VQE on quantum magnetism

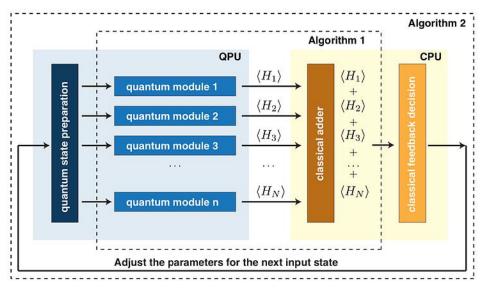
Panagiotis Constantinidis - TUC 2/2024

Presentation contents

- VQE outline and the variational principle
- The ansatz

Optimization strategies

- VQE applied on a cube
- 1D quantum phase transition
- VQE for a Kagome lattice



OPU --- evaluates

CPU → optimizes

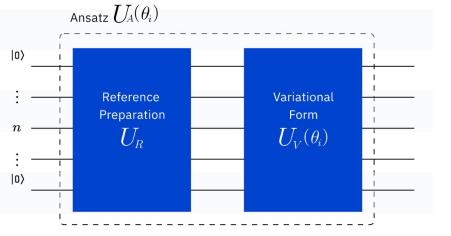
Similar to neural networks?

The algorithm follows an iterative process by evaluating some expectation value on a parameterized quantum circuit. The parameters are then to be optimized by a classical subroutine.

$$\langle \hat{\mathbf{H}} \rangle \equiv \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \ge E_0$$

It can be proven easily that the we can't go wrong by taking the expectation value.

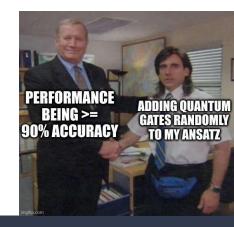
Since it will be greater or equal to the exact ground energy.



Defines the optimization landscape!

It's difficult to come up with or design one...

The variational form is the main part. The reference preparation is optional but might give a significant boost.



Optimizers

Local: they focus on a singular point of the landscape Global: opposite from local but take more resources

Gradient based: they rely on derivative evaluations in order to progres

Gradient free: distinguishes function values in different points

COBYLA: global and gradient free QNGD: local and gradient based

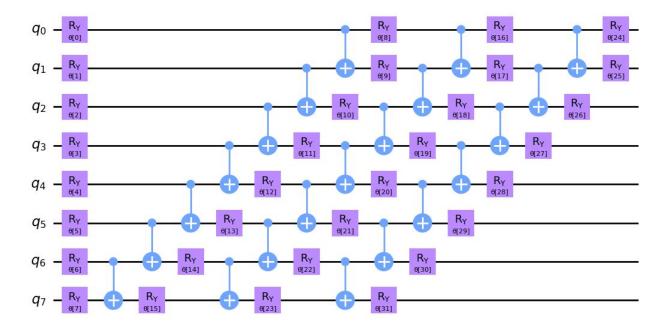
Barren plateaus: gradients vanish exponentially to the circuits complexity. It is proven that this affects also gradient free optimizers. Bootstrapping: utilizing previous statistical knowledge in order to head start the optimizer.

$$\mathbf{a}_{n+1} = \mathbf{a}_n - \gamma
abla F(\mathbf{a}_n)$$
 that's not QNGD

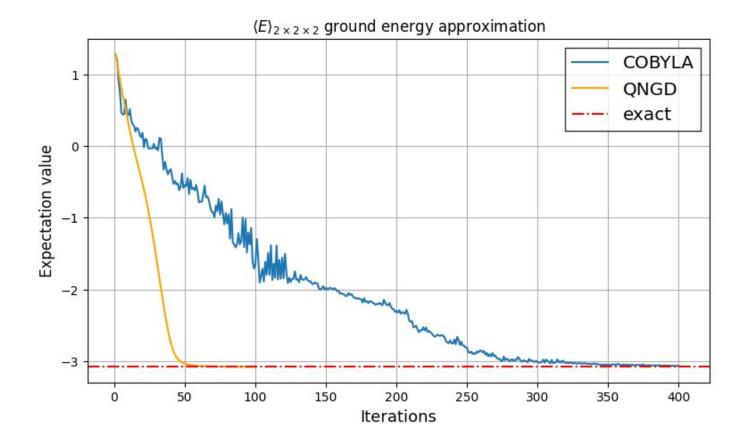
QNGD is a form of gradient that is independent of the parameterization (not to be confused with the ansatz).

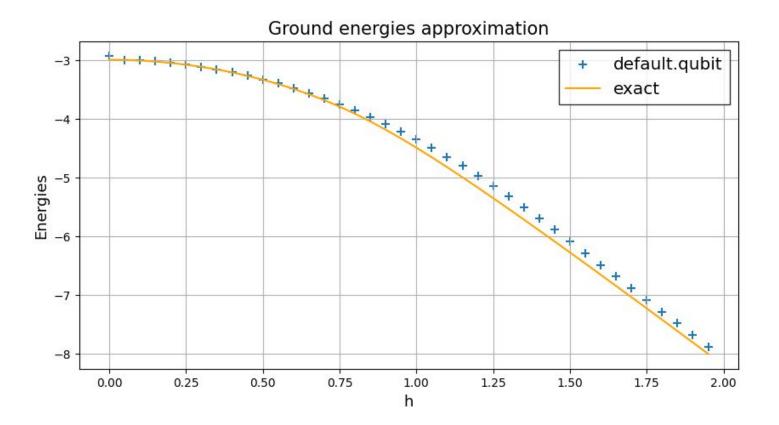
Maps functions to probability distributions and computes their distance (via KL divergence).

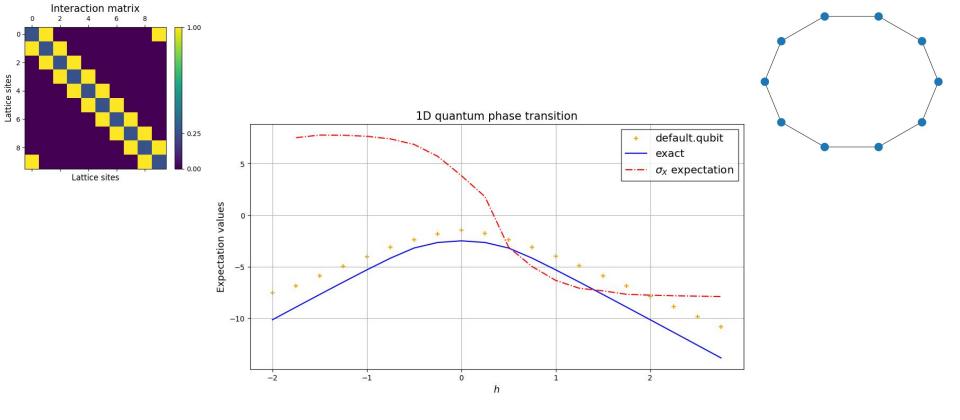
$$\hat{\mathbf{H}} = -\sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \frac{1}{4} \sum_i \hat{\sigma}_i^x$$



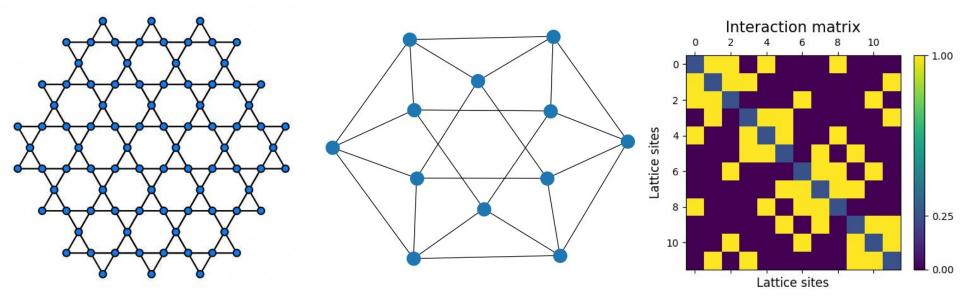
The ansatz preserves only real amplitudes while the reverse linear entanglement is equivalent to full.

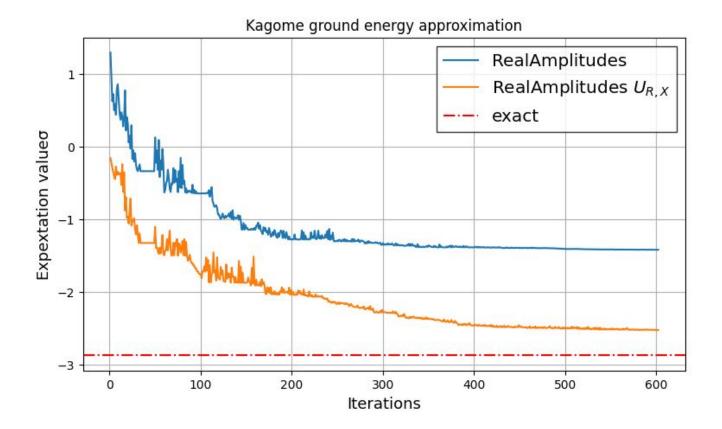






The Kagome's lattice intriguing geometric is includes triangles arranged in a hexagonal pattern.





Questions?

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Ever thought of Ising sounds?

https://www.youtube.com/watch?v=mD-0VpNSJA0

References

https://arxiv.org/abs/1304.3061