Title: Alleviating the sign structure of quantum states

Speakers: Giacomo Torlai

Collection: Machine Learning for Quantum Design

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Abstract: The sign structure of quantum states - the appearance of â€œprobabilityâ€• amplitudes with negative sign - is one of the most striking contrasts between the classical and the quantum world, with far-reaching implications in condensed matter physics and quantum information science. Because it is a basis-dependent property, one may wonder: is a given sign structure truly intrinsic, or can it be removed by a local change of basis? In this talk, I will present an algorithm based on automatic differentiation of tensor networks for discovering non-negative representations of many-body wavefunctions. I will show some numerical results for ground states of a two-leg triangular Heisenberg ladder, including an exotic Bose-metal phase.

Alleviating the Sign Structure of Quantum States

Giacomo Torlai

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Flatiron Institute

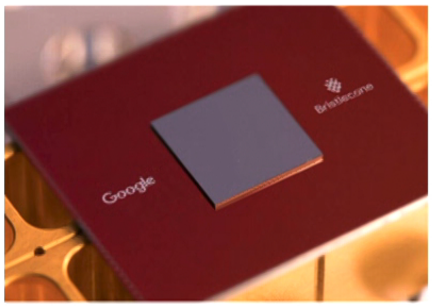
FLATIRON INSTITUTE
Division of Simons Foundation

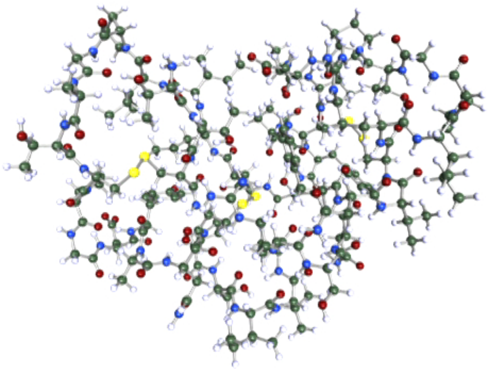
Machine Learning for Quantum Design

Perimeter Institute for Theoretical Physics
July 8th 2019

Sign Structure of Quantum States

$$\text{Sign}\,\langle\boldsymbol{\sigma}|\Psi\rangle$$






PERIMETER

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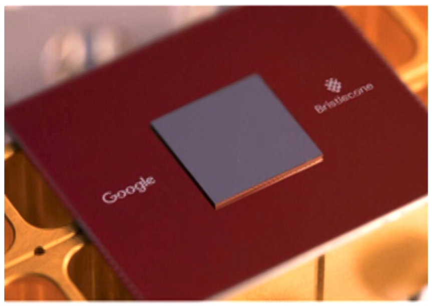
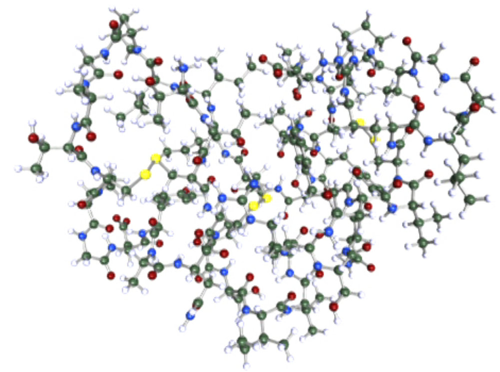




How to classify its complexity?

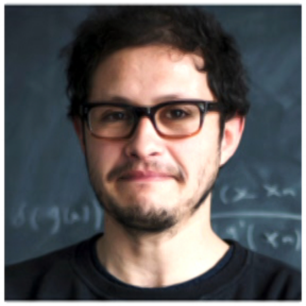
How to ged rid of it?

When is it intrinsic?

Relationship with entanglement?

Quantum Monte Carlo?

Collaborators



Juan Carrasquilla
Vector Institute & UW

Matthew Fishman
Flatiron Institute

Roger Melko
Perimeter Institute & UW

Matthew Fisher
UCSB

Path integrals

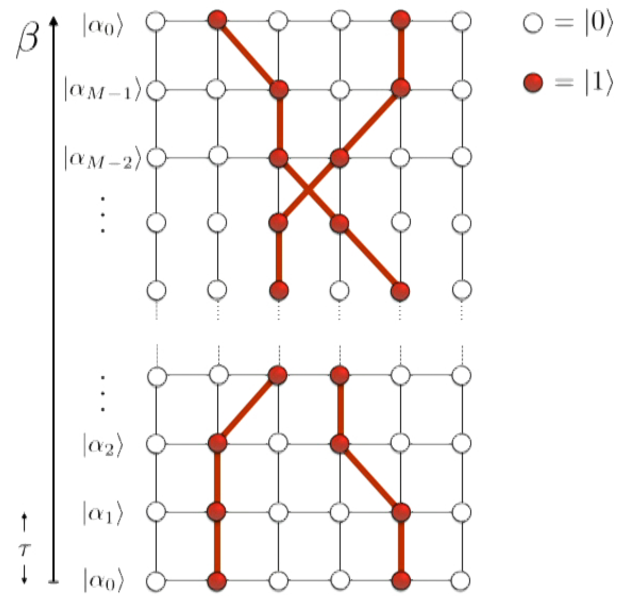
(d+1) representation of the quantum partition function:

$$Z = \sum_{\alpha_0} \cdots \sum_{\alpha_{M-1}} \langle \alpha_0 | e^{-\tau \hat{H}} | \alpha_1 \rangle \langle \alpha_1 | e^{-\tau \hat{H}} | \alpha_2 \rangle \dots \langle \alpha_{M-1} | e^{-\tau \hat{H}} | \alpha_0 \rangle$$

$$= \sum_{\{\boldsymbol{\alpha}\}} W(\{\boldsymbol{\alpha}\}) \qquad W(\{\boldsymbol{\alpha}\}) \Longrightarrow \text{Weight of a world-line.}$$

"Positive-definite" path integrals:

$$\langle \alpha_k | e^{-\tau \hat{H}} | \alpha_{k+1} \rangle \approx \hat{\mathcal{I}} - \tau \langle \alpha_k | \hat{H} | \alpha_{k+1} \rangle \geq 0 \quad \Longrightarrow \quad W(\{\boldsymbol{\alpha}\}) \geq 0 \;\; \forall \{\boldsymbol{\alpha}\}$$



Path integrals

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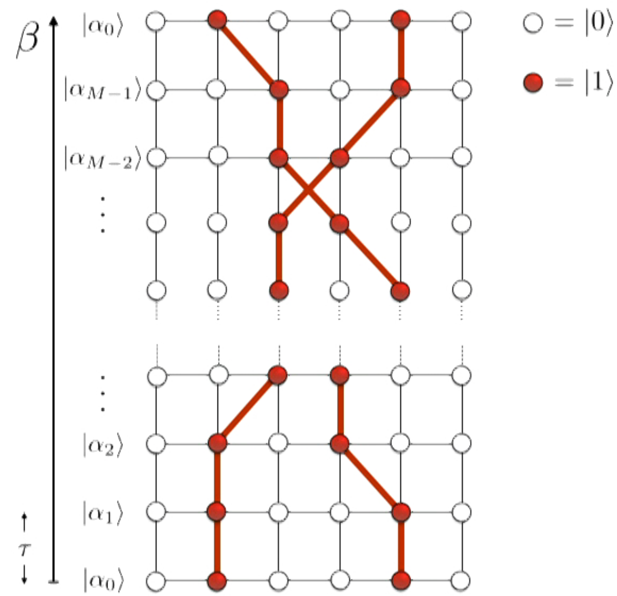

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Quantum Monte Carlo

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{A}\right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}}\right)} = \frac{\sum_{\{\boldsymbol{\alpha}\}} W(\{\boldsymbol{\alpha}\}) A(\{\boldsymbol{\alpha}\})}{\sum_{\{\boldsymbol{\alpha}\}} W(\{\boldsymbol{\alpha}\})}$$

Sample world-lines $\{\boldsymbol{\alpha}_k\}$ according to probability $W(\{\boldsymbol{\alpha}\})$

The sign problem of Quantum Monte Carlo

If the weights are both positive and negative, sample from the absolute value:

$$\langle \hat{A} \rangle = \frac{\sum_{\{\alpha\}} W(\{\boldsymbol{\alpha}\}) A(\{\boldsymbol{\alpha}\})}{\sum_{\{\alpha\}} W(\{\boldsymbol{\alpha}\})} = \frac{\sum_{\{\alpha\}} |W(\{\boldsymbol{\alpha}\})| \mathrm{Sign}(W(\{\boldsymbol{\alpha}\})) A(\{\boldsymbol{\alpha}\})}{\sum_{\{\alpha\}} |W(\{\boldsymbol{\alpha}\})| \mathrm{Sign}(W(\{\boldsymbol{\alpha}\}))} = \frac{\langle \hat{A}\, \mathrm{Sign} \rangle}{\langle \mathrm{Sign} \rangle}$$

Loh, Gubernatis, Scalettar, White, Scalapino and Sugar (1990)
Henelius and Sandvik (2000)
Troyer and Wiese (2005)

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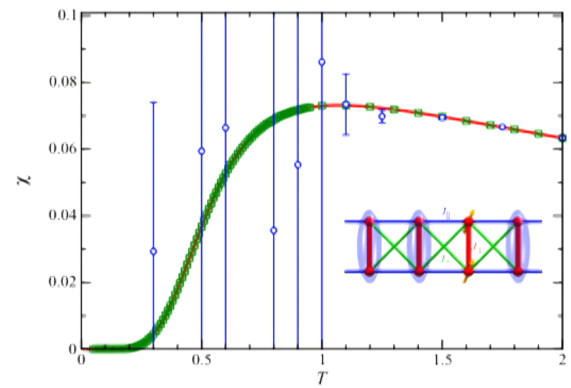
But… $\frac{\Delta \mathrm{Sign}}{\langle \mathrm{Sign} \rangle} \approx \frac{e^{\beta N \Delta f}}{\sqrt{N_{mc}}}$ 

Sign structure: $\mathrm{Sign}\, W(\{\boldsymbol{\alpha}\})$

Honecker *et al* (2016)



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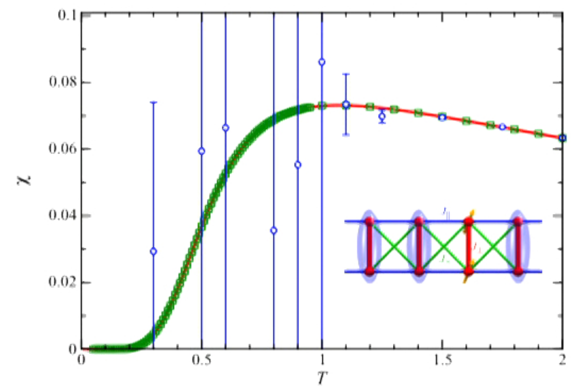

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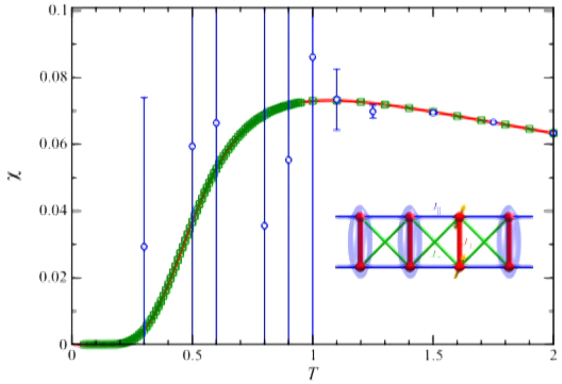

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Generic solution is NP-hard.

Specific solutions
Partial alleviation

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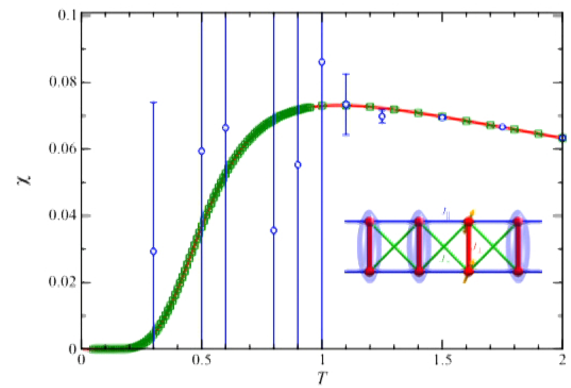

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Specific solutions
Partial alleviation

Meron cluster
Fermion Bag
…
Change of basis

Chandrasekharan and Wiese (1999)
Nakamura (1997)
Umrigar, Toulouse, Filippi, Sorella and Hennig (2007)
Huffman and Chandrasekharan (2014)
Alet, Damle and Pujari (2016)

The sign problem ~~of Quantum Monte Carlo~~

Impossibility of capturing underlying physics with classical representation.

The sign problem ~~of Quantum Monte Carlo~~

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Ground state limit: $e^{-\beta \hat{H}} \approx |\Psi\rangle\langle\Psi|$ $\quad |\Psi\rangle = \sum_{\boldsymbol{\sigma}} \Psi(\boldsymbol{\sigma})|\boldsymbol{\sigma}\rangle$ $\quad \Psi(\boldsymbol{\sigma}) = \langle\boldsymbol{\sigma}|\Psi\rangle$ $\quad |\boldsymbol{\sigma}\rangle = |\sigma_1, \ldots, \sigma_N\rangle$

Sign structure: $\mathrm{Sign}(\Psi(\boldsymbol{\sigma}))$ $\quad \Psi(\boldsymbol{\sigma}) \geq 0 \ \forall |\boldsymbol{\sigma}\rangle \Rightarrow \langle \mathrm{Sign}(\Psi(\boldsymbol{\sigma})) \rangle = 1$ $\quad \Psi(\boldsymbol{\sigma}) \Longleftrightarrow P(\boldsymbol{\sigma})$ "Classical"

The sign problem ~~of Quantum Monte Carlo~~

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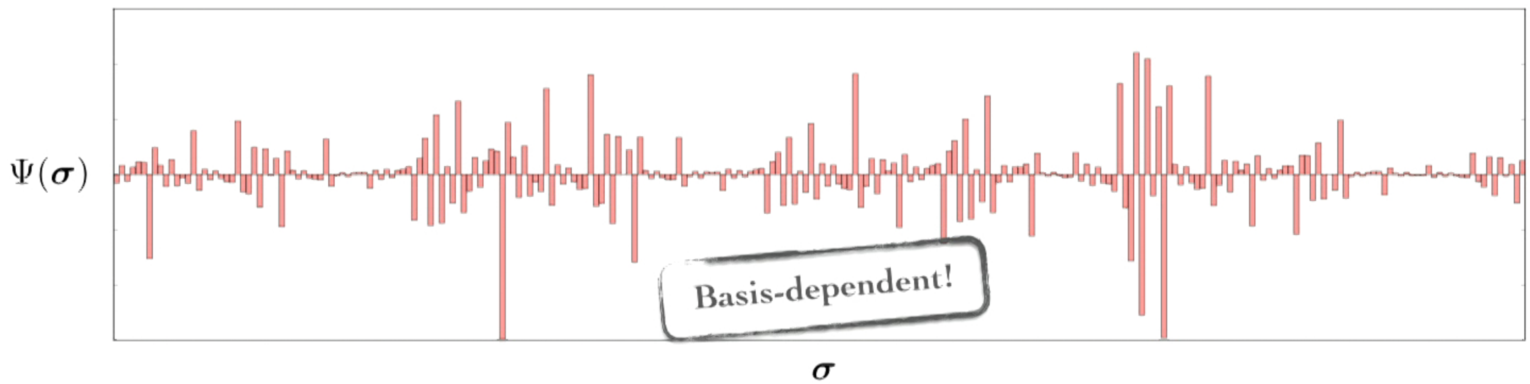
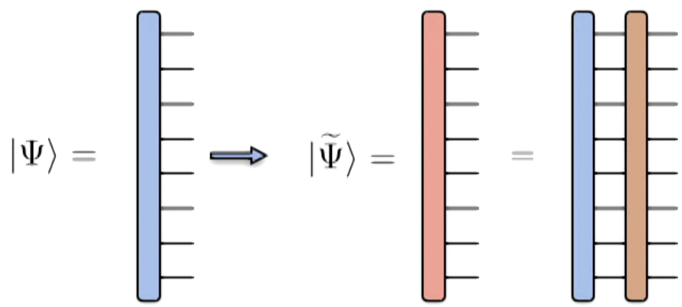


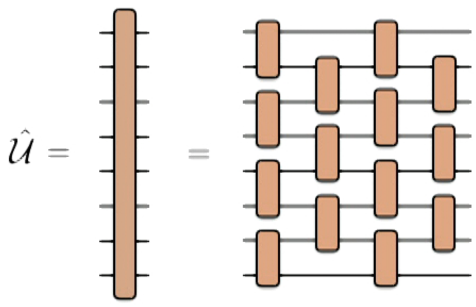
Wavefunction positivization

Let's change the basis with a unitary transformation $\hat{\mathcal{U}}$ so that: $\widetilde{\Psi}(\boldsymbol{\sigma}) \geq 0$ $\widetilde{\Psi}(\boldsymbol{\sigma}) = \langle \boldsymbol{\sigma} | \hat{\mathcal{U}} | \Psi \rangle$

Generally:



Unitary compiled into local quantum gates

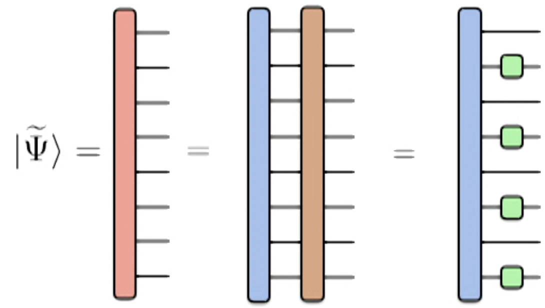


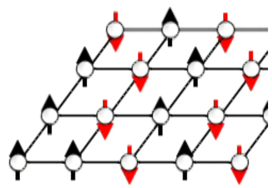
Wavefunction positivization

Quantum anti-ferromagnets

Bipartite lattice: $\mathrm{Sign}\big(\Psi(\boldsymbol{S}^z)\big) = (-1)^{N_A^{\uparrow}}$ (Marshall and Peierls, 1955)

Change of basis: $\hat{\mathcal{U}}_{MS} = \bigotimes_{j\in A} e^{i\pi\hat{\sigma}_j^z}$





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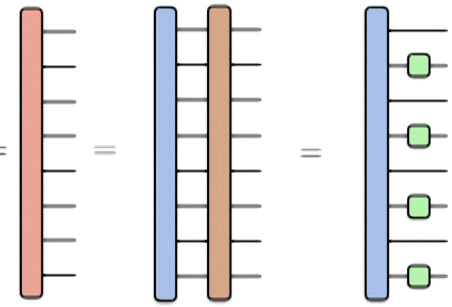
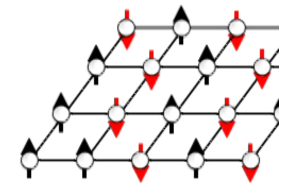
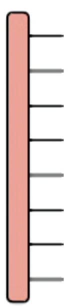
$|\widetilde{\Psi}\rangle =$

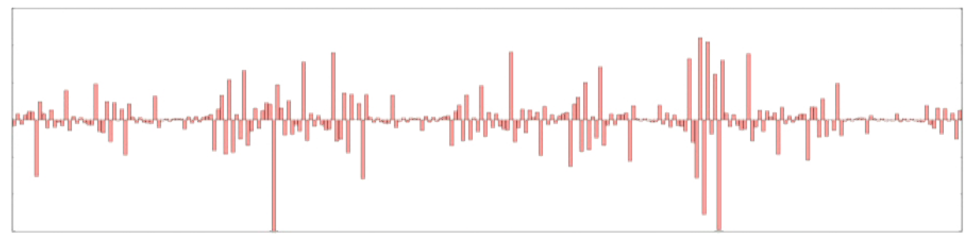




Apparent or intrinsic?

$|\Psi\rangle$





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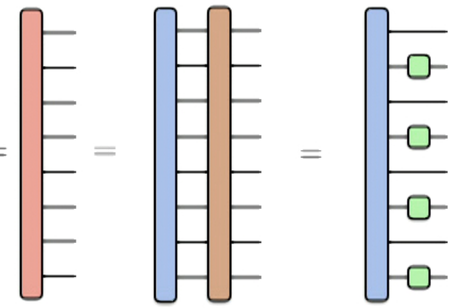
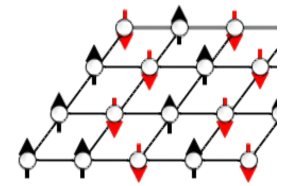
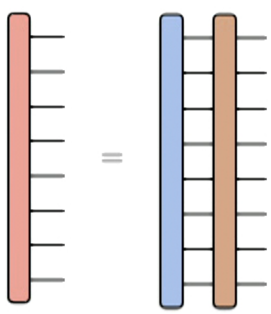
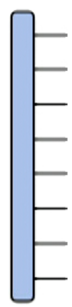
$|\widetilde{\Psi}\rangle =$ 

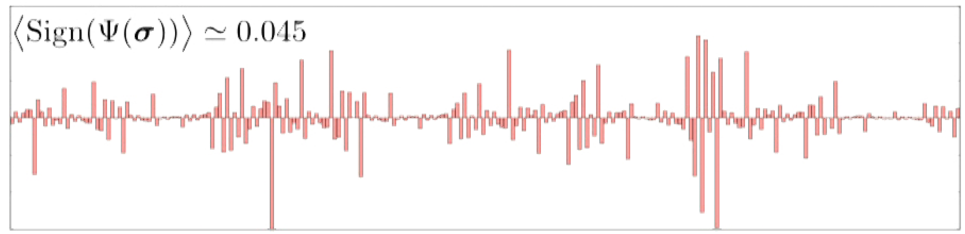


Apparent or intrinsic?

$|\Psi\rangle = \hat{\mathcal{U}}(\boldsymbol{\theta})\,|\Psi_0\rangle$



$|\Psi_0\rangle =$ 

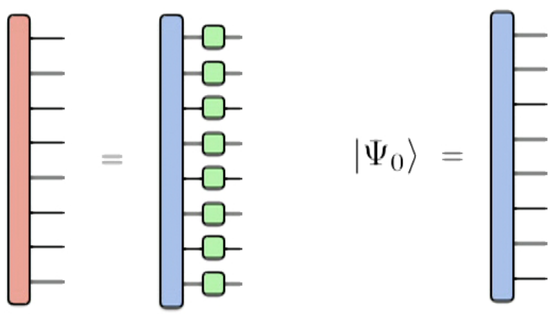


Wavefunction positivization

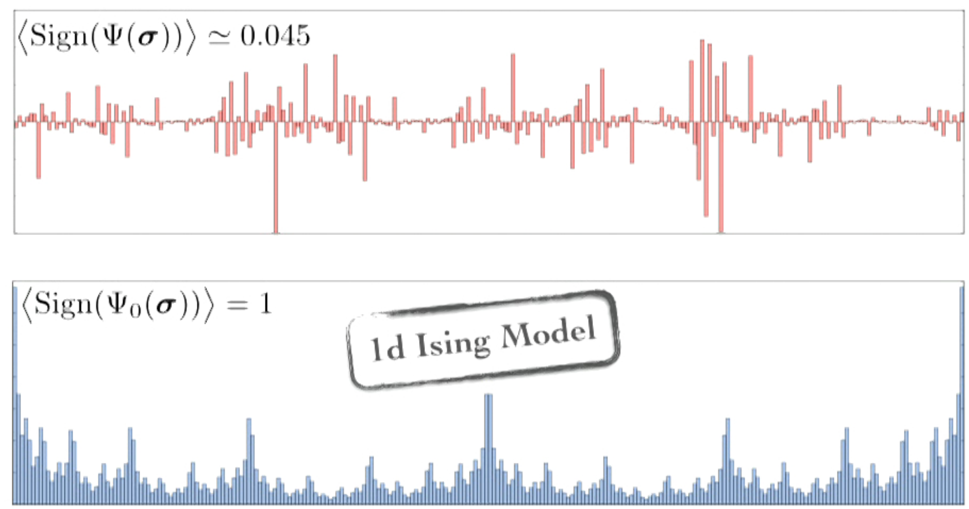
How would you even know?

Apparent or intrinsic?

$$|\Psi\rangle = \bigotimes_j \hat{R}_y(\theta_j)\,|\Psi_0\rangle$$



Positive state a few gates away.



Automating insights

Autonomous search of local bases that positivize wavefunctions

Ingredients

Appropriate representation

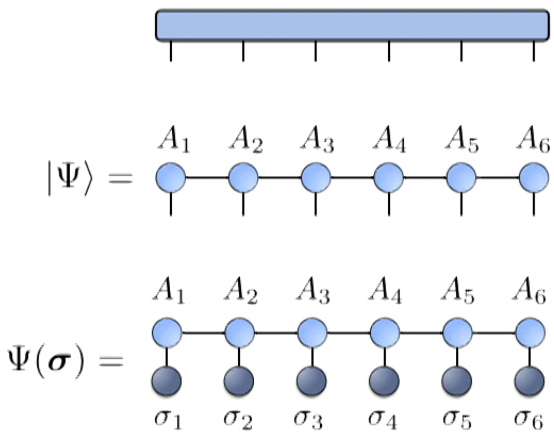
Good cost function

Adequate software

1. Tensor network representation

Input wavefunction = Matrix Product State

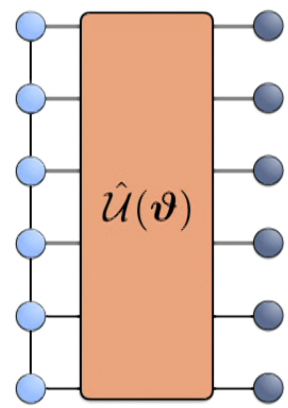
$$|\Psi\rangle = \sum_{\boldsymbol{\sigma}} A_1^{\sigma_1} A_2^{\sigma_2} \ldots A_N^{\sigma_N} |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle$$

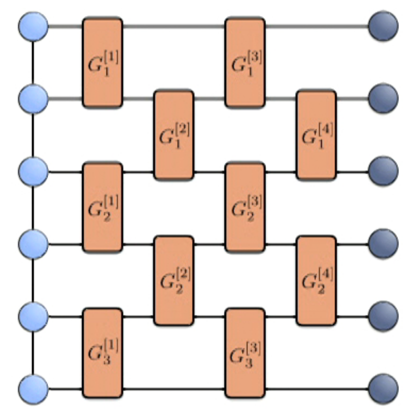


Local unitary transformation = Quantum Circuit

$$\boldsymbol{\vartheta} = \{\boldsymbol{\vartheta}^{[1]}, \boldsymbol{\vartheta}^{[2]}, \ldots\}$$

$$\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}) = \langle \boldsymbol{\sigma} | \hat{\mathcal{U}}_{\boldsymbol{\vartheta}} | \Psi \rangle \qquad \hat{G}_k^{[\ell]} = e^{-i\hat{\Gamma}_k^{[\ell]}}$$



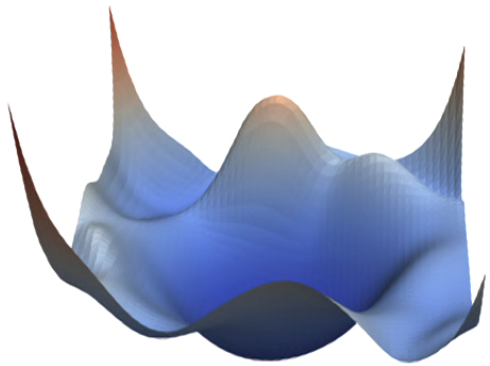


2. The cost function

Definition

We require the following conditions at the output of the circuit:

$$\mathrm{Sign}\big(\mathbb{R}\mathrm{e}\big[\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})\big]\big) = 1 \qquad \mathbb{I}\mathrm{m}\big[\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})\big] = 0 \quad \forall\ |\boldsymbol{\sigma}\rangle$$



Most conveniently expressed as averages over the output distribution:

$$\sum_{\boldsymbol{\sigma}} |\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})|^2 \big|\mathbb{I}\mathrm{m}\big[\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})\big]\big| = 0 \quad \text{and} \quad \sum_{\boldsymbol{\sigma}} |\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})|^2 \mathrm{Sign}\big(\mathbb{R}\mathrm{e}\big[\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})\big]\big) = 1$$

Cost function: $\mathcal{C}(\boldsymbol{\vartheta}) = \sum_{\boldsymbol{\sigma}} |\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})|^2 \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})$ $\qquad$ $\mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}) = \gamma\big|\mathbb{I}\mathrm{m}\big[\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})\big]\big| - (1-\gamma)\mathrm{Sign}\big(\mathbb{R}\mathrm{e}\big[\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})\big]\big)$

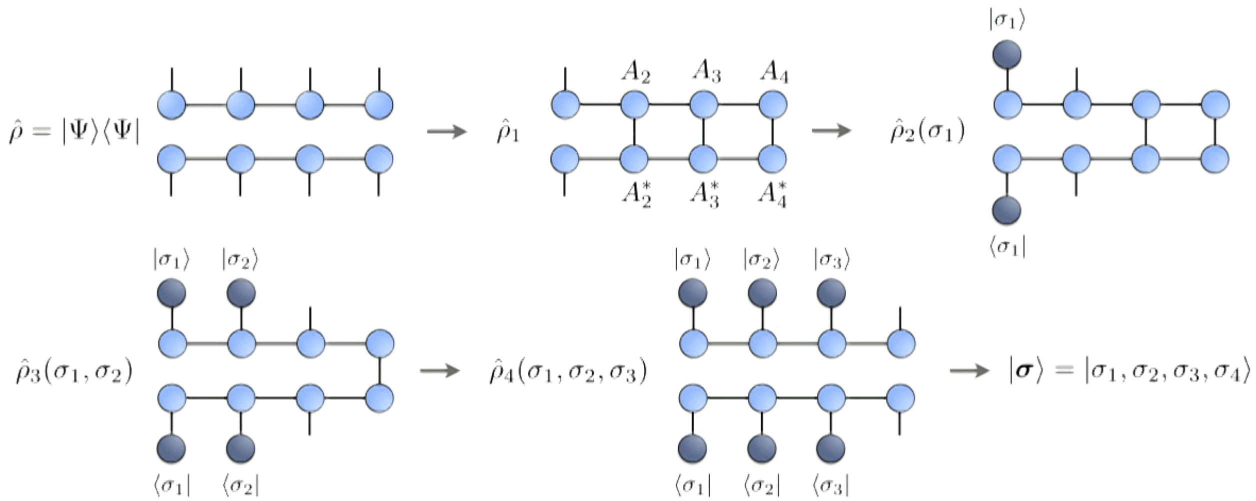
Discover the optimal parameters by minimization: $\boldsymbol{\vartheta}^* = \underset{\boldsymbol{\vartheta}}{\mathrm{argmin}}\, \mathcal{C}(\boldsymbol{\vartheta})$

Example: Gradient Descent $\qquad \boldsymbol{\vartheta} \to \boldsymbol{\vartheta} - \eta\, \mathcal{G}(\boldsymbol{\vartheta}) \qquad \mathcal{G}(\boldsymbol{\vartheta}) = \nabla_{\boldsymbol{\vartheta}} \mathcal{C}(\boldsymbol{\vartheta})$

2. The cost function

Computation

Approximate with average over finite samples: $\mathcal{C}(\boldsymbol{\vartheta}) = \sum_{\boldsymbol{\sigma}} |\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})|^2 \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}) \approx \widetilde{\mathcal{C}}(\boldsymbol{\vartheta}) = \frac{1}{M} \sum_{\boldsymbol{\sigma}_j} \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j)$



3. Differentiable programming

Automatic differentiation

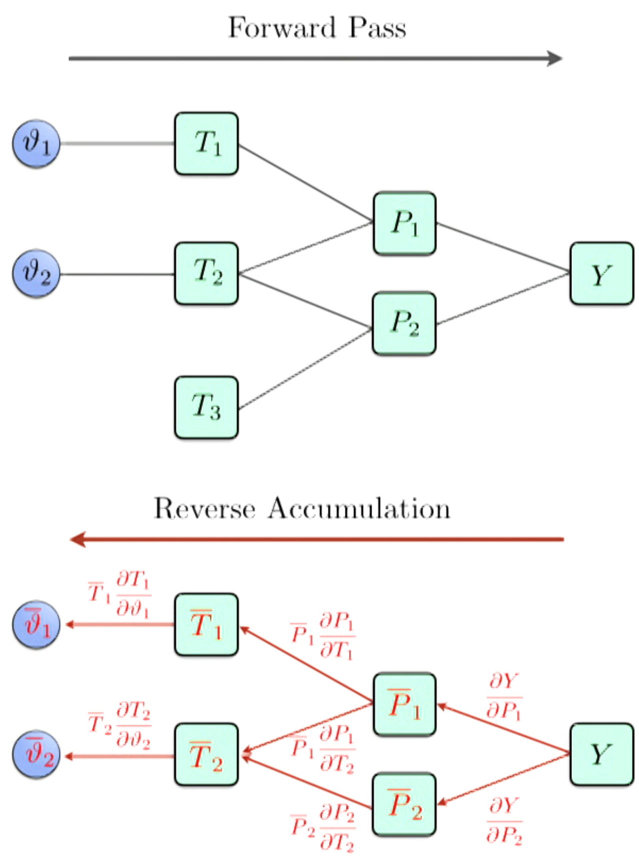
Build a computational graph:

$$\boldsymbol{\vartheta} \to T_1 \to T_2 \to \cdots \to T_n \to \mathcal{C}(\boldsymbol{\vartheta})$$

Compute derivative from the output:

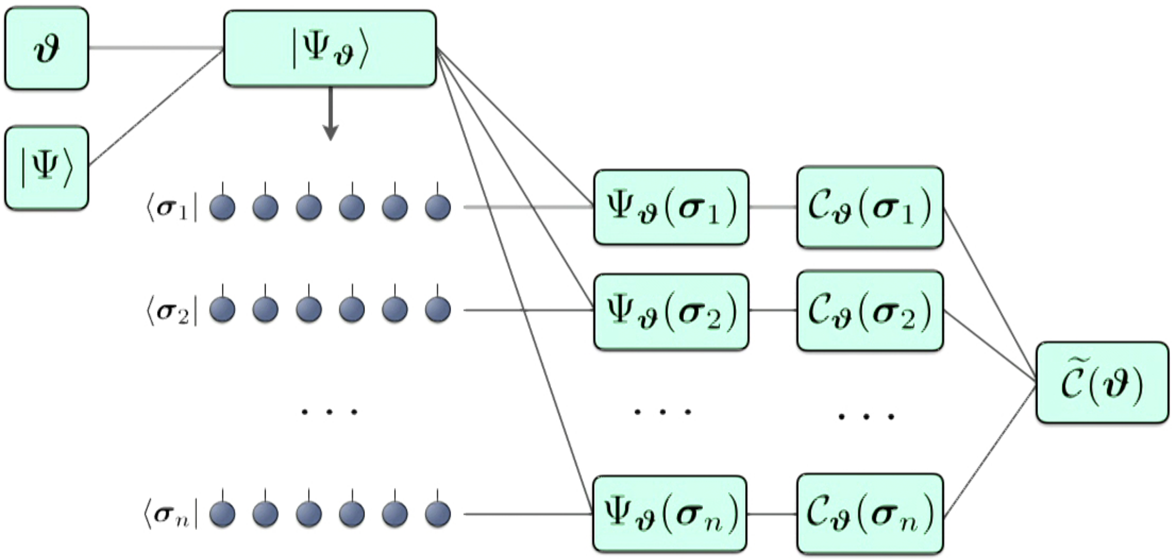
$$\frac{\partial \mathcal{C}(\boldsymbol{\vartheta})}{\partial \boldsymbol{\vartheta}} = \frac{\partial Y}{\partial T_n} \frac{\partial T_n}{\partial T_{n-1}} \cdots \frac{\partial T_2}{\partial T_1} \frac{\partial T_1}{\partial \boldsymbol{\vartheta}}$$

$$\overline{T}_j = \sum_{i \in \mathcal{N}(j)} \overline{T}_i \frac{\partial T_i}{\partial T_j}$$



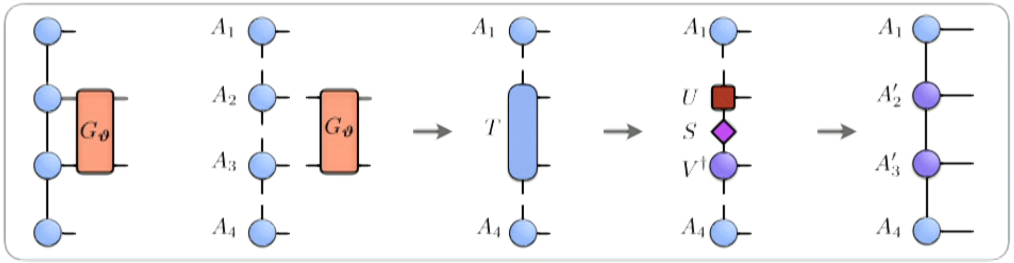
The computational graph

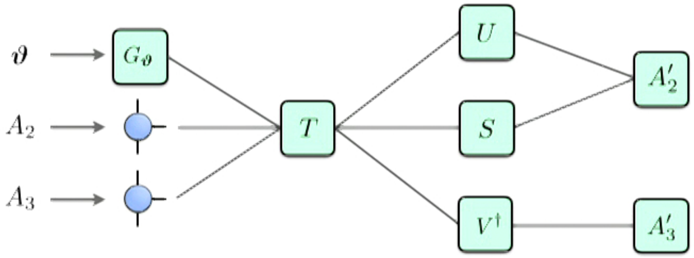
Approximate cost function: $\mathcal{C}(\boldsymbol{\vartheta}) \approx \widetilde{\mathcal{C}}(\boldsymbol{\vartheta}) = \frac{1}{M}\sum_{\boldsymbol{\sigma}_j} \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j)$ $\{\boldsymbol{\sigma}_j\} \sim p_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}) = |\Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma})|^2$ (perfect sampling)

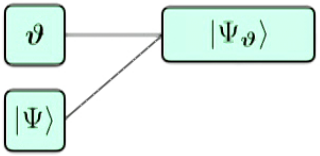


The computational graph

Forward pass: output state

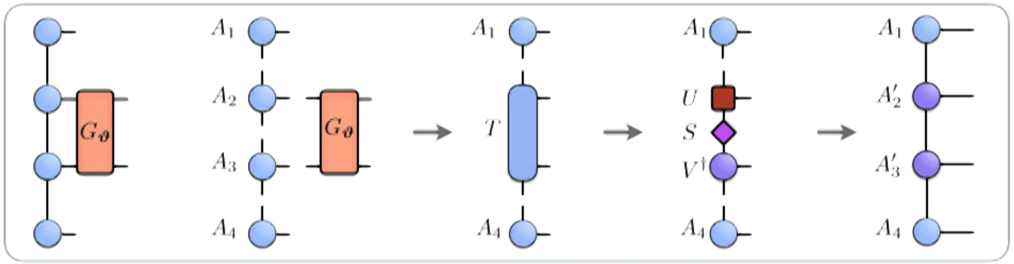


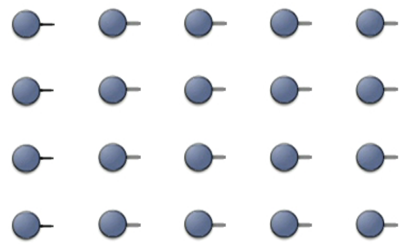


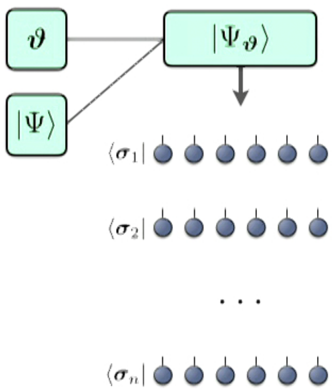


The computational graph

Forward pass: sampling

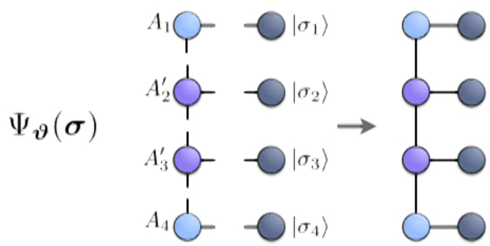


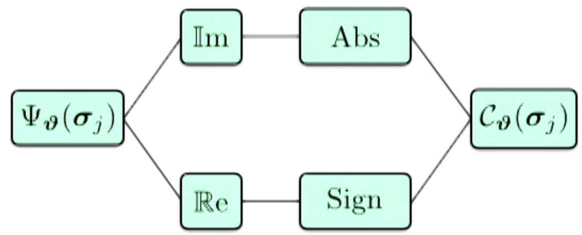


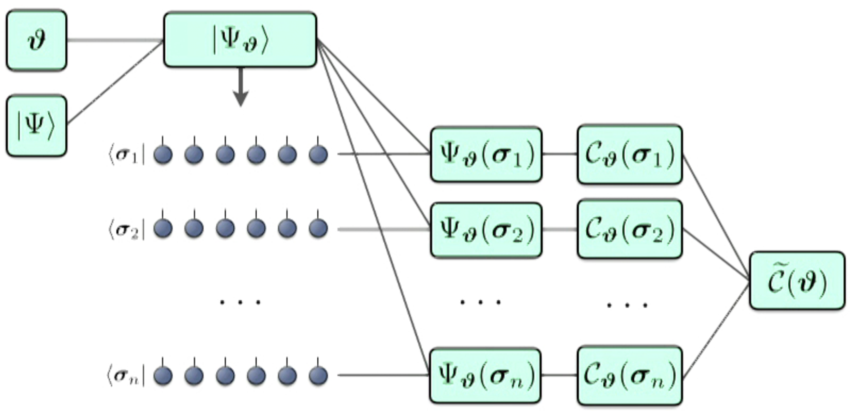


The computational graph

Forward pass: cost evaluation







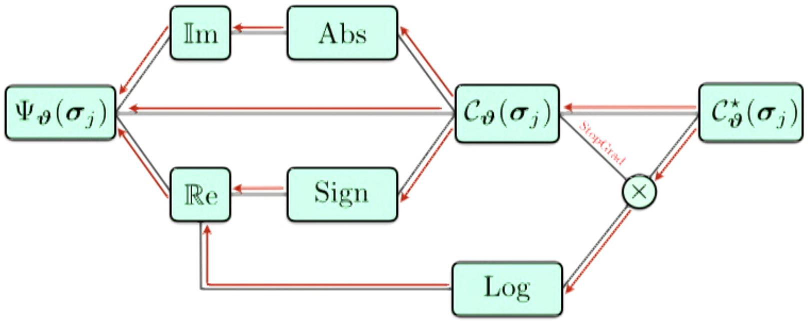
The computational graph

Backward pass

Note: $\nabla_{\vartheta}\widetilde{\mathcal{C}}(\vartheta) = \frac{1}{M}\sum_{\sigma_j}\nabla_{\vartheta}\mathcal{C}_{\vartheta}(\sigma_j) \neq \mathcal{G}(\vartheta) = \nabla_{\vartheta}\mathcal{C}(\vartheta)$

$$\mathcal{G}(\vartheta) \approx \widetilde{\mathcal{G}}(\vartheta) = \frac{1}{M}\sum_{\sigma_j}\Big[\nabla_{\vartheta}\mathcal{C}_{\vartheta}(\sigma_j) + 2\,\mathcal{C}_{\vartheta}(\sigma_j)\mathbb{R}\mathrm{e}\big[\nabla_{\vartheta}\log\Psi_{\vartheta}(\sigma_j)\big]\Big]$$

$$\mathcal{C}^{\star}_{\vartheta}(\sigma_j) = \mathcal{C}_{\vartheta}(\sigma) + 2\{\mathcal{C}_{\vartheta}(\sigma)\}_{\mathrm{ng}}\,\mathbb{R}\mathrm{e}\big[\log\Psi_{\vartheta}(\sigma)\big]$$



Problem: No stable AD software with SVD gradients of complex-valued tensors.

The computational graph

Backward pass

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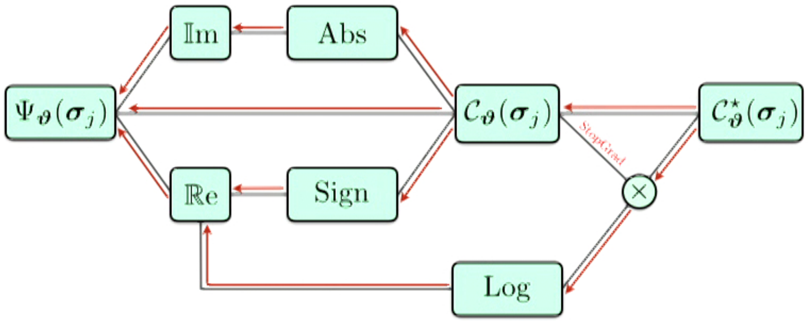

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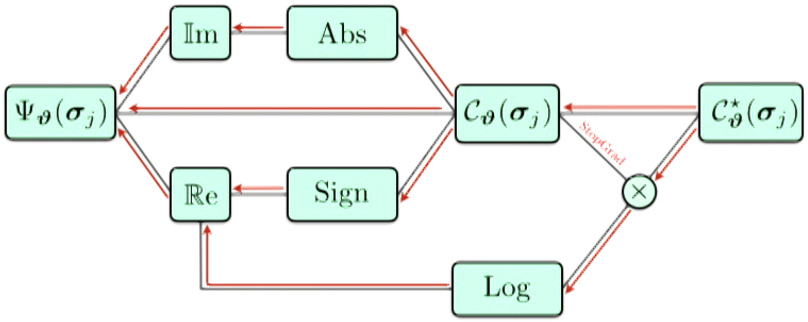
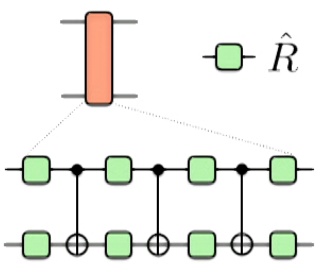
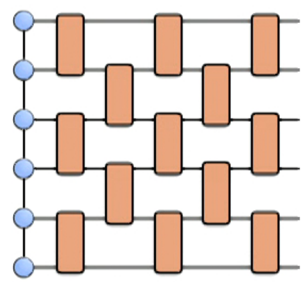


Problem: No stable AD software with SVD gradients of complex-valued tensors.

Two-qubit gate decomposition



Inefficient

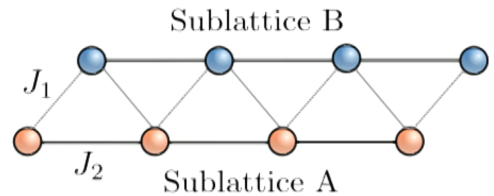


Numerical experiments

Two-leg triangular Heisenberg ladder

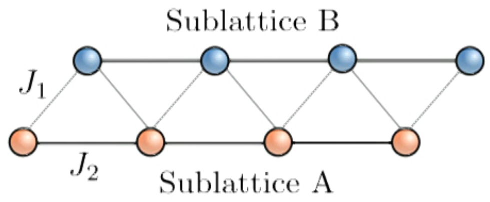
$$\hat{H} = J_1 \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + J_2 \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+2} + \frac{J_{\text{ring}}}{2} \sum_j \hat{\boldsymbol{P}}_{j,j+1,j+3,j+2} + h.c.$$

$$|\boldsymbol{S}^z\rangle = |S_1^z, \dots, S_N^z\rangle \qquad \hat{\boldsymbol{P}}_{i,j,k,l}|S_i^z, S_j^z, S_k^z, S_l^z\rangle = |S_l^z, S_i^z, S_j^z, S_k^z\rangle$$



Numerical experiments

Two-leg triangular Heisenberg ladder



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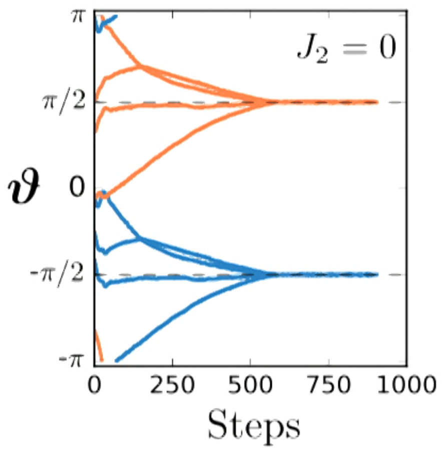
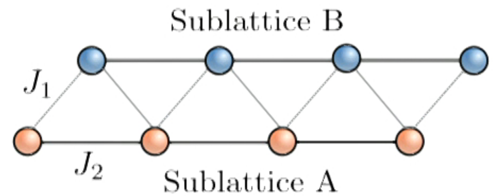
$$|\boldsymbol{S}^z\rangle = |S_1^z, \ldots, S_N^z\rangle \qquad \hat{\boldsymbol{P}}_{i,j,k,l}|S_i^z, S_j^z, S_k^z, S_l^z\rangle = |S_l^z, S_i^z, S_j^z, S_k^z\rangle$$

Marshall Sign



Numerical experiments

Two-leg triangular Heisenberg ladder



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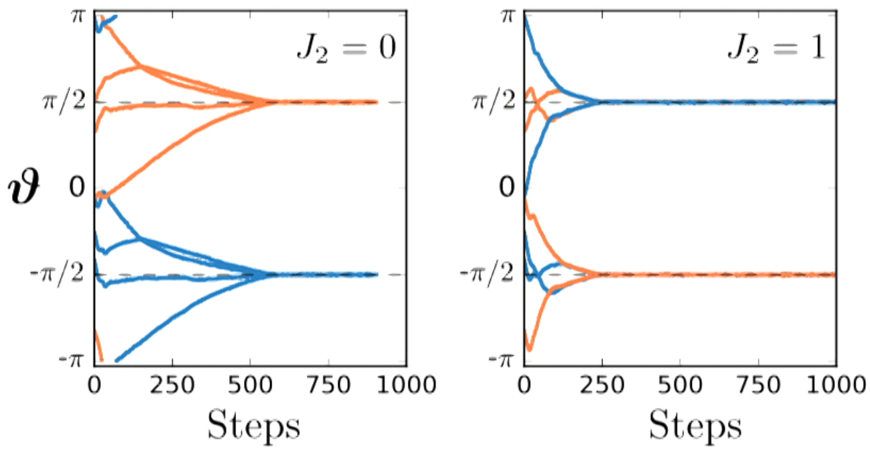
$$|\boldsymbol{S}^z\rangle = |S^z_1, \ldots, S^z_N\rangle \qquad \hat{\boldsymbol{P}}_{i,j,k,l}|S^z_i, S^z_j, S^z_k, S^z_l\rangle = |S^z_l, S^z_i, S^z_j, S^z_k\rangle$$

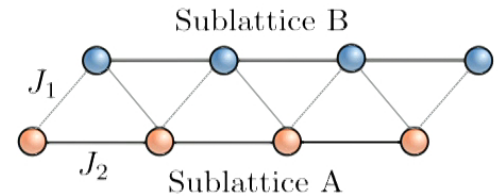
Marshall Sign



Numerical experiments

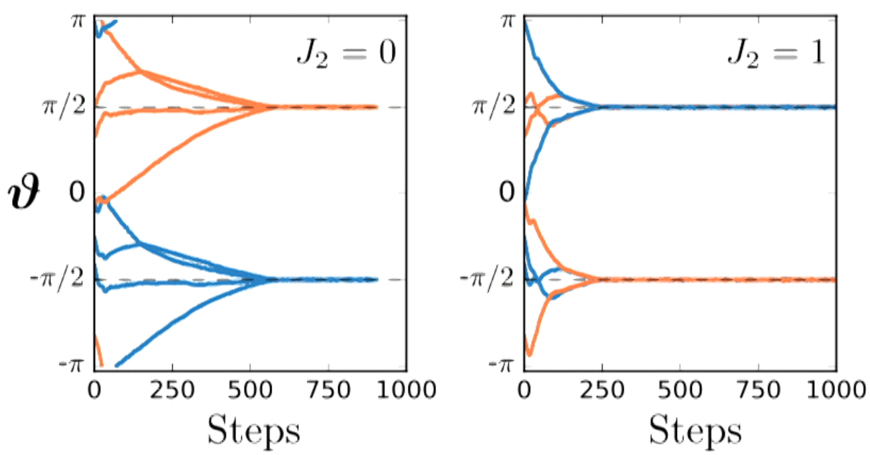
Two-leg triangular Heisenberg ladder

$$\hat{H} = J_1 \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + J_2 \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+2} + \frac{J_{\text{ring}}}{2} \sum_j \hat{\boldsymbol{P}}_{j,j+1,j+3,j+2} + h.c.$$

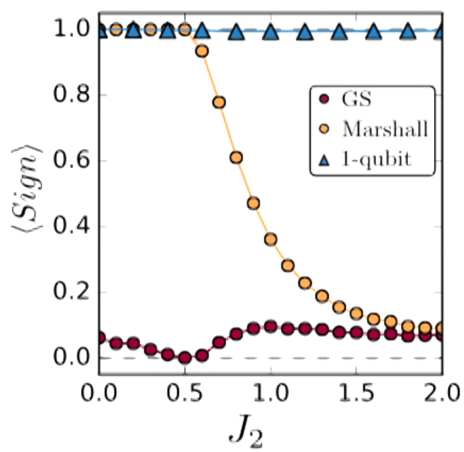


$$|\boldsymbol{S}^z\rangle = |S^z_1, \ldots, S^z_N\rangle \qquad \hat{\boldsymbol{P}}_{i,j,k,l}|S^z_i, S^z_j, S^z_k, S^z_l\rangle = |S^z_l, S^z_i, S^z_j, S^z_k\rangle$$

Marshall Sign

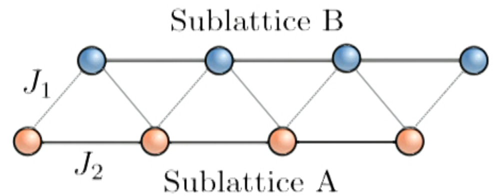


J1-J2



Numerical experiments

Two-leg triangular Heisenberg ladder



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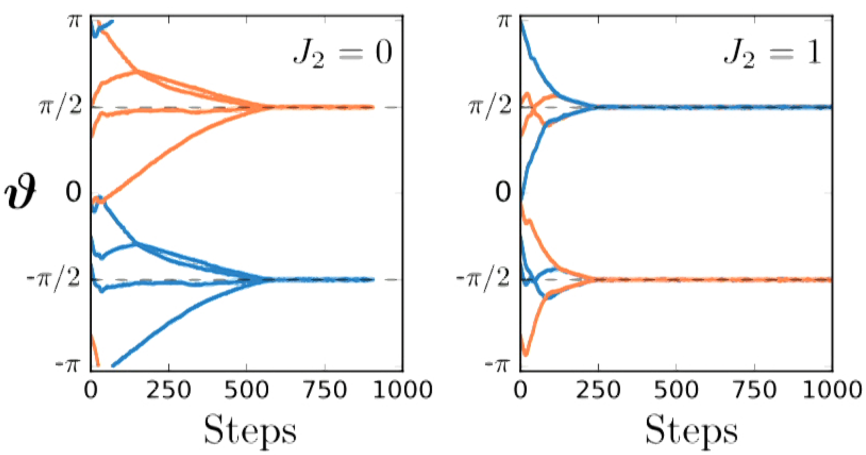
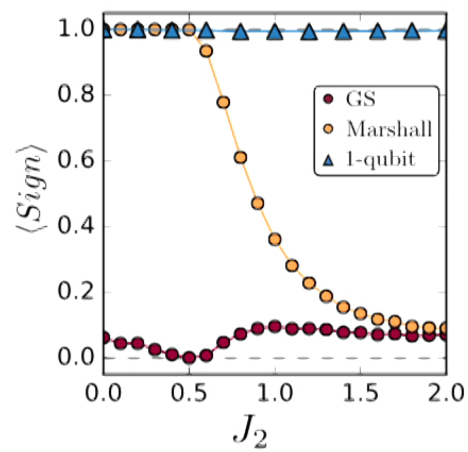
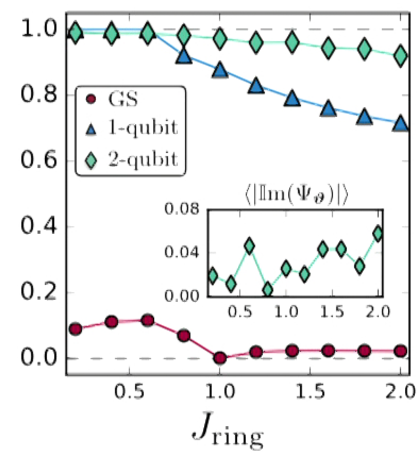


J1-J2



Bose Metal



Conclusions

Automated approach to discover non-negative representations of many-body wavefunctions.

Algorithm exploits automatic differentiation of tensor networks

Need stable AD primitives for complex-valued tensors.

Directions:

- Classification of the complexity = scaling of the depth with system size.
- Entanglement of positivization
- Positivization of path integrals

GT, J Carrasquilla, MT Fishman, RG Melko and MPA Fisher - arXiv:1906.04654

D Hangleiter, I Roth, D Nagaj and J Eisert - arXiv:1906.02309
R Levy and BK Clark - arXiv:1907.02076

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