Outline

This project consists of two parts. Part 1 contains 10 mandatory questions, each marked out of 1, and comprises 20% of the final mark for the project. In part 2 you can choose one of 4 topics — this comprises 80% of the final mark for the project, and is marked out of 10.

The deadline for both parts of the project is the beginning of the lecture on the 17th of April 2020.

Part 1

1. What is the average size (locality, or weight) of a single transformed fermionic creation or annihilation operator under the a) Jordan-Wigner, b) Bravyi-Kitaev, and c) JKMN transformation?

2. Write down the Hamiltonian for the (fermionic) Hubbard model on a 1-dimensional chain.

3. Transform the above Hamiltonian onto a qubit basis via the Jordan-Wigner transformation.

4. Write down the commutation relations for

   - fermionic creation and annihilation operators.
   - Majorana operators.

5. What is the scaling of the number of terms in the Hamiltonian with the system size for the a) Hubbard model, b) Heisenberg model, c) Electronic structure problem?

6. What is the scaling of the number of parameters in the UCC ansatz truncated to a) singles, b) singles and doubles?

7. Write a formula for elements of the fermionic 1-RDM in terms of the fermionic 2-RDM in an N-particle system. Hint: states of an N-particle system are eigenstates of the number operator $\sum_i \hat{n}_i$.

8. Prove the Hellman-Feynman theorem — that $\frac{\partial}{\partial\lambda}\langle\Psi_j|H|\Psi_j\rangle = \langle\Psi_j|\frac{\partial H}{\partial\lambda}|\Psi_j\rangle$. State any assumptions you require on $|\Psi_j\rangle$ (you will need to make at least one!).

Part 2

Topic 2.A. Hamiltonian variational ansatze.
In this project you will implement and optimize the Hamiltonian variational ansatz of Wecker, Hastings and Troyer for the Hubbard model on a 2×2 lattice

Literature:

- `https://arxiv.org/abs/1507.08969`.

Objectives and tasks:

- Learn and understand the Hamiltonian variational ansatz.
  - What is the problem that is being solved?
  - What is the motivation for this choice of variational ansatz?
  - For which systems do the authors suggest this ansatz might be preferable?
- Understand the Hubbard model on a square lattice.
  - How many nearest neighbours does each site connect to on an infinite lattice?
  - How many nearest neighbours does each site connect to on a 2×2 lattice?
  - Write h_h, h_v, and h_U (defined below Eq. 2) in terms of creation and annihilation operators for a 2×2 lattice.
  - How many qubits are required to represent the Hubbard model on a single site?
  - What is the non-interacting Hamiltonian for this system?
- Provide an implementation of the Hamiltonian variational ansatz for the Hubbard model
  - Write a function to generate hermitian terms in h_h, h_v and h_U.
  - Write a function to generate the non-interacting and interacting Hamiltonians.
  - Write a function to generate circuits implementing $e^{i\theta h}$ terms given the above. Remember to leave θ a free parameter, and transform from fermions into qubits.
  - Write a function to generate the Hamiltonian variational ansatz using the above sub-functions.
  - Write a function to generate the non-interacting starting state using the above (the openfermioncirq.prepare_gaussian_state function may be relevant here).

- Implement the VQE using the above, measure the energy at $t = 1$ and $U = 2$, and compare performance to the result found in ArXiv:1507.08969 as a function of the step size S. Be careful with optimization!

The report should contain:

1. A description of the Hamiltonian and system being studied.
2. A description and explanation of the algorithm and quantum-classical hybrid scheme.
3. An implementation of the ansatz and evaluation of performance (preferably in a jupyter notebook)

For 7+: optimize the circuit ordering such two of the three steps of the ansatz run in constant time (it will not be possible to do this for all 3 steps). Split the hopping parameter t into a horizontal hopping t_h and vertical hopping t_v, and map out the ansatz convergence, energy, and electron-electron correlators $\langle \hat{c}^\dagger_{i,\sigma} \hat{c}^\dagger_{j,\sigma'} \rangle$ as t_v/t_h goes from $0 \to \infty$.

For 10: compare the Hamiltonian variational ansatz to the MP2-ordered UCC ansatz of arXiv:1701.02691 or the perturbative heirarchy of arXiv:1907.08157 and determine which has faster convergence on a 4×2 lattice.

Topic 2.B. Obtaining excited state energies via eigenstate witnessing. In this project you will implement the eigenstate witnessing algorithm of Santagati *et al* for the H_2 molecule.

Literature:

- `https://arxiv.org/abs/1611.03511`.

Objectives and tasks:

- Learn and understand the WAVES protocol
  - What is the main purpose of the WAVES protocol?
  - How does the WAVES protocol achieve this?
  - How is the cost function of the WAVES protocol measured?
  - What are the excitation operators (eq. 10) used for in the WAVES protocol?
- Provide an implementation of the WAVES protocol to find ground and excited states of the H2 molecule
  - Write a function to generate the Hamiltonian of the H_2 molecule (choose your favourite bond distance).
  - Write a function to generate the Trotterized parametrized Hamiltonian ansatz (Eq. 7).
  - Write a function to calculate an appropriate value of t based on the non-interacting part of the H_2 Hamiltonian.
  - Write a function to generate a circuit for time evolution under the full H_2 Hamiltonian for time t, conditional on an ancilla qubit.
  - Combine the above functions to implement step 1 of the WAVES protocol.
  - Write a function to generate excitation operators for the H_2 molecule.
  - Combine this with the above to implement step 2 of the WAVES protocol.

The report should contain:

1. A brief description of the WAVES protocol and what it achieves.
2. An implementation (preferably in a jupyter notebook) of the WAVES protocol on the H_2 molecule to find the ground state and excited state manifold.

For 8+: Implement IPEA on the obtained ground and excited states and determine the accuracy of the resulting energies.
For 10: Compare the WAVES protocol to other protocols for finding excited states in terms of cost to implement and accuracy obtained.

Topic 2.C. Time evolution of the triton toy model.
In this project you will investigate the time evolution of the triton toy model for neutrino-nucleus scattering.

Literature:

- `https://arxiv.org/abs/1911.06368` (in particular Sec. III).

Objectives and tasks:

- Learn and understand the triton toy model
  - Write down the general triton toy model in a fermionic representation.
  - What is the physical interpretation of this model?
  - Write down the representation of the triton toy model Hamiltonian with 2 particles and $N_f = 2$ modes in the limiting case $V = -4U$.
  - What does each qubit correspond to in this case? Which state corresponds to having both particles on the same site as the nuclei?
  - Is this a first-quantized or second-quantized representation?
  - Write the representation of the triton toy model Hamiltonian with 2 particles and $N_f = 2$ modes when $V \neq 4U$ (in Pauli operators).
- Use a variational quantum eigensolver to approximate the ground state of the triton toy model
  - Write a function to implement the state preparation routine used by Roggero *et al* (eq. 32).
  - Write a function to generate the triton toy model Hamiltonian for different values of t, U and V.
  - Optimize the VQE at different values of t, U, and V, and compare the error in the energy of the ground state.
- Measure the time dynamics of the ground state
  - Write a function to implement time evolution by Trotterization (either naively or via the methods used in the text).
  - Write a function to estimate the probability of finding both particles on the same site as the nuclei (3-body contact function) after a period of time evolution.
  - Combine these functions with the previously-optimized VQE, and compare the results to Fig.7 of the main text.

The report should contain:

1. A description of the triton toy model and its mapping onto qubits.
2. A description of the state preparation and time evolution algorithms, and identification of all sources of error.
3. Code (preferably in a jupyter/ipython notebook) to simulate time evolution on the triton model and measure and plot the 3-body contact function as a function of time.

For 8+: Use quantum phase estimation to prepare the ground state, and multiple Trotter steps in the time evolution. See how both adjustments change the time dynamics.
For 10: Investigate the linear response of this model using the methods of ArXiv:1804.01505.

Topic 2.D. Determining excited state spectra via the quantum subspace expansion.

In this project you will use the quantum subspace expansion of McClean *et al* to determine the excited state spectra of the H_4 molecule.

Literature:

- `https://arxiv.org/abs/1603.05681`.

Objectives and tasks:

- Learn and understand the quantum subspace expansion
  - What is the primary aim of this quantum algorithm?
  - What needs to be done for this algorithm over and above a regular VQE?
  - What do McClean *et al* suggest as an appropriate choice of excitation operators for a fermionic system?
  - What is the cost of this algorithm?
  - Does this algorithm have any secondary desirable effects?
- Investigate the H_4 molecule
  - Generate the Hamiltonian for the H_4 molecule in a rectangular geometry with sides of length l_h and l_v.
  - Plot the (Full-CI) ground state energy and the Hartree-Fock energy as a function of l_v with $l_h = 1$ Angstrom fixed.
  - When is this molecule weakly-correlated? When is it strongly-correlated?
- Determine the ground state of the H_4 molecule using the UCC ansatz
  - Write a function to generate the UCC ansatz for 8 qubits (remember to keep parameters free!)
  - Write a function to prepare the initial Hartree-Fock starting state
  - Optimize the VQE at various values of l_v (again with $l_h = 1$ fixed) and compare the variational energy with the Full-CI and Hartree-Fock energies.
- Determine excited states with the quantum subspace expansion
  - Write a function to measure the overlap and linear response Hamiltonian from the converged variational wavefunction.
  - Write a function to solve the generalized eigenvalue problem using the overlap and LR Hamiltonian.

- Plot the obtained excited state energies against the Full-CI values as a function of l_v with $l_h = 1$ Angstrom fixed.

The report should contain:

1. A description of the QSE, what it achieves, and its cost to implement.
2. Code (preferably a jupyter or ipython notebook) that studies the H_4 molecule using the QSE, and compares the result to the Full-CI and HF energies.

For 10: Implement the MP2 subroutine of ArXiv:1701.02691 to order the terms in the VQE, and study the energy in a square H_4 lattice as a function of the MP2 cut-off. Extend this concept to a ordering and cut-off of the excitation operators in the QSE, and determine how interchangeable the two are in terms of energy errors.