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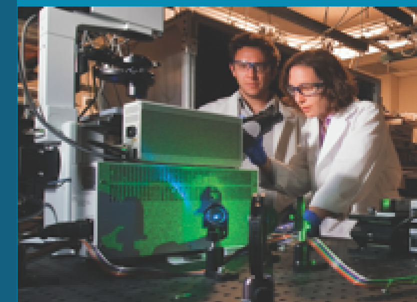
Beating Random Assignment for Approximating Quantum 2-Local Hamiltonian Problems



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Quantum Bits Live in a Sphere

State space

Classical bit: (bit)

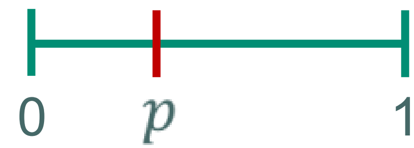
OR

+1 = Head   -1 = Tail

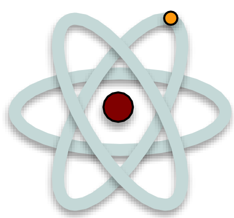
{+1, -1}

Prob. bit: (p-bit)

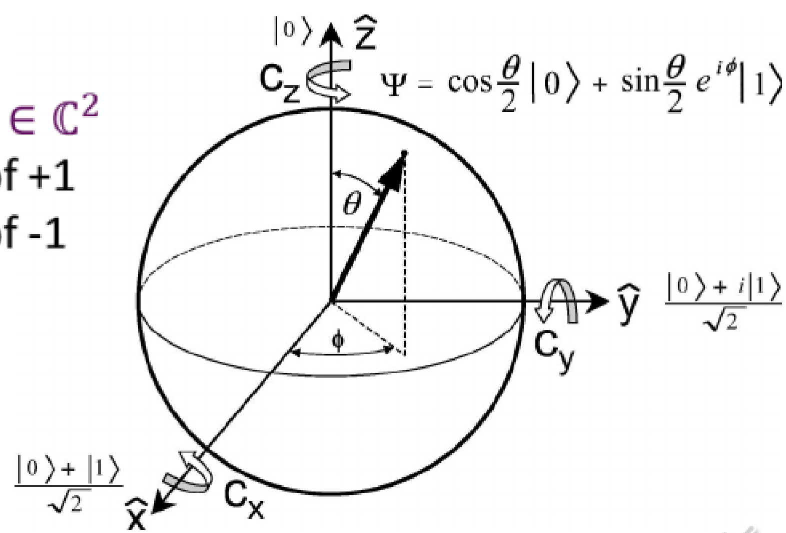
+1 with probability p
-1 with probability 1-p



Quantum bit: (qubit)



$\alpha|+1\rangle + \beta|-1\rangle \in \mathbb{C}^2$
$|\alpha|^2$-probability of +1
$|\beta|^2$-probability of -1



How to describe a Generic distribution of qubits?

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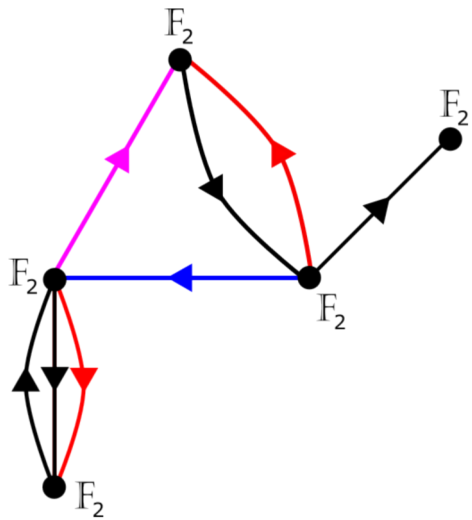
Classical and Quantum Combinatorial Optimization

Classical



- Edges correspond to non-linear functions on vertices

$$f = \sum_{(j \to k) \in E} f_{jk}(v_j, v_k)$$

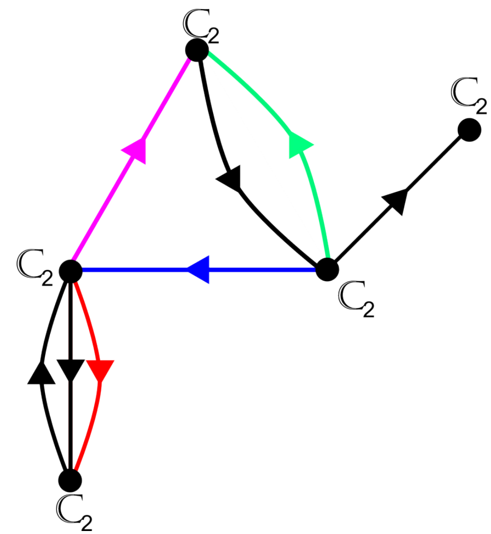
- Task is to find

$$\max_{\mu} \mathbb{E}_{\mu}[f]$$

- **Example** Max Cut

$$f_{jk}(v_j, v_k) = v_j + v_k - 2 v_j v_k$$

Quantum (2-Local Hamiltonian Problem)



- Optimizing over tensor product

$$\mathbb{F}_2^{\oplus n} \leftrightarrow \mathbb{C}_2^{\otimes n}$$

- Edge functions now linear, obj is the same

$$\max_{\rho} \mathbb{E}_{\rho}[f] \approx \max_{\rho} Tr\left[\sum_{(j \to k) \in E} h_{jk} \rho\right]$$

- h_{jk} has "non-trivial" part only on j and k:

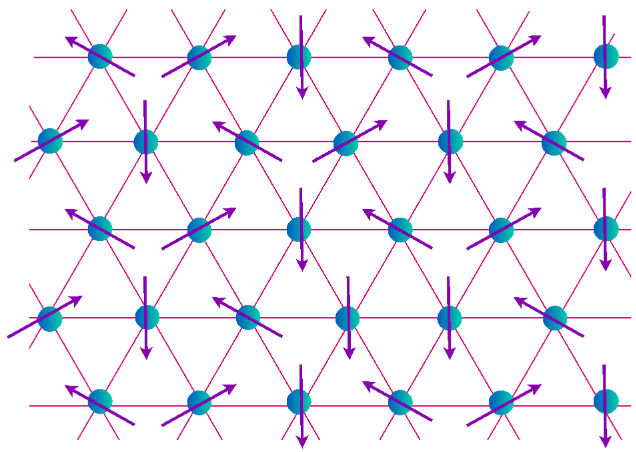
$$h_{12} = O_{12} \otimes \mathbb{I}_3 \otimes \cdots \otimes \mathbb{I}_n$$

- **Find largest e-value of exp. large matrix from a local description**

Motivation

Possible Energies for Physical systems

- Heisenberg model is fundamental for describing quantum magnetism, superconductivity, and charge density waves. We consider generalization of this problem



Anti-ferromagnetic Heisenberg model: roughly neighboring quantum particles aim to align in opposite directions. This kind of Hamiltonian appears, for example, as an effective Hamiltonian for so-called Mott insulators.
[Image: Sachdev, arxiv:1203.4565]

Complexity Theory

- 2-Local Hamiltonian problem is QMA complete -> **If we shouldn't expect to solve it, how well can we approximate it?**
- Field of Classical Approximation Algorithms very developed. **Very few results giving rigorous approx. algs. for quantum problems.**

Approximation Algorithms and Ansatze

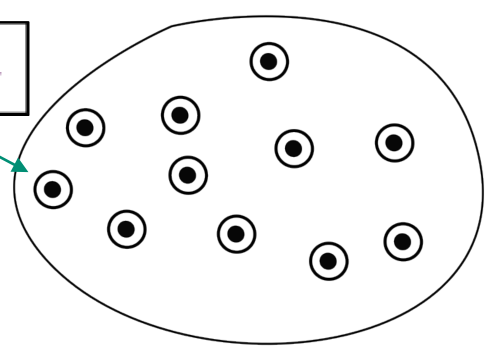
$$\frac{Alg(\{h_{ij}\})}{\lambda_{max}(H)} \geq \alpha$$

Runs in poly time in n,
provable guarantee independent of instance

- Unlike classical combinatorial opt. not clear what “kind” of description is best
- **Ansatz**- “kind” of quantum state the algorithm outputs.
- **Example: Product State Ansatz**

$$\rho_i = \frac{I + \alpha_i X_i + \beta_i Y_i + \gamma_i Z_i}{2}$$

$$= \prod$$



- Analogy: Independent Coin Flips
- Overall distribution of independent variables can be specified with marginals

Assumptions

Assumption	Reference
Graph-Dependent Assumption	[Bansal, Bravyi, Terhal, 07'], [Gharibian, Kempe, 12'], [Brandao, Harrow, '16], [Harrow, Montanaro, '17]
Quantum Max Cut	[Gharibian, Parekh, '19], [Anshu, Gosset, Morenz, '20] [PT '21] (x2)
Traceless	[Bravyi, Gosset, Koenig, Temme, '18]
Projectors	[Hallgren, Lee, P. '20] [This work]

- No "universal" approximation algorithm: generalizes max ind. set [Wocjan, Beth '03]
- Just like classical, people study 2-Local HP with assumptions
- **For us: 2-Local terms are projectors**, **i.e.** $h_{12} = P_{12} \otimes \mathbb{I}_3 \otimes \cdots \otimes \mathbb{I}_n$
  - Assume further the rank of each h_{ij} is the same
  - 3 cases of interest corresponding to rank of P_{ij}

Our Contributions

Thm For **bipartite** traceless we get

$$\alpha = \frac{2\, ln(1+\sqrt{2})}{3\, \pi}$$

Thm If each $h_{(i \to j)} = P_{\{i,j\}} \otimes \mathbb{I}_{[n] \setminus \{i,j\}}$ where $rank(P) = k$, there is an approx. alg. obtaining factor:

$$\alpha(k) = \begin{cases} 0.387 \;\; if \;\; k = 1 \\ 0.585 \;\; if \; k = 2 \\ 0.764 \; if \; k = 3 \end{cases}$$

Thm If in addition each P is "strictly quadratic", we obtain the following approx. factors:

$$\alpha(k) = \begin{cases} 0.467 \;\; if \;\; k = 1 \\ 0.639 \;\; if \; k = 2 \\ 0.805 \;\; if \; k = 3 \end{cases}$$

Trivial (Random) Assignment:

$$\alpha(k) = \begin{cases} 1/4 \;\; if \;\; k = 1 \\ 1/2 \;\; if \;\; k = 2 \\ 3/4 \;\; if \;\; k = 3 \end{cases}$$

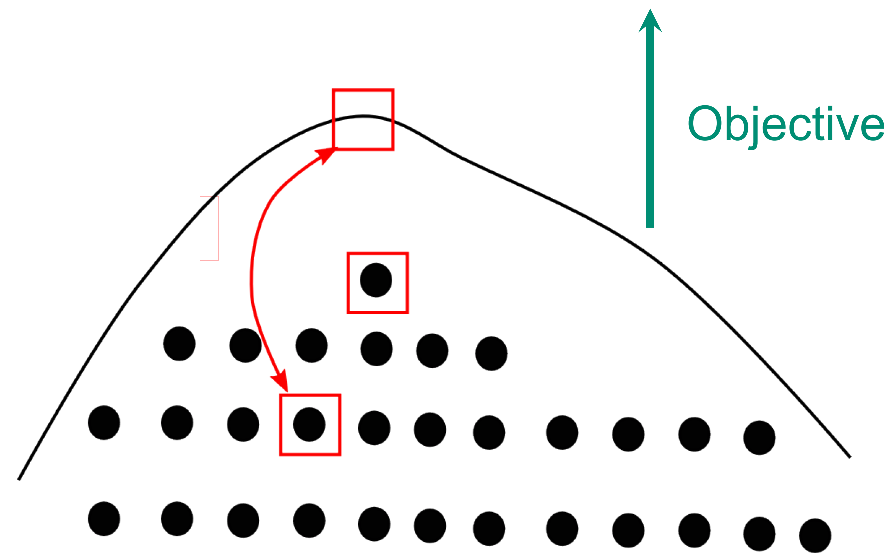
How Does the Approx. Alg. Work?

Classical Rounding-

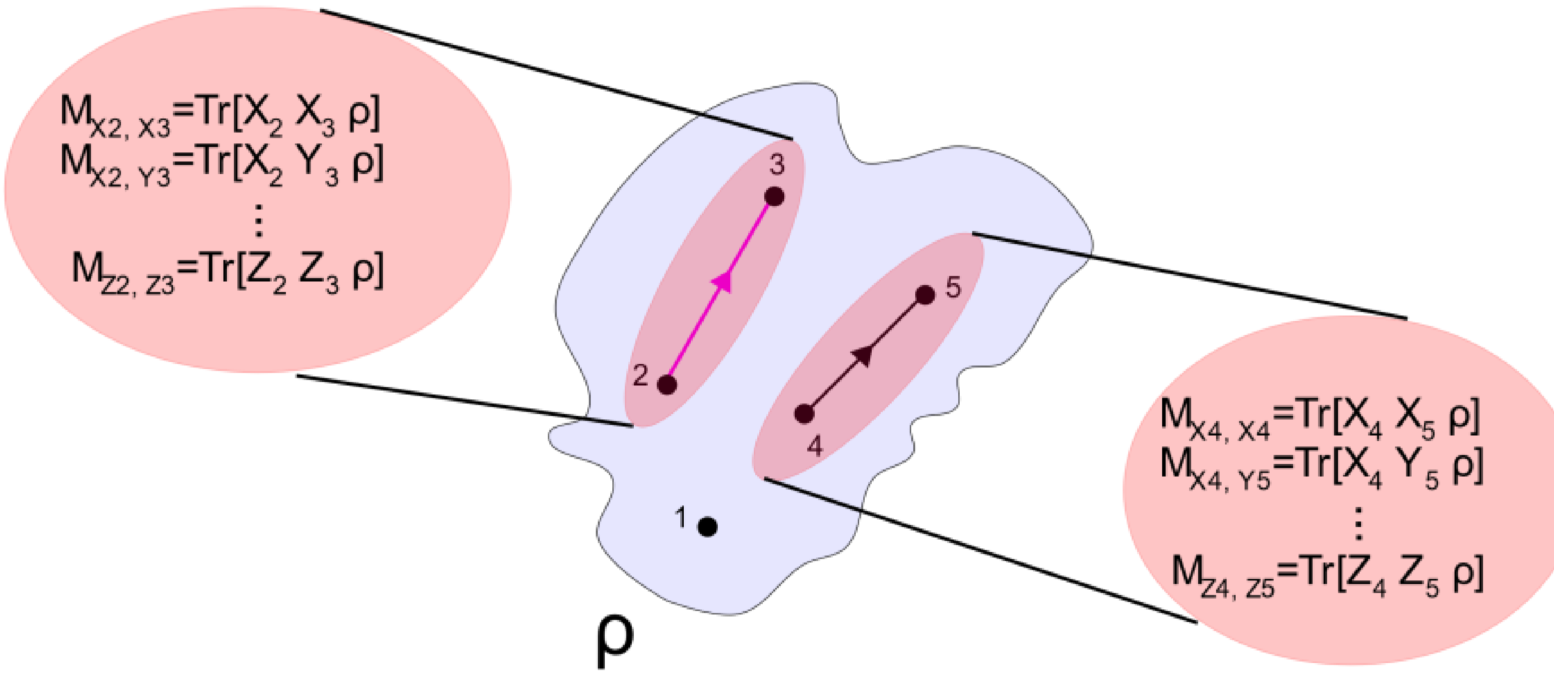
- Relax NP-hard optimization problem
- Use solution of relaxation to get element in $\mathbb{F}_2^n$
- Analyze loss in obj. from rounding

Quantum Rounding

- Problem is exp. large SDP
- Can we relax this to polynomially large SDP?



Relaxation



- Define **Moment Matrix** $M \in \mathbb{C}^{3n\times 3n}$

$$M_{\sigma j,\eta l} = Tr\left[\,\sigma_j \eta_l \rho\right] : \ \sigma, \eta \in \{X, Y, Z\}$$

- Pauli basis is complete, this description captures all **2-Local** statistics ⇒ Given **only** the moment matrix, we could calculate the objective

The SDPs

- Hence, could equivalently optimize over M:

$$\max \sum_e Tr(C^e M)$$

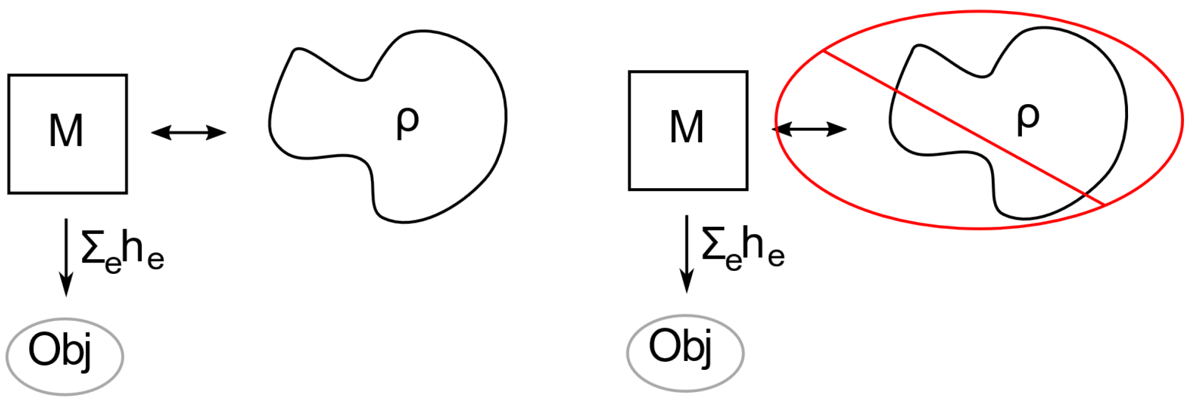
$$s.t. \, M_{\sigma j, \eta l} = Tr(\sigma_j \eta_l \rho)$$

$$\rho \in \mathcal{D}(2^n), \qquad M \in \mathbb{R}^{3n \times 3n}, \succcurlyeq 0$$

$v^T M v = Tr(T^2 \rho) \geq 0$

For non-imaginary entries

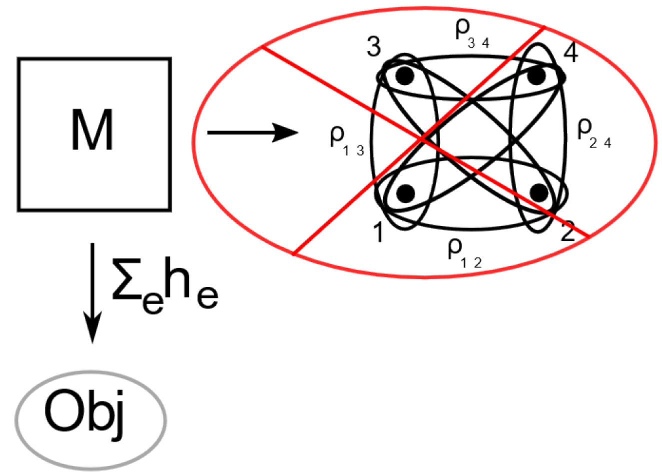
- **Haven't really done anything at this point**
  - Equivalent to original SDP, merely represented 2-Local part redundantly
  - Can "forget" correspondence to get poly-sized SDP!



The SDPs

- **The catch**? In SDP, marginals will be globally inconsistent
- Otherwise, we would be solving a QMA-hard problem!
- M may not even be consistent with a set of 2-local marginals
- SDP we study forces with property with additional variables
- Slight tightening of the 1st level of the quantum Lasserre Hierarchy

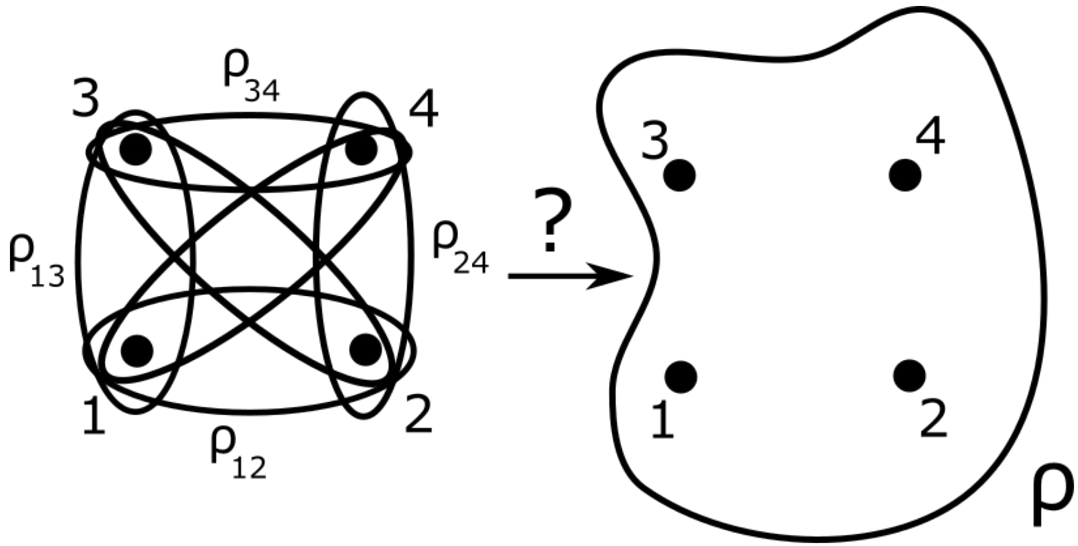
[Lasserre '01]
[Pironio, Navascués, Acìn, '10]



$$\max \sum_e Tr(C^e M)$$
$$s.t.\, M_{\sigma j, \eta l} = Tr(\sigma_j \eta_l \rho) \forall \sigma, j, \eta, l$$
$$M_{ij,ij} = 1, M_{ij,ik} = 0$$
$$Tr(\rho_{ij}) = 1 \,\forall i, j$$
$$M \succcurlyeq 0, \rho_{ij} \succcurlyeq 0 \,\forall i, j$$
$$M \in \mathbb{R}^{3n \times 3n}, symmetric$$
$$\rho_{ij} \in \mathbb{C}^{4 \times 4}, Hermitian \,\forall i, j$$

What does the SDP give us?

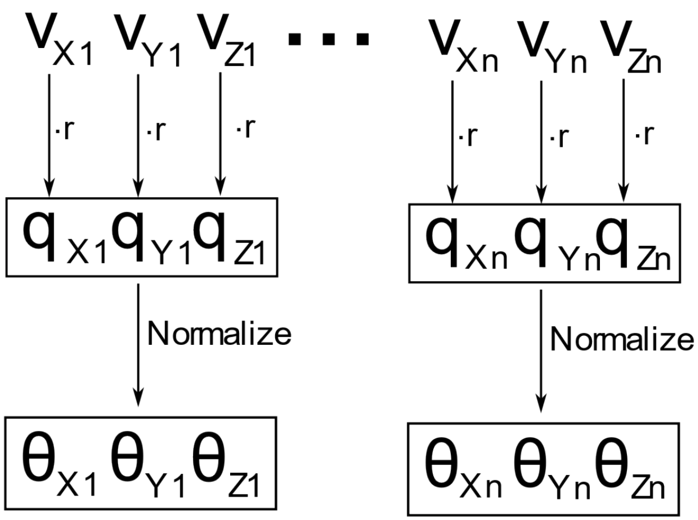
- M^*- optimal solution to SDP
  - Cholesky decomposition- $\{v_{\sigma j}\}$ such that $M_{\sigma j,\eta l} = v_{\sigma j}^T v_{\eta l}$.
  - Statistics corresponding to a non-physical density matrix
  - However, objective of M **upper bounds** optimal density matrix
- $\{v_{\sigma j}\}$ represents unphysical statistics, can we **round to** a physical state with these vectors? Maybe a Bloch vector?
- Rounding to Bloch vectors would **guarantee** "physical-ness"



“Hyperplane” Rounding

- Let $r \sim \mathcal{N}(0, \mathbb{I})$. If we could take $\theta_{\sigma j} = v_{\sigma j} \cdot r$:
  - $\mathbb{E}[(v_{\sigma j} \cdot r)(v_{\eta l} \cdot r)] = \mathbb{E}[v_{\sigma j}^T r\, r^T v_{\eta l}] = v_{\sigma j}^T v_{\eta l}$
- We would get approx. factor 1! But this is unphysical, need to normalize:
- **Procedure**
  - Take $q_{\sigma j} = v_{\sigma j} \cdot r \;\forall \sigma, j$
  - Normalize: $\theta_{\sigma j} = \frac{v_{\sigma j} \cdot r}{\sqrt{\sum_\eta (v_{\eta j} \cdot r)^2}}$
  - Output:

$$\rho = \prod_i \left(\frac{\mathbb{I} + \sum_\sigma \theta_\sigma \sigma_i}{2} \right)$$



$$\theta_{X1} = \frac{q_{X1}}{\sqrt{q_{X1}^2 + q_{Y1}^2 + q_{Z1}^2}}$$

Analysis

- Evaluate the expected approx. factor edge by edge:

$$\mathbb{E}\left[Tr\left(\sum_e h_e\ \rho\right)\right] = \sum_e \mathbb{E}[Tr(h_e\ \rho)]$$

- If $\frac{\mathbb{E}[Tr(h_e\ \rho)]}{Tr[M\ C^e]} \geq \alpha$ for all e, then $\sum_e \mathbb{E}[Tr(h_e\ \rho)] \geq \alpha\ \sum_e Tr[M\ C^e]$
- Reduce edge to **standard form** which depends on the rank of h_e
- Given this standard form, use **Hermite polynomials** to calculate the expectation:
  - $f(z), g(z)$ functions of normal r.v.'s $\mathcal{N}(0, \mathbb{I})$
  - $\Rightarrow \mathbb{E}[f(z)g(z)] = \sum_\mu \hat{f}_\mu \hat{g}_\mu$
  - $\theta_{\sigma i}$ function of $r \sim \mathcal{N}(0, \mathbb{I})$

Future Work

- **Optimizing proof methods?** proven approximation factors are strict lower bounds on performance of alg., we suspect it is possible to prove actual performance with better techniques
- **1-Local vs. 2-Local?** We suspect alg. has same performance when 1-local terms are included
- **Genuinely entangled Ansatz?**
- **Approximation alg. making crucial use of quantum circuit?**