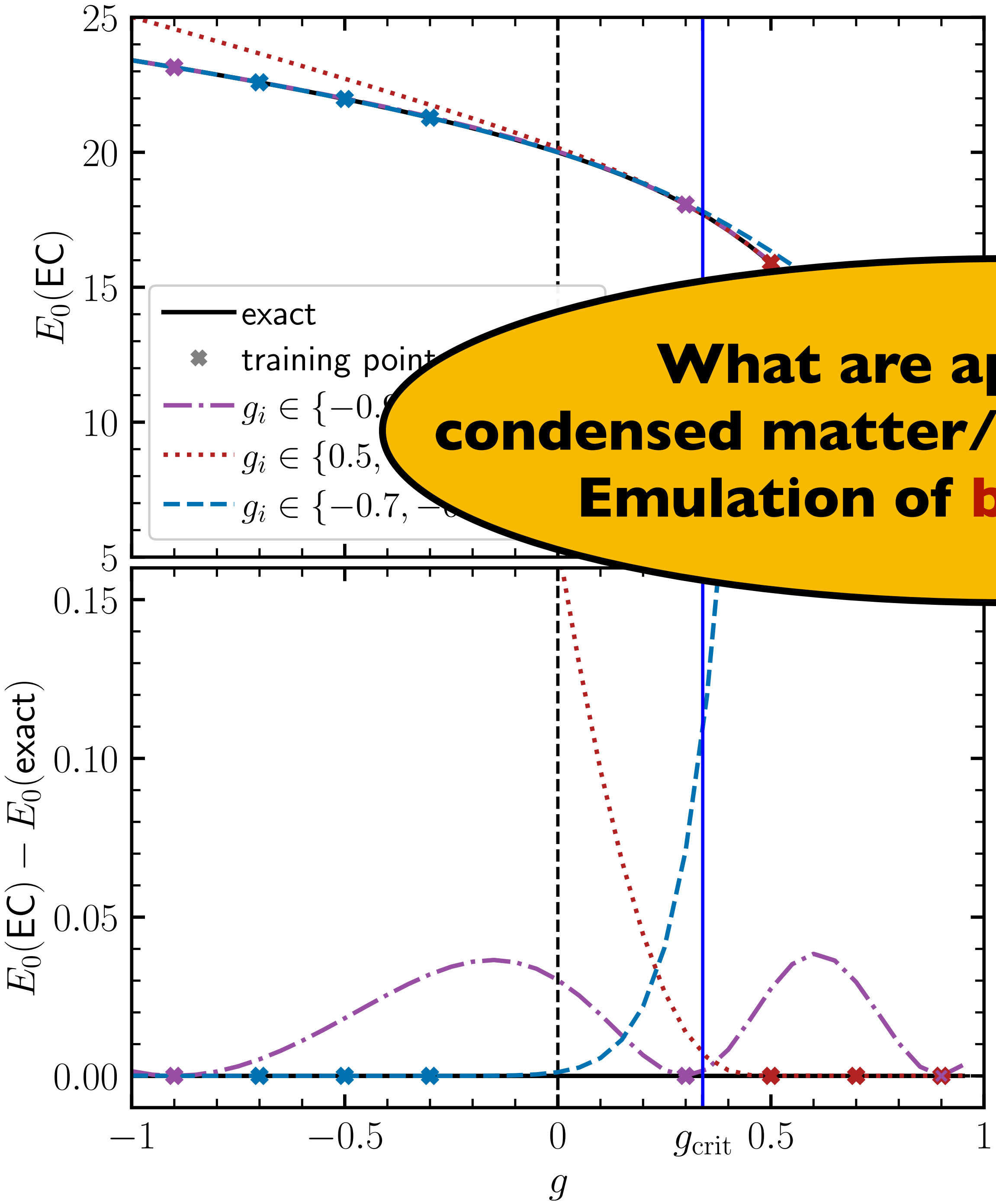
- Introduction of **different training manifolds**: normal, superfluid, mixed
- One-sided training manifolds are **unreliable for non-trained regime**
- Mixed training manifold **yields consistent prediction** for all couplings

Selection of appropriate training vectors crucial!

similar study using DMRG:
Baran, Nichita, PRB (2023)

Performance of the EC emulator

EC emulator using different training sets



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What are applications in condensed matter/quantum chemistry?
Emulation of bond stretching?

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Conclusions

Pairing Hamiltonian as many-body testbed

- Integrable Richardson solution for arbitrary system size
- Emergence of critical coupling separating normal and superfluid phase
- Breakdown of conventional many-body expansions

Lesson: Hartree-Fock-based schemes are doomed to fail

Implications on many-body frameworks

- Capture static correlations via spontaneous symmetry breaking
- Account for dynamic correlations using many-body expansion
- Parametric dependence can be efficiently emulated

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Lesson: Hartree-F

Take-home message:
Schematic models reveal key correlations relevant for realistic applications.

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