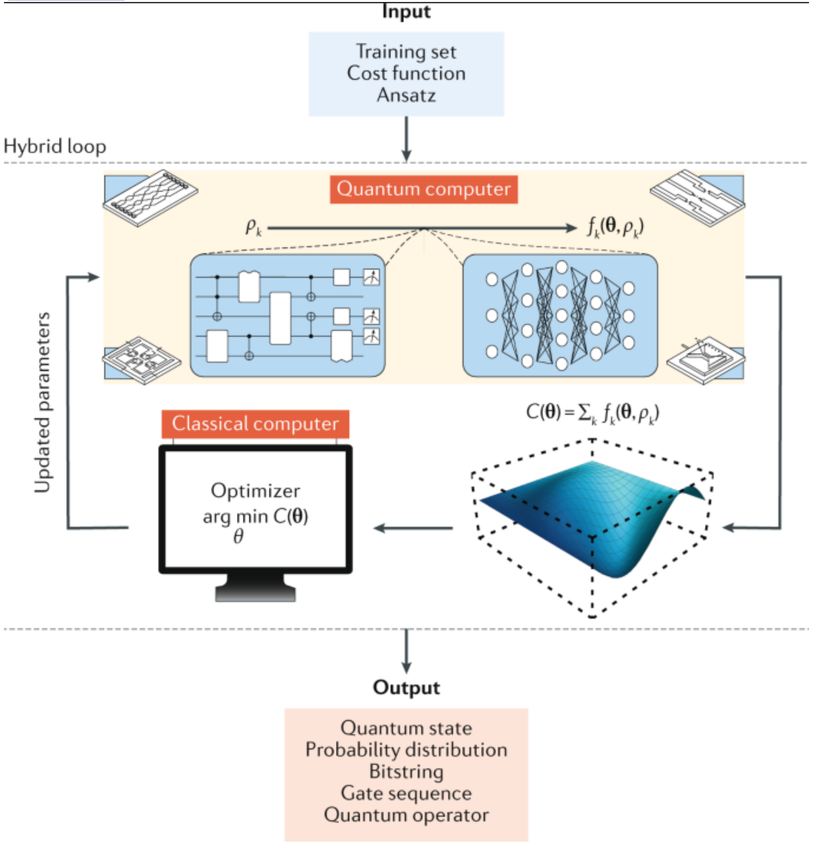
#27 Add Qiskit Nature demonstrations for physics problems

Qiskit Advocate Mentorship Program - Fall 2021

Mentors: Steve Wood and Soham Pal

Mentees: Siddhartha and José Victor

VQE

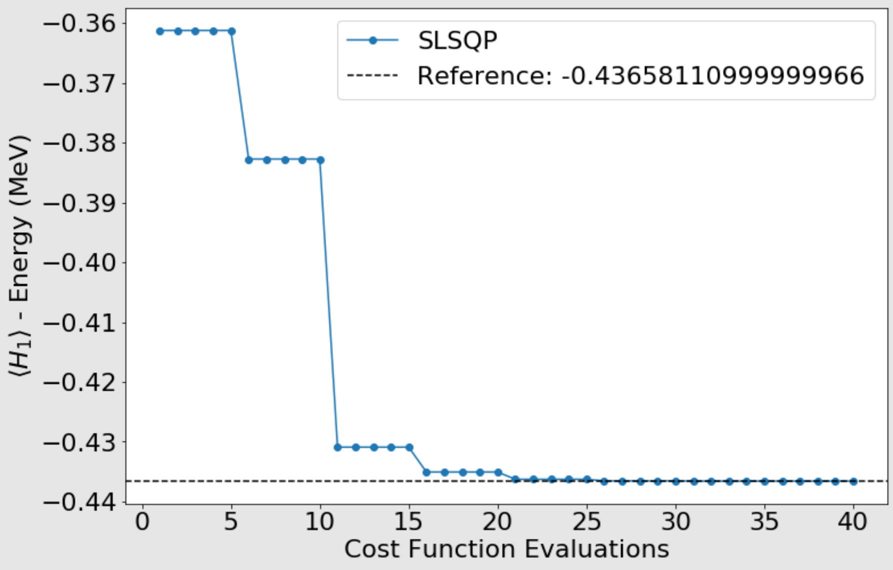


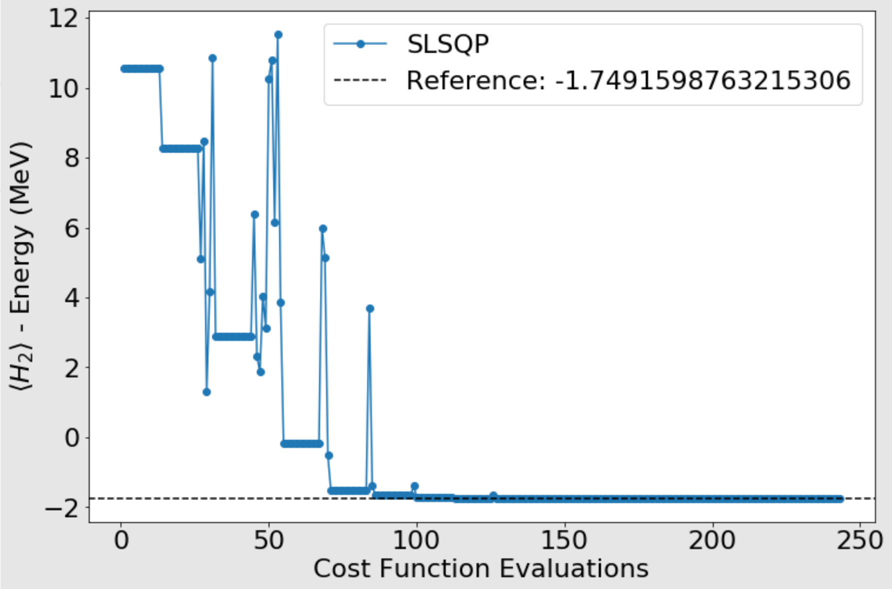
Cerezo, M., Arrasmith, A., Babbush, R. *et al.* Variational quantum algorithms. *Nat Rev Phys* 3, 625–644 (2021).

Binding energy between the proton and the neutron inside Deuteron nucleus

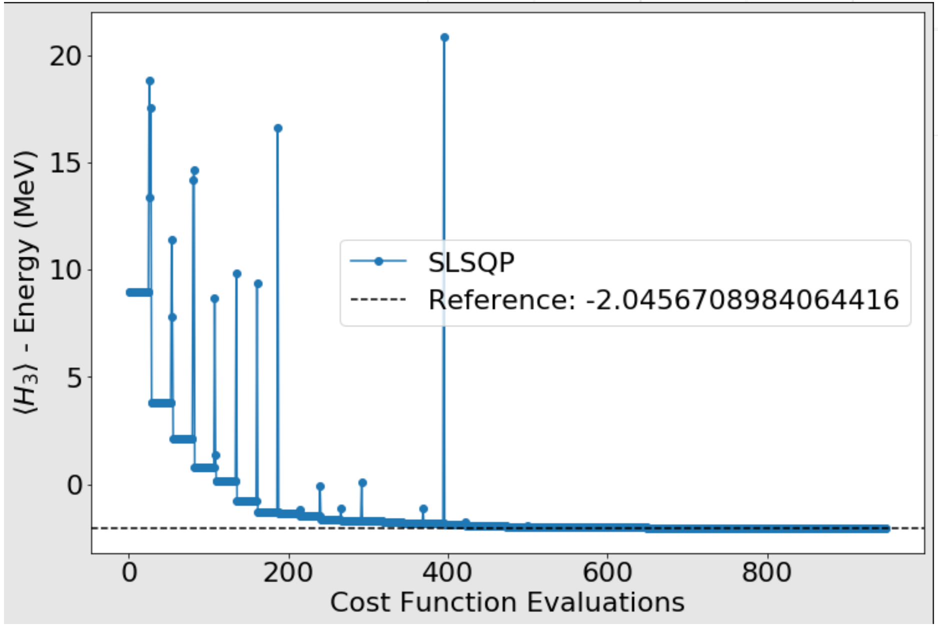
$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^{\dagger} a_n .$$

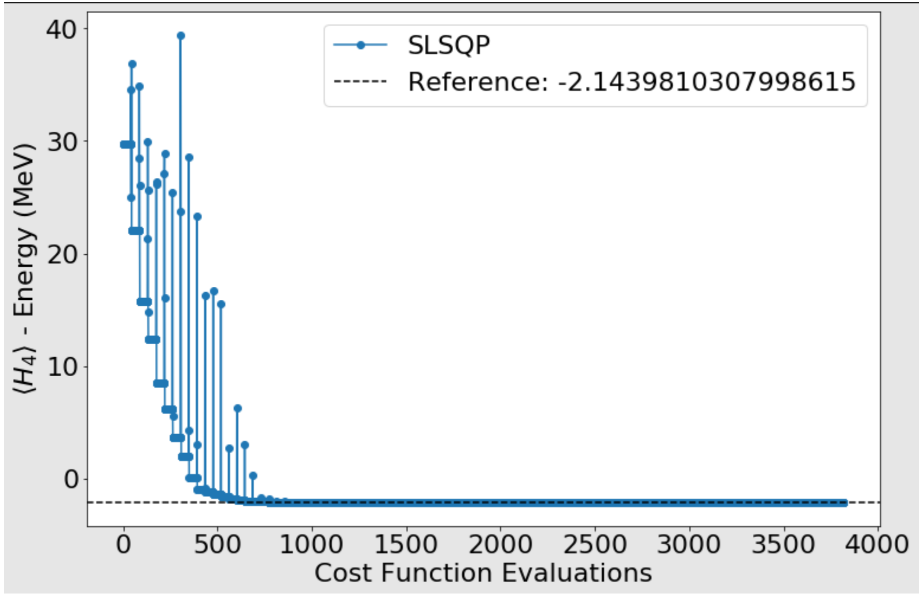
$$H_2 = 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304\,(X_0X_1 + Y_0Y_1)\,,$$
$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119\,(X_1X_2 + Y_1Y_2)\,.$$





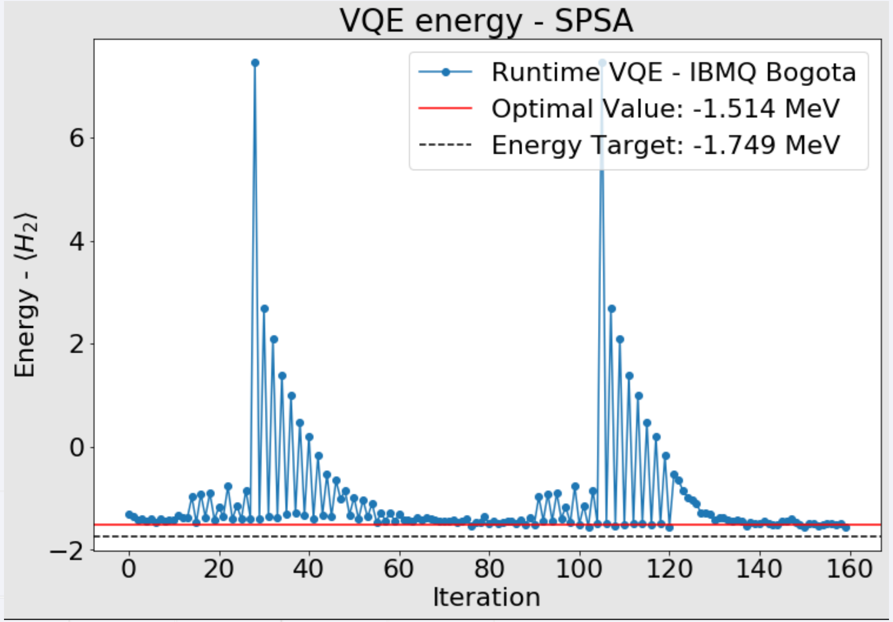
More results





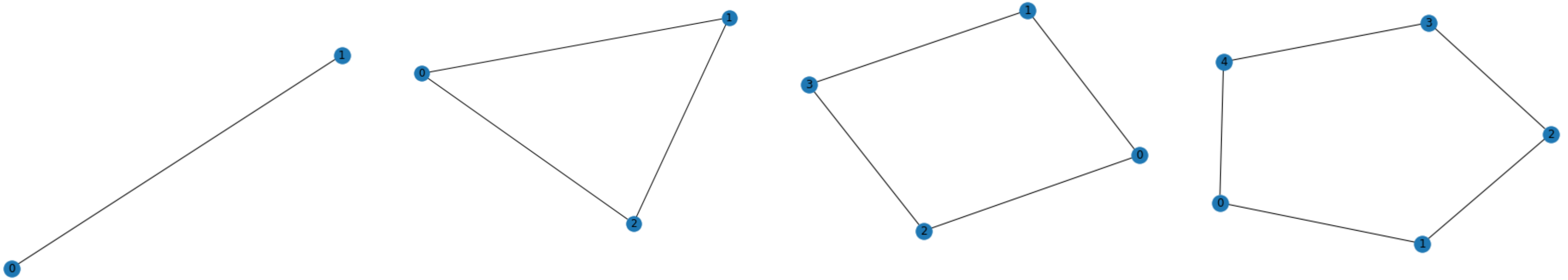
Usefuls Qiskit tools for the Deuteron problem

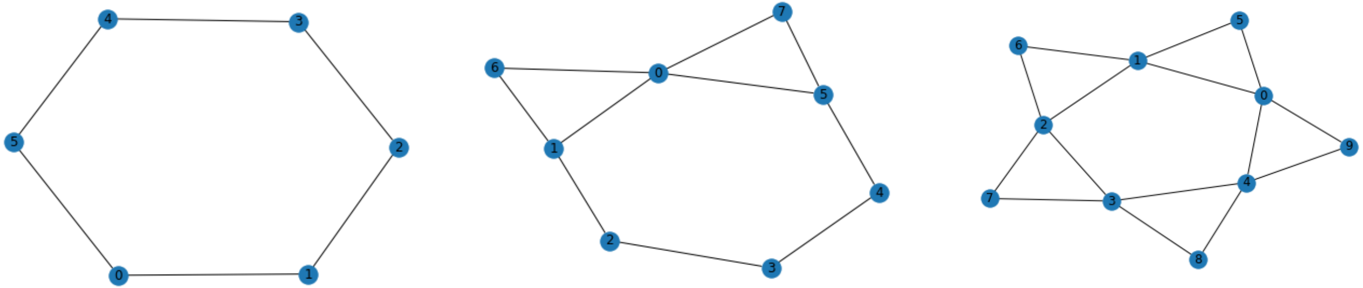
- FermionicOp
  For writing the Hamiltonian in terms of creation and annihilation operators (e.g. using sparse labels).
- QubitConverter and JordanWignerMapper
  For the process of conversion of a Hamiltonian written in terms of creation and annihilation operators to a Hamiltonian written in terms of Pauli operators.
- VQE
  For the computation of the binding energy (optimal_value).
- VQEProgram
  Allows highly efficient execution of the VQE on a real quantum device.
- Z2 symmetries
  Since the Hamiltonian has Z2 symmetry, we can reduce the problem by 1 qubit.



Heisenberg model on different lattice configurations

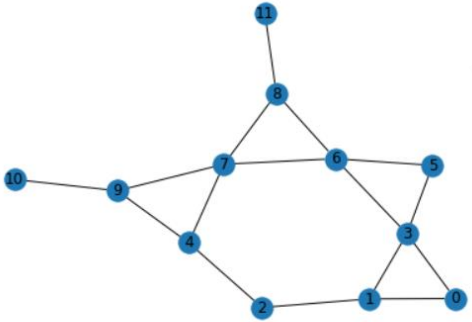
$$H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle i,j \rangle} X_i X_j + Y_i Y_j + Z_i Z_j$$



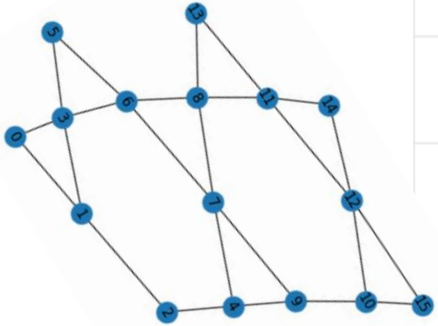


Higher Kagome lattice configurations

$$H=\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j=\sum_{\langle i,j\rangle}X_iX_j+Y_iY_j+Z_iZ_j$$



12 qubits

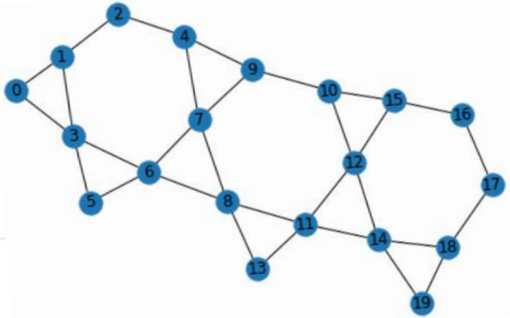


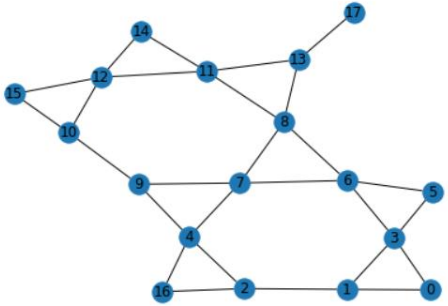
16 qubits

(2^16 x 2^16) matrix

~ 64 GiB of memory

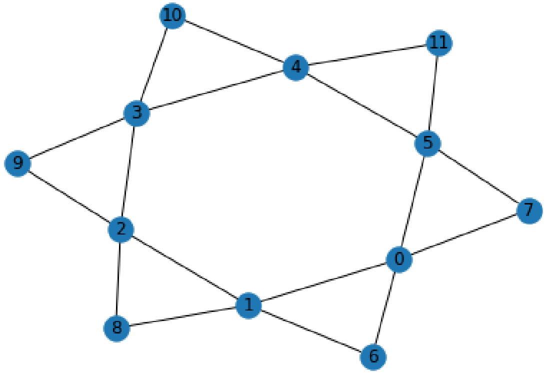
20 qubits

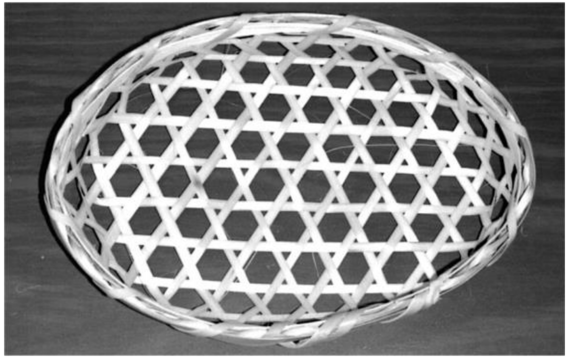




18 qubits

Kagome lattice

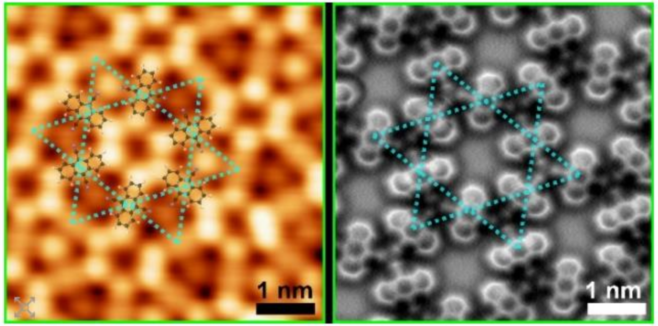




2D MATERIALS | RESEARCH UPDATE

Kagome geometry produces magnetism in a 2D organic material

29 Oct 2021 Isabelle Dumé

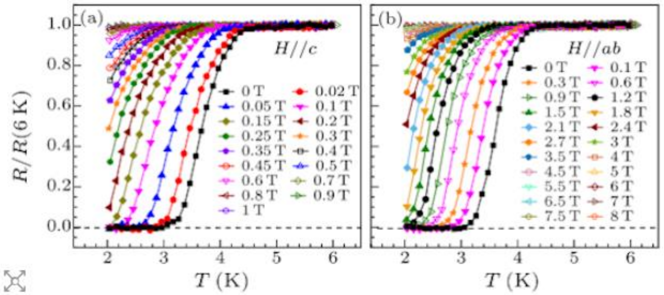


The star-like "kagome" structure of the molecules in this 2D metal-organic material (shown in an STM image on the left and a non-contact AFM image on the right) produces strong electronic interactions. (Courtesy: FLEET)

ADVANCED MATERIALS | RESEARCH UPDATE

Unusual superconductivity appears in a Kagome metal

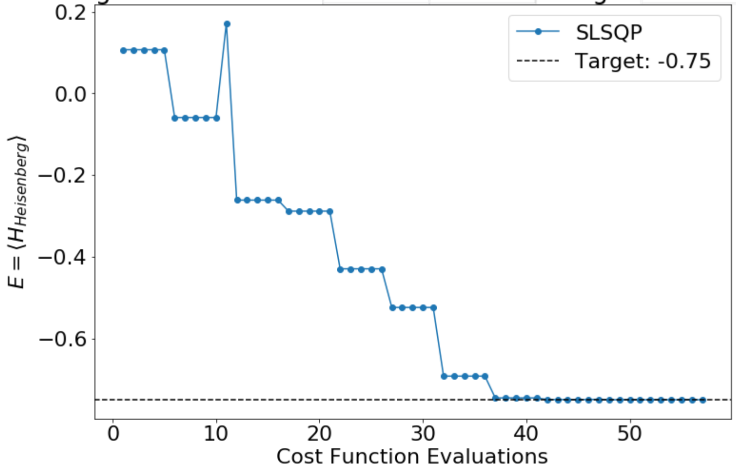
06 Jul 2021 Isabelle Dumé



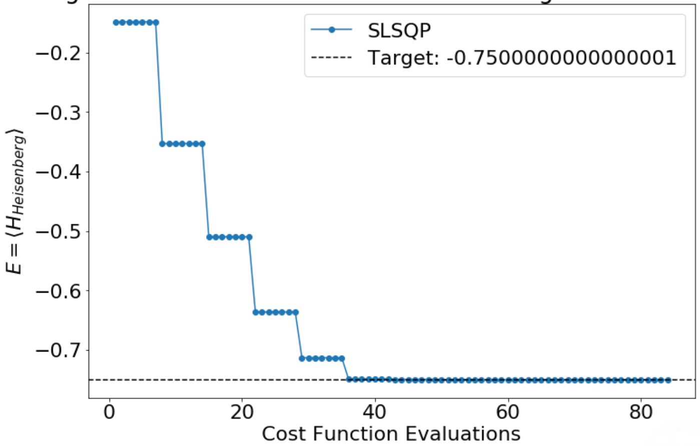
The normalized resistance under magnetic fields and anisotropic upper critical magnetic fields of the CsV_3Sb_5 single crystal. (Credit: *Chinese Physics Letters*)

Results

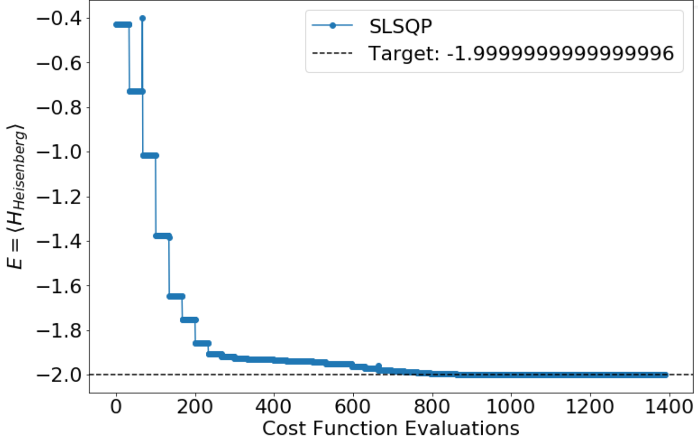
Energy convergence for the Hamiltonian of Heisenberg Model in the line lattice



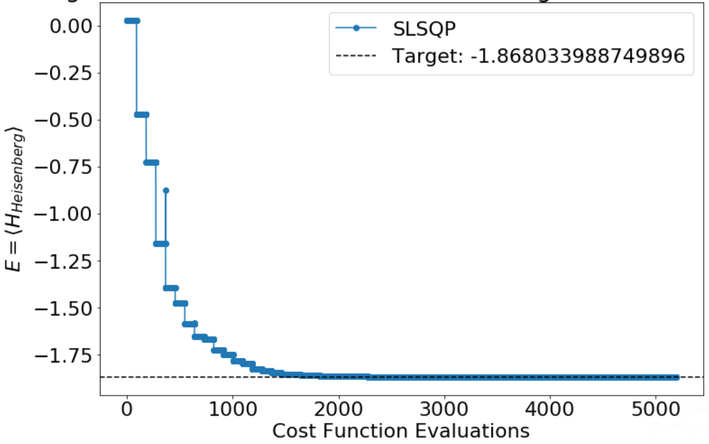
Energy convergence for the Hamiltonian of Heisenberg Model in the triangle lattice



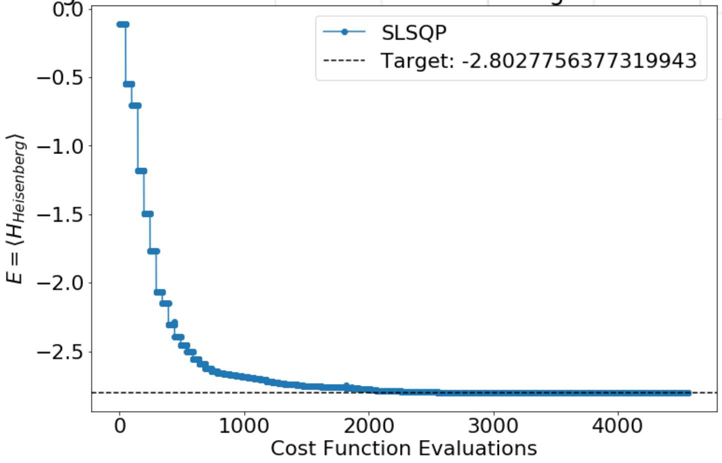
Energy convergence for the Hamiltonian of Heisenberg Model in the square lattice



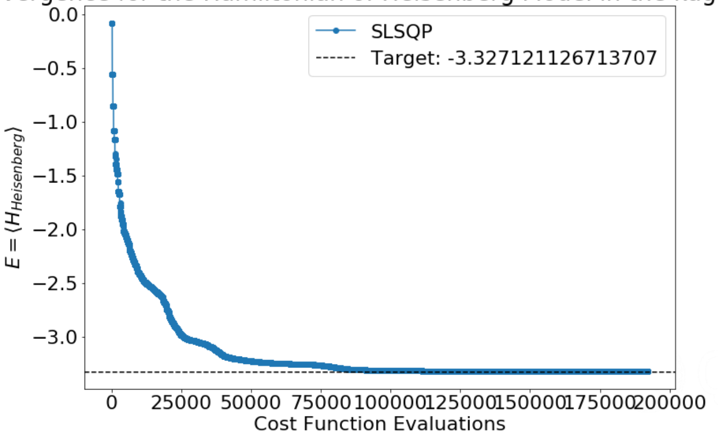
Energy convergence for the Hamiltonian of Heisenberg Model in the pentagon lattice



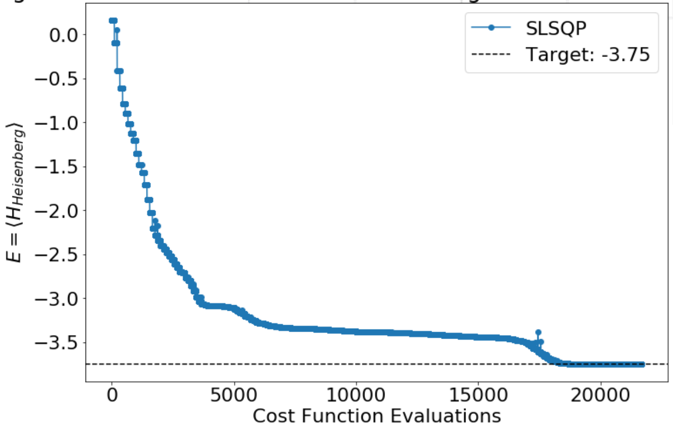
Energy convergence for the Hamiltonian of Heisenberg Model in the hexagon lattice



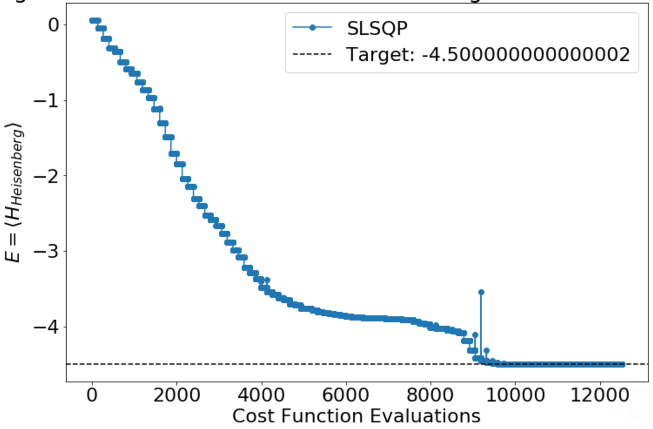
Energy convergence for the Hamiltonian of Heisenberg Model in the kagome_8q lattice



Energy convergence for the Hamiltonian of Heisenberg Model in the five-pointed star lattice



Energy convergence for the Hamiltonian of Heisenberg Model in the kagome_12q lattice



Creating an ansatz for lattice problems with first order interactions

$$\hat{H} = -\frac{1}{2}\sum_{j=1}^{N}(J_x\sigma_j^x\sigma_{j+1}^x + J_y\sigma_j^y\sigma_{j+1}^y + J_z\sigma_j^z\sigma_{j+1}^z + h\sigma_j^z)$$

- Adiabatic Theorem

$H_0 \longrightarrow H_t$

$|\psi_0\rangle \longrightarrow |\psi_t\rangle$

- $H(t) = H_0(1-\frac{t}{T}) + H\frac{t}{T}$
- Trotterization:

$e^{-iH_0\Delta t}\, e^{-iH\Delta t}$

Time evolution $\longleftrightarrow$ Ansatz

$\Delta t = \frac{t}{N}$

$U(t) = \prod_{i=1}^{N} e^{-iH_0\Delta t}\, e^{-iH\Delta t} \longleftrightarrow U(\vec{\theta}) = \prod e^{-i\theta_0 H_0}\, e^{-i\theta H}$

More flexible and easier ansatz

$$H = \sum_{i=1}^{m} H_i \quad \ni \quad \text{if } H_i = \sum_{j=1}^{m_i} h_{ij} \quad \text{then} \quad [h_{ip}, h_{iq}] = 0$$

$$\Rightarrow \quad e^{-i\delta t H} \sim \prod_{i=1}^{m} e^{-i\delta t H_i}$$

And WLOG we can take H_0 to be any of the H_i.

Time Evolution $\longleftrightarrow$ Circuit Ansatz

$$U(t) = \prod_{i=1}^{N} e^{-i\delta t H_0} \prod_{j=1}^{m} e^{-i\delta t H_j} \quad \longleftrightarrow \quad U(\vec{\theta}) = \prod_{i=1}^{\#\text{layers}} \prod_{j=1}^{m} e^{-i\theta_{ij} H_j}$$

2-qubit gate ansatz

$$H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle i,j \rangle} X_i X_j + Y_i Y_j + Z_i Z_j$$

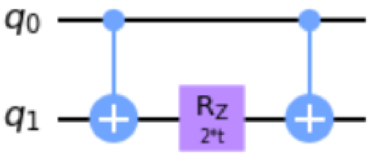
Find full commuting sectors

$$H = \sum H_i \quad \left(\text{e.g. } \begin{aligned} H_1 &= X_1X_2 + X_2X_3 \ldots \\ H_2 &= Y_1Y_2 + \ldots \\ H_3 &= Z_1Z_2 + \ldots \end{aligned} \right.$$

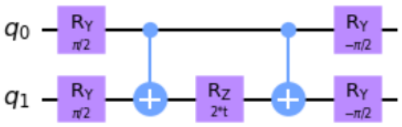
$$e^{-i\vec{\theta} H_i} = \prod e^{-i\theta_{ij} h_j}$$

$$h_j = \sigma_j^k \sigma_j^k$$

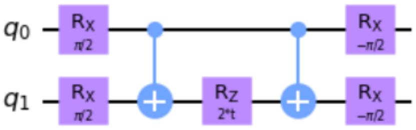
$$e^{-itZ_0Z_1} =$$



$$e^{-itY_0Y_1} =$$

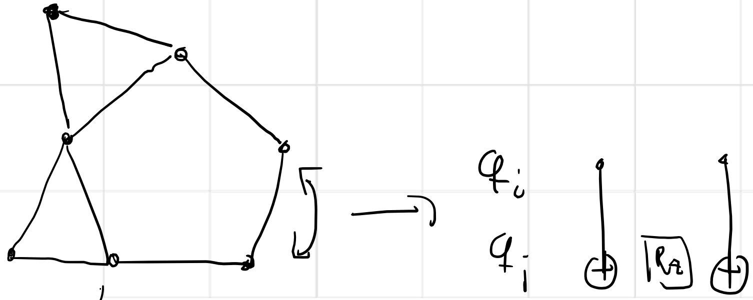


$$e^{-itX_0X_1} =$$



Advantages and results

- Entanglement needed only for first neighbours



map lattice into Hardware configuration (reduce swaps)

- Use basic rotation gates

- Gives a good approximation and fast (runs of < 2 hours) for the ground state

8 qubit energy error < 4%

10 qubit energy error < 10%

Usefuls Qiskit tools for the Heisenberg model problem

- Pauli and PauliOp
  For writing the Hamiltonian in terms of Pauli operators.

- VQE
  For the computation of the ground state energy (optimal_value).

- Retworkx
  Allows the creation of the graph that represents the lattice configuration.

- Z2 Symmetries
  Heisenberg's Hamiltonian has the trivial symmetry $\sigma_i \rightarrow -\sigma_i$ (the problem is that we don't know which is the correct sector)

Final product

We want to construct two tutorials explaining in detail how we use Qiskit tools to tackle the physical problems that we chose.

We also want to give some feedback about our experience to help in the construction of new tools in Qiskit Nature.

Thank you!