COMPUTING CLASSICAL PARTITION FUNCTIONS: FROM ONSAGER AND KAUFMAN TO QUANTUM ALGORITHMS

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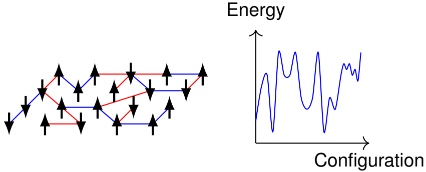
The Context

Optimization, Partition Functions and Quantum Computers

THE CONTEXT

Classical Problems...



- **Binary Optimization** (QUBO/MaxCut) is **hard**
- Many Classical Approaches:
  - Heuristic Exact Solvers (e.g. Gurobi, QuBowl)
  - Hardware Solvers (e.g. Ising Machines)
  - Monte Carlo (e.g. Simulated Annealing)
  - More...
- State-of-the-art: $\sim 10^4$ vertices (sparse graphs)

THE CONTEXT

- **Binary Optimization** (QUBO/MaxCut) is **hard**
- Quantum Approaches:
  - Quantum Annealing (D-Wave)
  - Variational Algorithms (QAOA, VQE)
  - Imaginary Time Evolution (VITE, QITE)
  - **And many more**

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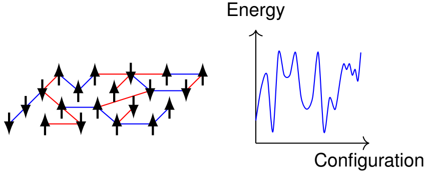
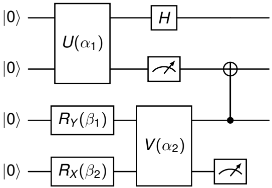


...with Quantum Solutions



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  - **And many more**
- Classical-to-Quantum Optimization Problem:

$$\{s_v\} \in \{0,1\}^M \to |\psi\rangle \in (\mathbb{C}^2)^{\otimes M}$$

$$\min_{\{s_v\}} H(\{s_v\}) \to \min_{\psi} \langle\psi|H|\psi\rangle$$

- State-of-the-art: $\sim 10^2 - 10^3$ qubits $\lesssim 10^4$

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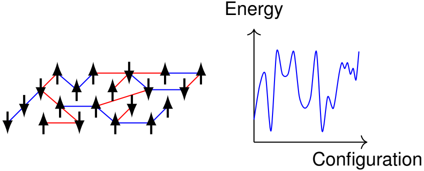

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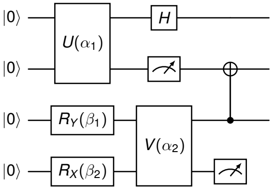

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- NISQ: Limited Memory (and Circuit Depth). Alternative road?

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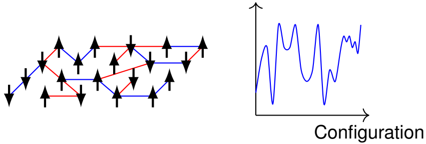

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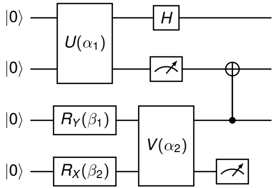

BEYOND OPTIMIZATION

- Physics-inspired approach:
  Finite temperature Ising models
- Still hard at finite temperature
- Classical Approaches:
  - Monte Carlo Methods
  - Tensor Networks
  - Hardware Solvers (Janus II)
  - And many more
- Alternative Classical-to-Quantum Mapping:
  Solution of 2D Ising Model

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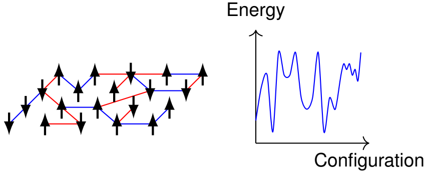

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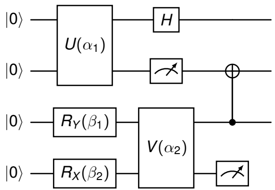

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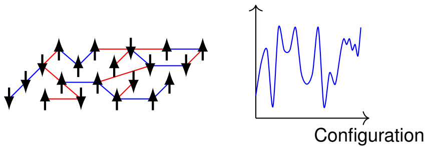

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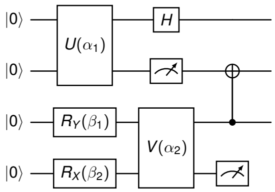

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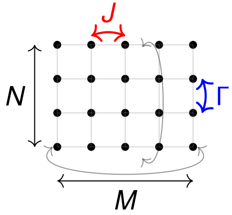
The Prelude

The Classical 2D Ising Model

THE PRELUDE - THE CLASSICAL 2D ISING MODEL

- **Classical** spins on a 2D lattice with $s_{v,k} = \pm 1$ and energy

$$E(\{s_{v,k}\}) = -\sum_{k=1}^{N}\sum_{v=1}^{M}(Js_{v,k}s_{v+1,k} + \Gamma s_{v,k}s_{v,k+1}), \ J,\Gamma > 0$$



- **Equilibrium** Properties, $p(\{s_{v,k}\}) \propto e^{-\beta E(\{s_{v,k}\})}$:
  1. Partition Function: $\mathcal{Z} = \sum_{\{s_{v,k}\}} e^{-\beta E(\{s_{v,k}\})}$
  2. Correlation Functions: $\langle s_{u,k}s_{u',k'}\rangle = \frac{1}{\mathcal{Z}}\sum_{\{s_{v,k}\}} s_{u,k}s_{u',k'}e^{-\beta E(\{s_{v,k}\})}$

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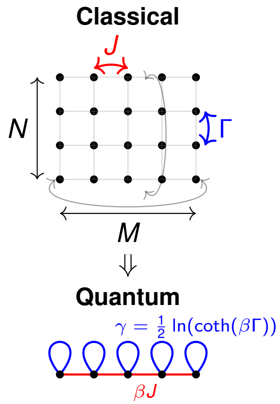
- **Transfer Matrix** Solution (Onsager 1944, Kaufman 1949):
  1. Partition Function: $\mathcal{Z} = c\,\mathrm{Tr}\left(\prod_{k=1}^{N} V\right)$, $V = e^{\beta J \sum_{v=1}^{M} Z_v Z_{v+1}}\, e^{\gamma \sum_{u=1}^{M} X_u}$
  2. Correlation Functions: $\langle s_{u,k} s_{u',k'} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}(V \cdots Z_u V \cdots Z_{u'} V \cdots V)$

- (Floquet) **Imaginary Time Evolution** of the Quantum Chain

- Only M qubits for $M \times N$ spins!



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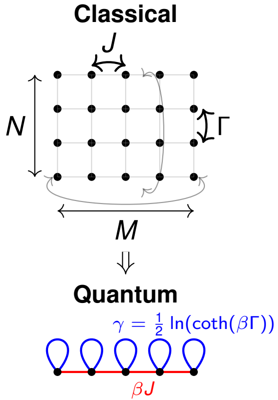

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- Diagonalization via **Representation Theory** of Lie Groups/Algebras:

(aka Jordan-Wigner and Free Fermions) $\rho : \mathrm{SO}(2M,\mathbb{C})^{\times 2} \mapsto \mathcal{M}(2^M,\mathbb{C})$

$$T = P\cdot\begin{pmatrix} t_1 & & \\ & \ddots & \\ & & t_{4M}\end{pmatrix}\cdot P^{-1} \mapsto V = \rho(T) = \rho(P)\begin{pmatrix} v_1 & & \\ & \ddots & \\ & & v_{2^M}\end{pmatrix}\rho(P^{-1}) \Rightarrow \mathcal{Z}$$

MOTIVATION AND OBJECTIVES

Motivation

1. Partition Functions as a **generalization** of optimization
2. **Qubit-efficient** Classical-to-Quantum Mapping for **2D Ising Model**[1]

Objectives

1. More **general models**? Kaufman-type/Lie-theoretic solution?
2. Can we (efficiently) implement it **on a quantum computer**?

[1] See also: Arad 2010, De las Cuevas 2011, Iblisdir 2014, Matsuo 2014

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A RESTRICTED CLASS OF ISING MODELS

- **Classical** spins $s_{v,k} = \pm 1$ on N *layers* of a graph $\mathbb{G}$:

$$E(\{s_{v,k}\}) = -\sum_{k=1}^{N} \left(\sum_{(u,v)\in E(\mathbb{G})} J_{uv}^{k} s_{u,k} s_{v,k} + \sum_{v\in V(\mathbb{G})} H_{v}^{k} s_{v,k} + \sum_{v\in V(\mathbb{G})} \Gamma_{v}^{k} s_{v,k} s_{v,k+1} \right)$$

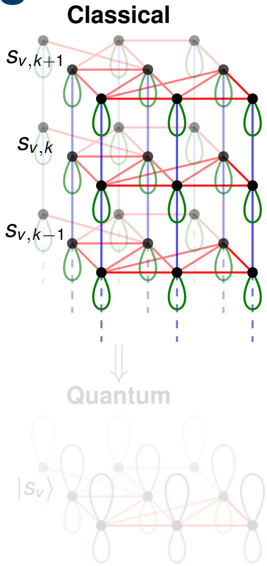
- Equilibrium Properties via Transfer Matrix (here $\Gamma_v^k > 0$):
  1. Partition Function (**Periodic Boundary**):

$$\mathcal{Z} = c\,\mathrm{Tr}\left(\prod_{k=1}^{n} V_k\right), \quad V_k = e^{\beta \sum_{(u,v)} J_{uv}^{k} Z_u Z_v} e^{\beta \sum_v H_v^k Z_v} e^{\sum_v \gamma_v^k X_v}$$

  2. Correlation Functions (**Periodic Boundary**):

$$\langle s_{u,k} s_{u',k'} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}(V_1 \cdots Z_u V_k \cdots Z_{u'} V_{k'} \cdots V_N)$$

- **Dimensional Reduction**: $M \times N$ classical spins to M qubits.
  - N^d spins on d-dim hypercube $\to N^{d-1}$ qubits on $d-1$-dim hypercube



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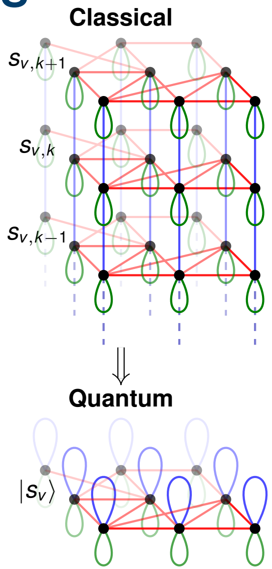

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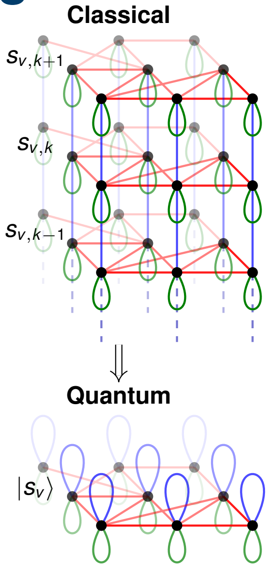

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  1. Additional terms: Square 2D, with fields $H_v^k \neq 0$;
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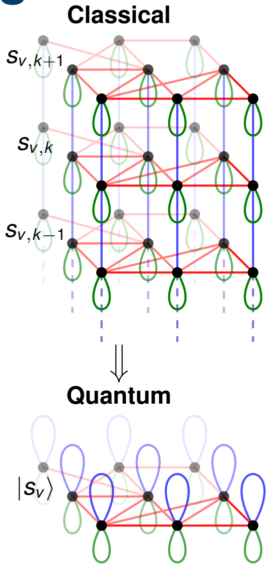
- Kaufman-type/Lie-theoretic solution?



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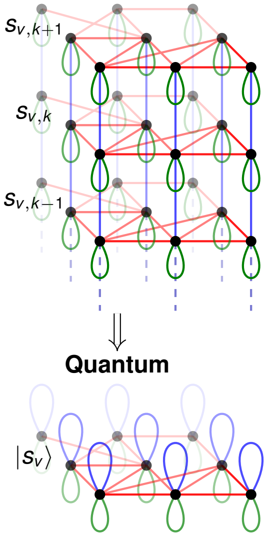
- Kaufman-type/Lie-theoretic solution?
  Exponential time/memory:
  1. For any graph $\mathbb{G}$, with fields, $\dim G_{\text{Lie}} = \mathrm{O}(4^M)$
  2. For any non-1D graph $\mathbb{G}$, no fields, $\dim G_{\text{Lie}} = \mathrm{O}(4^M)$ (1)



(1) Real-imaginary correspondence based on the work of Kazi/Larocca/Farinati/Coles/Cerezo/Zeier (Unpublished)

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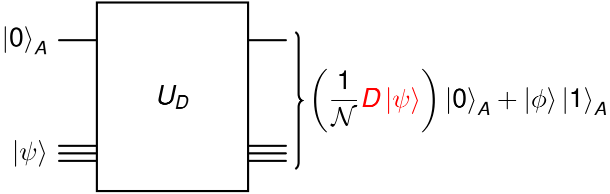
- Probabilistic Approach: **Block Encodings**[2]



- Introduce non-unitarity via **ancillas and (weak) measurements**

[2]See also: Martyn 2021, Zhu 2023, Arad 2010.

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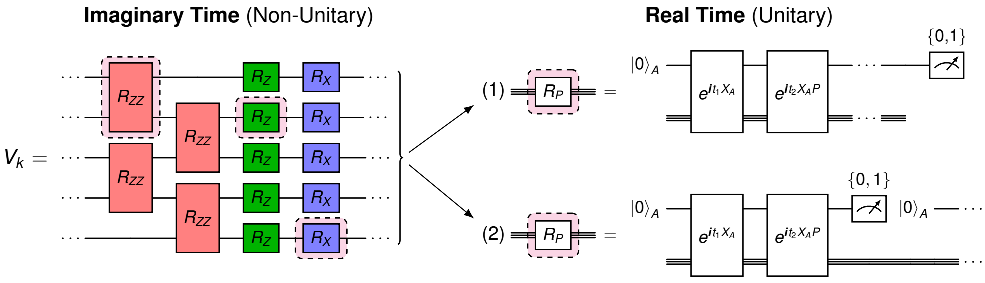


$R_P = e^{\tau P}, \; P \in \{Z_u Z_v, Z_u, X_v\}$

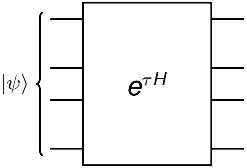
(1) Many ancillas, end-of-circuit measurements

(2) Few ancillas, mid-circuit measurements with reset

HOW TO IMPLEMENT IMAGINARY TIME EVOLUTION?

- Transfer Matrix V_k is **not unitary**! No direct implementation on quantum computers
- Deterministic Approach: **Unitary Approximation** (Open Boundary)
  1. Variational Imaginary Time Evolution (McArdle, 2019) as subroutine:

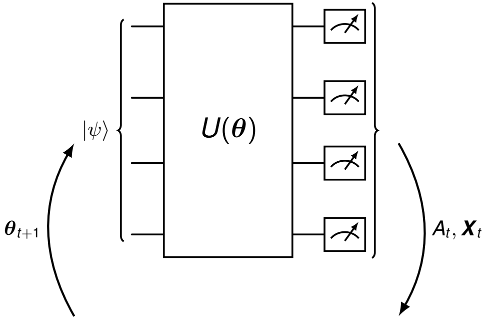
Imaginary Time (Non-Unitary)



$$H \in \left\{ \sum_{(u,v)} J_{uv} Z_u Z_v,\ \sum_v H_v Z_v,\ \sum_v \gamma_v X_v \right\}$$

$\approx$

Real Time (Unitary)



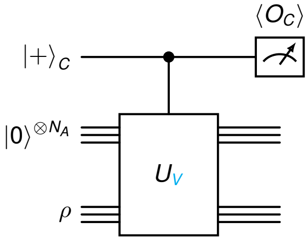
$$\delta_\tau \| (\partial/\partial_\tau + H - E_\tau) |\psi(\tau)\rangle \| = 0 \Rightarrow \dot{\boldsymbol{\theta}} = A^{-1} \cdot \boldsymbol{X}$$

COMPUTATION ON A QUANTUM COMPUTER

- **Many-ancilla** Block-Encoding
(Periodic Boundary: $\rho \propto \mathbb{1}$, Open Boundary: $\rho = (|+\rangle\langle+|)^{\otimes M}$)

  1. Partition Function via **Hadamard Test** with
  $\Pi_0^C + \Pi_1^C U_V$, $V = \prod_k V_k$:

$$\mathcal{Z} = c\,\mathrm{Tr}(\rho V) = c'(\langle X_C\rangle - i\,\langle Y_C\rangle)$$



  2. Expectation values via Hadamard Test with
  $\Pi_0^C + \Pi_1^C U_{V'}$, $V' = V_1 \cdots Z_u V_k \cdots Z_{u'} V_{k'} \cdots V_N$:

$$\langle s_{u,k} s_{u',k'}\rangle = \frac{\mathrm{Tr}(\rho V')}{\mathrm{Tr}(\rho V)} = \frac{\langle X_C\rangle' - i\,\langle Y_C\rangle'}{\langle X_C\rangle - i\,\langle Y_C\rangle}$$

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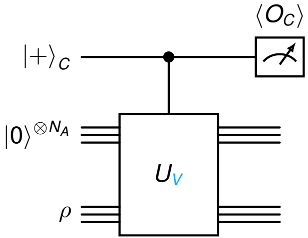

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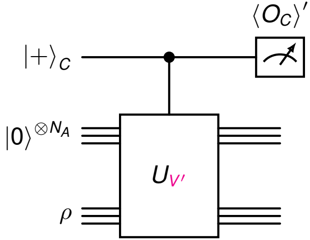

COMPUTATION ON A QUANTUM COMPUTER

- **Few-Ancilla** Block-Encoding (Stochastic Circuit)
  (Periodic Boundary: $\rho \propto \mathbb{1}$, Open Boundary: $\rho = (|+\rangle\langle+|)^{\otimes M}$)

  1. Partition Function via **Hadamard Test** with
     $\Pi_0^C + \Pi_1^C V$, $V = \prod_k V_k$:

$$\mathcal{Z} = c\,\mathrm{Tr}(\rho V) = c' \frac{\langle X_C\rangle - \boldsymbol{i}\,\langle Y_C\rangle}{1 + \langle Z_C\rangle}$$

  2. Expectation values via Hadamard Test with
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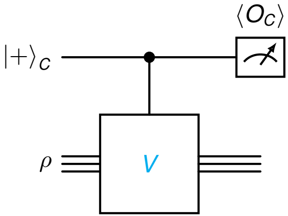

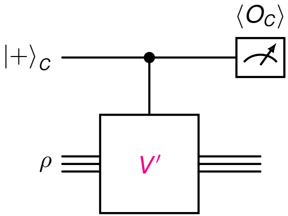

COMPUTATION ON A QUANTUM COMPUTER

- **Unitary** Approximation
  (Open Boundary: $\rho = (|+\rangle\langle+|)^{\otimes M}$)

1. Partition Function via **Hadamard Test** with
   $U(\theta^*) \approx \Pi_0^C + \Pi_1^C V, \; V = \prod_k V_k$:

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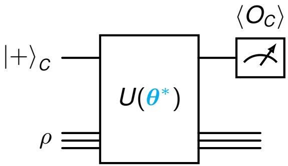

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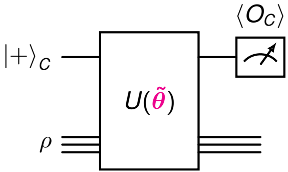

SUMMARY AND OUTLOOK

1. Transfer Matrix mapping for **equilibrium classical** systems **on quantum** systems:
   - Dimensional Reduction
   - Works **beyond standard 2D**.
   - **No Kaufman-type solution** beyond standard 2D

2. Quantum Computer **implementations** suitable for **NISQ**:
   - **Block encodings**: Polynomial depth, Variable number of ancillas
   - **Unitary Approximation**: No ancillas, Model-dependent depth

- **Approximation Scale**?
- **General inter-layer** interactions?
- Role of **Symmetries**? Lie-theoretic properties?

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Thanks!

To appear in ReAQCT '24 Proceedings

LIE THEORY IN A NUTSHELL

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First steps

How to determine $\mathfrak{g}$?

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  one can go from a Lie algebra to another (with $\mathfrak{g}_{\mathbb{C}} = \tilde{\mathfrak{g}}_{\mathbb{C}}$):

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- Special cases: **one compact** and **one split** real form.

LIE ALGEBRA CLASSIFICATION

Conjecture

The ”thermal” Lie algebra $\mathfrak{g} = \langle \{Z_u Z_v\}_{(u,v)\in E(G)}, \{X_v\}_{v\in V(G)} \rangle_{\text{Lie}}$ for classical layers of arbitrary graphs G (no fields) is the **split real form** of the Multi-Angle QAOA ansatz.

(**Imaginary Time**) Disordered Ising model on:

- 2D Rectangular lattice with periodic boundary conditions: $\mathfrak{g} = \mathfrak{so}(M, M) \oplus \mathfrak{so}(M, M)$
- 3D (even) Cubic lattice Ising model: $\mathfrak{g} = \mathfrak{sp}(2^{M-1}, \mathbb{R}) \oplus \mathfrak{sp}(2^{M-1}, \mathbb{R})$

(**Real Time**) Multi-Angle QAOA on[1]:

- Cycle Graph: $\mathfrak{g} = \mathfrak{so}(2M) \oplus \mathfrak{so}(2M)$
- (Even) Bipartite Graph: $\mathfrak{g} = \mathfrak{sp}(2^{M-1}) \oplus \mathfrak{sp}(2^{M-1})$

[1](Unpublished) Work by Kazi/Larocca/Farinati/Coles/Cerezo/Zeier, 2024

LIE ALGEBRA CLASSIFICATION

Result #1

The ”thermal” Lie algebra $\mathfrak{g} = \langle \{Z_u Z_v\}_{(u,v)\in E(G)}, \{X_v, Z_v\}_{v\in V(G)} \rangle_{\text{Lie}}$ for classical layers of any connected graph G (with fields) is $\mathfrak{sl}(2^M, \mathbb{R})$, $M = |V|$.

Result #2

The ”thermal” Lie algebra $\mathfrak{g} = \langle \{Z_u Z_v\}_{(u,v)\in E(G)}, \{X_v\}_{v\in V(G)} \rangle_{\text{Lie}}$ for classical layers of arbitrary graphs G (no fields) has the **same dimension** as that of the Multi-Angle QAOA ansatz.