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A lattice gauge theory ground state calculation through subspace diagonalization

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Work in collaboration with
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Manuscript in preparation. All results are preliminary

QuantHEP 2025 - Berkeley, CA - October 2, 2025

Why we want the ground state of LGTs

Vacuum properties
- Phase diagram
- Correlation length

As an initial state
- Single-particle excitations
- Quench

$|\Omega\rangle$

Dependency on constraints
- Response to static probe charges
- Boundary, topology, ...

Spectrum
- If excited states are buildable

Quantum subspace diagonalization

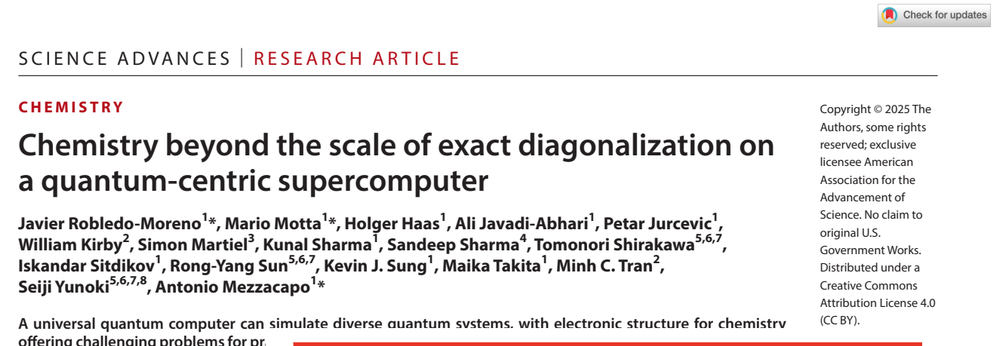
Idea:

Reduce the dimension of Hamiltonian

↓

Classically diagonalize

- Hamiltonian projected onto subspace containing the ground state
- Quantum used to identify the subspace
- Several approaches (sample-based, Krylov, sample-based Krylov)



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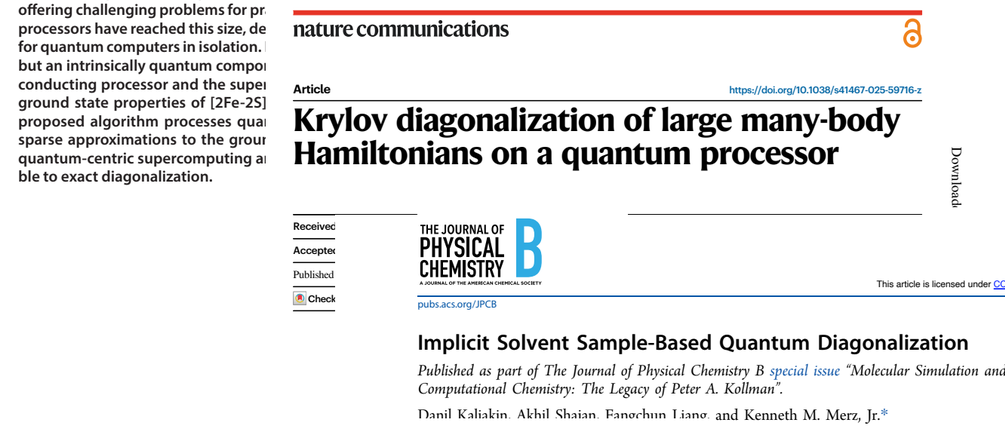
SCIENCE ADVANCES | RESEARCH ARTICLE

CHEMISTRY

Chemistry beyond the scale of exact diagonalization on a quantum-centric supercomputer

Javier Robledo-Moreno[1]*, Mario Motta[1]*, Holger Haas[1], Ali Javadi-Abhari[1], Petar Jurcevic[1], William Kirby[2], Simon Martiel[3], Kunal Sharma[1], Sandeep Sharma[4], Tomonori Shirakawa[5,6,7], Iskandar Sitdikov[1], Rong-Yang Sun[5,6,7], Kevin J. Sung[1], Maika Takita[1], Minh C. Tran[2], Seiji Yunoki[5,6,7,8], Antonio Mezzacapo[1]*

A universal quantum computer can simulate diverse quantum systems, with electronic structure for chemistry offering challenging problems for pr processors have reached this size, de for quantum computers in isolation. but an intrinsically quantum compo conducting processor and the supe ground state properties of [2Fe-2S] proposed algorithm processes qua sparse approximations to the grou quantum-centric supercomputing a ble to exact diagonalization.



nature communications

Article

https://doi.org/10.1038/s41467-025-59716-z

Krylov diagonalization of large many-body Hamiltonians on a quantum processor

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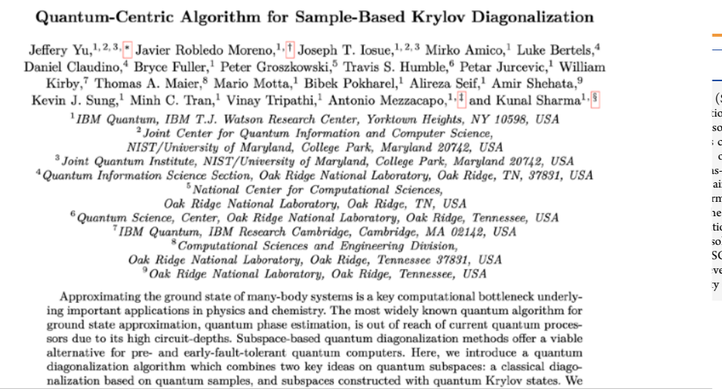
Article

Implicit Solvent Sample-Based Quantum Diagonalization

Published as part of The Journal of Physical Chemistry B special issue "Molecular Simulation and Computational Chemistry: The Legacy of Peter A. Kollman".

Danil Kaliakin, Akhil Shajan, Fangchun Liang, and Kenneth M. Merz, Jr.*



Quantum-Centric Algorithm for Sample-Based Krylov Diagonalization

Jeffery Yu,[1,2,3,*] Javier Robledo Moreno,[1,†] Joseph T. Iosue,[1,2,3] Mirko Amico,[1] Luke Bertels,[4] Daniel Claudino,[4] Bryce Fuller,[1] Peter Groszkowski,[5] Travis S. Humble,[6] Petar Jurcevic,[1] William Kirby,[7] Thomas A. Maier,[8] Mario Motta,[1] Bibek Pokharel,[1] Alireza Seif,[1] Amir Shehata,[9] Kevin J. Sung,[1] Minh C. Tran,[1] Vinay Tripathi,[1] Antonio Mezzacapo,[1,‡] and Kunal Sharma[1,§]

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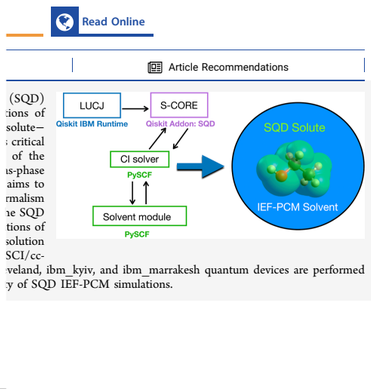
Approximating the ground state of many-body systems is a key computational bottleneck underlying important applications in physics and chemistry. The most widely known quantum algorithm for ground state approximation, quantum phase estimation, is out of reach of current quantum processors due to its high circuit-depths. Subspace-based quantum diagonalization methods offer a viable alternative for pre- and early-fault-tolerant quantum computers. Here, we introduce a quantum diagonalization algorithm which combines two key ideas on quantum subspaces: a classical diagonalization based on quantum samples, and subspaces constructed with quantum Krylov states. We



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Article Recommendations

(SQD) ions of solute– critical of the s-phase aims to rmalism e SQD tions of solution SCI/cc-

LUCJ

Qiskit IBM Runtime

S-CORE

Qiskit Addon: SQD

CI solver

PySCF

Solvent module

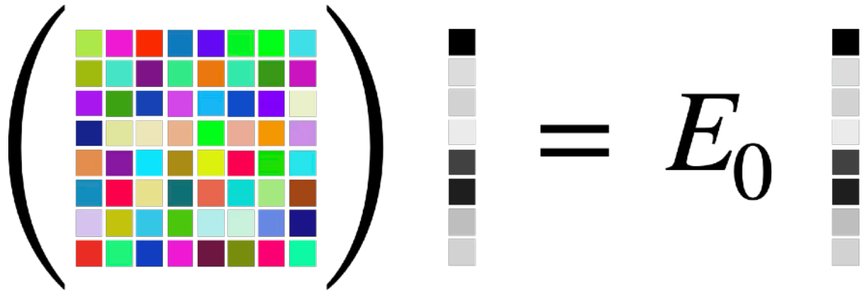
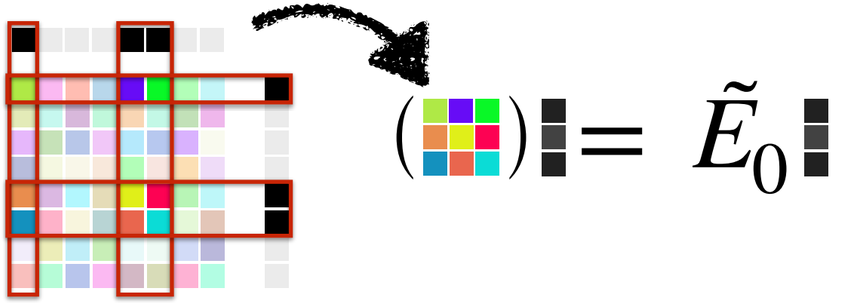
PySCF

SQD Solute

IEF-PCM Solvent

veland, ibm_kyiv, and ibm_marrakesh quantum devices are performed y of SQD IEF-PCM simulations.

Sample-based diagonalization

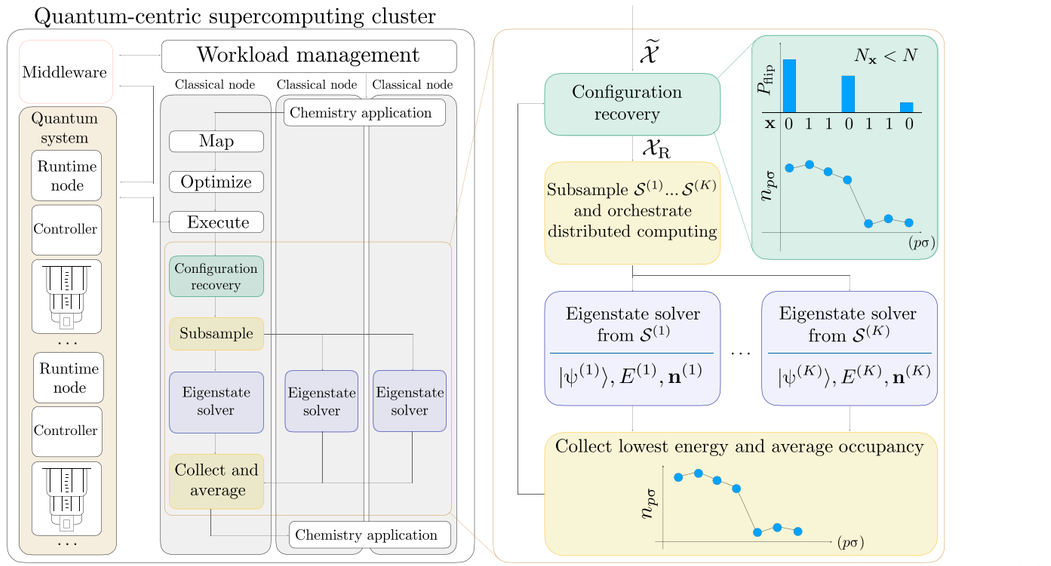
If  then 

where $\tilde{E}_0 \gtrsim E_0$

Steps

- Prepare an approximate ground state (via variational method etc.)
- Sample the state
- Configuration recovery
- Projection & diagonalization

More later



Robeldo-Moreno et al. Sci. Adv. 11

Sample-based Krylov diagonalization

Given a state $|\psi_0\rangle$ s.t. $\langle\Omega|\psi_0\rangle \neq 0$,

$$|\Omega\rangle \in \lim_{D\to\infty} \mathrm{span}\left\{U^n|\psi_0\rangle\right\}_{n=0}^{D}$$

where $U = e^{-iH\Delta t}$ for some Δt.

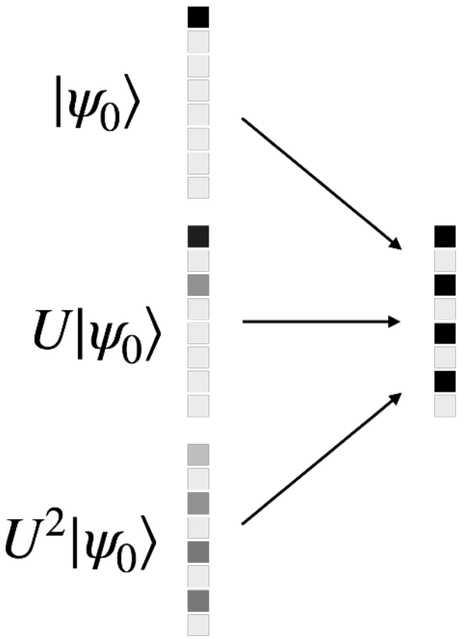
Krylov space

Sample from all Krylov basis states

→ Ground state should be in the subspace

Advantage:

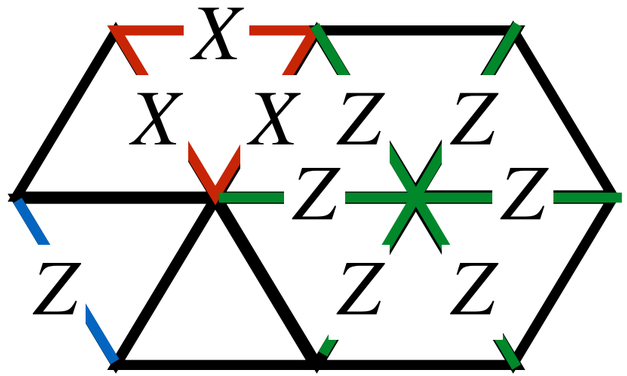
- Initial state can be simple
- Only need time evolution circuits



The system: 2D triangular pure $\mathbb{Z}_2$ LGT

$$H = -\sum_{e\in\mathscr{E}} Z(e) - \lambda \sum_{p\in\mathscr{P}} \prod_{e\in\partial p} X(e) = H_E + H_M$$

edges (↑ $e\in\mathscr{E}$) plaquettes (↑ $p\in\mathscr{P}$)



Gauss's law:

$$G_n|\psi\rangle = g_n|\psi\rangle \quad (g_n = \pm 1)$$

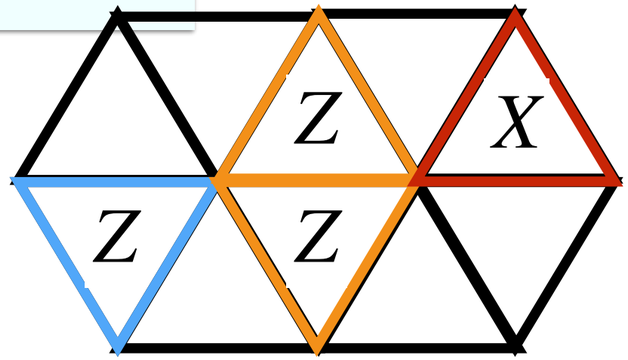
$$G_n = \prod_{e\in\partial v_n} Z(e)$$

- Pure Z_2 → g_n are static charges
  - There can only be even number of -1s
- Edges are the only dynamic d.o.f.
  - $2^{|\mathscr{E}|}$-dim Hilbert space (with gauge redundancy)

Dual: Hexagonal Ising model

$$H = -\sum_{e\in\mathscr{E}_{\text{bulk}}} s_e Z(p_e^{(l)})Z(p_e^{(r)}) - \sum_{e\in\mathscr{E}_{\text{bnd}}} s_e Z(p_e) - \lambda \sum_{p\in\mathscr{P}} X(p)$$

$s_e = \pm 1$ determined by $\{g_n\}$ (static charges)

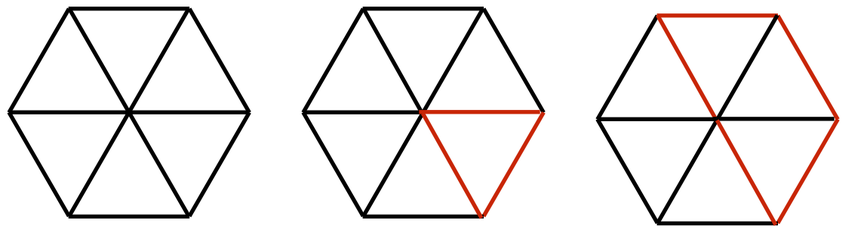


- Gauss's law is solved at the Hamiltonian level
  → No gauge redundancy
- Plaquettes (→ Ising spins) are the dynamical d.o.f.

  Basis: plaquette "excitations" (= Wilson loops) over some base state

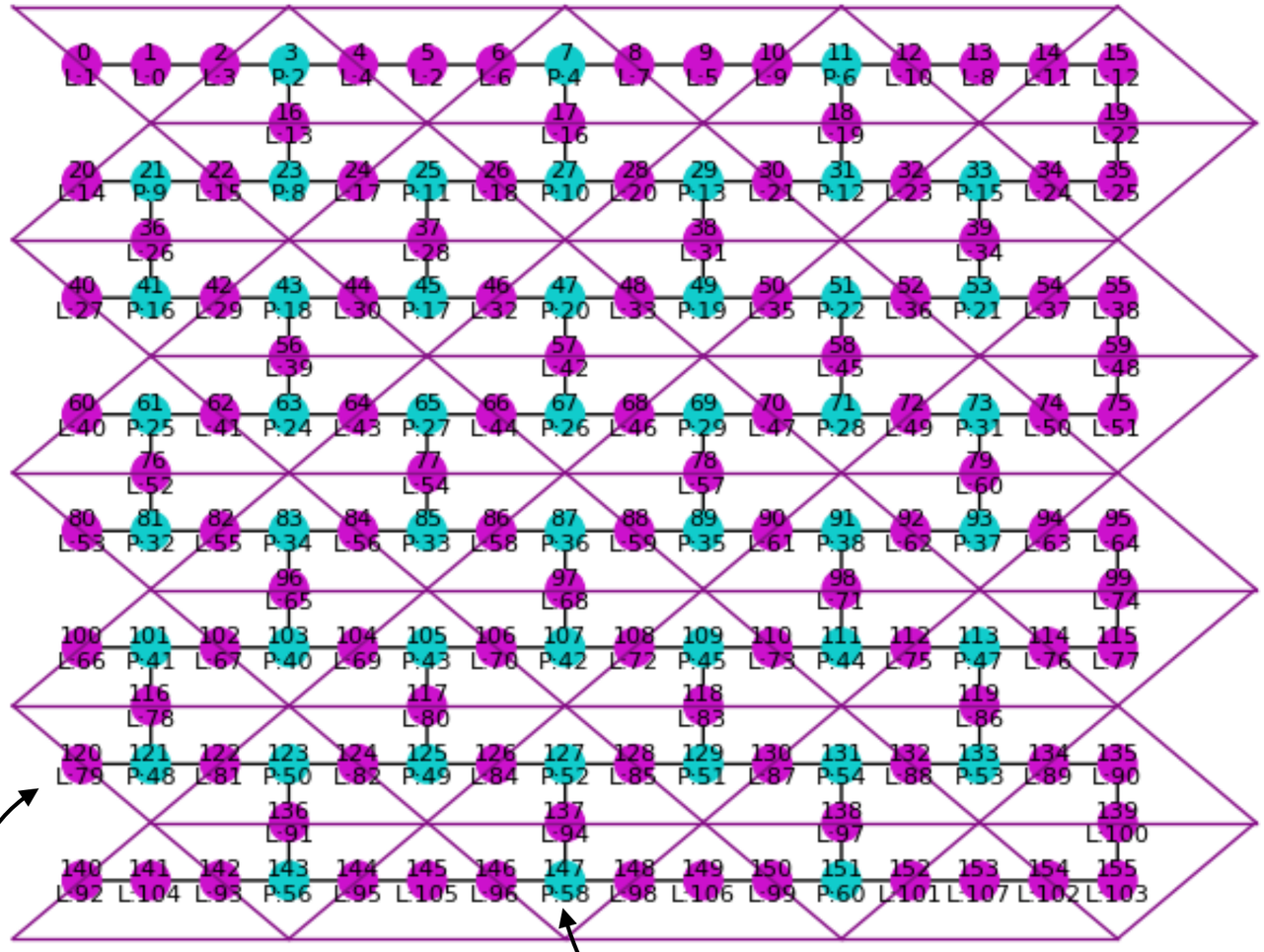
  → $2^{|\mathscr{P}|}$-dim Hilbert space

NB: DMRG works well even for >200 spins



Triangular pure $\mathbb{Z}_2$ LGT ❤ heavy hex

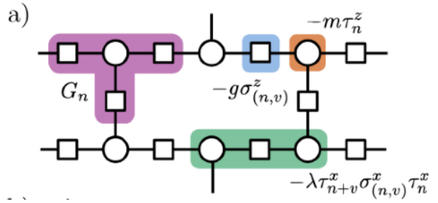
ibm_pittsburgh (Heron r3 - 156 qubits)



Link qubits = dynamic d.o.f.

Plaquette qubits = ancillae

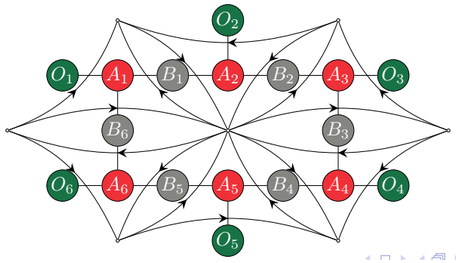
cf.



$$H = -m\sum_{\boldsymbol{n}} \tau^z_{\boldsymbol{n}} - g\sum_{(\boldsymbol{n},\boldsymbol{v})} \sigma^z_{(\boldsymbol{n},\boldsymbol{v})} - \lambda\sum_{\boldsymbol{n},\boldsymbol{v}} \tau^x_{\boldsymbol{n}+\boldsymbol{v}}\sigma^x_{(\boldsymbol{n},\boldsymbol{v})}\tau^x_{\boldsymbol{n}}.$$

Cobos et al. arXiv:2507.08088

also

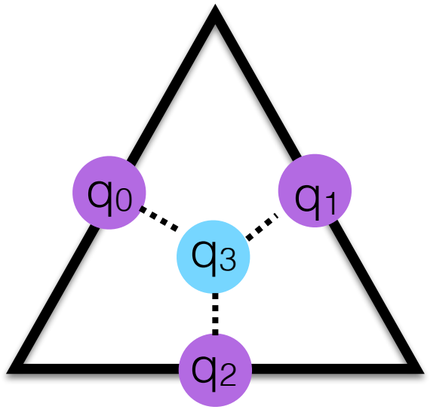


$$H = \sum_{\triangle} H_{\triangle} = -J\sum_{\triangle}[U_{\triangle} + U^{\dagger}_{\triangle} - \lambda(U_{\triangle} + U^{\dagger}_{\triangle})^2].$$

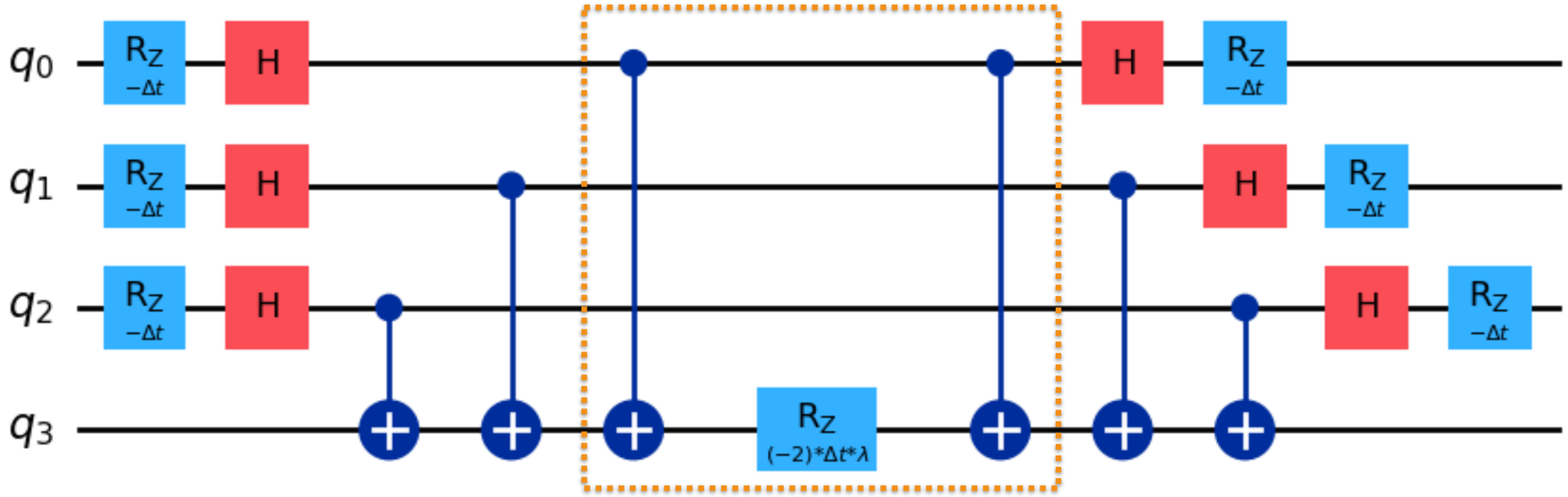
Banerjee et al. PRR 4

"Here we consider a U(1) quantum link model on a triangular lattice, ... that ideally matches the heavy hexagonal topology of the Eagle chip."

Triangular pure $\mathbb{Z}_2$ LGT ❤ heavy hex



$$U_E\left(\frac{\Delta t}{2}\right)\, U_B(\Delta t)\, U_E\left(\frac{\Delta t}{2}\right)$$



$R_{zz}(-2\lambda\Delta t)$ → continuous-angle gate

156-qubit Trotter (2nd-order) step:

- 448 CZ + 128 R_{ZZ}
- depth 22

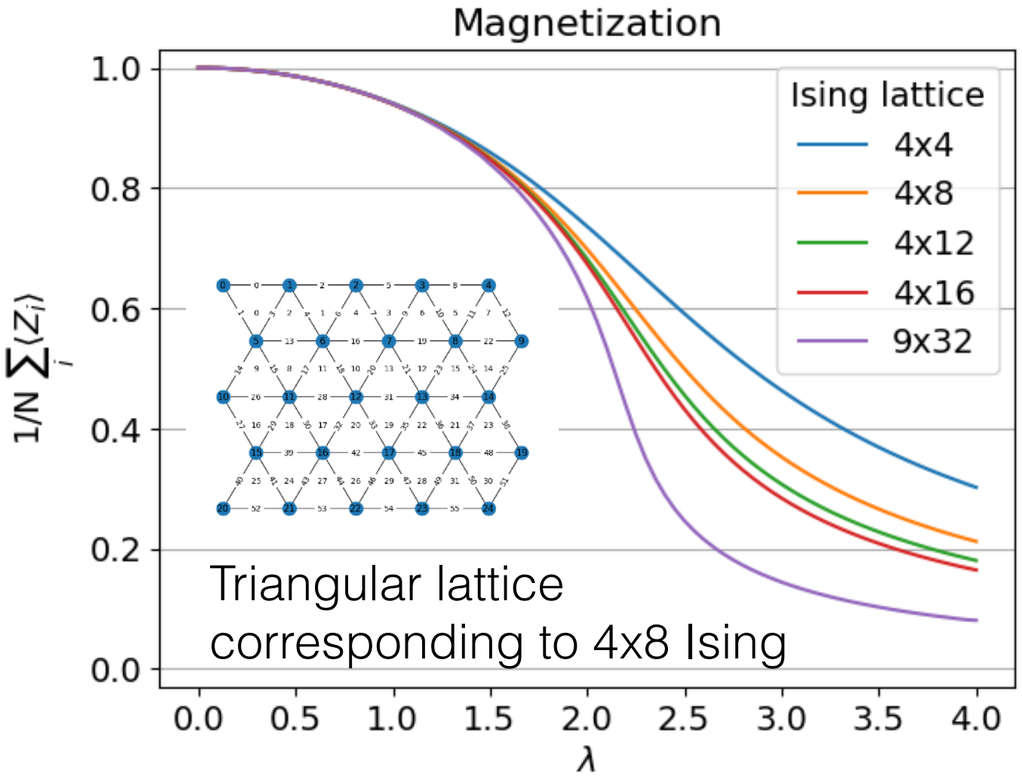
Sparsity of the ground state

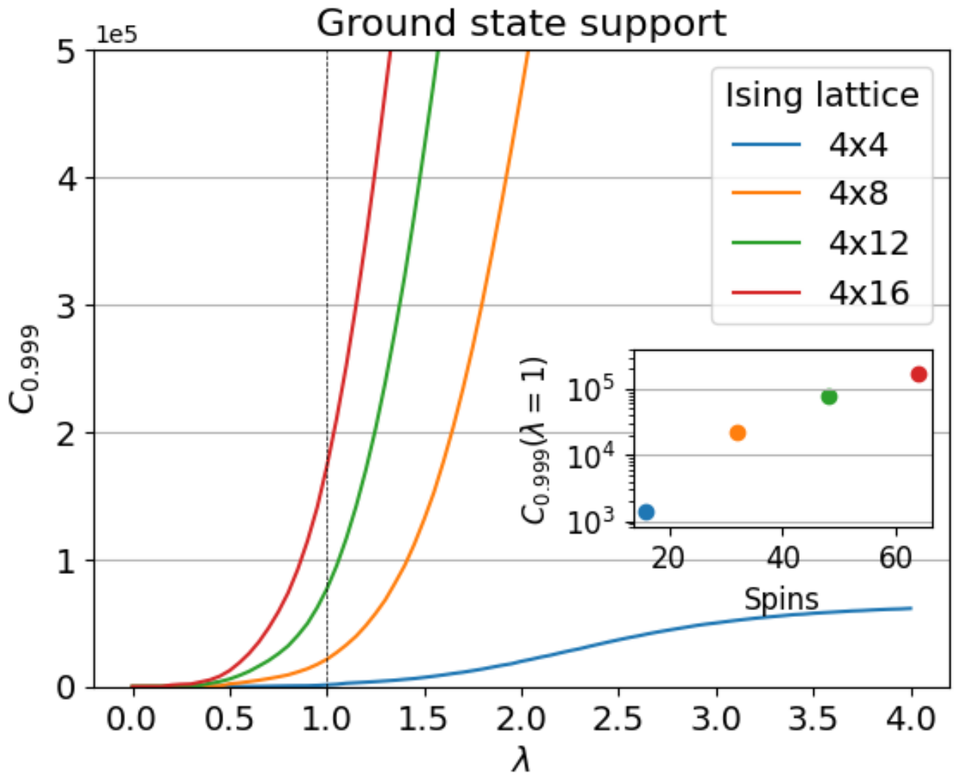
Ground state must be sparse in Z basis for SKQD to work

→ Need to be in weak-coupling ($\lambda \lesssim 1$) regime

$$C_{0.999} = \mathrm{argmin}_n \left(\sum_{i=0}^{n-1} |c_i|^2 > 0.999 \right)$$

|amplitude|² in descending order





SKQD in practice

We need to sample $U|\psi_0\rangle, U^2|\psi_0\rangle, \ldots, U^D|\psi_0\rangle$,
with $U = \exp(-iH\Delta t)$.

- What are good D and Δt values?
- How do we deal with errors?

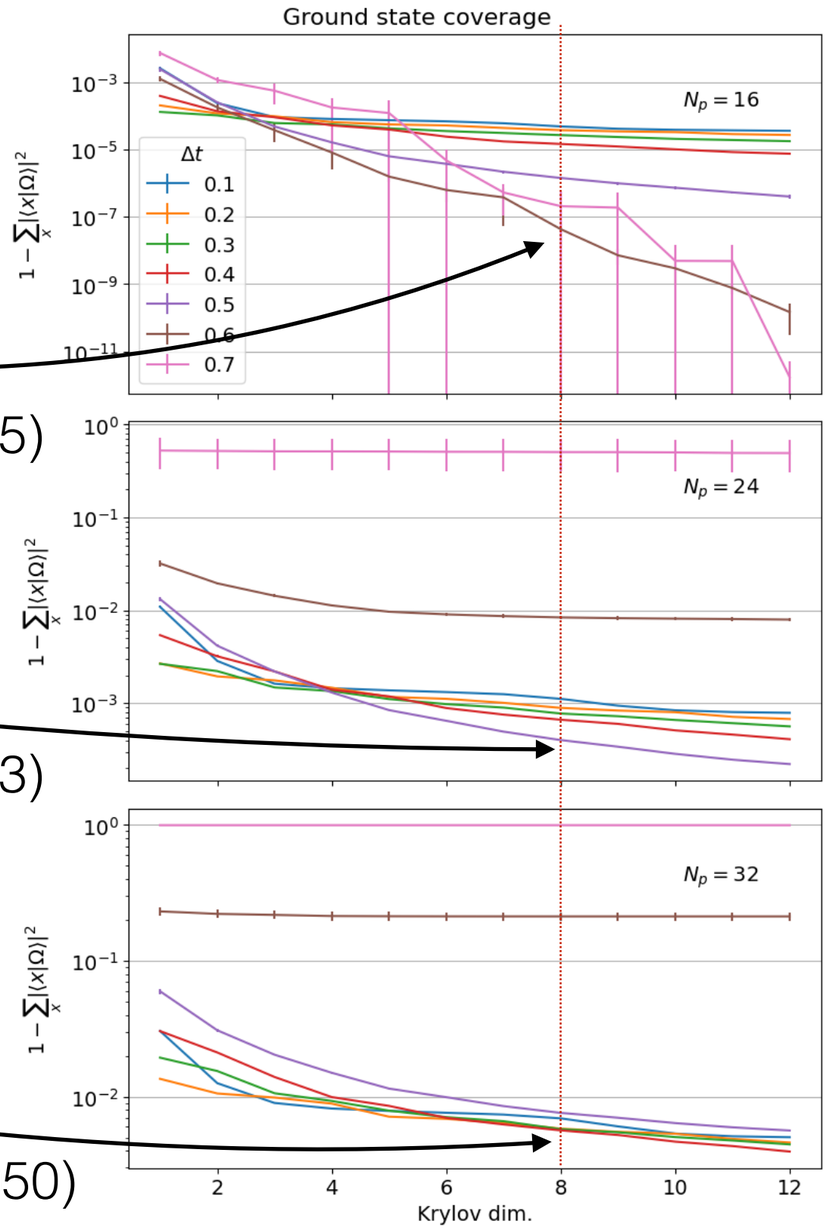
D and Δt:

Theoretically, $(\Delta t)_{\text{opt}} = \pi/\|H\|$[1]

→ for $\lambda = 1$, $(\Delta t)_{\text{opt}} \sim 0.8/N_p$

But practical $(\Delta t)_{\text{opt}}$ is known to be ~10x

Chose (arbitrarily) $D = 8$ & $\Delta t = 10/N_p$



Δt=0.4
(0.8/32=0.025)

Δt=0.5
(0.8/24=0.033)

Δt = 0.6
(0.8/16 = 0.050)

$1 - \sum_{x \in S} |\langle x|\Omega\rangle|^2$ S: simulator samples
$|\Omega\rangle$: DMRG

[1] Epperly et al., 10.1137/21M145954X

Configuration recovery

Bits are flipped by errors in the obtained samples.
How can we know what we were supposed to have observed?

Task:
Device a case-specific procedure to generate the support of Krylov states using observed bitstrings as hints

Use symmetries, constraints, ...

Example from the chemistry paper:

$$|1001\rangle \rightarrow \{|1001\rangle, |1010\rangle, |0101\rangle, |0110\rangle\}$$

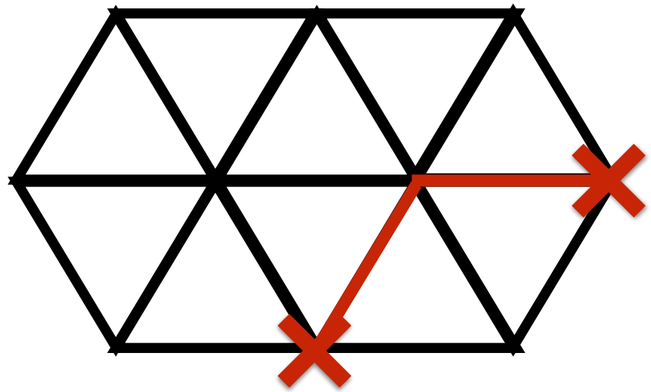
(Electron number / Total spin / Z spin conservation)

Having more states is OK
as long as basis size is classically tractable

Configuration recovery for Z2 LGT

$$G_n|\psi\rangle = g_n|\psi\rangle \quad (g_n = \pm 1)$$

$$G_n = \prod_{e \in \partial v_n} Z(e)$$



Gauss's law expressed in Z basis → Can check on bitstrings

Violation events = “syndromes” in QEC-speak

→ Use tools from QEC to correct bit flips on links

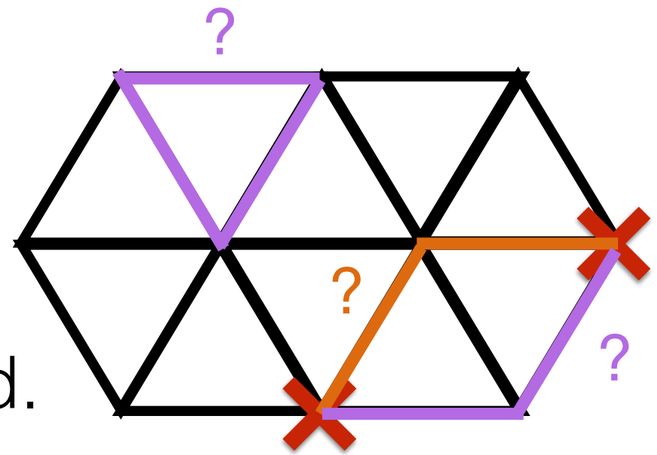
Minimum-weight perfect matching (MWPM)

= Find shortest paths between pairs of error detection events

MWPM is not enough

Syndrome measurements can only catch deviations into a different charge sector.

→ MWPM proposes one physical state, but states with arbitrary Wilson loops are all equally valid.



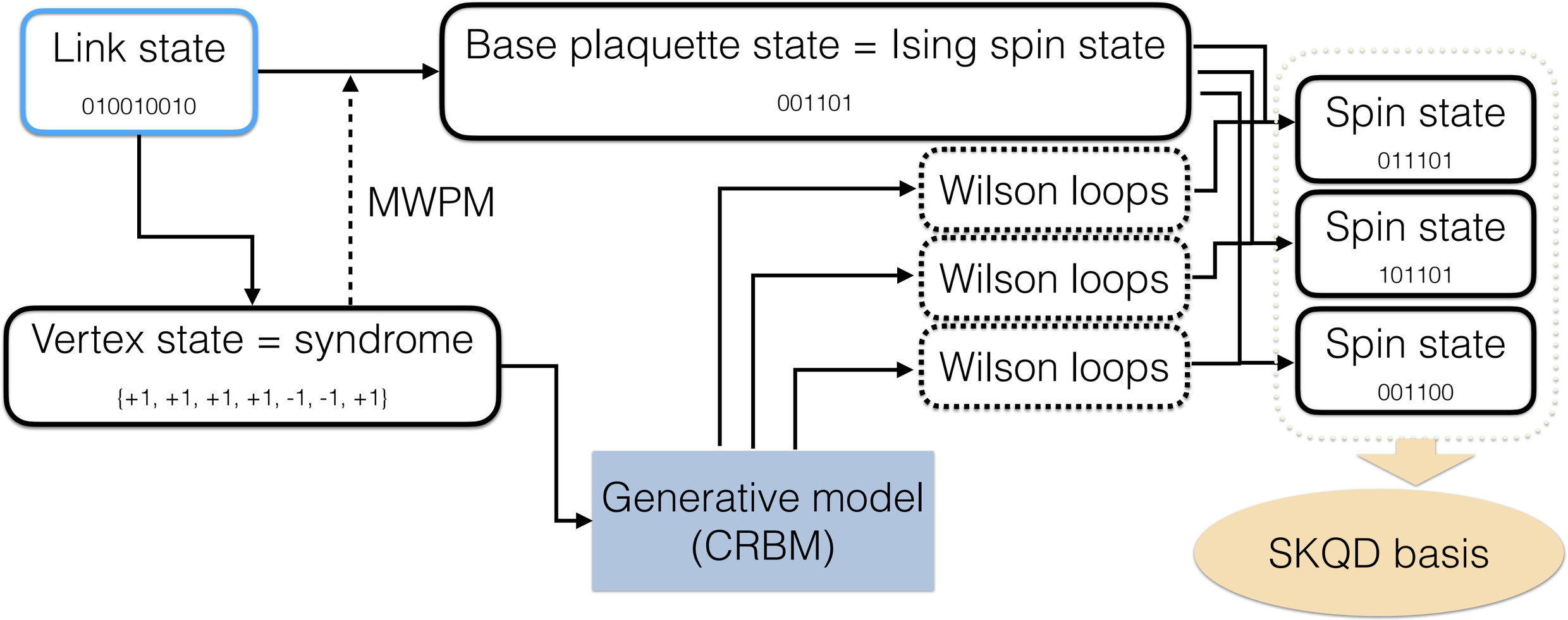
i.e. All possible physical states

How to include the correct state in the SKQD basis

- Random plaquette excitations → ✘
- Informed guesses through an error model → Use a generative model

Configuration recovery flow

For each shot:



Conditional restricted Boltzmann machine

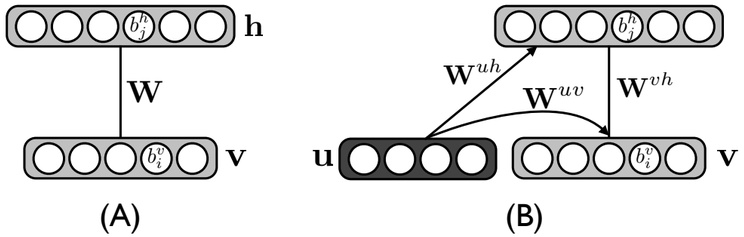


Figure 1: Illustration of an RBM (A) and a conditional RBM (B).

Mnih et al. 1202.3748

Restricted Boltzmann machine

Boltzmann machine with 2 ("v" and "h") layers.

Given a set of binary vectors $\mathbf{X} = \{\mathbf{x_i}\}$, maximize

$$\prod_{\mathbf{x}_i \in \mathbf{X}} p(\mathbf{x}_i) = \prod_{\mathbf{x}_i \in \mathbf{X}} \sum_{\mathbf{h}} e^{-E(\mathbf{x}_i, \mathbf{h}; W, \mathbf{a}, \mathbf{b})} / Z$$

where

$$E(\mathbf{v}, \mathbf{h}; W, \mathbf{a}, \mathbf{b}) = -\mathbf{v}^T W \mathbf{h} - \mathbf{a} \cdot \mathbf{v} - \mathbf{b} \cdot \mathbf{h}$$

and $Z = \sum_{\mathbf{vh}} e^{-E}$.

RBM as a generative model

Can generate events via MCMC:

$\mathbf{v} \leftarrow$ Random binary vector

for a large number:

$\mathbf{h} \sim p(\mathbf{h} \mid \mathbf{v})$

$\mathbf{v} \sim p(\mathbf{v} \mid \mathbf{h})$

end for

return $\mathbf{v}$

Conditional RBM

Probabilities depend on external $\mathbf{u}$

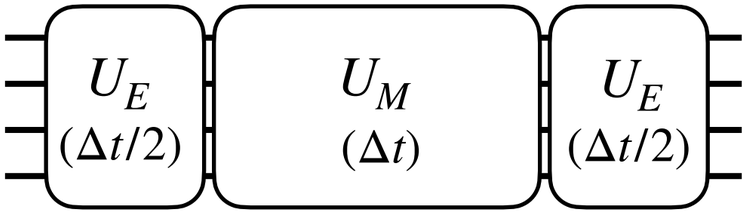
→ $\mathbf{u}$: syndromes, $\mathbf{v}$: Wilson loops

CRBM training

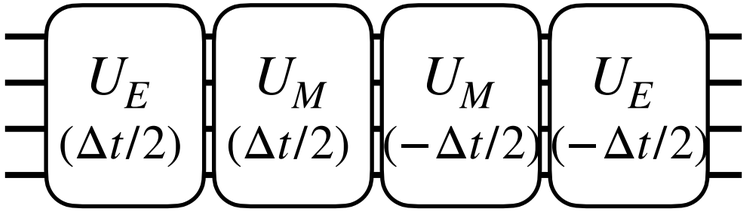
Training dataset from forward-backward circuits

- Circuit structure identical to 2nd-order Trotter
- Correct final state known (000..0)
  → All Wilson loops are due to bit flips

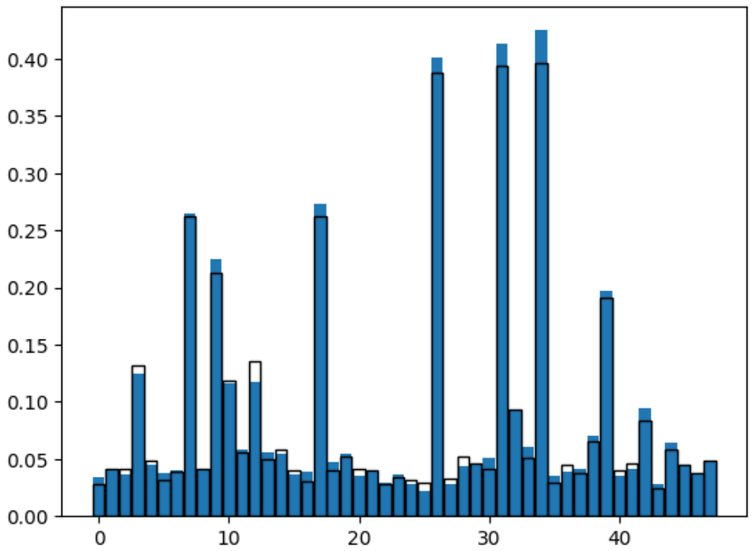
For each shot, extract $\mathbf{u}$ and $\mathbf{v}$ after MWPM correction



2nd-order Trotter



Forward-backward



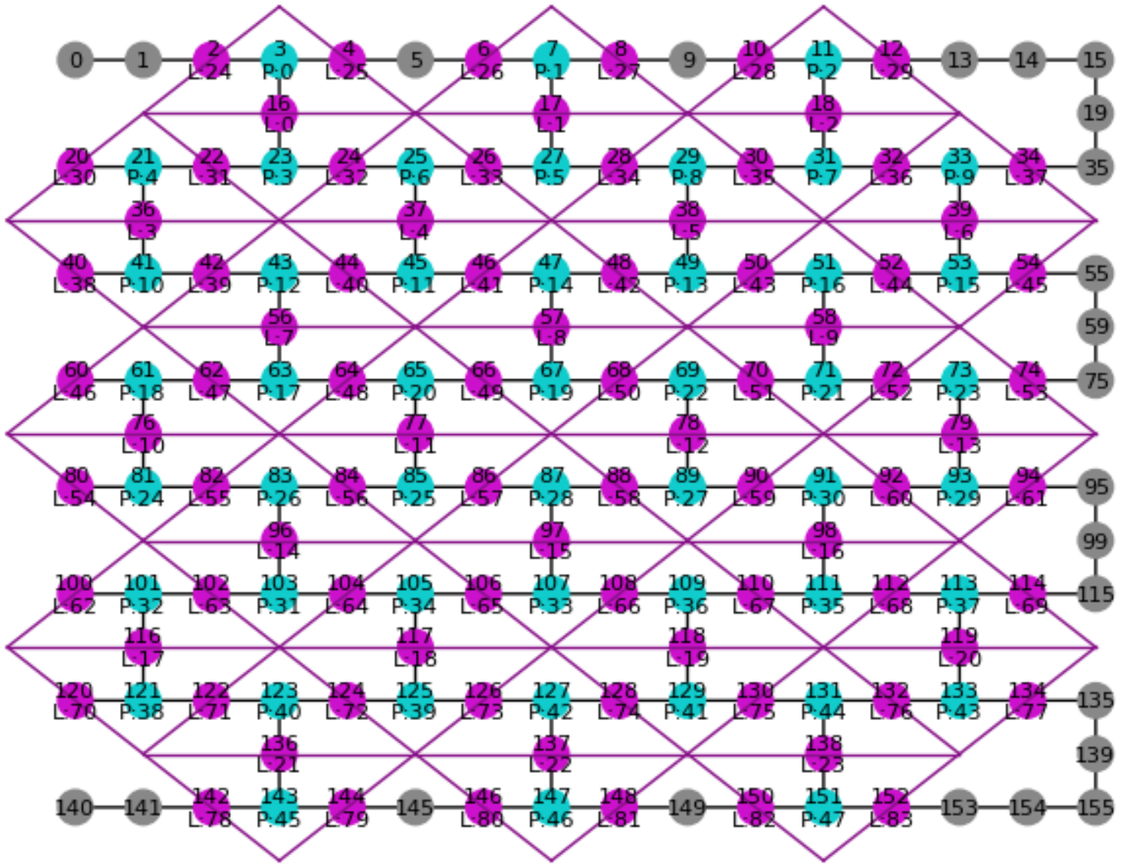
arbitrary bitstring indices

Blue: generated data
Black: test data

Energy with configuration recovery

Full-QPU model result not yet available

Smaller model (48 plaquettes) on ibm_pittsburgh



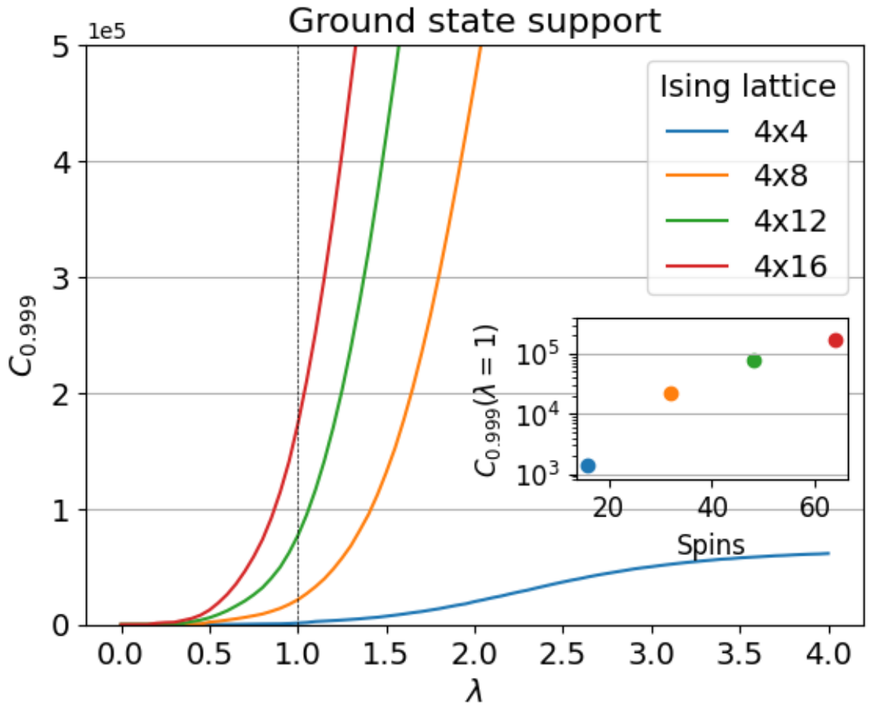
	E_0 (λ=0.8)	ΔE_{DMRG}
MWPM only	-87.981	1.162
With CRBM samples	-88.271	0.872
DMRG	-89.143	0

SKQD basis size (reduced Hamiltonian dim.) ~ 5.5M

Scaling and generalization

Not easy to scale the method up

- Support of ground state grows ~exponentially with lattice size
  → Lower λ
- $(\Delta t)_{\text{opt}}$ scales inversely with lattice size
  → More Trotter steps



Way forward

- Better use of (quasi-) translational / rotational symmetry?
- Larger λ with smaller lattice?
- Apply the method to LGT with Abelian Gauss's law?

Conclusion & outlook

- Applied sample-based quantum Krylov diagonalization to LGT
- Triangular $\mathbb{Z}_2$ pure LGT maps well onto heavy-hex lattice
  - Is dual to hexagonal Ising model
- Ground state of Triangular $\mathbb{Z}_2$ LGT is sparse if not too close to λ_c
- Studied optimal SKQD parameters with DMRG and circuit simulation
- Demonstrated a novel configuration recovery procedure based on a generative model (CRBM)
  - Should work if LGT has Abelian Gauss's law
  - Energy estimation improves with configuration recovery
- We can compute the ground state; now look into physics..
  (Potential curve, string breaking / roughening, approach to phase transition, ...)