Entanglement-inspired variational quantum circuits

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Motivation

Goal: Efficiently simulate quantum systems with quantum computers
Problem: Current NISQ devices are noisy and only few qubits are available (*Quantum 2, 79 (2018)*)
Approach I: Circuit cutting

- Technique for dividing a circuit into smaller sub-circuits
- Decreasing the hardware demands and potentially mitigating errors introduced through gate operations
- Classical information exchange of the different sub-circuits is costly
- Only reasonable to use this method if few cuts are sufficient in order to divide the circuit efficiently

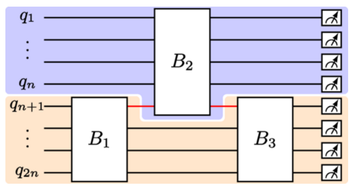


Fig. 1: Circuit cutting (*Phys. Rev. Lett. 125, 150504 (2020)*)

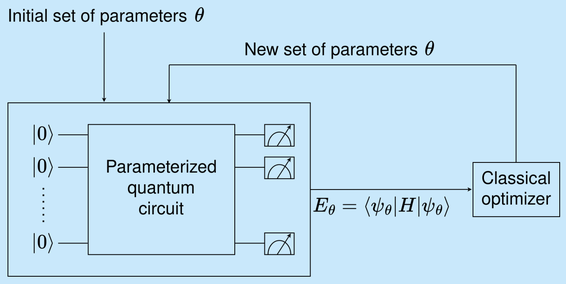
- **In which systems is it useful to apply this method and how can we design circuits that adhere to this principle?**

Approach II: Preparation of initial state

- Use entanglement information about system
- Include long-range entanglement in the initial state of the VQE by building singlets
- **Can we achieve a better convergence compared to a VQE initialized with a product state?**

Method: Variational quantum eigensolver (VQE)

- VQE (*Nature Reviews Physics 3, 625 (2021)*) tries to approximate the ground state of a system
- Optimizing parameters of a quantum circuit with several quantum-classical optimization loops



Model I: transverse-field Ising chain

Model

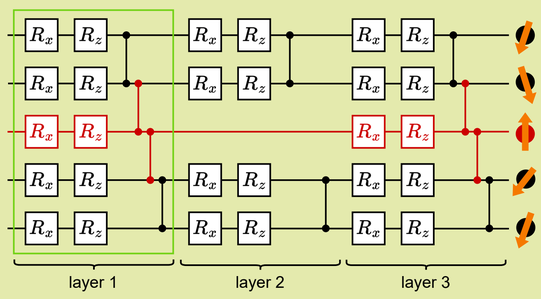
Want to find system that can be properly described by an ansatz that needs few cuts to be divided
→ Use system that has separate structure itself:

- Study behaviour of quantum critical spin chain (here: finite chain with odd number of spins)
- Add impurity by applying a magnetic field to central spin
- Fixing central spin leads to separation of left and right part of chain

- Transverse-field Ising model (TFIM): $H_{\mathrm{TFIM}} = \sum_i \left(-\sigma_i^z\sigma_{i+1}^z + h^x\sigma_i^x\right) + h_0^z\sigma_0^z$
  - $h^x = -1.0$ is disordering magnetic field
  - Last term describes the impurity at the central spin of the chain

Parametrized quantum circuit

- Consisting of x-rotation, z-rotation and R_{zz} gates as depicted
- Using open boundary conditions
- Focus on influence of different numbers and positions of entangling gates on accuracy depending on number of layers
- Circuit cutting: want to find circuit which can be divided by few cuts while still giving a certain accuracy



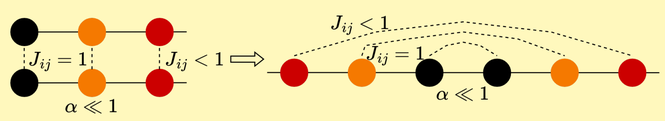
- To reduce number of cuts necessary, we reduce number of entangling gates
- Vary number of layers in which gates are applied to central spin/ qubit
- Notation: $x = $ ["layers including gates applied to central spin"], i.e., $x = [1, 3]$ in example

Model II: spin-ladder chain

Model

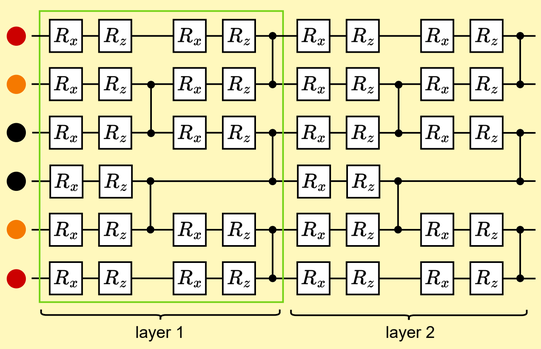
System with entanglement across spins that are several sites apart from each other

- Spin-ladder chain: $H_{\mathrm{SL}} = \sum_{i,j=n-(i-1)} \left(J_{ij}\vec{S}_i\vec{S}_j\right) + \alpha\sum_i \left(\vec{S}_i\vec{S}_{i+1}\right)$
  - $\alpha \ll 1$
  - $J_{ij} = 1$ except for one coupling (the two spins with the largest distance)
  - First sum is chosen such that we effectively describe a spin ladder mapped to a 1D system



Parametrized quantum circuit

- Consisting of x-rotation, z-rotation and R_{zz} gates as depicted
- Using open boundary conditions
- Usually $|0\rangle^{\otimes n}$ is used as initial state of VQE
- We use initial state which consists of singlets between all spins coupled by J_{ij}



Results I: Energy

Fig. 2: Varying x

- Variationally optimized energy E' for different number of layers while varying x for 9 spins
- Compared to exact energy E: $\varepsilon_{\mathrm{rel}} = \left(E - E'\right)/E$
- Accuracy converges to plateau for finite length of x
- Value of plateau depends on absolute number of entangling gates
- By adding layer to x, plateau value improves

Fig. 3: Plateau values

- Plateau values for different number of x with and without impurity for different system sizes
- By increasing number of layers in x, the accuracy increases for all chain lenghts

Without impurity

- Difference of accuracy for different number x decreases with increasing system size

With impurity

- Decreasing difference not visible due to reaching machine precision
- For larger system sizes only a single entangling gate with the central spin is needed to achieve high accuracy
- Even better accuracy than without impurity with $3x$

Conclusion I (a)

- **Possible to read off the number of cuts necessary to achieve a desired accuracy with a VQE calculation**
- Possible to estimate a priori the needed number of entangling gates depending on impurity strenghts when constructing a VQE solution for another system

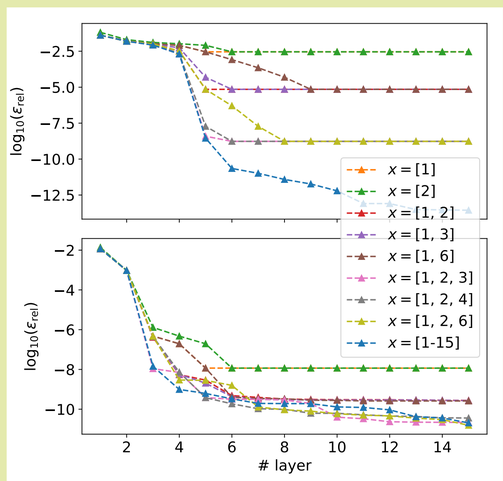


Fig. 2: Accuracy depending on depth of circuit for $h_0^z = 0.0$ (top) and $h_0^z = -10.0$ (bottom).

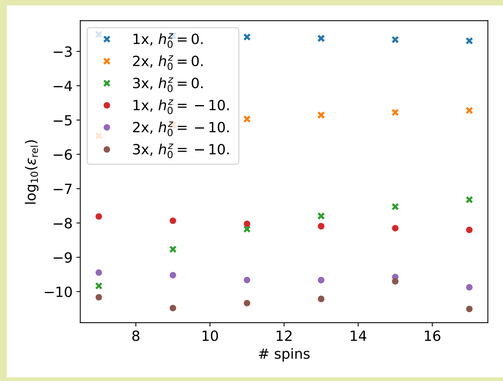


Fig. 3: Plateau values for different number of x.

Results I: Entanglement

To better understand improvement of accuracy with increasing impurity

- Reduced density matrix: $\rho_{\mathrm{A}} = \mathrm{Tr}_{\mathrm{B}}|\psi\rangle\langle\psi|$
  - A is left half and B right half (including central spin) of chain
- Entanglement entropy: $S = -\mathrm{Tr}(\rho_{\mathrm{A}}\ln(\rho_{\mathrm{A}}))$

Fig. 4: Accuracy compared to entanglement

- Accuracy of energy for varying h_0^z for $1x$ and $2x$ in comparison to the entanglement entropy
- With increasing magnetic field the entanglement entropy of the two parts of the chain decreases

Conclusion I (b)

- **Accuracy increases in the same way as S decreases only with slightly different slope**

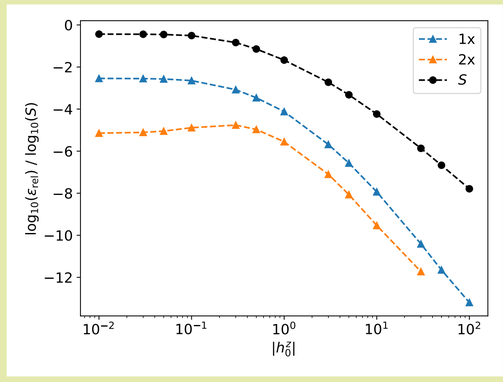


Fig. 4: Accuracy in relation to entanglement for varying h_0^z for 9 spins.

Results II: Energy

Fig. 5: Varying α

- Logarithmic accuracy of energy for system of 6 spins
- Comparison of ansatz with $|0\rangle^{\otimes n}$ as initial state with initial state prepared as singlet state for varying α
- Accuracy of energy for singlet initial state improves when decreasing the value α
- Accuracy of energy calculated with product initial state reaches a plateau at third layer
- The more α deviates from J_{16}, the more layers are needed to get to exact solution

Fig. 6: Varying impurity

- J_{16}, the coupling of the longest dimer, is varied
- Value of plateau is connected to value of impurity
- Ansatz with product initial state has problems to find small contribution of impurity singlet
- With a smaller impurity value it takes more layers to leave that plateau and to converge to exact value

Conclusion II

- **By preparing the initial state we can find a better solution with only few layers**
- How much better this solution is depends on purity of singlet state
- Preparation of initial state makes it possible to better converge to exact value when a long-range interaction small compared to other couplings is present

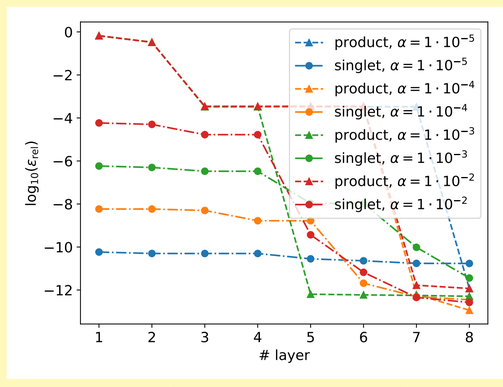


Fig. 5: Accuracy for product and singlet initial state depending on depth of circuit for $J_{16} = 0.001$ and varying α.

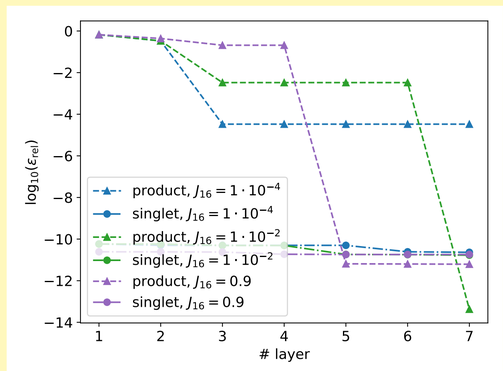


Fig. 6: Accuracy for product and singlet initial state depending on depth of circuit for $\alpha = 1 \cdot 10^{-5}$ and varying J_{16}.

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