

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 "probability" 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**

Center for Computational Quantum Physics  
Flatiron Institute

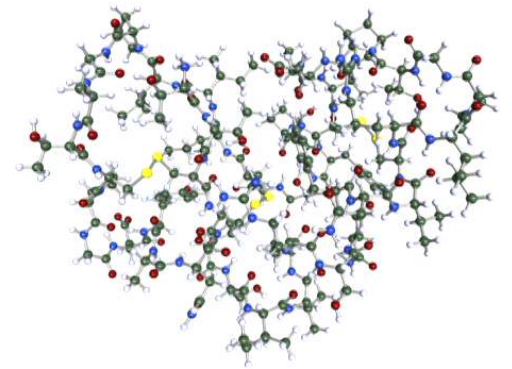


Machine Learning for Quantum Design

Perimeter Institute for Theoretical Physics  
July 8th 2019

# Sign Structure of Quantum States

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





# Sign Structure of Quantum States

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



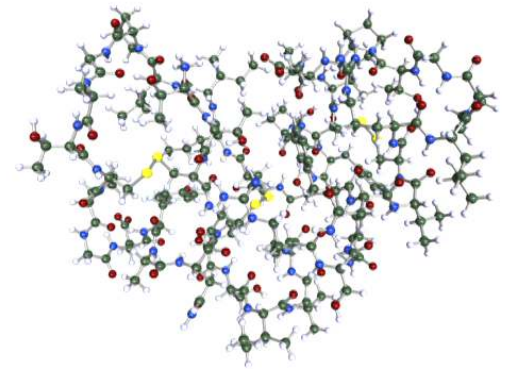
How to classify its complexity?

How to get rid of it?

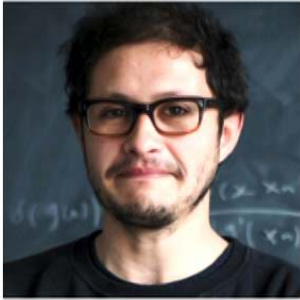
When is it intrinsic?

Relationship with entanglement?

Quantum Monte Carlo?



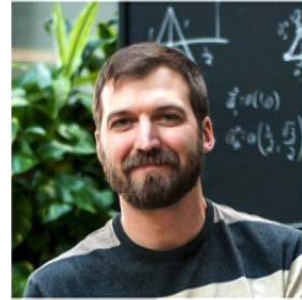
## Collaborators



Juan Carrasquilla  
Vector Institute & UW



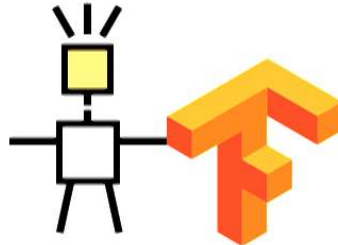
Matthew Fishman  
Flatiron Institute



Roger Melko  
Perimeter Institute & UW



Matthew Fisher  
UCSB



# Path integrals

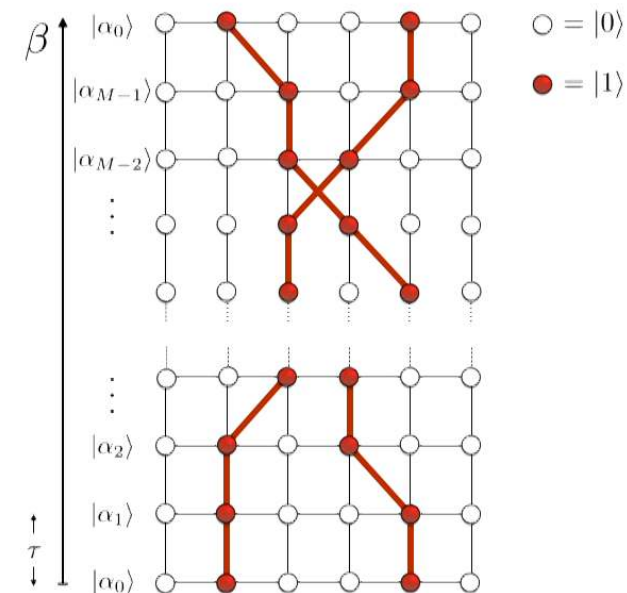
(d+1) representation of the quantum partition function:

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

$$= \sum_{\{\alpha\}} W(\{\alpha\}) \quad W(\{\alpha\}) \Rightarrow \text{Weight of a world-line.}$$

“Positive-definite” path integrals:

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



# Path integrals

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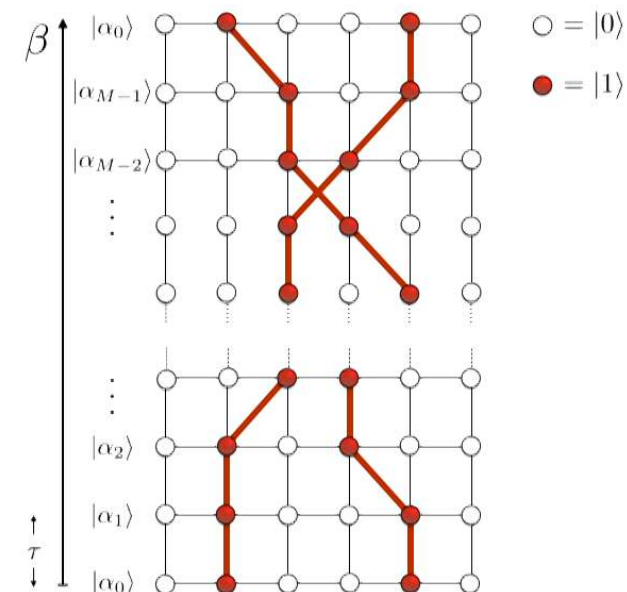
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## Quantum Monte Carlo

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

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



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# The sign problem of Quantum Monte Carlo

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

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

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

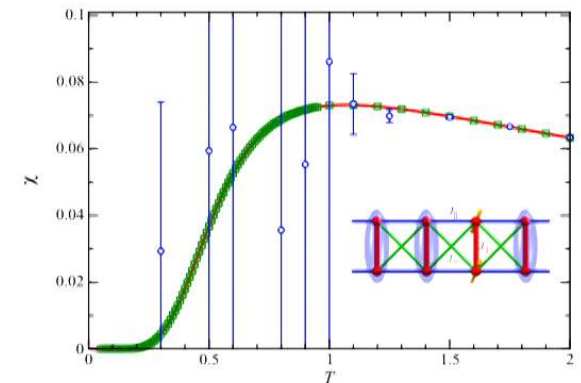
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But...  $\frac{\Delta \text{Sign}}{\langle \text{Sign} \rangle} \approx \frac{e^{\beta N \Delta f}}{\sqrt{N_{mc}}}$   Sign structure:  $\text{Sign } W(\{\alpha\})$

Honecker *et al* (2016)



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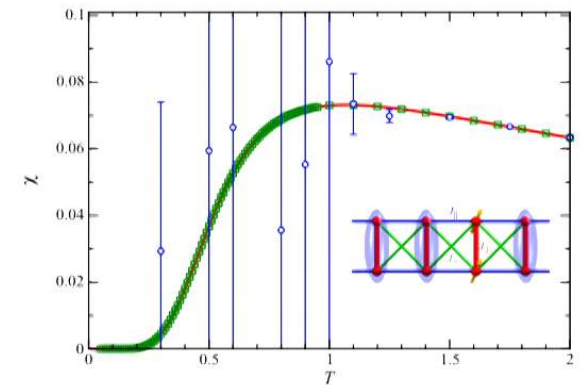
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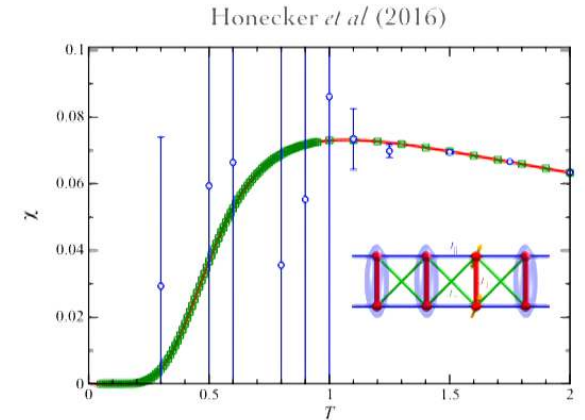
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 Generic solution is NP-hard.

 Specific solutions  
Partial alleviation



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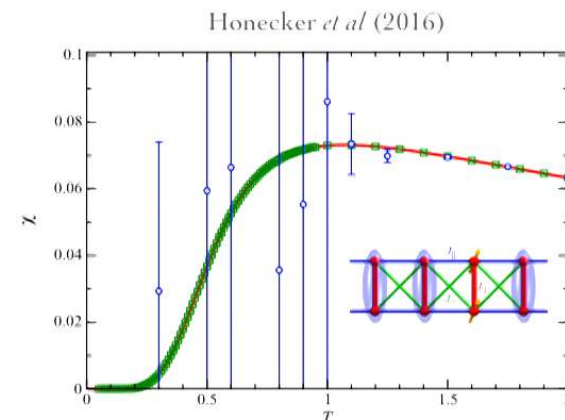


Loh, Gubernatis, Scalettar, White, Scalapino and Sugar (1990)  
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 Specific solutions  
 Partial alleviation



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)

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# The sign problem of ~~Quantum Monte Carlo~~

Impossibility of capturing underlying physics with classical representation.

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

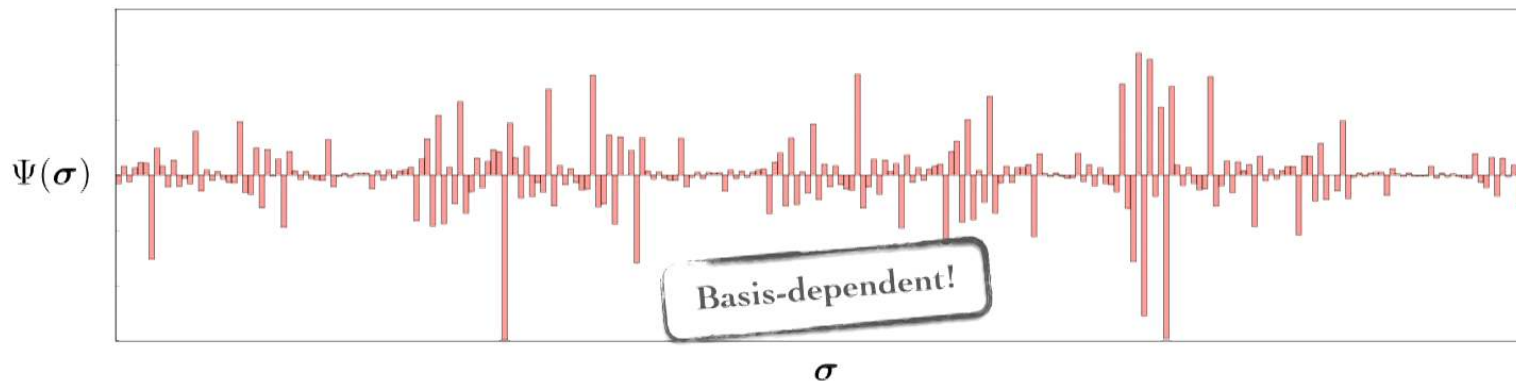
Sign structure:  $\text{Sign}(\Psi(\sigma))$      $\Psi(\sigma) \geq 0 \ \forall |\sigma\rangle \Rightarrow \langle\text{Sign}(\Psi(\sigma))\rangle = 1$      $\Psi(\sigma) \longleftrightarrow P(\sigma)$  "Classical"

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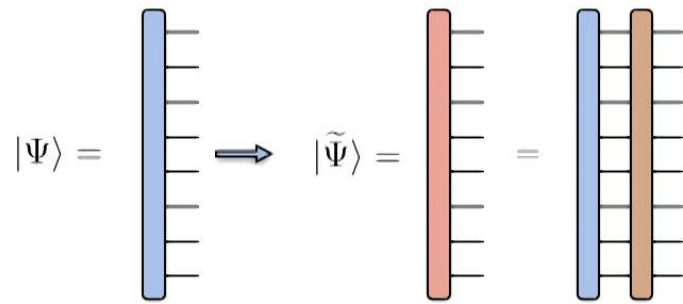
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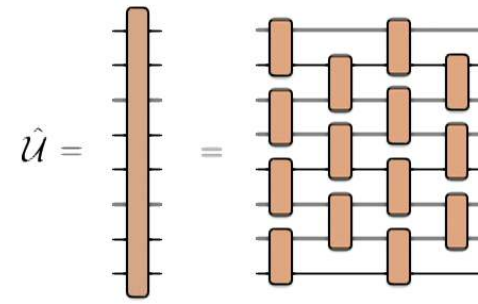
# Wavefunction positivization

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

Generally:



Unitary compiled into local quantum gates

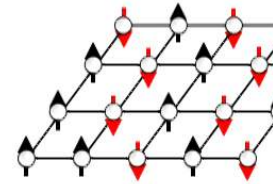
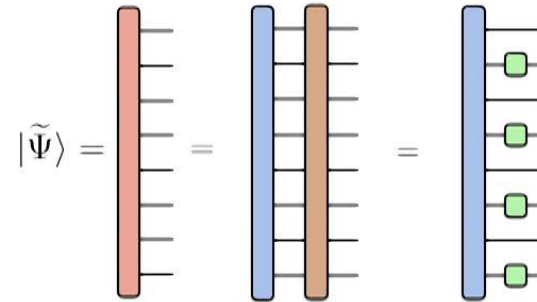


# Wavefunction positivization

## Quantum anti-ferromagnets

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

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

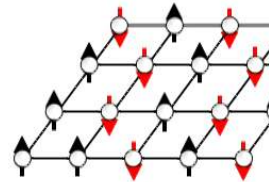
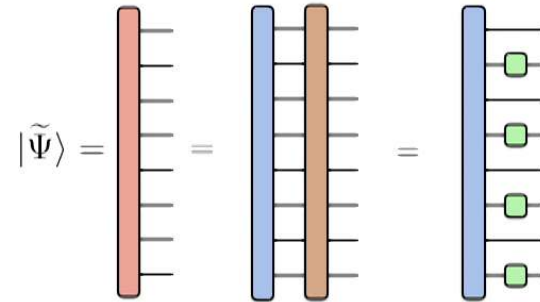


# Wavefunction positivization

## Quantum anti-ferromagnets

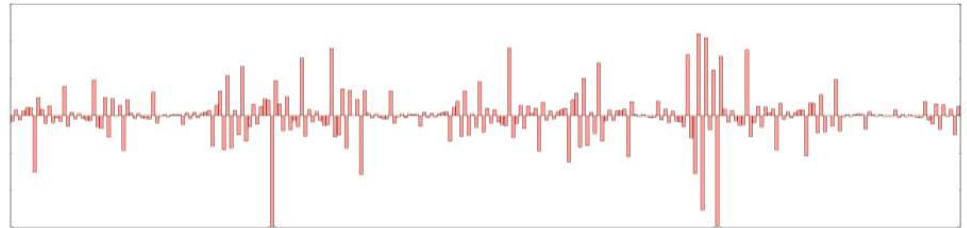
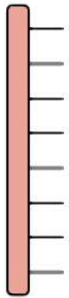
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## Apparent or intrinsic?

$|\Psi\rangle$

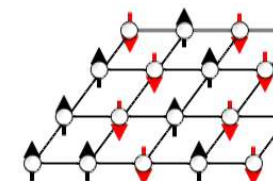
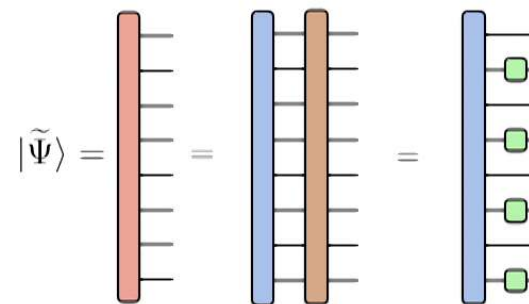


# Wavefunction positivization

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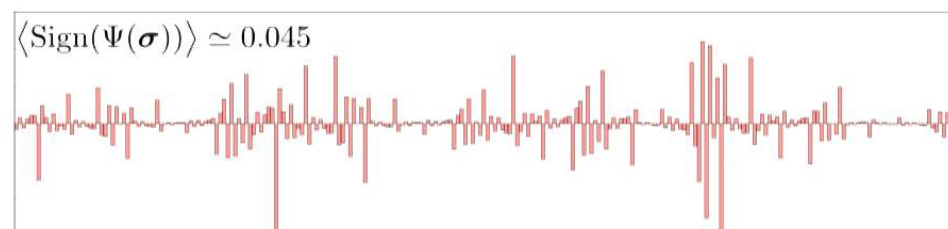
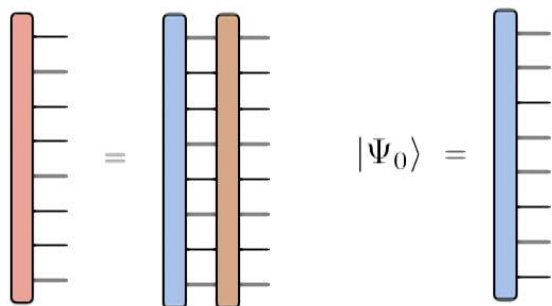
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## Apparent or intrinsic?

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

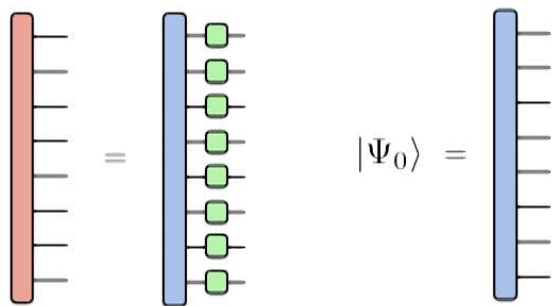


# Wavefunction positivization

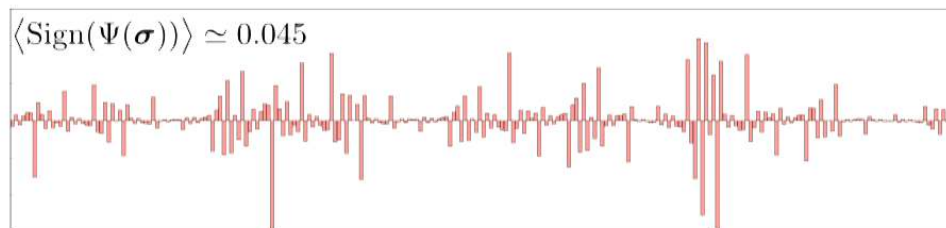
How would you even know?

Apparent or intrinsic?

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



Positive state a few gates away.



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## Automating insights

**Autonomous search of local bases that positivize wavefunctions**

### Ingredients

Appropriate representation

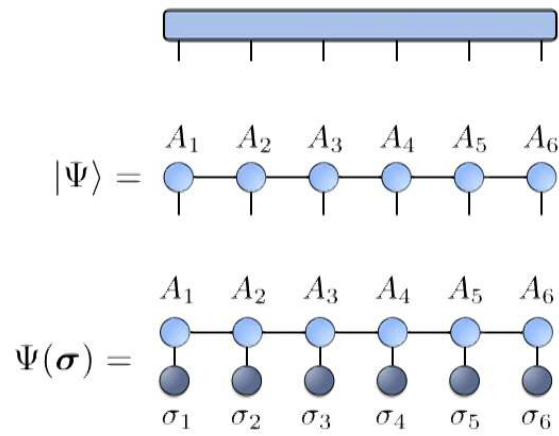
Good cost function

Adequate software

# 1. Tensor network representation

Input wavefunction = Matrix Product State

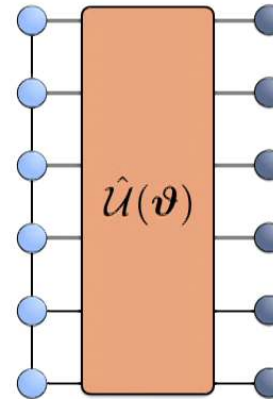
$$|\Psi\rangle = \sum_{\sigma} A_1^{\sigma_1} A_2^{\sigma_2} \dots A_N^{\sigma_N} |\sigma_1, \sigma_2, \dots, \sigma_N\rangle$$



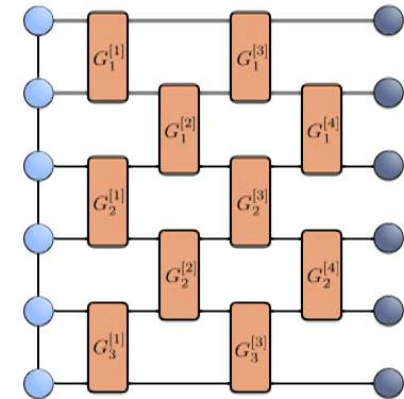
Local unitary transformation = Quantum Circuit

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

$$\Psi_{\vartheta}(\sigma) = \langle \sigma | \hat{U}_{\vartheta} | \Psi \rangle$$



$$\hat{G}_k^{[\ell]} = e^{-i\hat{\Gamma}_k^{[\ell]}}$$



## 2. The cost function

### Definition

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

$$\text{Sign}(\text{Re}[\Psi_{\vartheta}(\sigma)]) = 1 \quad \text{Im}[\Psi_{\vartheta}(\sigma)] = 0 \quad \forall |\sigma\rangle$$

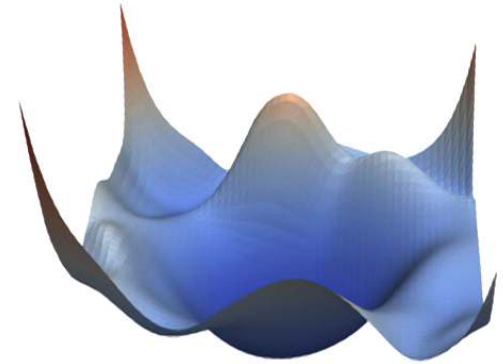
Most conveniently expressed as averages over the output distribution:

$$\sum_{\sigma} |\Psi_{\vartheta}(\sigma)|^2 |\text{Im}[\Psi_{\vartheta}(\sigma)]| = 0 \quad \text{and} \quad \sum_{\sigma} |\Psi_{\vartheta}(\sigma)|^2 \text{Sign}(\text{Re}[\Psi_{\vartheta}(\sigma)]) = 1$$

$$\text{Cost function: } \mathcal{C}(\vartheta) = \sum_{\sigma} |\Psi_{\vartheta}(\sigma)|^2 \mathcal{C}_{\vartheta}(\sigma) \quad \mathcal{C}_{\vartheta}(\sigma) = \gamma |\text{Im}[\Psi_{\vartheta}(\sigma)]| - (1 - \gamma) \text{Sign}(\text{Re}[\Psi_{\vartheta}(\sigma)])$$

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

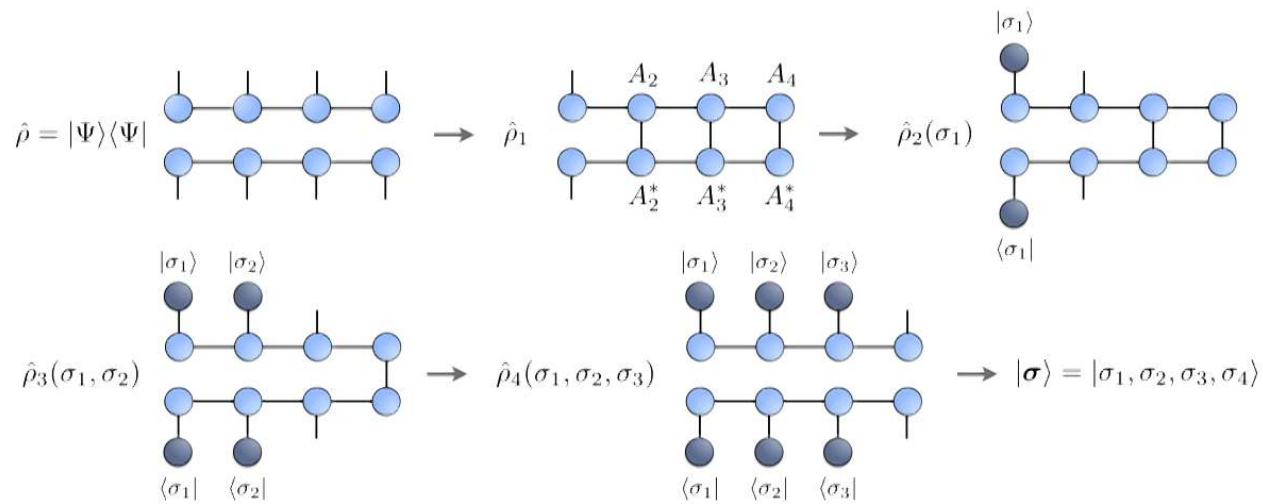
Example: Gradient Descent  $\vartheta \rightarrow \vartheta - \eta \mathcal{G}(\vartheta) \quad \mathcal{G}(\vartheta) = \nabla_{\vartheta} \mathcal{C}(\vartheta)$



## 2. The cost function

### Computation

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



# 3. Differentiable programming

## Automatic differentiation

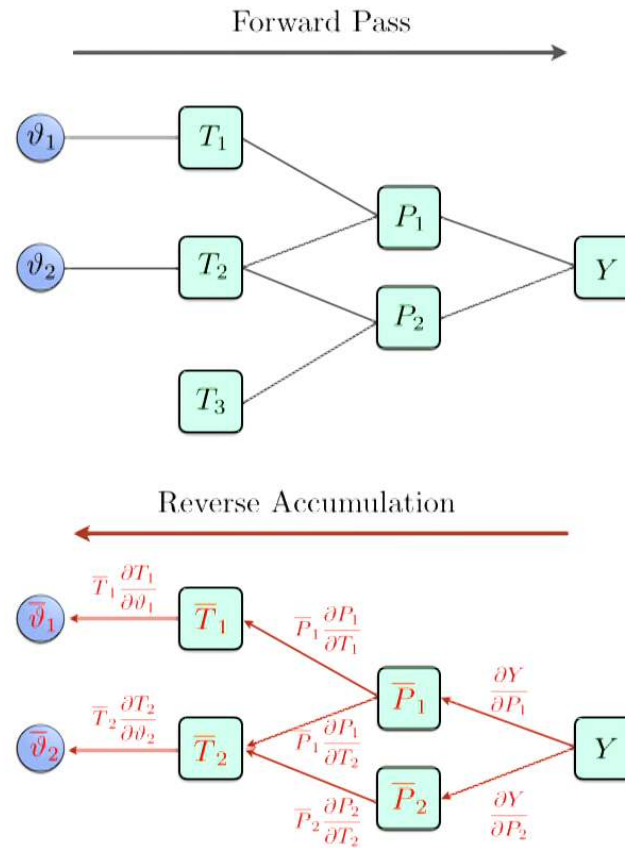
Build a computational graph:

$$\boldsymbol{\vartheta} \rightarrow T_1 \rightarrow T_2 \rightarrow \dots \rightarrow T_n \rightarrow \mathcal{C}(\boldsymbol{\vartheta})$$

Compute derivative from the output:

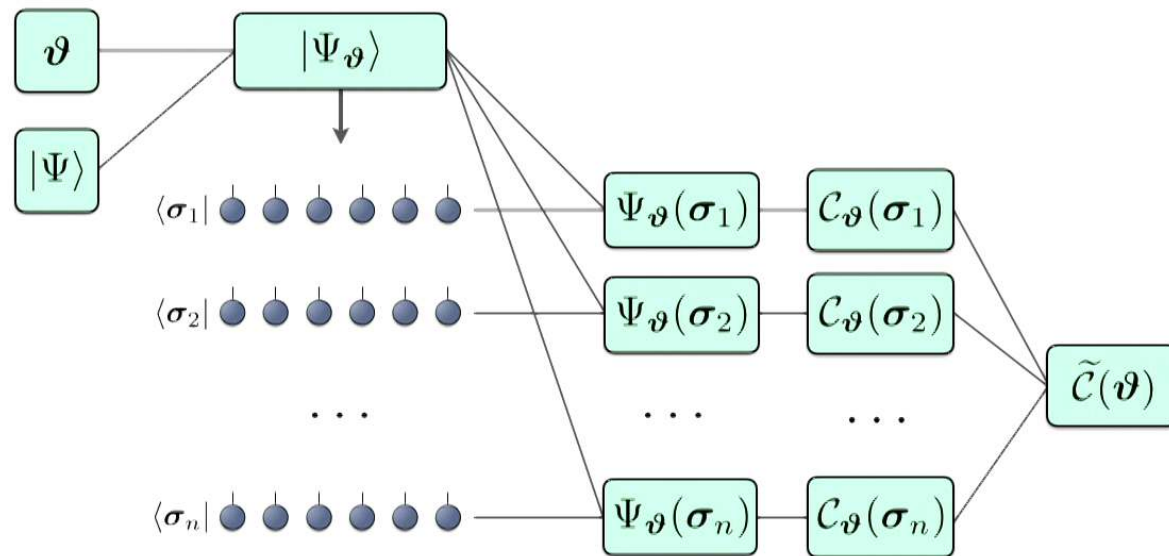
$$\frac{\partial \mathcal{C}(\boldsymbol{\vartheta})}{\partial \boldsymbol{\vartheta}} = \frac{\partial Y}{\partial T_n} \frac{\partial T_n}{\partial T_{n-1}} \dots \frac{\partial T_2}{\partial T_1} \frac{\partial T_1}{\partial \boldsymbol{\vartheta}}$$

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



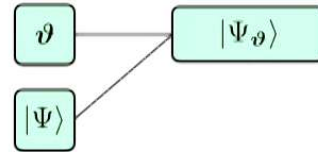
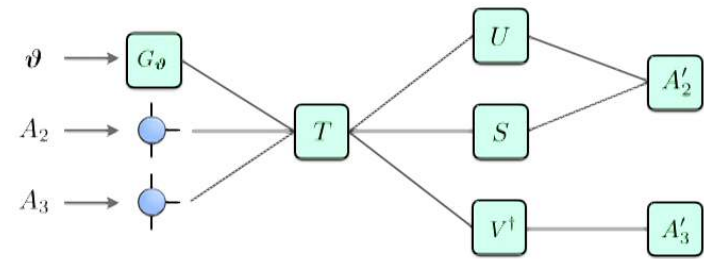
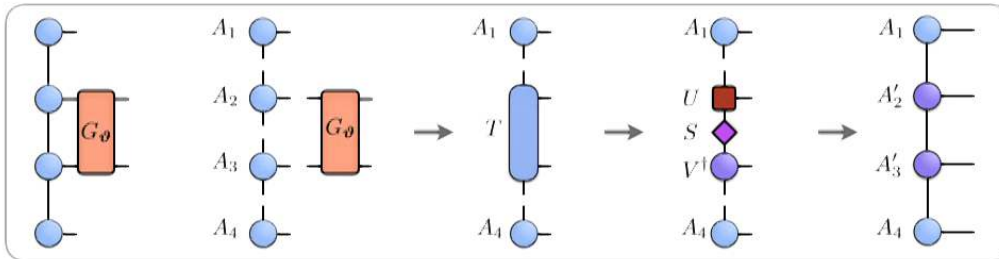
# The computational graph

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



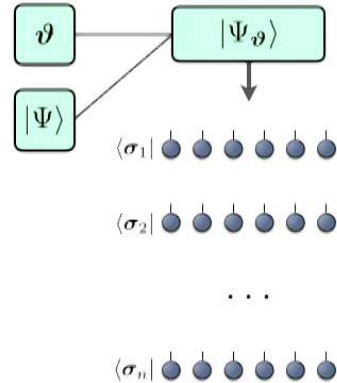
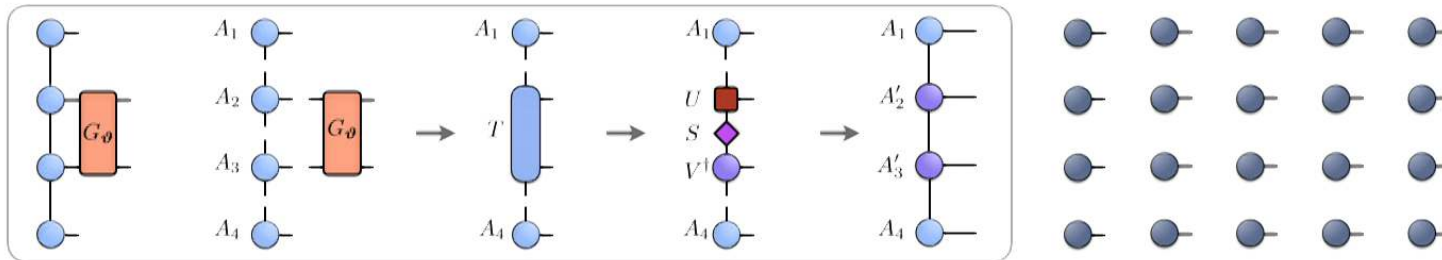
# The computational graph

Forward pass: output state



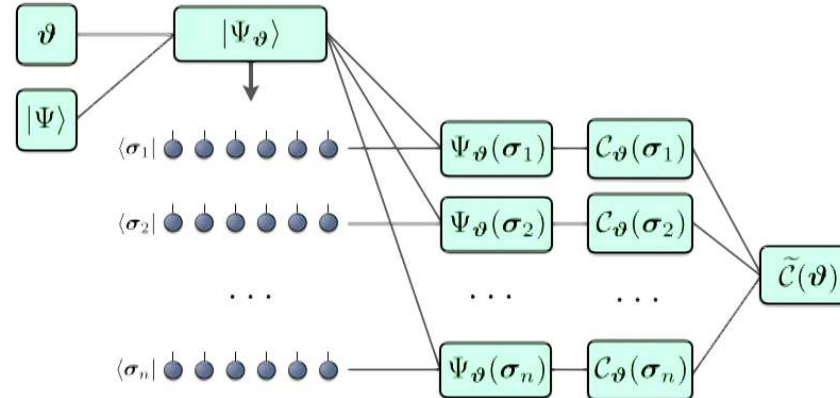
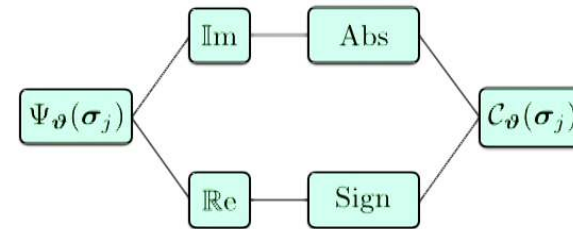
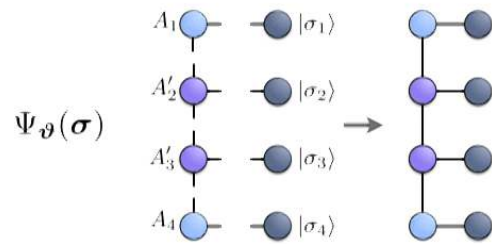
# The computational graph

Forward pass: sampling



# The computational graph

Forward pass: cost evaluation



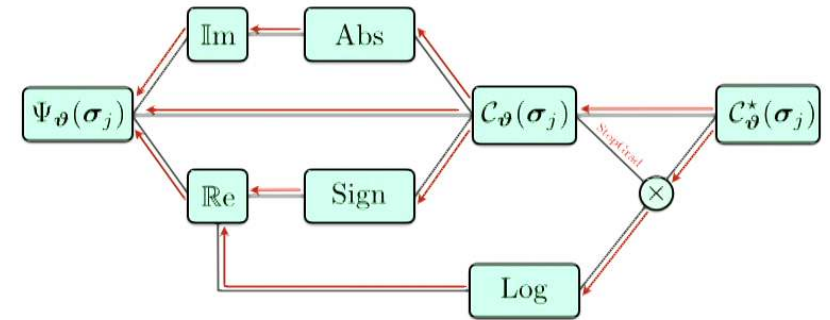
# The computational graph

## Backward pass

Note:  $\nabla_{\boldsymbol{\vartheta}} \tilde{\mathcal{C}}(\boldsymbol{\vartheta}) = \frac{1}{M} \sum_{\boldsymbol{\sigma}_j} \nabla_{\boldsymbol{\vartheta}} \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) \neq \mathcal{G}(\boldsymbol{\vartheta}) = \nabla_{\boldsymbol{\vartheta}} \mathcal{C}(\boldsymbol{\vartheta})$

$$\mathcal{G}(\boldsymbol{\vartheta}) \approx \tilde{\mathcal{G}}(\boldsymbol{\vartheta}) = \frac{1}{M} \sum_{\boldsymbol{\sigma}_j} \left[ \nabla_{\boldsymbol{\vartheta}} \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) + 2 \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) \operatorname{Re}[\nabla_{\boldsymbol{\vartheta}} \log \Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j)] \right]$$

$$\mathcal{C}_{\boldsymbol{\vartheta}}^*(\boldsymbol{\sigma}_j) = \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) + 2 \{ \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) \}_{\text{ng}} \operatorname{Re}[\log \Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j)]$$



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

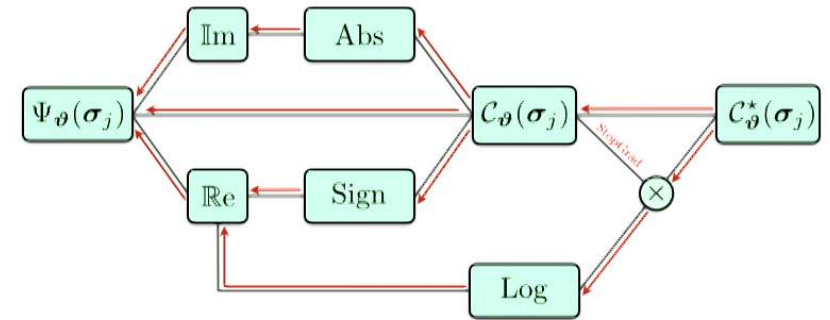
# The computational graph

## Backward pass

Note:  $\nabla_{\boldsymbol{\vartheta}} \tilde{\mathcal{C}}(\boldsymbol{\vartheta}) = \frac{1}{M} \sum_{\boldsymbol{\sigma}_j} \nabla_{\boldsymbol{\vartheta}} \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) \neq \mathcal{G}(\boldsymbol{\vartheta}) = \nabla_{\boldsymbol{\vartheta}} \mathcal{C}(\boldsymbol{\vartheta})$

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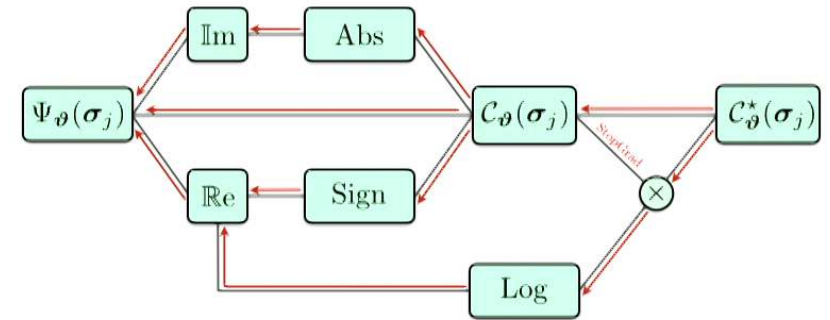
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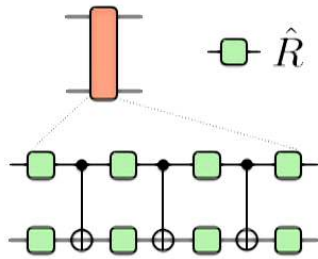
$$\mathcal{G}(\boldsymbol{\vartheta}) \approx \tilde{\mathcal{G}}(\boldsymbol{\vartheta}) = \frac{1}{M} \sum_{\boldsymbol{\sigma}_j} \left[ \nabla_{\boldsymbol{\vartheta}} \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) + 2 \mathcal{C}_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j) \operatorname{Re}[\nabla_{\boldsymbol{\vartheta}} \log \Psi_{\boldsymbol{\vartheta}}(\boldsymbol{\sigma}_j)] \right]$$

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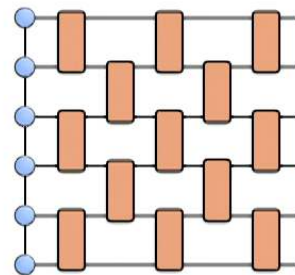


**Problem:** No stable AD software with SVD gradients of complex-valued tensors.

Two-qubit gate decomposition



Inefficient

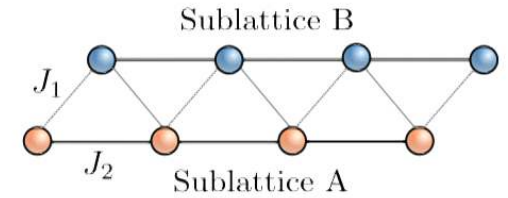


# Numerical experiments

## Two-leg triangular Heisenberg ladder

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

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

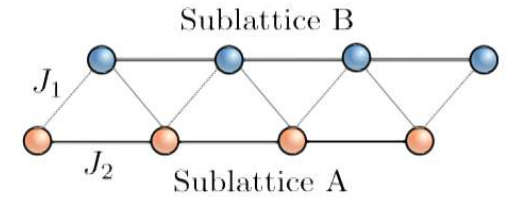


# Numerical experiments

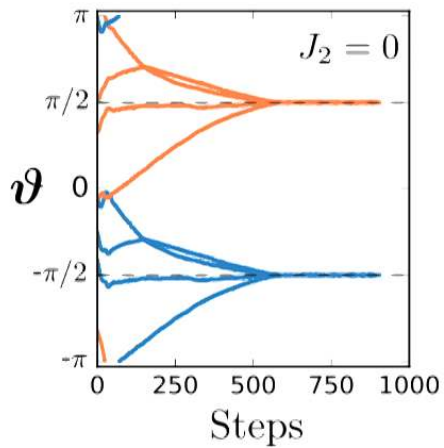
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## Marshall Sign

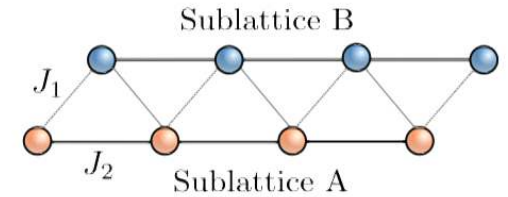


# Numerical experiments

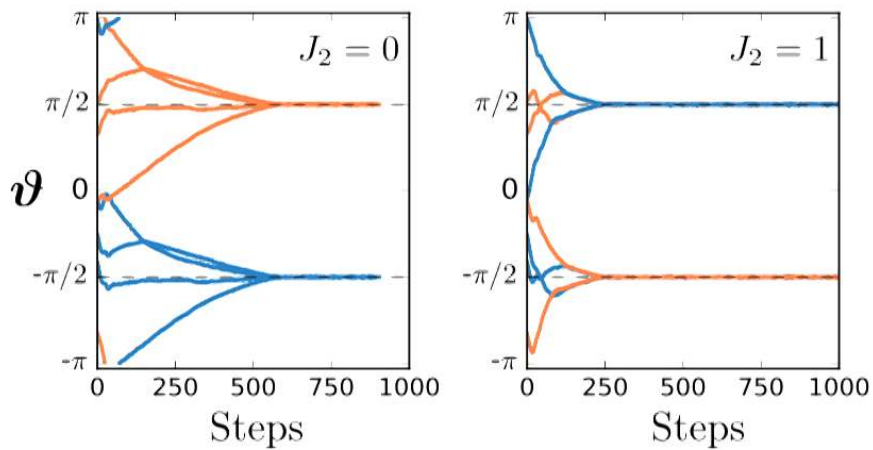
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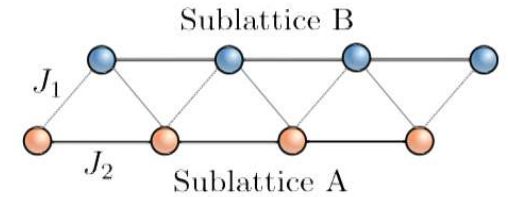


# Numerical experiments

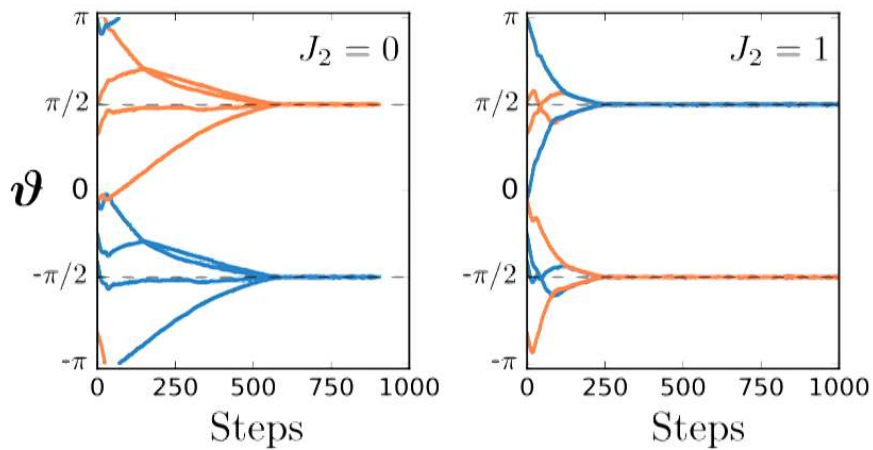
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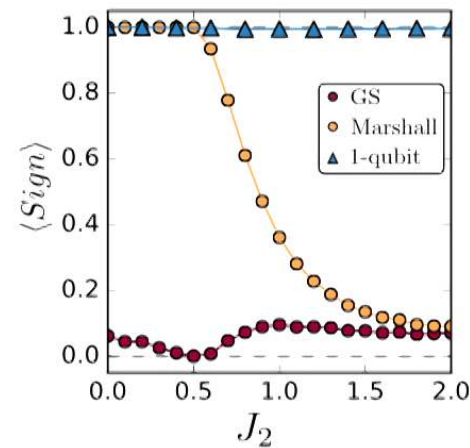
$$|S^z\rangle = |S_1^z, \dots, S_N^z\rangle \quad \hat{P}_{i,j,k,l} |S_i^z, S_j^z, S_k^z, S_l^z\rangle = |S_l^z, S_i^z, S_j^z, S_k^z\rangle$$



### Marshall Sign



### J1-J2



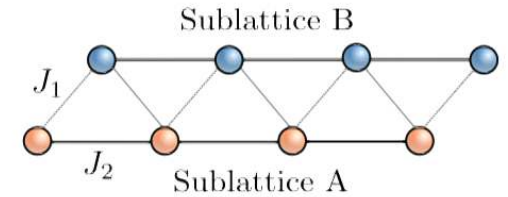
# Numerical experiments

## Two-leg triangular Heisenberg ladder

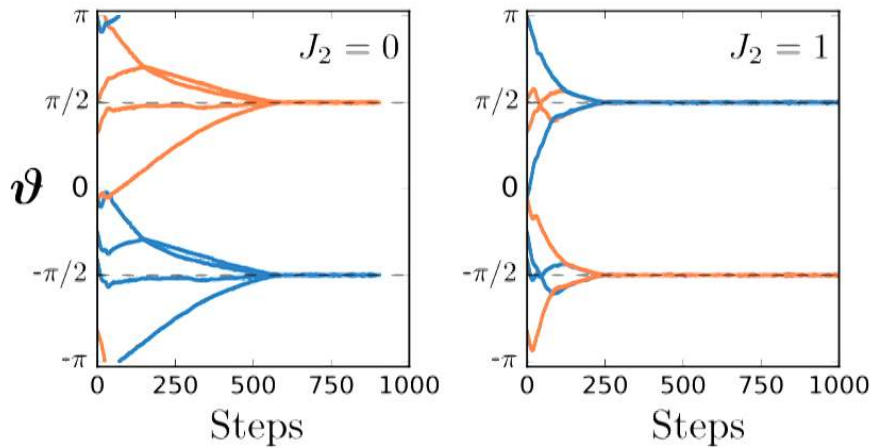
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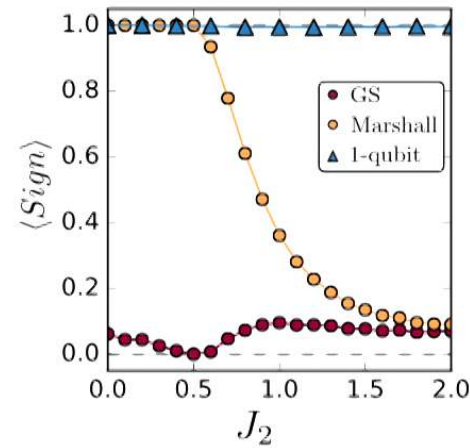
$$\hat{P}_{i,j,k,l} |S_i^z, S_j^z, S_k^z, S_l^z\rangle = |S_l^z, S_i^z, S_j^z, S_k^z\rangle$$



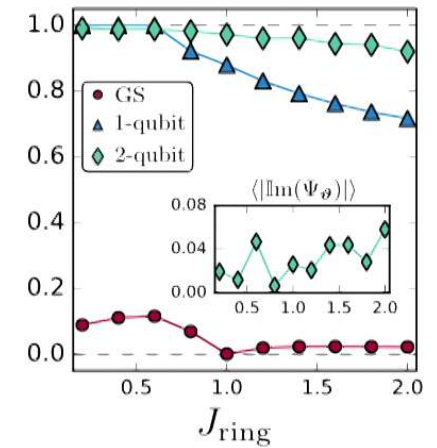
### Marshall Sign



### J1-J2



### Bose Metal



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## 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