Quantum Fourier Transform

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Why UCCSD?

A key requirement of quantum gates is that they "preserve the norm" when acting on states i.e. they are unitary. The coupled cluster opertor e^T by itself is not unitary. To make it unitary, we have to introduce $T^\dagger$.

$$U(\vec{t}) = e^{T-T^\dagger} = e^{\sum_j t_j(\tau_j - \tau_j^\dagger)}$$

Here τ_j are the excitation operators and t_j are the corresponding cluster amplitudes.

How do we map this operator $e^{T-T^\dagger}$ to quantum gates?

Recall that encoding methods were evaluated based on their efficiency in performing "electronic operations". Well the excitation operators of the form $\tau_j - \tau_j^\dagger$ are really a bunch of creation and annhilation operators. In the JW mapping or the BK mapping, these turn out to be simply a linear combination of pauli matrices. But isn't $\tau_j - \tau_j^\dagger$ enclosed within an exponential i.e $e^{\tau_j - \tau_j^\dagger}$? Well there are quantum algorithms to convert the "exponentiation of pauli matrices" into much simpler rotation and CNOT gates.

$$\Psi_{CISD} = (1 + T_1 + T_2)\Phi_0 = \Phi_0 + T_1\Phi_0 + T_2\Phi_0$$

$$\Psi_{CCSD} = e^{T_1+T_2}\Phi_0 = \Phi_0 + T_1\Phi_0 + (T_1^2 + T_2)\Phi_0 + (T_1T_2 + T_1^3)\Phi_0 + ...$$

$$|11\rangle$$

$$a_i a_j + a_j a_i = 0$$
$$a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0$$
$$a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}$$

$$|\alpha|^2 + |\beta|^2 = 1$$

$$
\begin{aligned}
|\psi_1\rangle &= \alpha\,|0\rangle + \beta\,|1\rangle \\
|\psi_2\rangle &= \alpha\,|00\rangle + \beta\,|1\rangle + \gamma\,|10\rangle + \delta\,|11\rangle \\
&\vdots \\
|\psi_n\rangle &= \sum_{i=1}^{2^n} \alpha_i \left|a_i^1 a_i^2 \cdots a_i^n\right\rangle
\end{aligned}
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\end{aligned}
$$

$$a^\dagger |0\rangle = |1\rangle$$
$$a |1\rangle = |0\rangle$$

What about phase estimation?

Quantum Phase Estimation is a very popular quantum algorithm which seems naturally suited for this task. By computing the phase of the eigenvalue, it finds the eigenvalue of the hamiltonian. However, it requires too many gates and is very costly, at least for NISQ devices. So, VQE uses a much more feasible method called hamiltonian averaging procedure instead of quantum phase estimation for measurement.

Where does the qubit hamiltonian come from?

First, using trotterization, we decompose the hamiltonian of the large system into a sum of local hamiltonians that act only on subsets of the system. Now these local hamiltonians are still made up of creation and annhilation operators. Converting them to pauli matrices, we have

$$H = \sum_i h_i O_i$$

where O is the tensor product of pauli matrices. And thus we have our qubit hamiltonian.

How do we measure the energy?

For every local hamiltonian, we have to run the whole quantum program multiple times to obtain the expectation value $\langle O_i \rangle$. When this is done for all local hamiltonians, the total energy is computed as a weighted sum of these expectation values.

$$E = \sum_i^M h_i \langle O_i \rangle$$