PHY3650 Paper

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Abstract

Quantum many body physics is a modern subdiscipline in quantum mechanics and condensed matter theory in which multiple particles composing of a single system are studied in conjunction as a whole. Unlike many problems found under extensive study in an undergraduate quantum mechanics course, the systems of interest usually range typically to more than three degrees of freedom, sometimes ranging to even the triple digits. This is largely because many of the problems in this field are used as models for the behaviour of electrons contained in some metallic surface. The way of finding analytic solutions to finding ground states of Hamiltonians of these models gets extremely tedious as the number of particles in the system increases (we will define these terms later). This has led research towards a direction in which one may prefer a numerical approach towards solving this problem, which is where quantum computing plays a role. In this paper aimed at a undergraduate audience informed of some basic principles in quantum computing and information theory, we show how to use quantum circuits and machine learning (sometimes this is called quantum machine learning) methods in order to find ground states of multiple particle systems in a slightly technical fashion. We use what we have learned in order to solve the problem of finding ground energy levels of a simple one dimensional lattice model: the one dimensional transverse field Ising model.

Basically a table of contents:

Theory and background information

We review some fundamental concepts behind quantum mechanics that should be familiar.

Solutions to the Schrodinger Equation

All isolated quantum systems must obey the Schrodinger Equation:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = H|\psi\rangle$$

Where H is the Hamiltonian or energy observable of the system. Physically speaking, because H is a hermitian operator, it must contain a spectral decomposition consisting of distinct eigenvecctors and eigenvalues that span the hilbert space.

$$H = \sum_i E_i |E_i\rangle\langle E_i|$$

Of particular interest to physicists is finding the energy states and levels of the Hamiltonian. This can be done analytically by using a diagonalization routine to the Hamiltonian. Once we know these energy states, we could calculate everything that we wish to know about a certain given system, be it expectation values with respect to certain observables, the time evolution of the system given some initial state, and etc.

Where $|E_i\rangle$ are referred to as the energy levels of the system . To see why, we take a look at the equation when the Hamiltonian is time-independent. If $|\psi_0\rangle$ is the initial state of the system at an initial reference $t = 0$, then a solution to the equation would be of the form:

$$|\psi_t\rangle = e^{-\frac{i}{\hbar}Ht}|\psi_0\rangle$$

Where the operator exponential is a unitary, which obeys the main postulates of quantum mechanics in that an isolated system must undergo unitary evolution. We sometimes call this exponential the time evolution operator. It has a similar spectral decomposition:

$$e^{-\frac{i}{\hbar}Ht} = \sum_j e^{-\frac{iE_j}{\hbar}t}|E_j\rangle\langle E_j|$$

Now if we suppose that our state initially started off as one of the eigenvectors of the Hamiltonian, then the state of the system as a function of time would then be

Variational Theorem

Variational Quantum Circuits

It is an arbitrary Unitary imposed upon the initial state

Variational Quantum Algorithm: Finding ground states of Hamiltonians

Let A ground state $|\psi_{\text{gs}}\rangle$ is an

Culiminary Example: Transverse Field Ising Model

We gather all of our knowledge of variational quantum algorithms in order to solve a simple problem: finding the energy ground state of the transverse field ising Hamiltonian. Our Hamiltonian of interest is:

$$H = -j \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

Where σ^z, σ^x are the Pauli matrices and the first sum is over adjacent qubit pairs. As an example to get the feel of what this looks like, consider an $N = 3$ system of qubits, then our Hamiltonian will be:

$$H = -j\left(\sigma_1^z \sigma_2^z + \sigma_2^z \sigma_3^z\right) - h\left(\sigma_1^x + \sigma_2^x + \sigma_3^x\right)$$

(include citation). Diagonalizing this is extremely difficult and scales even longer with the dimension of the hilbert space, which is $\dim(\mathcal{H}) = 2^N$ once we reach to two orders of magnitude, one may as well shoot darts with a blindfold in order to guess the ground state, which is exactly what we are going to do. For this example, we build the following.

We build the following ansatze circuit, where one layer of the circuit is shown:

The analytical expression for the ground state energy of a transverse model is:

$$E_{\text{gs}} = \frac{2N}{\pi} |h + j| \mathcal{E}\left(\frac{4hj}{(h+j)^2}\right)$$

(Insert here our experimental data, we could get a plot of the energy level of the ith iteration on the vertical axis and the amount of iterations at the horizontal axis.)

Concluding Remarks

All of what we have covered so far has only been a scrape of the iceberg. Given that the field has emerged from the past twenty years, the future of its forward direction is largely optimistic as the technological implementation of near-fault-tolerant quantum devices reaches our fingertips. We hope that these references provide future readers into more indepth topics.