Chapter 4

Quantum Simulation

Many body system has various types of particle and their interaction terms are also different. Due to many interactions, it is a difficult task to simulate a many body system on classical computers. However classical computers has able to simulate a certain limit of few body system. Here quantum computers may provide a way to simulate these system as it has more processing power. As of an kick start of this field, two body system has simulated on quantum computers and further many body system will simulated. In this thesis, we start with deuteron as two body system and try to simulate it. For quantum simulation, variational quantum eigensolver (VQE) technique has been proposed. This VQE takes input as particle and its hamiltonian, and by using a optimizer it try to get minimum energy which is the ground state energy of this hamiltonian.

4.1 Variational Quantum Eigensolver

Variational Quantum Eigensolver (VQE) is a hybrid algorithm, and as input it needs Hamiltonian of the system. VQE is designed to find the ground state energy of the system by estimating the eigenvalue (energy) of this hamiltonian. After eigenvalue calculation an optimizer is used to get it's lowest value (ground state energy). The Hamiltonian we have is in fermionic operator (creation and annihilation operator) form, to use this Hamiltonian in VQE, it needs to be encoded the hamiltonian into pauli operators form. Why we chooses to get hamiltonian into pauli operator form has simple answer that quantum computers has gates as pauli matrices, so we can easily calculate hamiltonian expectation value using quantum computing. To

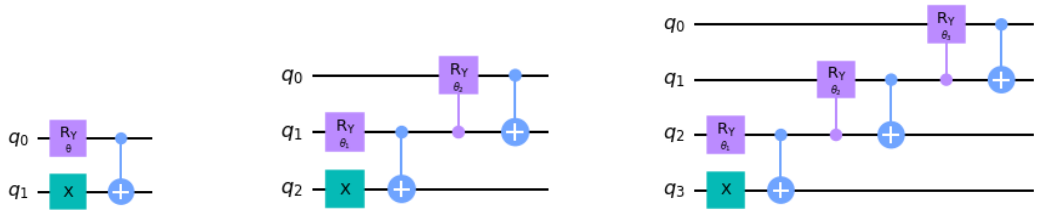
encode these fermionic operators into spin or pauli operators, there are methods for encoding *i.e.,* Gray Code, Bravyi-Kitaev and One-Hot encoding [12]. One-Hot encoding will be used in our work through Jordan-Wigner transformation. After encoding this hamiltonian into pauli operators form or into qubit form, we take an arbitrary state ψ and take expectation value of hamiltonian in this state. In quantum mechanics the expectation value of a operator with respect to a state is always greater then or equal to its lowest eigenvalue and the state should be normalized.

$$a_0 = \langle\psi|\mathrm{H}|\psi\rangle$$

$a_0 \geq a_{min}$, here a_{min} is lowest eigenvalue of operator and a_0 is the expectation value of operator with respect to $|\psi\rangle$ state . The arbitrary state has variational parameter θ, and using classical optimizer we try to get minimum value of this expectation value. This process repeated until we achieved lowest eigenvalue. a_θ is expectation value of parameterized state.

$$a_\theta = \langle\psi(\theta)|\mathrm{H}|\psi(\theta)\rangle$$

The parameterized state $|\psi(\theta)\rangle$ in quantum circuit has been created by applying unitary transformation on initial state $|0\rangle$ as $\mathrm{U}(\theta)|0\rangle = |\psi(\theta)\rangle$, this unitary transformation has combination of quantum gates. Rotational gates around y axis (R_y), controlled not gates, and X gates have been used here and the quantum circuit diagram of state preparation is in figure 4.1 according to number of qubit.



(a) (b) (c)

Figure 4.1: Quantum circuit for variational ansatz for N = 2, 3, 4

The hamiltonian in pauli operator form is used in quantum circuit by applying pauli gates. We take expectation values of all pauli strings in the hamiltonian that is measured. For measurement of pauli strings in hamiltonian, we have to choose

what value of measured quantities we should accept and which one we should not. for single qubit, the expectation value of Z in measurement is taken in arbitrary state $|\psi\rangle$. Since the Z is a form of hamiltonian, so this expectation value is in the form of energy and written as:

$$E_\psi(Z) = \langle\psi|Z|\psi\rangle = \langle\psi|(|0\rangle\langle 0| - |1\rangle\langle 1|)|\psi\rangle$$

$$= \langle\psi|0\rangle\langle 0|\psi\rangle - \langle\psi|1\rangle\langle 1|\psi\rangle$$

$$= |\langle 0|\psi\rangle|^2 - |\langle 1|\psi\rangle|^2$$

$$= P_{|\psi\rangle}(0) - P_{|\psi\rangle}(1)$$

Here $P_{|\psi\rangle}(0)$ is the probability that state $|\psi\rangle$ is measured to be $|0\rangle$, So if 0 measured C_0 times and 1 measured C_1 times out of total measurements. Expectation value of Z is

$$E_\psi(Z) = \frac{C_0 - C_1}{C_0 + C_1}$$

now for expectation value of X

$$E_\psi(X) = \langle\psi|X|\psi\rangle = \langle\psi|HZH|\psi\rangle$$

$$= \langle H^\dagger\psi|Z|H\psi\rangle = \langle H\psi|Z|H\psi\rangle$$

$$= E_{H\psi}(Z)$$

$$= P_{H|\psi\rangle}(0) - P_{H|\psi\rangle}(1)$$

Here $P_{H|\psi\rangle}(0)$ is probability that state $H|\psi\rangle$ is measured to be $|0\rangle$, here we have prepare state $|\psi\rangle$ and apply hadamard gate on it.
For expectation value of Y it can be written as $Y = SXS^\dagger = SHZHS^\dagger$

$$E_\psi(Y) = \langle\psi|SHZHS^\dagger|\psi\rangle$$

$$= \langle H^\dagger S^\dagger\psi|Z|HS^\dagger\psi\rangle$$

$$= \langle HS^\dagger\psi|Z|HS^\dagger\psi\rangle = E_{HS^\dagger|\psi\rangle}(Z)$$

$$= P_{HS^\dagger|\psi\rangle}(0) - P_{HS^\dagger|\psi\rangle}(0)$$

Here we have to prepare a state $|\psi\rangle$ and apply hadamard and $S^\dagger$ gate. For 2 qubit

XX expectation value is

$$E_\psi(XX) = \langle\psi|XX|\psi\rangle = \langle\psi|(HZH)\otimes(HZH)|\psi\rangle$$

$$= \langle H^\dagger H^\dagger\psi|Z\otimes Z|HH\psi\rangle$$

$$= \langle HH\psi\,|(|0\rangle\langle 0| - |1\rangle\langle 1|)\otimes(|0\rangle\langle 0| - |1\rangle\langle 1|)|\,HH\psi\rangle$$

$$= \langle HH\psi|(|00\rangle\langle 00| - |01\rangle\langle 01| - |10\rangle\langle 10| + |11\rangle\langle 11|)|HH\psi\rangle$$

$$= P_{HH|\psi\rangle}(00) - P_{HH|\psi\rangle}(01) - P_{HH|\psi\rangle}(10) + P_{HH|\psi\rangle}(11)$$

Other combination of XY and ZZ can be calculated same way and for more number of qubit we can use this calculation and choose the results that we have to take. This results are used by classical optimizer to choose a set of parameters for which eigenvalue is minimized. for better optimization, the state should be close to ground state. This parameterized state is also called variational ansatz and it depends on encoding and corresponding transformation.

4.2 Deuteron Problem

Deuteron as two body system consist a proton and a neutron. Ground state energy calculation of deuteron will establish the concept of quantum simulation and it can be used to simulate heavier nuclei. For VQE input, we use a Hamiltonian from pionless effective field theory [15, 16] and have to work on discrete variable representation. For more detail one can look appendix A. Hamiltonian for deuteron is,

$$\mathrm{H}_N = \sum_{n,n'=0}^{N-1} \langle n'|\mathrm{T}+\mathrm{V}|n\rangle a^\dagger_{n'} a_n$$

Kinetic energy matrix element and potential energy matrix element from [14] are

$$\langle n'|\mathrm{T}|n\rangle = \frac{\hbar\omega}{2}\left[\left(2n+\frac{3}{2}\right)\delta^{n'}_n - \sqrt{n\left(n+\frac{1}{2}\right)}\delta^{n'+1}_n - \sqrt{(n+1)\left(n+\frac{3}{2}\right)}\delta^{n'-1}_n\right],$$

$$\langle n'|\mathrm{V}|n\rangle = V_0\delta^0_n\delta^{n'}_n.$$

Here, $V_0 = -5.68658111$ MeV, $a^\dagger_{n'}$ and a_n is creation and annihilation operator and n′ and n are state of harmonic oscillator and N is dimension of oscillator. Values

of T and V can be directly use from above equations of energy matrix elements. This harmonic oscillator hamiltonian operator is fermionic as is consists fermionic creation and annihilation operator. In second quantization form the hamiltonian is

$$\mathrm{H} = \sum_{ij} h_{ij} a_i^\dagger a_j$$

here this h_{ij} is :

$$h_{ij} = \langle i|T + V|j\rangle = \int \phi_i(r) \left[\frac{\hbar^2}{2m}\nabla^2 + V(r)\right] \phi_j(r) dr$$

here $\phi_i(r)$ or $|i\rangle$ represent the basis of system. So we calculate h_{ij} manually and $a^\dagger a$ will be evaluated by quantum computing. But $a^\dagger a$ can not be directly calculate by quantum computing. Basis state and operator has to be mapped into qubit's basis state and qubit operations. Qubit basis states are $|0\rangle$ and $|1\rangle$ and a state can be represented as $\psi_q = a|0\rangle + b|1\rangle$ and for n-qubit system

$$\psi_q^n = \otimes \prod_{j=0}^{n-1} (a_j|0\rangle + b_j|1\rangle)$$

For quantum computing we have to map ψ_f into ψ_q and mapping decide some factor of computing as number of qubits, number of operations and circuit depth. In JW transformation a single qubit will be assign of one basis state $|i\rangle$.
The quantum spin with S = 1/2 can describe by fermions as $|\downarrow\rangle = f^\dagger|0\rangle$ and $|\uparrow\rangle = |0\rangle$. Spin up and down states of single spin corresponds to empty fermion states and single occupied state. We can take the analogy from fermionic operator and spin-1/2 Pauli operators can transform as $\sigma^+ \equiv f$ and $\sigma^- \equiv f^\dagger$ [17]. The spin-1/2 Pauli operator is σ^x, σ^y and σ^z and representation of spin lowering and raising operator is

$$\sigma^+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$\sigma^- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

σ_j defined as Pauli spin operator acting on state j or site j, spin raising and lowering

operator σ_j^+ and σ_j^- in terms of x and y component of spin operator is

$$\sigma_j^+ = (\sigma_j^x + \iota\sigma_j^y)/2$$

$$\sigma_j^- = (\sigma_j^x - \iota\sigma_j^y)/2$$

The anti-commutator relation of σ_j^+ and σ_j^- is $\{\sigma_j^+, \sigma_j^-\} = 1$, which is expected as from fermionic operator follows the same relation for same site, but on different site fermionic operator has $[f_j^\dagger, f_k] = 0$ for $j \neq k$ and spins are unlike the fermions on different site anti-commutation. To have the analogy from fermions, we have to get fermion commutation relations from spin operators. This can be done by taking a new set of operators which is a transformation of fermionic operator defined as :

$$a_j^\dagger = e^{\left(+\iota\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)}.f_j^\dagger$$

$$a_j = e^{\left(-\iota\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)}.f_j$$

$$a_j^\dagger a_j = f_j^\dagger f_j$$

We just added a phase factor called string which is determined by number of occupied fermionic modes in $k = 1, ..., j-1$ and phase factor can be written as

$$e^{\left(+\iota\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)} = \prod_{k=1}^{j-1} e^{+\iota\pi f_k^\dagger f_k} = \prod_{k=1}^{j-1}(1 - 2f_k^\dagger f_k) = \prod_{k=1}^{j-1}(\sigma_k^z)$$

Here $\sigma_k^z = 1 - 2f_k^\dagger f_k$. The canonical anti-commutation relation is $\{a_j^\dagger, a_j\} = 1$, $\{a_j^\dagger, a_k^\dagger\} = 0$ and $\{a_j, a_k\} = 0$ and followed by spin operator, So now we can take the analogy

$$\sigma_j^+ = e^{\left(-\iota\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)}.a_j$$

$$\sigma_j^- = e^{\left(+\iota\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)}.a_j^\dagger$$

$$\sigma_j^z = 1 - 2a_j^\dagger a_j$$

Here $a_j^\dagger a_j = f_j^\dagger f_j$ is number operator which can have value of 0 and 1. Now to map fermionic operator in spin operator we use these above transformation as from σ^z,

$$a_j^\dagger a_j = \frac{(1 - \sigma_j^z)}{2} = \frac{(I - Z_j)}{2}$$

We will use the notations σ_j^x, σ_j^y and σ_j^z as X_j, Y_j and Z_j respectively which represent the X, Y and Z quantum gate on j-qubit.

$$a_j^\dagger a_k = \frac{1}{4}(\sigma_j^x - \iota\sigma_j^y)(\sigma_k^x + \iota\sigma_k^y)$$

$$a_j a_k^\dagger = \frac{1}{4}(\sigma_j^x + \iota\sigma_j^y)(\sigma_k^x - \iota\sigma_k^y)$$

adding these two terms

$$a_j^\dagger a_k + a_j a_k^\dagger = \frac{1}{2}(\sigma_j^x\sigma_k^x + \sigma_j^y\sigma_k^y) = \frac{1}{2}(X_jX_k + Y_jY_k)$$

we can simply write that the Jordan-Wigner transformation of fermionic operators to quantum computing as :

$$a_j^\dagger \to \frac{1}{2}\left[\prod_{k=0}^{j-1} Z_k\right](X_j - \iota Y_j)$$

$$a_j \to \frac{1}{2}\left[\prod_{k=0}^{j-1} Z_k\right](X_j + \iota Y_j)$$

In our fermionic hamiltonian there are two types of terms according to operators and we can transform it into spin operator suitable for quantum computing by

$$h_{jj}a_j^\dagger a_j = \sum_j \frac{h_{jj}}{2}(1 - Z_j)$$

$$h_{jk}(a_j^\dagger a_k + a_k^\dagger a_j) = \frac{h_{jk}}{2}\left(\prod_{p=k+1}^{j-1} Z_p\right)(X_jX_k + Y_jY_k)$$

where h_{jj} and h_{jk} are from fermionic hamiltonian mention above.
for N=1, We calculate spin operator Hamiltonian H_1 :

$$\mathrm{H}_1 = \langle 0|\mathrm{T} + \mathrm{V}|0\rangle a_0^\dagger a_0$$

$$= (\langle 0|\mathrm{T}|0\rangle + \langle 0|\mathrm{V}|0\rangle)a_0^\dagger a_0$$

$$= \frac{\langle 0|\mathrm{T}|0\rangle}{2}(I - Z_0) + \frac{\langle 0|\mathrm{V}|0\rangle}{2}(I - Z_0)$$

taking value of $\langle 0|\mathrm{T}|0\rangle$ and $\langle 0|V|0\rangle$ from kinetic and potential energy matrix

$$\mathrm{H}_1 = \frac{3\hbar\omega}{8}(I - Z_0) + \frac{V_0}{2}(I - Z_0)$$

taking the value of $\hbar\omega = 7$ MeV, the reason for taking this value will be discussed in next section on variational calculation.

$$\mathrm{H}_1 = 2.625(I - Z_0) - 2.48432(I - Z_0) = 0.218291(Z_0 - I)$$

For N=2

$$\begin{aligned}
\mathrm{H}_2 &= \langle 0|T + V|0\rangle a_0^\dagger a_0 + \langle 0|T + V|1\rangle a_0^\dagger a_1 + \langle 1|T + V|0\rangle a_1^\dagger a_0 + \langle 1|T + V|1\rangle a_1^\dagger a_1 \\
&= \langle 0|T|0\rangle a_0^\dagger a_0 + \langle 0|V|0\rangle a_0^\dagger a_0 + \langle 0|T|1\rangle a_0^\dagger a_1 + \langle 1|T|0\rangle a_1^\dagger a_0 + \langle 1|T|1\rangle a_1^\dagger a_1 \\
&= \frac{3\hbar\omega}{8}(I - Z_0) + \frac{V_0}{2}(I - Z_0) - \frac{\hbar\omega}{4}\sqrt{\frac{3}{2}}(X_0X_1 + Y_0Y_1) + \frac{7\hbar\omega}{8}(I - Z_1) \\
\mathrm{H}_2 &= 5.9067I + 0.218291Z_0 - 6.125Z_1 - 2.143304(X_0X_1 + Y_0Y_1)
\end{aligned}$$

From similar way we can transform for N=3,4, and so on and value of

$$\begin{aligned}
\mathrm{H}_3 = {} & 15.531709I + 0.218291Z_0 - 6.125Z_1 - 9.625Z_2 - 2.143304(X_0X_1 + Y_0Y_1) \\
& - 3.9133119(X_1X_2 + Y_1Y_2)
\end{aligned}$$

$$\begin{aligned}
\mathrm{H}_4 = {} & 28.656709I + 0.218291Z_0 - 6.125Z_1 - 9.625Z_2 - 13.125Z_3 \\
& - 2.143304(X_0X_1 + Y_0Y_1) - 3.9133119(X_1X_2 + Y_1Y_2) - 5.670648(X_2X_3 + Y_2Y_3)
\end{aligned}$$

Now we can use this hamiltonian in VQE and can estimate the expectation value and optimize it for ground state energy. Results from VQE is in table 4.1 .

H_N	Energy
H_1	-0.436 MeV
H_2	-1.749 MeV
H_3	-2.045 MeV
H_4	-2.143 MeV

Table 4.1: Ground state energy of deuteron for increasing the dimension of harmonic oscillator

Since this is for only N=4, for higher number of N our results are more better, but we have limitation in number of qubit. Extrapolation technique is used here for this problem, however if more number of qubits is available then results would be more precise without extrapolating. In next section we talk about extrapolation and required parameters for it.

4.3 Variational Calculation in Harmonic Oscillator Basis

The harmonic oscillator basis offers an expansion basis that is widely used in nuclear structure computations, but due to restricted computational resources, the basis must be truncated before computation. An extrapolation result to an infinite basis size is required in this computation. Truncating a harmonic oscillator basis has two variables, dimension of harmonic oscillator basis N and harmonic oscillator energy parameter $\hbar\omega$. Variational calculation utilize to estimate these variables, so we can define the size of expansion basis or model space. These two variables are associated with two momentum cutoff known as Ultraviolet momentum cutoff and Infrared momentum cutoff. Ultraviolet momentum cutoff related to the energy of the highest harmonic oscillator level in harmonic oscillators, whereas infrared cutoff (λ) corresponds to the lowest allowable momentum difference between single particle orbitals.

The truncated space defined by N and $\hbar\omega$ can now be considered a model space characterised by two momentum. The Ultraviolet momentum

$$\Lambda = \sqrt{m_N(N + 3/2)\hbar\omega}$$