More irreps, fewer regrets: Symmetries and subspace methods in quantum algorithms

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In this talk

1. Some facts about symmetry breaking and restoration

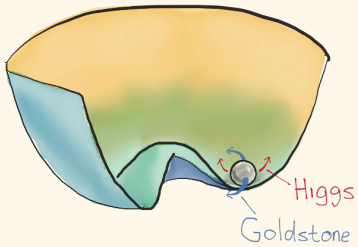
2. Handling symmetries on a quantum computer
   - What's up with quantum?
   - Some remedies

3. Configuration-mixing schemes
   - Configuration mixing in a nutshell
   - Encoding schemes and resources reduction
   - Illustration on a toy model

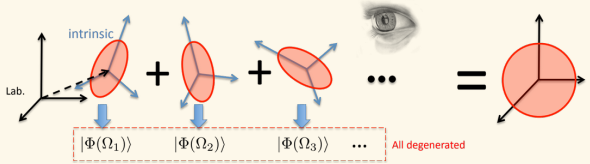
1 Symmetry breaking & restoration

Symmetries: fact-dumping

- *Fact #1:* symmetries of the Hamiltonian do *not* dictate symmetries of the eigenstates, even for finite N [1]
- *Fact #2*: Broken symmetries are restored in finite time
- Breaking symmetries is *natural*, but they should be restored to be consistent
- Some examples: pairing correlation, rotational modes



💡 Practical implications: symmetry-breaking ansatzes w. restoration can achieve better descriptions than symmetry-conserving, sometimes at lower costs



(Courtesy D. Lacroix)

2 Handling symmetries on a quantum computer

To break or not to break?

Phys. Rev. C 110.064320 (2024)

With Jing Zhang & Denis Lacroix

Symmetry restoration on QC: previous works

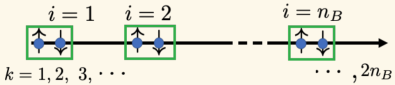
Most applications from chemistry/cond. mat.: e^-, with spin $\uparrow$ / $\downarrow$

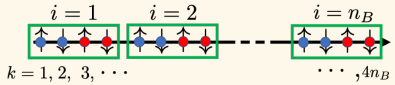
Symmetries: S^2, S_z, N, Π

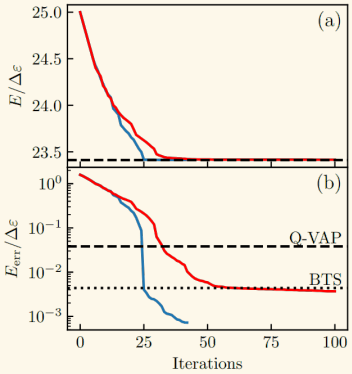
Atomic nuclei: n & p (isospin $\uparrow$ / $\downarrow$) $\times$ spin: 4 fermions species

Symmetries: $S^2, S_z, T^2, T_z, N_n, N_p, \Pi_n, \Pi_p$

- More symmetries can be broken
- Restoration becomes more expensive
- Restoration is harder to control
- Some quantum algorithms:
  - Quantum phase estimation
  - Grover-like symmetry amplification
  - Linear comb. of unitaries
  - Classical shadows
  - Configuration mixing: GCM







Symmetry restoration on QC: neutron-proton pairing

$$H = \sum_{i=1}^{n_B} \varepsilon_i \left[\left(\nu_i^\dagger \nu_i + \nu_{\bar{i}}^\dagger \nu_{\bar{i}} \right) + \left(\pi_i^\dagger \pi_i + \pi_{\bar{i}}^\dagger \pi_{\bar{i}} \right) \right] - \sum_{T_z=-1,0,1} g_V(T_z) \mathcal{P}_{T_z}^\dagger \mathcal{P}_{T_z} - \sum_{S_z=-1,0,1} g_S(S_z) \mathcal{D}_{S_z}^\dagger \mathcal{D}_{S_z}$$

Channels	Description	Operators
$T_z = \pm 1$	Electronic-like	$\mathcal{P}_{-1}^\dagger, \mathcal{P}_{+1}^\dagger$
$T_z = 0, S_z = 0$	Pure np w/ diff. spins	$\mathcal{P}_0^\dagger, \mathcal{D}_0^\dagger$
$S = 0$	Electronic + np w/ diff. spins	$\mathcal{P}_{-1}^\dagger, \mathcal{P}_0^\dagger, \mathcal{P}_{+1}^\dagger$
All	Like+unlike+mixed	All six

$$\mathcal{P}_1^\dagger = \sum_i \nu_i^\dagger \nu_{\bar{i}}^\dagger$$
$$\mathcal{P}_{-1}^\dagger = \sum_i \pi_i^\dagger \pi_{\bar{i}}^\dagger$$
$$\mathcal{P}_0^\dagger = \frac{1}{\sqrt{2}} \sum_i \left[\nu_i^\dagger \pi_{\bar{i}}^\dagger + \pi_i^\dagger \nu_{\bar{i}}^\dagger \right]$$
$$\mathcal{D}_1^\dagger = \sum_i \nu_i^\dagger \pi_i^\dagger$$
$$\mathcal{D}_{-1}^\dagger = \sum_i \nu_{\bar{i}}^\dagger \pi_{\bar{i}}^\dagger$$
$$\mathcal{D}_0^\dagger = \frac{1}{\sqrt{2}} \sum_i \left[\nu_i^\dagger \pi_{\bar{i}}^\dagger - \pi_i^\dagger \nu_{\bar{i}}^\dagger \right]$$

Methodology

ADAPT-VQE algorithm [2]:

- Initial state $|\Psi_0\rangle$
- $\left|\Psi_{n+1}\right\rangle = e^{i\theta_{n+1}\hat{A}_{n+1}}|\Psi_n\rangle = \prod_{j=0}^{n} e^{i\theta_j \hat{A}_j}|\Psi_0\rangle$
- $\hat{A}_{n+1}$ selected from a pool $\left\{\hat{A}^{(k)}\right\}$ by maximising the gradient of the energy

$$\frac{\partial E_{n+1}}{\partial \theta_{n+1}} = i\left\langle \Psi_n \right| \left[\hat{H}, \hat{A}^{(k)}\right] \left| \Psi_n \right\rangle$$

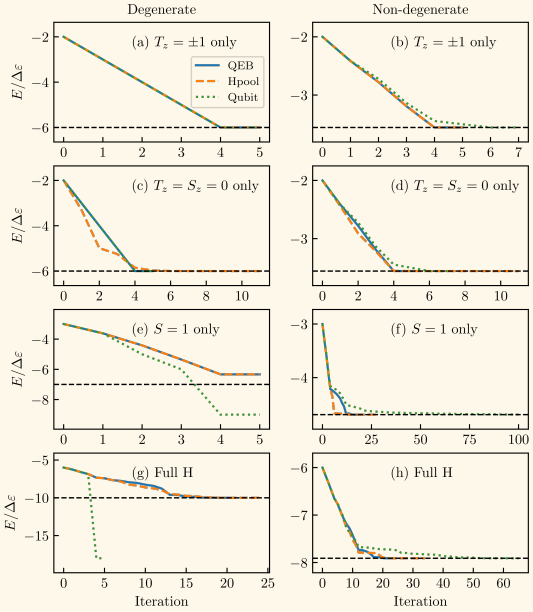
- Some variants:
  - select one, opt one
  - select one, opt all
  - select k, opt k [3]

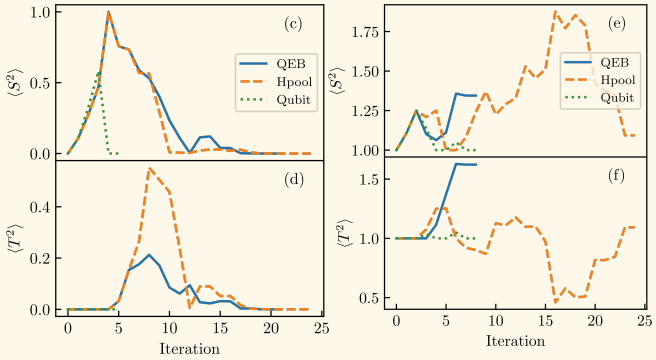
Operator pools:

	Particle number	**Seniority**	**Parity**
Hamiltonian	✓	✓	✓
Excitations	✓	✗	✓
Qubits	✗	✗	✓

	$n_B = 2$	$n_B = 3$	$n_B = 4$
Hamiltonian	14	30	52
Excitations	98	561	1940
Qubits	140	990	3640

Results: Convergence issues



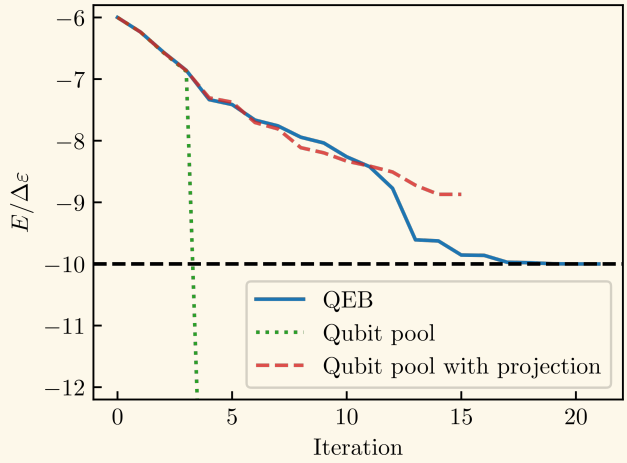


- Spontaneous SB
- GS degeneracies
- Initial state

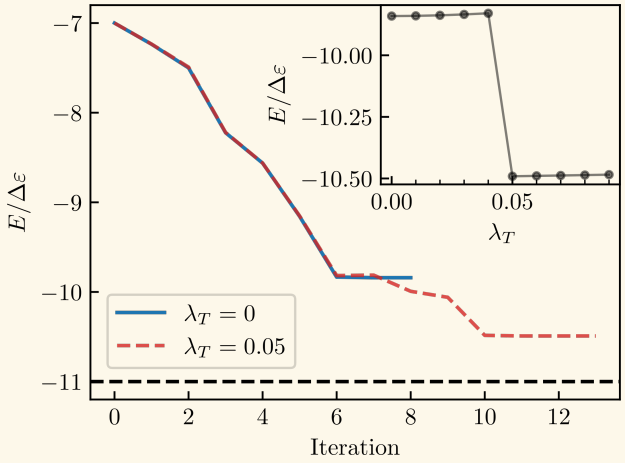
- Breaking S, T, is OK
- Breaking particle number is tricky

Results: Standard remedies

Projection

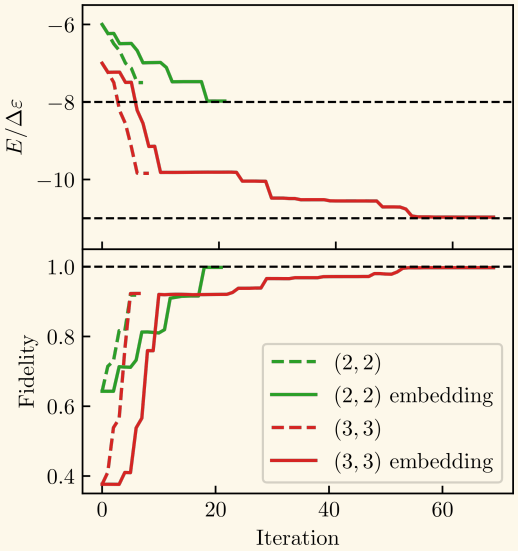


Penalty

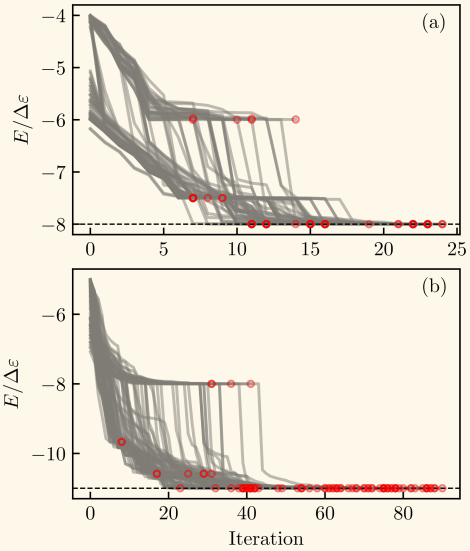


Results: Alternative methods

Embedding



Randomisation



3 Configuration-mixing schemes

Restoring symmetries, reducing quantum resources, and all that

Phys. Rev. C 109, 024327 (2023)

With Denis Lacroix

Configuration-mixing in a nutshell

Typical quantum algos: work on a single state $\left|\Psi_f\right\rangle = U|\Psi_i\rangle$

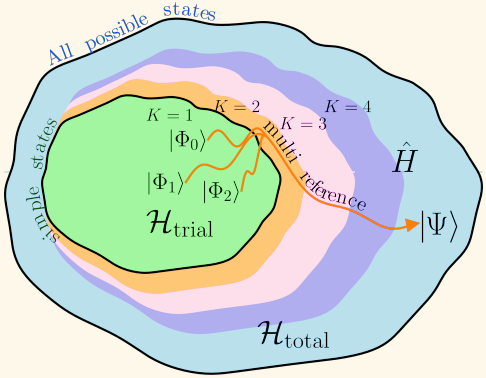
Pitfals: ansatz depth, symmetry, barren plateaus, etc

💡 Quantum subspace expansion (Review: [4]): many-body inspired method mixing reference states

$$\left|\Psi_j\right\rangle = \sum_{k=0}^{K-1} f_{k,j}|\Phi(\boldsymbol{q}_k)\rangle$$

$$\Rightarrow \boldsymbol{H}|\Psi\rangle = E\boldsymbol{S}|\Psi\rangle, \text{with } \boldsymbol{O}_{kk'} = \left\langle \Phi(\boldsymbol{q}_k)\middle|\hat{O}\middle|\Phi(\boldsymbol{q}_{k'})\right\rangle$$

- $\{\boldsymbol{q}\}$: "generator coordinates". Real time evolution, spatial deformation, etc
- $\{|\Phi\rangle\}$: "generator states". Note: construction not necessarily operator-based
- Common choice: $|\Phi(\boldsymbol{q_k})\rangle = e^{-i\hat{H}_C t_k}|\Psi_0\rangle$



Note: in some sense, special case of the Generator Coordinate Method (Hill & Wheeler (1953)) [5]

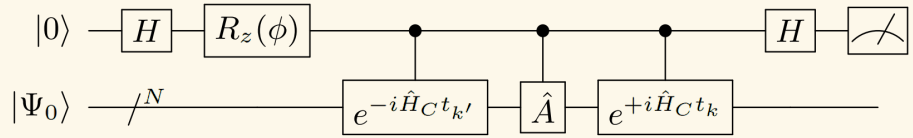
Configuration-mixing in a nutshell (ii)

Cool features:

- Improved eigenstates description (ground and low-lying) (Parrish & McMahon (2019) [6])
- Qubits reduction: very timely for QC, link with tensor networks (YBT & D. Lacroix (2023) [7])
- Systematic symmetry restoration (YBT & D. Lacroix (2023) [7]), YBT (2025) [8])
- Performance guarantees (Epperly et al. (2021)) [4]

Main difficulty: estimate $\boldsymbol{H}_{kk'} = \left\langle \Psi_0 \middle| e^{i\hat{H}_C t_k} \hat{H}_C e^{-i\hat{H}_C t_{k'}} \middle| \Psi_0 \right\rangle$

Done with Hadamard tests (here $\hat{A} = \hat{H}_C$):



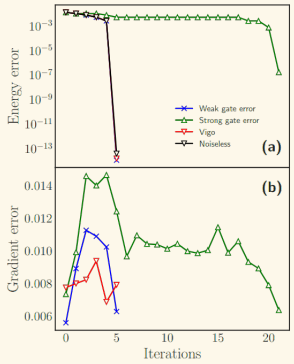
- Moderate resources-per-circuit overhead wrt single-reference. Total # of terms $\propto K$ or K^2
- Several variants, see [8]

Hamiltonian and encodings

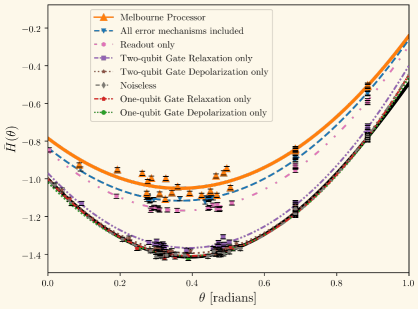
Likpin-Meshkov-Glick Hamiltonian: now a standard testbed for many-body quantum algorithms

$$H = \frac{\varepsilon}{2}\sum_{p=1}^{N}\sum_{\sigma}\sigma a^{\dagger}_{p\sigma}a_{p\sigma} + \frac{V}{2}\sum_{pp'}^{N}\sum_{\sigma} a^{\dagger}_{p\sigma}a^{\dagger}_{p'\sigma}a_{p-\sigma}a_{p'-\sigma}, \quad \chi = \frac{V(N-1)}{\varepsilon}$$

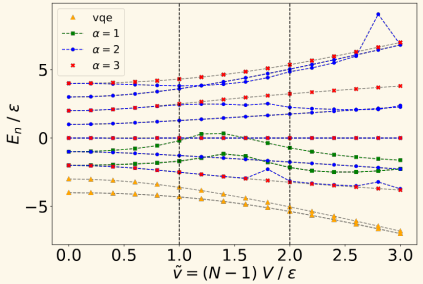
Jordan-Wigner: 1 state $\leftrightarrow$ 1 qubit



SU(2): 2 states $\leftrightarrow$ 1 qubit



$J-$scheme + Π basis: N states $\leftrightarrow \log_2(N)$ qubits



Reducing quantum resources: the factorisation trick

$$H = \frac{\varepsilon}{2}\sum_{\alpha}^{N} Z_\alpha + \frac{V}{4}\sum_{\alpha,\beta}^{N}\left(X_\alpha X_\beta - Y_\alpha Y_\beta\right)$$

- Symmetries of H: permutation, parity
- Permutation: coherent states $|\Omega\rangle = \left[R_y(\omega)|0\rangle\right]^{\otimes N}$ make an over-complete basis of the relevant $\mathcal{H}$

💡 Decompose eigenstates as $|\Psi\rangle_j = \sum_{k=0}^{K-1} f_{k,j}|\Omega_k\rangle$

- The $|\Omega_k\rangle$ don't have well-defined parity, but $|\Omega_k\rangle \pm |-\Omega_k\rangle)$ do!

Matrix elements factorise: with $p_{kk'} \equiv \langle\Omega_k|P|\Omega_{k'}\rangle$,

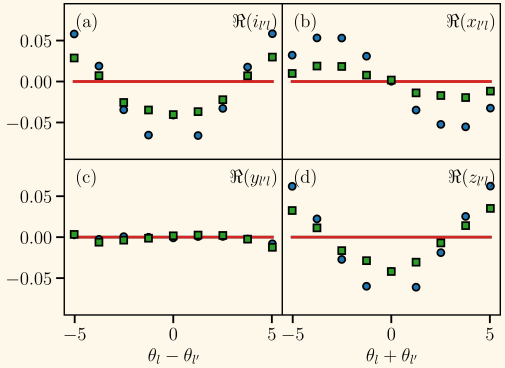
$$\boldsymbol{H}_{kk'} = \langle\Omega_k|H|\Omega_{k'}\rangle = \frac{\varepsilon N}{2} i_{kk'}^{N-2}\left[i_{kk'}z_{kk'} + \frac{\chi}{2}\left(x_{kk'}^2 - y_{kk'}^2\right)\right]$$

$$\boldsymbol{S}_{kk'} = \langle\Omega_k|\Omega_{k'}\rangle = i_{kk'}^N$$

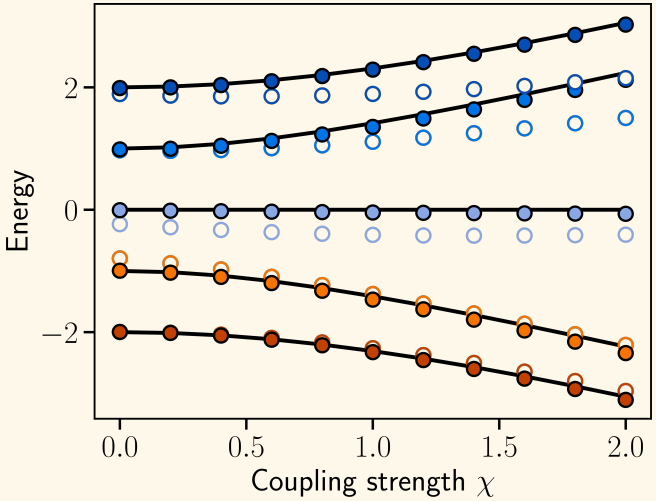
Results

N particles $\rightarrow N+1$ angles

- 10^5 shots per matrix element
- Ran on IBM Lagos backend



- Empty dots: raw results
- Filled dots: extrapolation & rescaling



Conclusions

What:

- Symm. breaking & restoration: straightforward for e^-, *much* less for np. Expecting similar mess for QCD
- Increased # of symmetries: delicate interplay between increased # of channels

Why:

- Unphysical degeneracies when s.p. energies are the same
- Initial state instrumental in convergence
- *Some* symmetries can be broken, but not *all*

Remedies:

- Embedding and iterative deflation
- Initial state randomisation
- Configuration mixing

Perspectives for QCD:

- Let's chat!

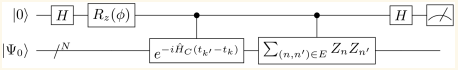

That's all Folks!

4 Some backups

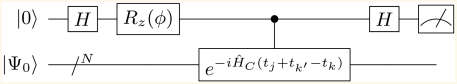
Kernels estimation

Goal: find the best way to estimate $\boldsymbol{H_{kk'}} = \left\langle \Psi_0 \middle| e^{i\hat{H}_C t_k} \hat{H}_C e^{-i\hat{H}_C t_{k'}} \middle| \Psi_0 \right\rangle$

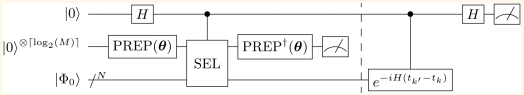
Pauli strings



Real-time evolution



Linear combination of unitaries



Method	CNOT	T	Anc.
Pauli	$\left(\sqrt{\rho}N\right)^5(L'+2)$	$4\left(\sqrt{\rho}N\right)^5(L'+1)\log_2\left(\frac{1}{\varepsilon}\right)$	1
RTE	$\rho N^2(L'+2)pC(p)$	$4\rho N^2(L'+1)\log_2\left(\frac{1}{\varepsilon}\right)pC(p)$	1
LCU	$\rho^3 N^6(L'+4)/\left(4\left\langle \hat{H}_C^2 \right\rangle\right)$	$\rho^3 N^6 L' \log_2\left(\frac{1}{\varepsilon}\right)/\left(4\left\langle \hat{H}_C^2 \right\rangle\right)$	$4\log_2(N)$

Truncation procedure

The Hill-Wheeler equation

$$\boldsymbol{H}|\Psi\rangle = E\boldsymbol{S}|\Psi\rangle$$

can be ill-conditioned when basis states are nearly linearly dependent.

Workaround: construct a smaller orthonormal basis.

- $\boldsymbol{S} = \boldsymbol{P}\boldsymbol{\Sigma}\boldsymbol{P}^\dagger, \text{remove vectors with eigenval} < e_{\text{cut}} \to \tilde{\boldsymbol{P}}$
- Solve $\widetilde{\boldsymbol{H}}|\tilde{\Psi}\rangle = \tilde{E}\tilde{\boldsymbol{S}}|\tilde{\Psi}\rangle$, with $\widetilde{\boldsymbol{H}} = \boldsymbol{P}\boldsymbol{H}\boldsymbol{P}^\dagger$ and $\tilde{\boldsymbol{S}} = \boldsymbol{P}\boldsymbol{S}\boldsymbol{P}^\dagger$
- Eigenstates can be reconstructed afterwards

$$|\tilde{\Psi}\rangle = \sum_j a_j|\tilde{\Phi}_j\rangle = \sum_k \left(\sum_j a_j \tilde{\boldsymbol{P}}_{k,j}\right)|\chi_k\rangle$$

Kernel-free QSE

Shifting $\hat{H}_C \to \hat{H}_C - E$, then

1. First option: Gaussian filter:

$$[U(t) - U(-t)]^K \propto \frac{1}{2^K} \sum_{k=0}^{K-1} C_K^k U((K-1-2k)t)$$
$$= e^{-Kt^2\left(\hat{H}_C - E\right)^2} + \mathcal{O}\left(t^4\left(\hat{H}_C - E\right)^4\right)$$

2. Second option: imaginary time evolution:

$$[(1+i)U(-t) + (1-i)U(t)]^K \propto \frac{1}{2^K} \sum_{k=0}^{K-1} C_K^k (1-i)^k (1+i)^{K-1-k} U((K-1-2k)t)$$
$$= e^{-Kt\left(\hat{H}_C - E\right)} + \mathcal{O}\left(t^2\left(\hat{H}_C - E\right)^2\right)$$

$\Rightarrow$ QSE can be used as a filter without even estimating the kernels

$\Rightarrow$ If the Hill-Wheeler eq. is solved, solutions are by construction better than 1. & 2.

Factorisation trick

(See YBT & D. Lacroix (2023))

If

$$H = \sum_{m=1}^{M} c_m P_m$$

$$|\Psi\rangle = \sum_{k=1}^{K} a_k |\Phi_k\rangle = \sum_{k=1}^{K} a_k |\varphi_k\rangle \otimes |\varphi'_k\rangle$$

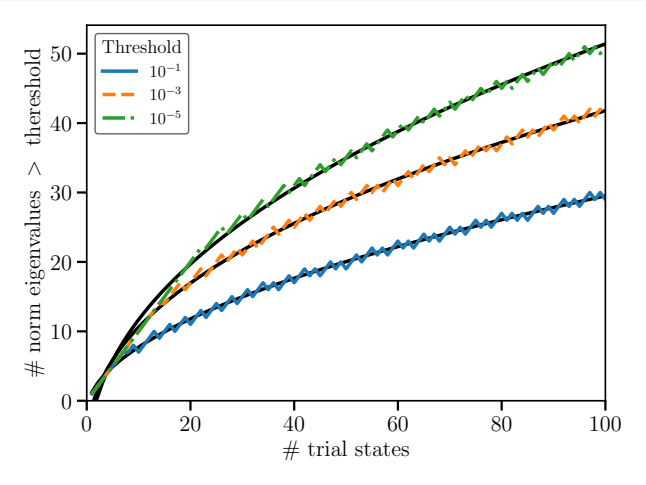
Then

$$S_{kk'} = \langle\varphi_k|\varphi_{k'}\rangle\langle\varphi'_k|\varphi'_{k'}\rangle$$

$$H_{kk'} = \sum_{m=1}^{M} c_m \langle\varphi_k|p_m|\varphi_{k'}\rangle\langle\varphi'_k|p'_m|\varphi'_{k'}\rangle, \quad \text{where } P_m = p_m \otimes p'_m$$

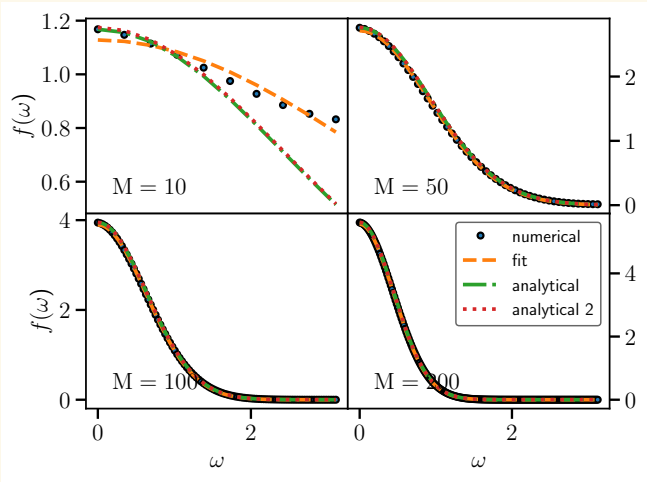
This generalises to any number of factors

Factorisation trick (ii)



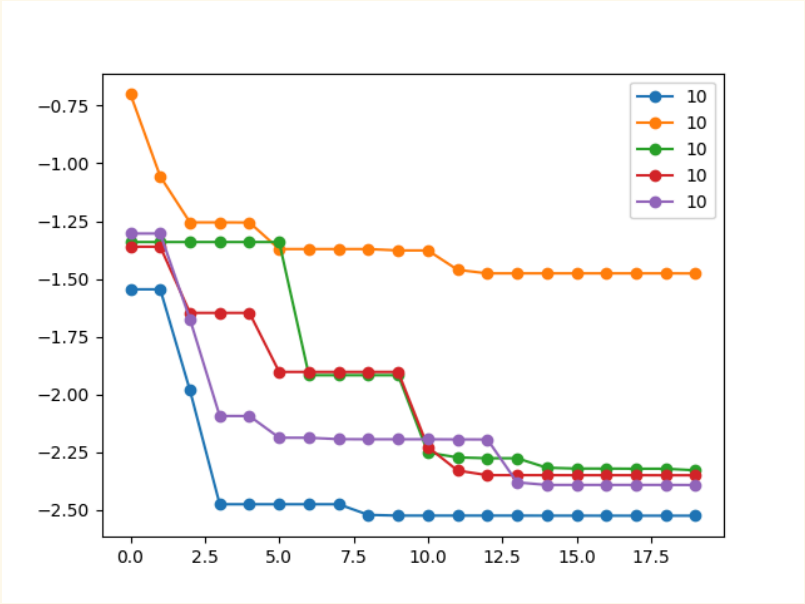
- Number of effective states $\propto \sqrt{\#\text{ trial states}}$
- Adjusting truncation threshold allows balancing dim of effective subspace and stability

Factorisation trick (iii)



- Gaussian spectrum cf Fourier analysis and asymptotic spectrum of Toeplitz matrices
- FWHM $\propto \frac{1}{\sqrt{M}}$: $\forall N$, can increase M to get a large enough space

Some optimisation traces

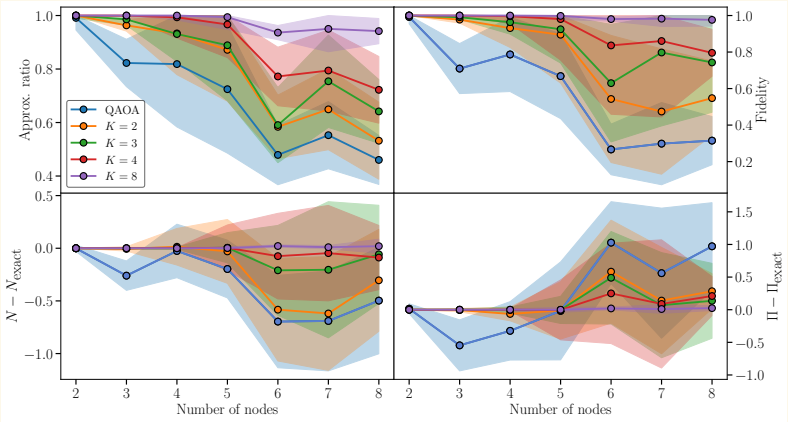


Some tests on MWIS

MIS: All edges have weight $w = 1$

MWIS: Edges are weighted.

Here, uniform random weights $1 \leq w \leq 2$. Each point: average over 14 Erdös-Rényi graphs.



Justifying some caveats

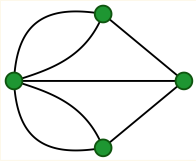
My computational means for [8]:

5 Subspace methods and combinatorial optimisation

Springer Proceedings of QUEST-IS

Methodology

Graph $G(V, E, w)$: vertices V, edges E, weights w



Graph optimisation on QC = finding GS of classical Ising-like Hamiltonians, e.g. for MIS:

$$n_i \to \hat{n}_i = \frac{I_i - Z_i}{2}$$

$$\Rightarrow \hat{H}_C = \sum_i w_i \hat{n}_i - \sum_{ij} w_{ij} \hat{n}_i \hat{n}_j$$

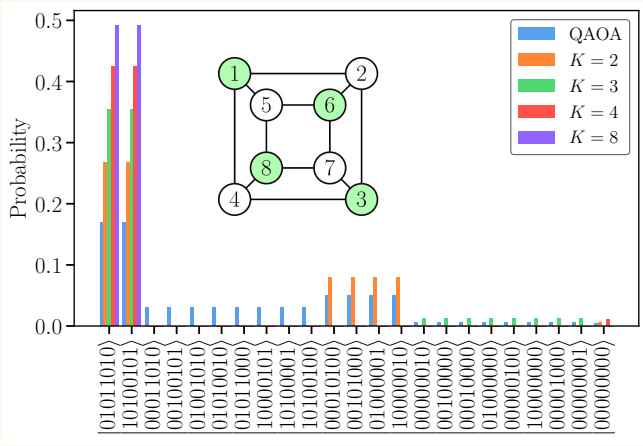
- Quantum Approximate Optimisation Ansatz:

$$U(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \prod_{\ell=1}^{L} e^{i\beta_\ell \hat{H}_M} e^{i\gamma_\ell \hat{H}_C}$$

- Here, $\hat{H}_M = \sum_i X_i$
- Initial state $|\Psi_0\rangle = |+\rangle^N$
- $L = 20$, optimised one-by-one
- GCM on top: $|\Phi_k\rangle = e^{-i\hat{H}_C t_k} |\Phi_0\rangle$
- Relevance metric: fidelity vs #gates (CNOT & T)

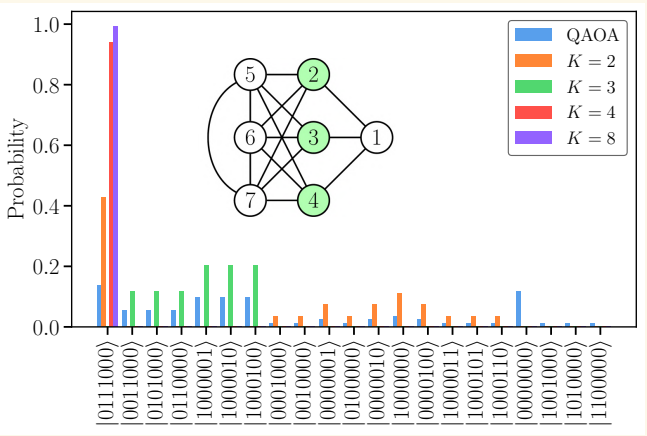
Results on simple graphs

"Easy" graph (small degree, solvable w/ greedy alg)



- QAOA: $\approx 35\%$, GCM: $\approx 98\%(K = 8)$

"Hard" graph (large degree, greedy alg fails)



- QAOA: $\approx 14\%$, GCM: $\approx 98\%(K = 8)$
- MIS found, except wrong parity at $K = 3$

Results on simple graphs (ii)

- Both MIS found

Application to Erdös-Rényi graphs

Erdös-Rényi graphs: N nodes, connect any pair with proba ρ (here $\rho =$1/2)

- ✓ NP hard
- ✓ Real-life relevance: resource allocation (smart grids, fault-resilient design), chemistry/pharma (reaction networks, epidemic spread)
- ✓ Common testbed in the QC community (E.g. Kim et al. (2024) [9], Zhao et al. (2024) [10], Leclerc et al. (2025) [11])

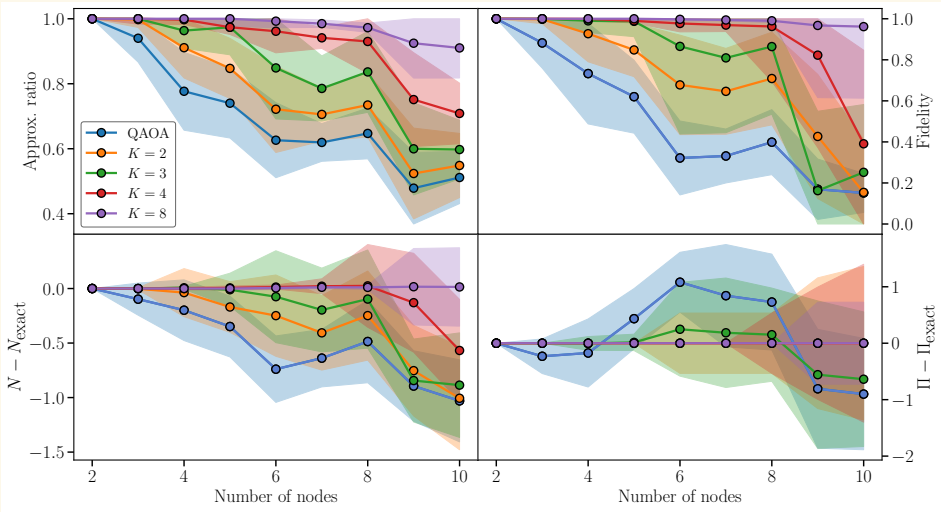
QAOA vs QSE comparison

- Fit fidelities w/ Fermi-Dirac

$$F_X(N) = \frac{\beta_X}{1 + e^{Na_X}}, \quad \text{compare } \left(\frac{\#\text{gates}}{F}\right)_{\text{QSE}} \text{ vs } \left(\frac{\#\text{gates}}{F}\right)_{\text{QAOA}}$$

- #gates depends on how matrix elements are evaluated (+ HW type & topology + physical error + QEC layers + ...)

Application to Erdös-Rényi graphs (ii)



- Systematically better:
  - Approx ratio
  - Fidelity
  - Hamming weight
  - Parity
- For $K = 8$, $N_* = 75$
- Each point: average over 14 Erdös-Rényi graphs

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