QUANTUM SIMULATIONS READING PROJECT

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ABSTRACT

Quantum simulation is a very interesting problem, while hard in nature to implement on classical computers one can find efficient ways to implement them in certain cases using quantum systems. Here we aim to explore algorithms for the execution of Hartree-Fock methods, configuration interactions, and coupled-cluster type calculations on quantum computers.

1   Review on Quantum Simulation

This section is made with reference to [2].

1.1   Introduction

The problem of creating a simulation of a quantum system is a famous and very difficult task. If one were to make use of a classical computer the resources required would scale exponentially. For example if one were to store a state of N spin 1/2 particles we would need to store 2^N numbers for the state and 4^N for the unitary evolution (this is about

4TB for $N = 40$).

There do exist certain classical stochastic methods which can be used for certain systems (specifically those where the functions being integrated do not change sign and vary slowly). The Quantum Monte Carlo methods offer a polynomial time implementation for the quantum many body simulation.

One of the alternatives to simulate quantum systems was proposed by Feynman. Bluntly put we use quantum systems to simulate quantum systems. The method described uses a mapping of the desired state and desired evolution to a state of the system and it's evolution. We denote the system state by $|\varphi\rangle$ and it goes from $|\varphi(0)\rangle$ to $|\varphi(t)\rangle$ with evolution $U = \exp(-\iota\hbar H_{sys}t)$. The simulator state $|\psi\rangle$ goes from $|\psi(0)\rangle$ to $|\psi(t)\rangle$ with evolution $U' = \exp(-\iota\hbar H_{sim}t)$. If we can create a mapping between the final and initial states and the evolution operator, we can simulate this system.

1.2 Digital and Analog Quantum Simulations

1.2.1 Digital Quantum Simulation

Here we make use of qubits for simulating the systems. Suppose we want to simulate spin 1/2 particles, we assign each particle to one qubit and we prepare our simulator state $|\psi(0)\rangle$ using the 1,0 convention for spin up and down respectively. For getting $|\psi(t)\rangle = \exp(-\iota\hbar Ht)|\psi(0)\rangle$ we apply the unitary $U = \exp(-\iota\hbar Ht)$ to our initial state by decomposing it into single qubit and two qubit gates (eg: U3 and CNOT gates are universal). This is referred to as DQS (digital quantum simulation) and since we can make a circuit for all unitaries, DQS is universal however we need not be able to find an efficient decomposition for all unitaries.

State preparation in general is a task which need not be efficient but in some cases there are convenient efficient algorithm. For example there is an algorithm for efficiently preparing a state of m electrons occupying n orbitals using recursion to reverse engineer the given state to the $|0\rangle^{\otimes(n)}$

For the actual evolution of state we use the Trotter's formula for dealing with systems of form $H = \sum_{i=1}^{n} H_i$ by using the fact that $\lim_{n\to\infty}(\prod_i \exp(H_i/N))^N = \exp(\sum_i H_i)$ since all the commutation terms are second order with $1/N$ hence in the limit go to zero so we break our unitary into small time steps to make sure that the error doesn't go large. The algorithms functions like this (reference: [3])

Inputs: The initial state $|\psi_0\rangle$ along with the Hamiltonian $H = \sum_{k=1}^{L} H_k$, the error range δ and time t_f for which we have to find $|\psi(t_f)\rangle$. Here $U_{\Delta t} = \prod_{k=1}^{L} \exp(-\iota\hbar H_k\Delta t)$

Outputs: The state $|\psi(\tilde{t}_f)\rangle$ such that $|\langle\psi(\tilde{t}_f)|\rangle|^2 < 1 - \delta$

Procedure:

1. Initialize state as $|\tilde{\psi_0}\rangle = |\psi_0\rangle$.
2. Iterative update $|\psi_{j+1}\rangle = U_{\Delta t}|\psi_j\rangle$.
3. $j = j + 1$; goto 2. while $j\Delta t < t_f$.
4. $|\psi(\tilde{t}_f)\rangle = |\tilde{\psi}_j\rangle$ final result

Runtime: This typically functions in $O(poly(1/\delta))$ operations. Here $U_{\Delta t}$ is a unitary which describes the approximate evolution over a time of Δt

Now comes the process of measurement. Generally for quantum systems this is done via quantum state tomography however those require resources that scale exponentially with the size of the system. To get around this estimation is done of correlation functions or spectra of operators.

1.2.2 Analog Quantum Simulation

In analog quantum simulation a real quantum system is used to simulate another quantum system and the real quantum system would be controllable hence one can make inferences about the simulated system using this possibly easier to control system by using mappings. The mappings are made as $H_{sim} = fH_{sys}f^{-1}$ where the initial state is transformed using f and we get the final state by transforming back with f^{-1}. Essentially we must note that H_{sim} and H_{sys} have the same eigenvalues for this to be a valid mapping. An example of hamiltonians like this would be a hamiltonian describing a gas of interacting bosonic atoms in a periodic potential and the bose-hubbard hamiltonian.

$$H_{sim} = -J\sum_{i,j}\hat{a}_i^\dagger\hat{a}_j + \sum_i \epsilon_i\hat{n}_i + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \tag{1}$$

$$H_{BH} = -J\sum_{i,j}\hat{b}_i^\dagger\hat{b}_j - \mu\sum_i \hat{n}_i + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \tag{2}$$

The bosonic atoms hamiltonian is described in 1 where $\hat{a}_j$ and $\hat{a}_j^\dagger$ are the bosonic annihilation and creation operators respectively and J is the hopping strength and U is the interaction strength. ϵ_i represents the energy offset. One can see that eq1 is quite similar to eq2. The μ eq2 is the chemical potential and that is pretty much the only difference. One can execute the bose-hubbard hamiltonian as described by eq2 using atoms in an optical potential. However there need not be a straightforward mapping in most situations. AQS does have quite some advantages over DQS such as the fact that state preparation would occur naturally as the system would naturally gravitate toward the equilibrium state normally. Also measurement can be done directly unlike the computational manipulation required in DQS.

1.3   Resource estimation

There is a general rule of thumb that to outperform a normal computer with a quantum computer one would need somewhere between 40 to 100 qubits. There are plenty of interesting things that can be done with about 10 qubits too from proof of concept simulations to even quantum chaos. However when you only need a few qubits you might as well use a classical computer. In DQS the estimate for representing N particles with pairwise potential would require n qubits for representing the wave function as a discrete variable and we would need m qubits for estimation of values to some precision. The coloumb potential can be calculated in $\mathcal{O}(N^2 m^2)$ steps which is clearly an exponential improvement from the classical way of calculation. There is however an overhead cost in for the gates as the step size decreases in trotterization.

It is stated that AQS has less stringent resource requirements and can procide useful results with classical computers. In AQS one can manipulate a larger number of particles with more resources for example hundreds of thousands of atoms have been trapped using only three laser beams.

In AQS effects of decoherence are generally believed to be less dramatic and is even suggested that it might be useful as a way of modelling decoherence of the simulated system. If the noise level naturally present in the simulator is lower than the simulated system one can artificially supplement the noise so that it faithfully mimics the simulated system. In principle one can make use of the natural symmetries present in the system so as to modify the effective decoherence using appropriate mappings. There are cases where fault tolerant methods are inefficient compare to trotter approximation such as finding the low lying spectrum of a pairing hamiltonian in an NMR implementation. Two qubit entaglement was found to be exponentially sensitive to both small changes in the hamiltonian and locations of the chosen qubits due to natural ordering introduced on the qubits by coding of the simulated system.

1.4   Physical Realizations

All physical systems that can be used as a quantum computer would also be a universal machine for DQS. However there are various quantum systems that can be used to implement AQS.

1.4.1   Atoms and Ions

Neutral atoms in optical lattices are well suited to mimic solid state systems. These optical potentials can be adjusted to change geometry and dimensionality of lattice like creating triangular or kagome lattices. These are quite flexible systems where there are several controllable parameters and there are both bosonic and fermionic elements that can be used here. A general Hubbard hamiltonian is written as

$$H = H_{hop} + H_{interaction} + H_{pot} + H_{internal} \tag{3}$$

One can simulate the Mott insulator-superfluid phase transition using this system by tuning the on-site interactions using Fresbach resonances. Continuous tunability of interaction strength allows one to enter a regime called the unitary regime where interaction strength is comparable to Fermi energy so we only have one energy scale in our system. Adressing individual atoms is a tough task however due to the best laser focusing widths are typically near the scale of lattice distance ($0.5 - 0.8 \mu m$)

One can even use these for DQS since one can make controlled operations by using a double optical potential with interaction between neighbouring atoms.

Using ions one can make multiple qubit gates by making use of their Coulumb repulsion and ion qubits tend to have much longer coherence times (in the order of seconds) and can also make sequences of high fidelity quantum gates.

The quantum states for trapped ions are mostly manipulated using resonantly driving transitions between internal states of the ions or resonantly driving sideband transitions involving the internal states and vibrational states of the ions in the trapping potential. The hamiltonian describing coupling between internal and vibrational modes due to laser driving at red-sideband frequency is the following

$$H = \iota\hbar\eta\Omega[\exp(\iota\varphi)\sigma_+ a - \exp(-\iota\varphi)\sigma_- a^\dagger] \tag{4}$$

Here Ω is the Rabi frequency of trasition between the internal states, σ_+ and σ_- are the two level atom transition operators. $a, a^\dagger$ are the ladder operators for the vibrational modes and ϕ is laser phase and η is the Lambe-Dicke

parameter. Using this one can realize quantum gates for DQS and even some hamiltonians for AQS. High fidelity one,two,three qubit (toffoli) gates have been implemented using this. Ions have generally been trapped using linear harmonic traps.

1.4.2 Nuclear and electronic spins

Nuclear spin qubits have long coherence times ($> 1s$) and high fidelity quantum gates of up to 12 qubits have been demonstrated. Here nuclear spins are manipulated using NMR (nuclear magnetic resonance). The general form of the hamiltonian is

$$H = -\hbar\gamma B \sum_i I_i^z + \sum_{i>j} J_{ij} I_i^z I_j^z \tag{5}$$

Here I is the angular momentum operator and J represents the spin-spin coupling coefficients. B is magnetic field and γ is the gyro-magnetic ratio. The different transitions between pairs of energy levels generally have distinct resonance frequencies which makes it possible to implement multi qubit gates using rf (radio frequency) pulses. Scaling is however a big issue here but can be possibly addressed by making use of nitrogen vacancy centers for strongly correlated systems.

Another system that is used are electron spins in semiconductor quantum dots. Quantum dots are semiconductor systems where excitations are confined in small regions in one or two dimensions and if they are roughly as wide as the wavelength of charge carrier they sort of have quantized levels similar to those of actual atoms. Readout can be manipulated both electrically and optically. They have decay times of $> 1s$. A hamiltonian for an array of quantum dots is given by

$$H = \sum_{j=1}^n \mu_B g_j(t) B_j(t) \cdot S_j + \sum_{1 \leq j < k \leq n} J_{jk}(t) S_j \cdot S_k \tag{6}$$

The first term comes form energy of applied magnetic field and the second term is exchange interaction due to virtual tunneling between quantum dots and S_j is spin of the electric charge quanta of the jth dot.

1.4.3 Superconducting circuits

There are many ways in which one can encode quantum information in superconducting circuits: number of super-conducting electrons on a small island, direction of current around a loop or in oscillatory states of the circuit. The circuit can be manipulated by applied voltages and currents. These have an advantage over real atoms since one can tailor characteristic frequencies, interaction strengths and so on much easily. Hamiltonian for N charge (flux) qubits biased at their symmetry points (optimal for quantum coherence) coupled capacitively is

$$H = -\sum_{i=1}^N \frac{\Delta_i}{2} \sigma_i^Z - \sum_{i,j} J_{ij} \sigma_i^Z \sigma_j^Z \tag{7}$$

Where Δ_i is level splitting and the J_{ij} is for coupling strength between i and j qubits. It must be noted that these are not two level systems however these additional levels could possibly be utilized for AQS for spin greater than 1/2.

1.4.4 Photons

Photons can carry quantum information over long distances and would hardly be affected by noise and decoherence and can encode qubits using polarization. One qubit gates can easily be realized using linear optical components however implementing two qubit gates for photonic systems are much more difficult. These have been used for many impressive tasks however like to calculate the possible fractional statistics of anyons using a six photon graph state, calculate the enrgy system of spectrum of hydrogen to 10 bits of precision and even simulate frustrated spin systems. These do have issues in flexibility and scalability so have a long way to go.

2 Hartree-Fock Theory

2.1 The formulae

The main aim here is calculations involving many electron systems in a pairwise potential. Using the Born-Oppenheimer approximation one can find the exact solutions for a hydrogen atom (or any one electron atom) however exact solutions cannot be found once we have more than one electron. The idea of the approximation is to consider

that nuclei are relatively stationary since electron movement is much faster. Let's first write the for an N electron system with N_{nucl} nuclei each with some Z_j atomic number at $\vec{R}_j$.

$$H^{el} = \sum_{i=1}^{N} \frac{p_i^2}{2m} - \sum_{i=1}^{N} \sum_{j=1}^{N_{nucl}} \frac{Z_j e^2}{|\vec{r}_i - \vec{R}_j|} + \sum_{i>j=1}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \tag{8}$$

Our aim is to solve $H \ket{\psi(1, 2, \ldots, N)} = E \ket{\psi(1, 2, \ldots, N)}$. We must note that this will be anti symmetric since it describes fermions. We will adopt the mean field approach where we assume particle's dynamics are decided by a mean field created by particles at rest. Another assumption is that each electron is described by a single electron wavefunction called the spin orbital which we represent as $\phi_i(x)$ which has both a spatial and spin component. The final solution is represented as a determinant called the slater determinant

$$\psi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = \frac{1}{\sqrt{N!}} \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \ldots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \ldots & \phi_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \ldots & \phi_N(x_N) \end{bmatrix} \tag{9}$$

The electrostatic potential felt by an electron occupying orbital $\phi_i(\vec{r})$ due to the mean field of remaining $N-1$ electrons would be

$$V_i(\vec{r}) = \sum_{j=1, j \neq i}^{N} \bra{\phi_j} \frac{e^2}{|\vec{r} - \vec{r'}|} \ket{\phi_j} \tag{10}$$

We also will define $V_{nucl}(\vec{r})$ which is the nuclear attraction potential felt by an electron at $\vec{r}$ then we have

$$V_{nucl}(\vec{r}) = \sum_{i=1}^{N_{nucl}} \frac{Z_i e^2}{|\vec{r} - \vec{R}_i|} \tag{11}$$

From this we get the Hartree equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{nucl}(\vec{r}) + V_i(\vec{r}) \right) . \phi_i(\vec{x}) = \varepsilon_i \phi_i(\vec{x}) \tag{12}$$

Clearly the nuclear attraction potential is a one eletron operator and the electrostatic potential is a two electron operator. The following equation shows the expectation values for one electron and two electron operators.

$$\bra{\Phi} O_1 \ket{\Phi} = \sum_i \bra{\phi_i} f \ket{\phi_i} = f_{ii}, O_1 = \sum_i f(\vec{r}_i) \tag{13}$$

$$\bra{\Phi} O_2 \ket{\Phi} = \frac{1}{2} \sum_j \sum_i (\bra{\phi_i \phi_j} g \ket{\phi_i \phi_j} - \bra{\phi_i \phi_j} g \ket{\phi_j \phi_i}), O_1 = \sum_{i,j} g(\vec{r}_i) \tag{14}$$

So the whole thing is reduced into an eigenvalue problem. We define the operators $h(\vec{r}_i) = \frac{p_i^2}{2m} + V_{nucl}(\vec{r}_i), V_H \ket{\phi_i} = \sum_{j=1}^{N} \bra{\phi_j} \frac{e^2}{r_{12}} \ket{\phi_j} \ket{\phi_i}$, $V_{ex} \ket{\phi_i} = \sum_{j=1}^{N} \bra{\phi_j} \frac{e^2}{r_{12}} \ket{\phi_i} \ket{\phi_j}$ and the problem reduces to the following eigenvalue problem

$$(h + V_H + V_{ex}) \ket{\phi_i} = \varepsilon_i \ket{\phi_i} \tag{15}$$

The total energy however is not simply the sum of all the orbital energies for the system and is actually $E_{HF} = \frac{1}{2} \sum_{i=1}^{N} (\varepsilon_i + h_{ii})$. We call the fock operator as $F = h + V_H + V_{ex}$.

2.2 Canonical transformations

This part is made with reference to supplementary materials provided in [1]. For solving the hartree fock equations and arriving at the assymetric state the state is variationally solved such that energy is stationary with respect to first order changes in the wavefunction and we start from an arbitrary orthogonal basis $\{\phi_i\}$. So we solve $\bra{\delta \psi} H \ket{\psi} = 0$. We assume the solution is represented as

$$\braket{r | \psi} = \bra{r} \prod_{i=1}^{n} a_i^\dagger \ket{vac} = \frac{1}{\sqrt{n!}} \det \begin{bmatrix} \chi_1(r_1) & \ldots & \chi_1(r_n) \\ \vdots & \ddots & \vdots \\ \chi_n(r_1) & \ldots & \chi_n(r_n) \end{bmatrix} \tag{16}$$

We will now index the states which are in the product wavefunction by i and those which aren't by a. We then can write the first order variation as $\langle\delta\psi| = \langle\psi| a_i^\dagger a_a \zeta$ where ζ is the first order variation in χ_i so we get the expression for the stationarity of the state as

$$\langle\psi| a_i^\dagger a_a H |\psi\rangle = 0 \tag{17}$$

We also have the one-body fermionic generators form a closed lie-algebra

$$[a_p^\dagger a_q, a_r^\dagger a_s] = \delta_{q,r} a_p^\dagger a_s - \delta_{p,s} a_r^\dagger a_s \tag{18}$$

The adjoint representation of an element of the algebra would be $\kappa = \sum_{p,q} \kappa_{p,q} a_p^\dagger a_q$ and it's commutators can be represented as $[\kappa, a_p^\dagger] = a_p^\dagger \kappa_{p,q}$ and $[\kappa, a_p] = a_p \kappa_{p,q}^*$. We then define similarity transformations on the ladder operators: $e^K a_p^\dagger e^{-K} = \sum_q a_q^\dagger u_{q,p}$, $e^K a_p e^{-K} = \sum_q a_q u_{q,p}^*$ and here u is the matrix given by the exponentiation of the coefficient matrix for the generator operator κ so it is $u = e^\kappa$.

Any rotation of the underlying basis can now be written with the similarity transform as

$$|\phi(\kappa)\rangle = e^K a_1^\dagger e^{-K} \ldots e^K a_n^\dagger e^{-K} = e^K |\psi\rangle \tag{19}$$

Now before we proceed we must note that the 2-RDM (reduced density matrix) can be obtained from the 1-RDM since

$$^1D_i^j = \langle\phi| a_j^\dagger a_i |\phi\rangle \tag{20}$$

$$^2D_{ij}^{pq} = \langle\phi| a_p^\dagger a_q^\dagger a_j a_i |\phi\rangle = {}^1D_i^{p1}D_j^q - {}^1D_i^{q1}D_j^p \tag{21}$$

Using expression of energy we get that we can express energy in terms of the 1-RDM purely since we can write the 2-RDM in terms of 1-RDM.

$$E(\kappa) = \sum_{ij} h_{ij} \langle\phi(\kappa)| a_i^\dagger a_j |\phi(\kappa)\rangle + \sum_{ijkl} V_{ijkl} \langle\phi| a_i^\dagger a_j^\dagger a_k a_l |\phi\rangle \tag{22}$$

$$= \sum_{ij} h_{ij} {}^1D_i^j + \sum_{ijkl} V_{ijkl} {}^2D_{lk}^{ij} \tag{23}$$

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