CaRBM: A Fixed-Depth Quantum Algorithm with Partial Correction for Thermal State Preparation

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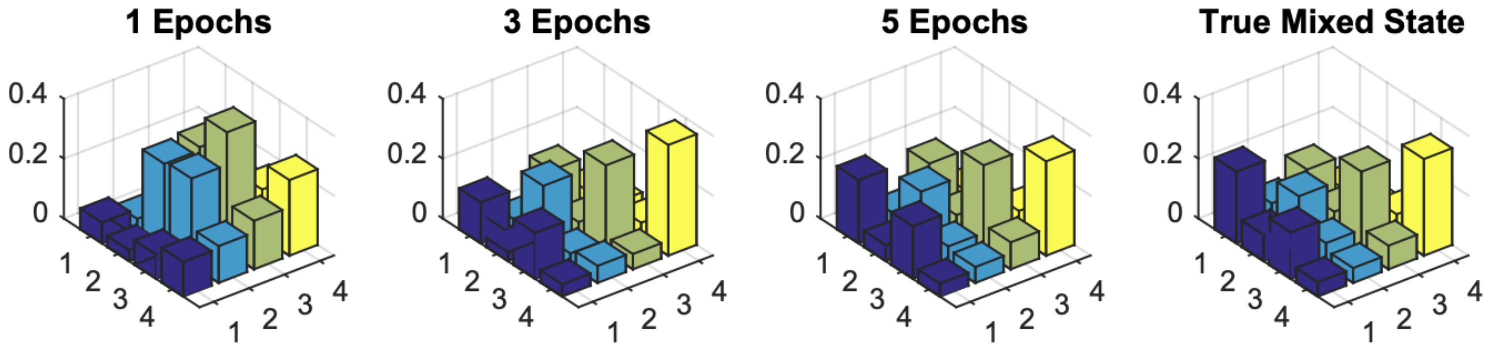
Speaker: Omar Alsheikh

O. Alsheikh et al., arXiv: 2603.17971

Thermal state preparation

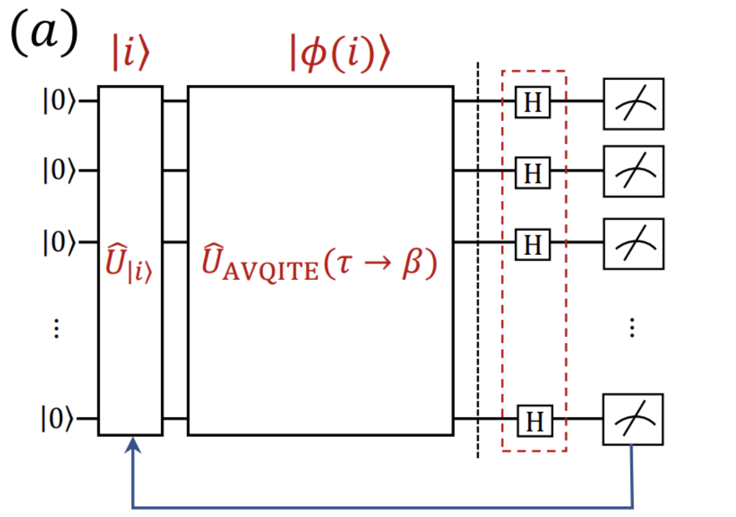
- State preparation is a key step in almost any quantum simulation.
- Any quantum system will eventually couple to an environment, and to simulate such open systems one needs to be able to prepare thermal (mixed) states.
- Thermal state preparation is used in quantum simulation, quantum machine learning, combinatorial optimization.



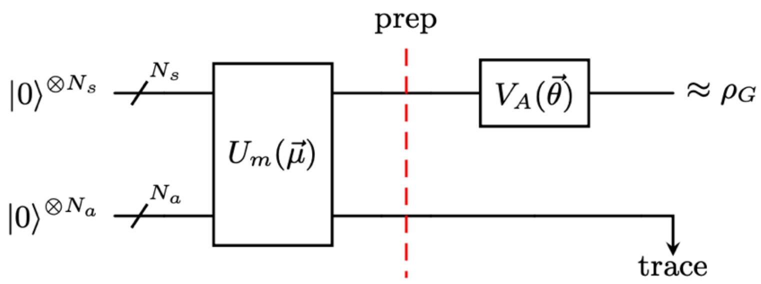
M. Kieferova and N. Wiebe, Physical Review A 96, 062327 (2017)

Thermal state preparation

- Two main approaches: Variational and imaginary time evolution (ITE).
- Variational algorithms face common issues like ansatz expressibility, high optimization cost, barren plateaus, as well as expensive entropy measurements.



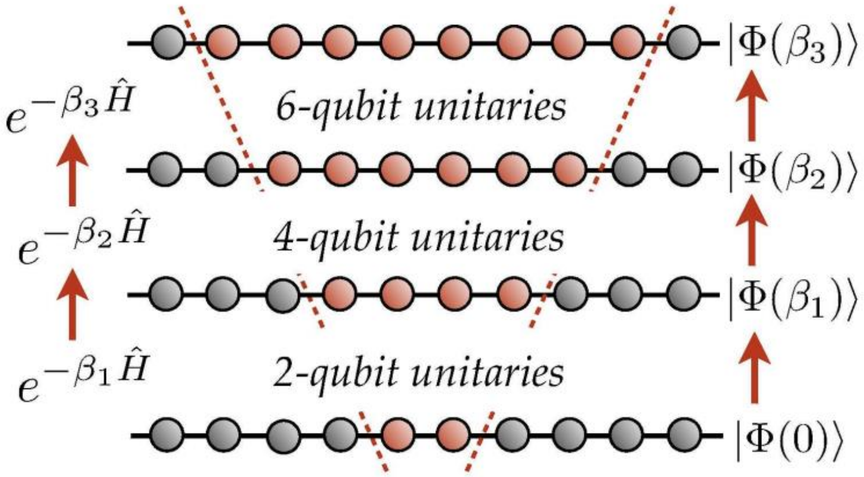
J. C. Getelina et al., SciPost Physics 15, 102 (2023)



B. Sambasivam et al., arXiv:2503.14490

Imaginary time evolution (ITE)

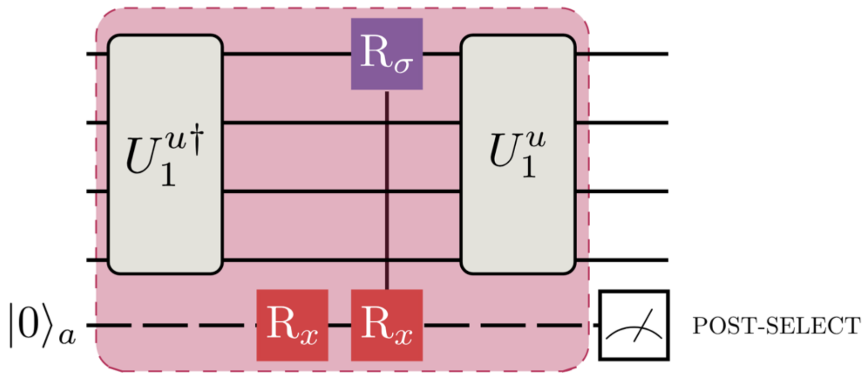
- ITE is non-unitary. Non-unitary operations are expensive on a quantum device.
- ITE is approximated by a series of unitary steps. This quickly gets expensive.
- It works best for short simulation times, and for initial states with minimal entanglement.



M. Motta et al., Nature Physics 16, 205 (2020)

ITE via block encoding

- A second approach to non-unitary dynamics is block encoding.
- The non-unitary operator is embedded inside a larger unitary matrix.
- We recover the required operation via post-selection.

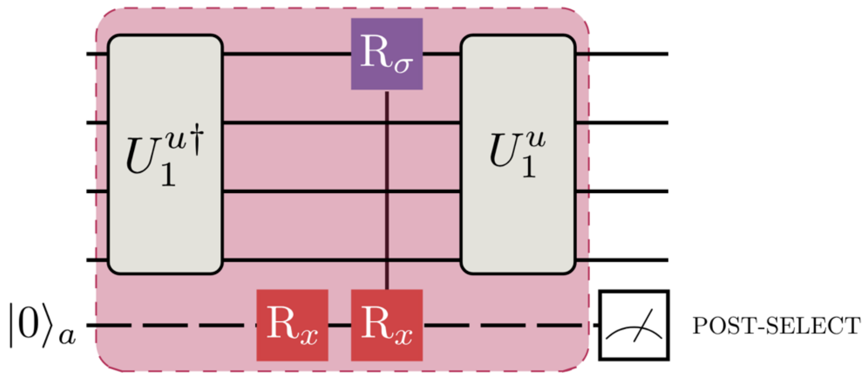


O. Alsheikh et al., arXiv: 2603.17971

$$U = \begin{bmatrix} A & \cdot \\ \cdot & \cdot \end{bmatrix}$$

RBM for ITE

- We employ a block-encoding scheme based on a neural network architecture known as a restricted Boltzmann machine (RBM) [1].
- Physical (visible) qubits are embedded into a larger system with ancillary (hidden) qubits.
- Non-unitary operations are obtained probabilistically.



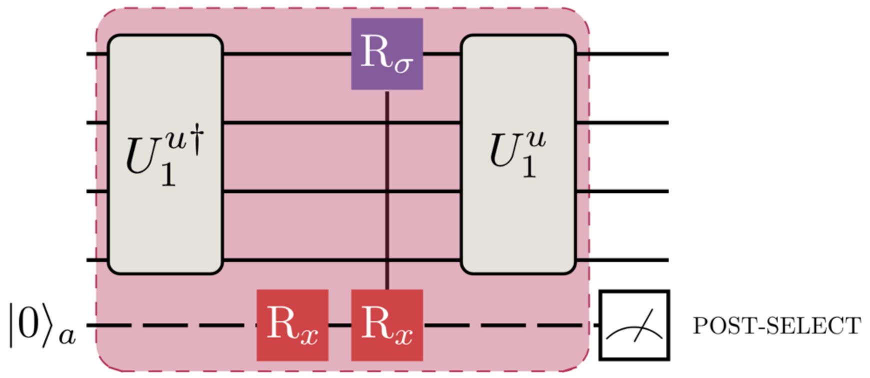
O. Alsheikh et al., arXiv: 2603.17971

$$
\begin{aligned}
e^{-\kappa\sigma_j}|\psi\rangle &= A\sum_{\tilde{h}=\pm 1} e^{-i(W\sigma_j+bI)\tilde{h}}|\psi\rangle \\
&= 2A\,\langle 0|_a\, e^{-i(W\sigma_j+bI)\otimes X_a}\,|\psi\rangle\otimes|0\rangle_a
\end{aligned}
$$

[1] E. Rrapaj and E. Rule, Physical Review Research 7, 013306 (2025).

RBM for ITE

- This simple version of RBM encoding only works if $\sigma_j \in \{I_j, X_j, Y_j, Z_j\}$
- For a general Hamiltonian given as a Pauli sentence, we need to find a product formula for $e^{-\beta H}$.
- We want to keep the number of post-selection processes as low as possible, so we pick a fixed-depth compilation protocol.

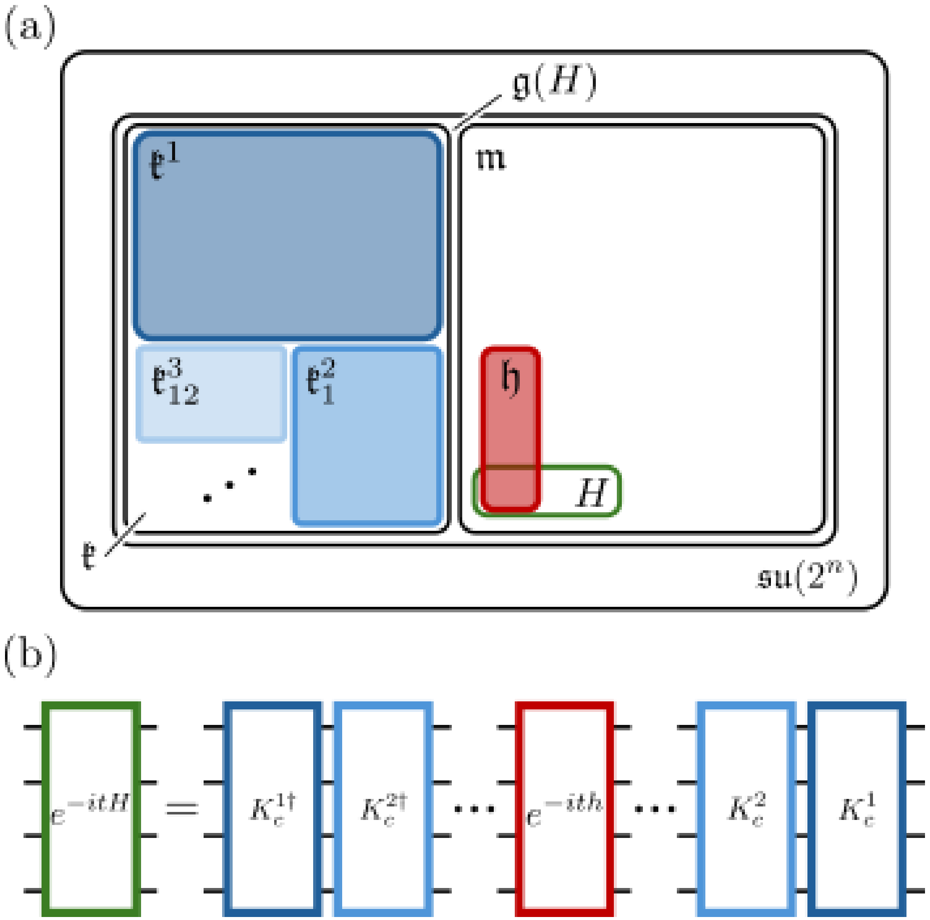


O. Alsheikh et al., arXiv: 2603.17971

$$e^{-\kappa\sigma_j}|\psi\rangle = A\sum_{\tilde{h}=\pm 1} e^{-i(W\sigma_j + bI)\tilde{h}}|\psi\rangle$$
$$= 2A\,\langle 0|_a\, e^{-i(W\sigma_j+bI)\otimes X_a}\,|\psi\rangle\otimes|0\rangle_a$$

Cartan Decomposition

- We use the algebraic structure of the Hamiltonian to get an exact, fixed-depth product formula [1,2].
- The time parameter appears in the Abelian part only.
- The algorithm can be extended to imaginary, or even complex, evolution.
- Each exponent can be transformed into a one-body operator, which is needed for efficient RBM implementation.

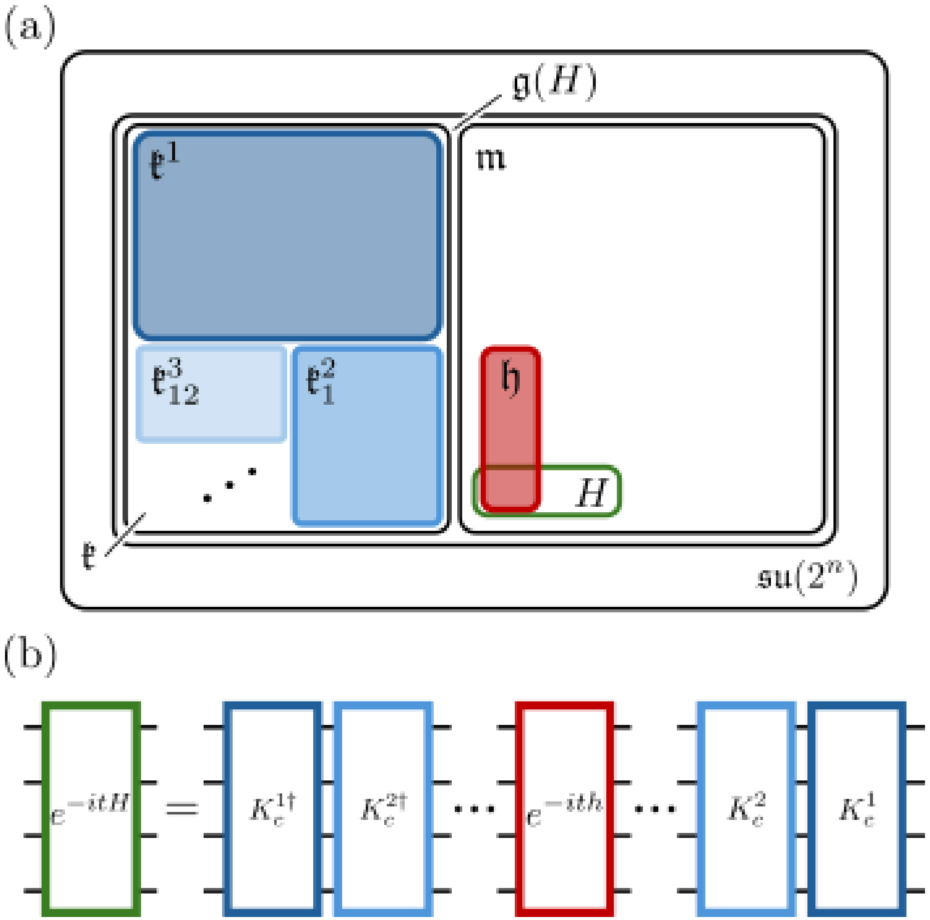


O. Alsheikh et al., arXiv: 2512.06070

[1] E. Kokcu et al., Physical Review Letters 129, 070501 (2022).
[2] **O. Alsheikh**, E. Kokcu, B. N. Bakalov, and A.F. Kemper, arXiv: 2512.06070.

Cartan Decomposition

- We take nested commutators of terms in the Hamiltonian to generate the dynamical Lie algebra $\mathfrak{g}(H)$.
- A specific Cartan decomposition is found.
- The Hamiltonian is "rotated" into an Abelian subalgebra. The unitary is found by solving an optimization problem.
- The cost function evaluation can be offloaded to quantum hardware.

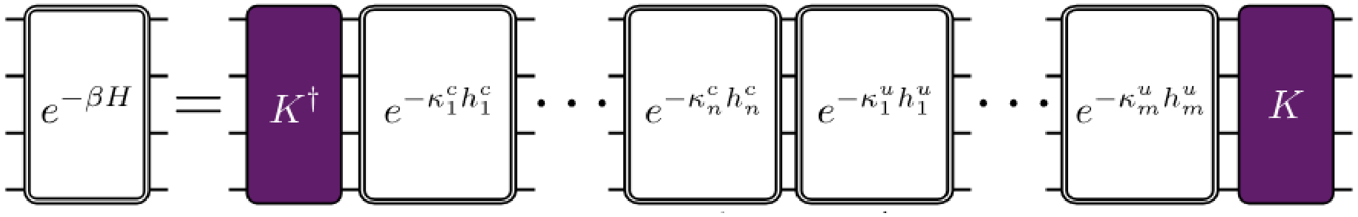


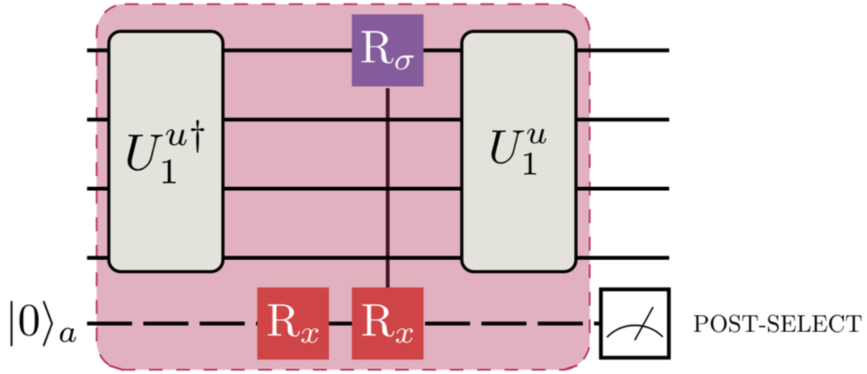
O. Alsheikh et al., arXiv: 2512.06070

[1] E. Kokcu et al., Physical Review Letters 129, 070501 (2022).
[2] **O. Alsheikh**, E. Kokcu, B. N. Bakalov, and A.F. Kemper, arXiv: 2512.06070.

CaRBM

- Given a spin Hamiltonian, find a Cartan decomposition.
- For every term in the Abelian part, apply the RBM identity and post-select to achieve ITE.

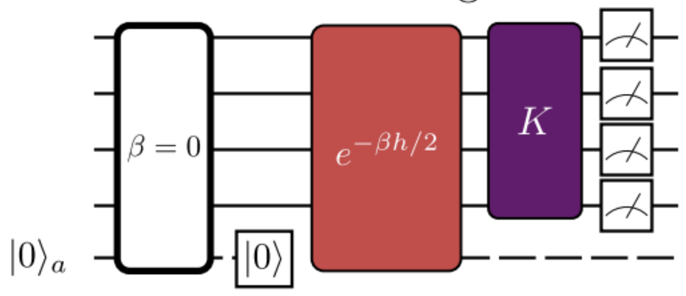




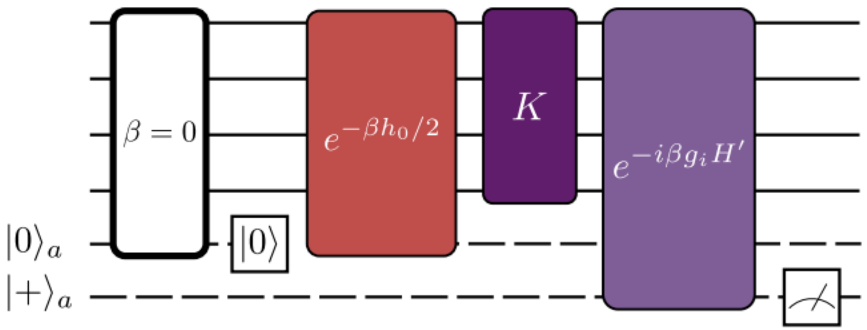
Thermal states

- One can prepare the fully mixed state and evolve with exp(-βH/2) to prepare the thermal state exp(-βH)/Z and find thermal averages.
- We can also do complex time evolution to find partition function zeros.

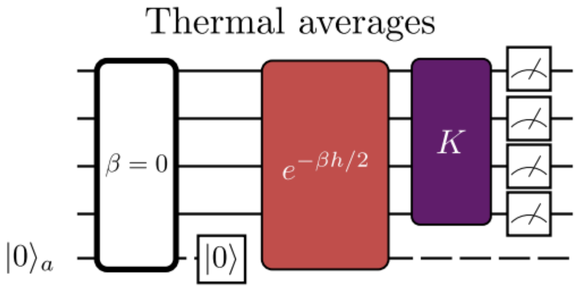
Thermal averages



Lee-Yang zeros



Thermal averages

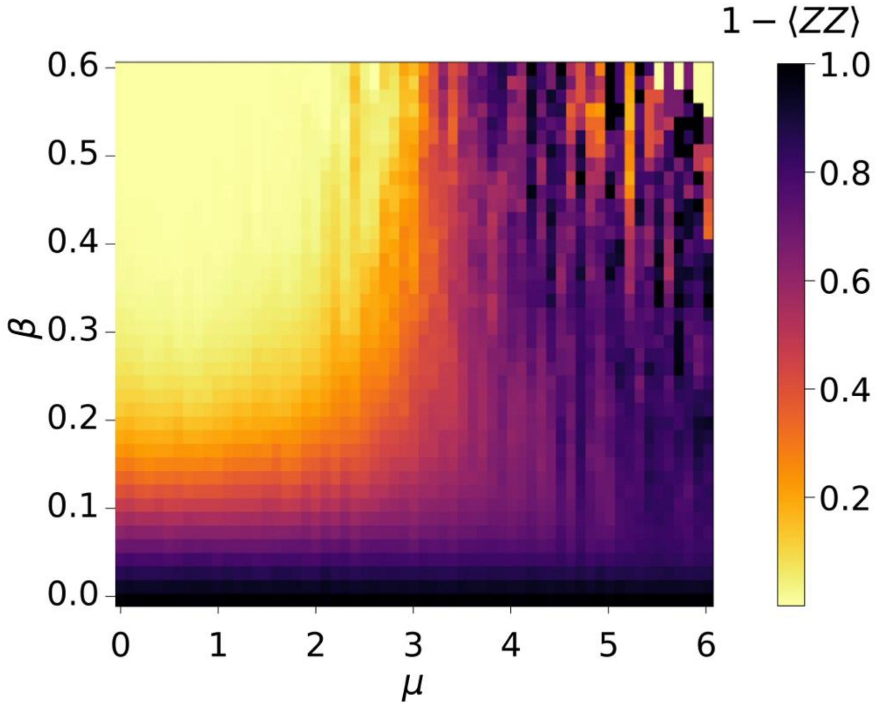


We run circuit simulations of the phase diagram of the Gross-Neveu model.

$$H_0 = \int dx\; i\bar{\psi}\alpha\partial_x\psi + m\bar{\psi}\beta\psi$$

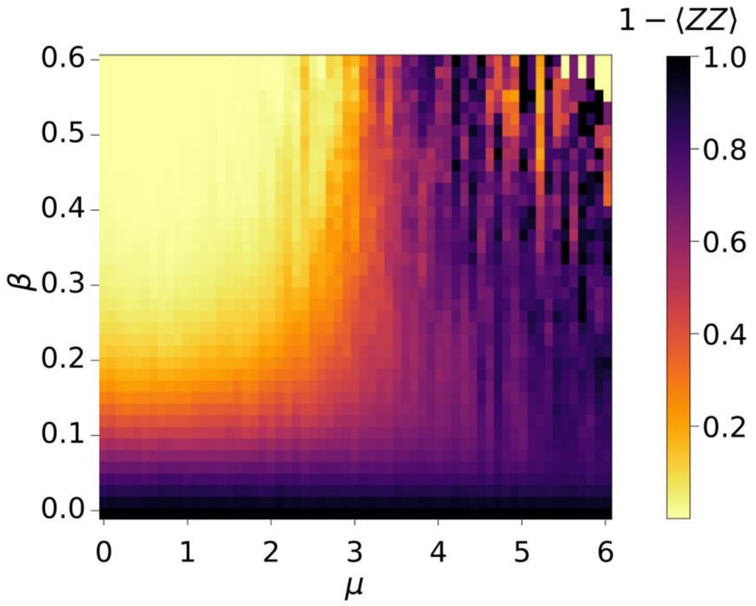
$$H_G = \int dx\; \frac{-G^2}{2}(\bar{\psi}\psi)^2$$

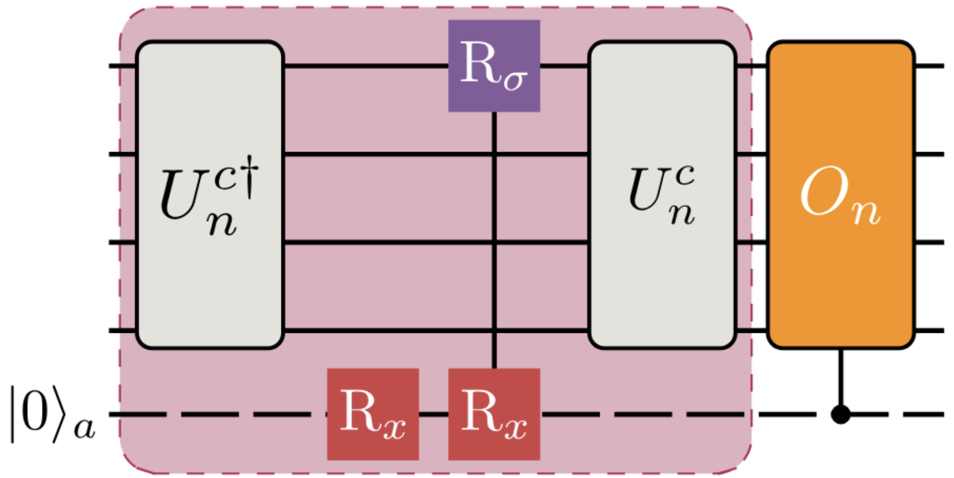
$$H_\mu = \int dx\; \mu\bar{\psi}\gamma\psi$$



RBM correction

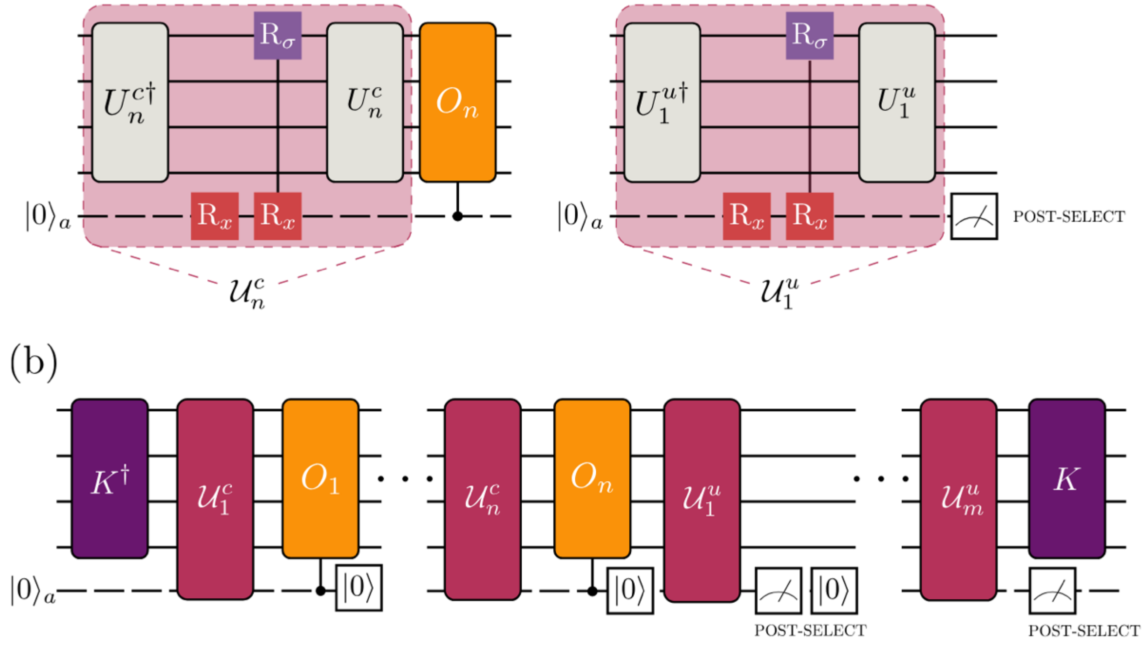
- Results are noisy due to diminishing success probabilities.
- We can find a particular RBM encoding for $e^{-\kappa\sigma}|\psi\rangle$ that, when it fails, gives us $e^{\kappa\sigma}|\psi\rangle$.
- We can correct this failed result by a controlled operation.



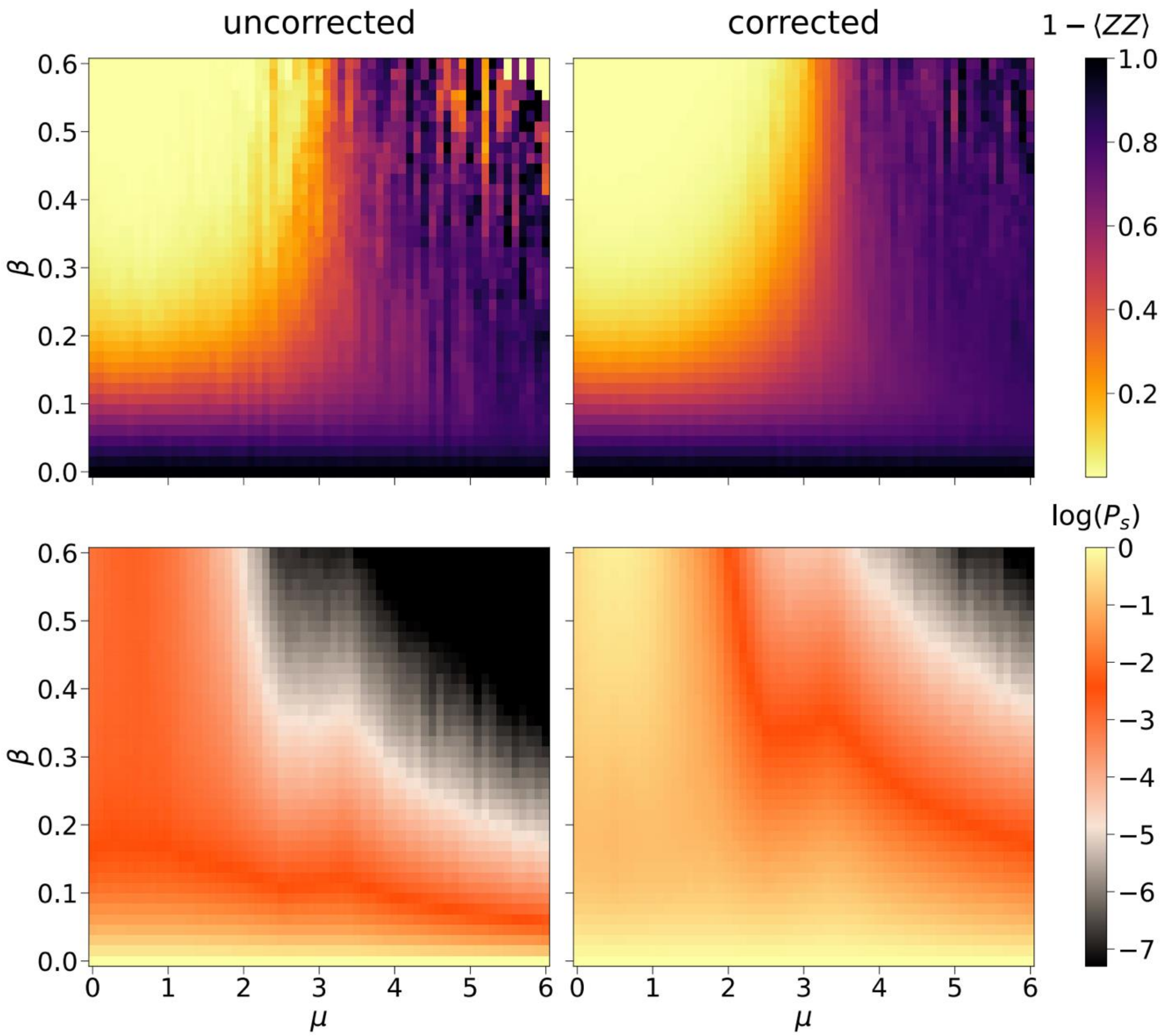


RBM correction

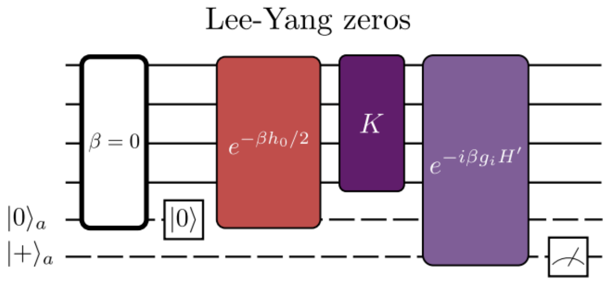
- To correct a given layer, the operator needs to commute with all the previous ITE layers.
- It also needs to keep $|\psi\rangle$ unchanged. Not an issue!
- Correct what you can and post-select the rest.



RBM correction



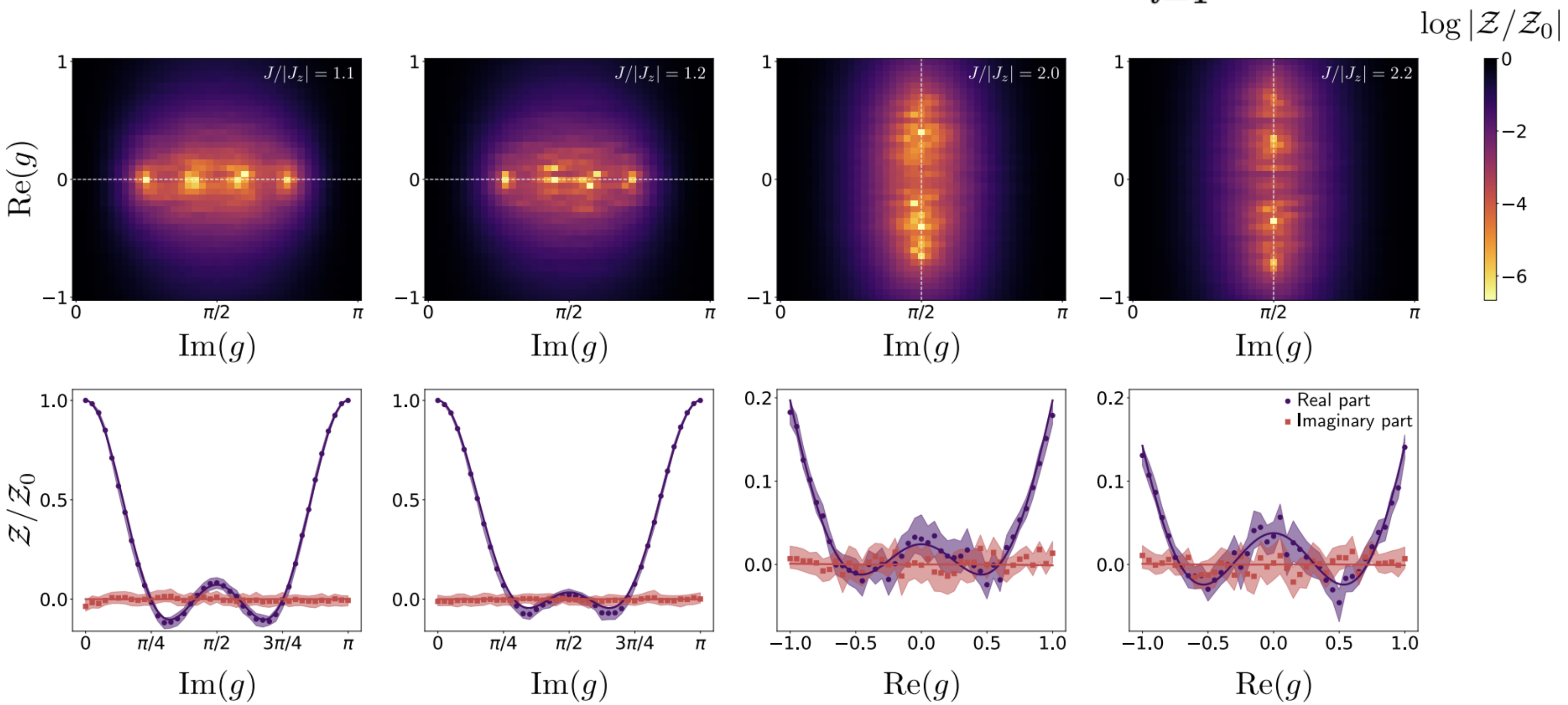
Lee Yang Zeros



We find the partition function zeros for the XXZ model in a complex magnetic field

$$H_s = -J\sum_{i=1}^{L-1}(X_iX_{i+1} + Y_iY_{i+1}) - J_z\sum_{i=1}^{L-1} Z_iZ_{i+1}.$$

$$H_B = g\sum_{i=1}^{L} Z_i$$



Conclusions

- CaRBM allows us to generate exact fixed depth circuits for ITE.
- We prepared thermal states and measured thermal averages and PF zeros.
- Well-rounded algorithm not limited by ansatz selection, low entanglement initial states. But lower success rate at low temperatures.
- We can correct some layers and get rid of some post-selection processes to enhance total acceptance rate.