PHY3650 Paper

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Abstract

Quantum many body physics is a vast subdiscipline in condensed matter theory and quantum chemistry that composes the study of multiparticle quantum systems and how macroscopic properties emerge from detailed descriptions of their dynamics. Many of the problems of interest involve finding ground states of conducting-surface and molecular systems, finding the time evolution of how a system changes from a known state and much more. Of particular problem under extensive research are the methods of finding ground-state solutions to these complicated systems, as most of them involve diagonalization of hamiltonian systems with matrices

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.

Theory and background information

We review some fundamental concepts behind quantum mechanics that should be familiar to the reader:

Quantum Systems

Quantum systems live in what is mathematically called a Hilbert Space. For most of the quantum systems that we are interested, particularly those that can be modeled and simulated via a quantum system, a Hilbert space $\mathcal{H}$ is a finite-dimensional vector space attached with an inner product (a generalization of a dot product from introductory classical mechanics). Because our Hilbert space is finite dimensional, it must have some sort of basis; better yet, because our inner product allows us to introduce notions of length and orthogonality, we can then assert ourselves orthonormal bases. For many physical problems, the orthonormal bases in our Hilbert space are typically associated with distinguishable states; as an example, for the familiar two qubit system, we usually use the well-called computational basis $\{|0\rangle, |1\rangle\}$ for typical calculation in a quantum system. For another system, say a spin-$\frac{1}{2}$ particle, the states that we can distinguish upon measurement are those of particles spinning up or those of spinning down, to which we relegate the symbols $\{|\uparrow\rangle, |\downarrow\rangle\}$ an arbitrary state of a quantum system can be described as a linear superposition of the distinguishable state elements of the system. We can write this as

$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

As an example of using the computational basis of the qubit system, where α and β are arbitrary complex numbers. A constraint that we have on deciding what is a state and what is not a state is that the state be normalized. This is so because we want to associate the modulus-squared of the coefficients of the linear combination as a probability amplitude.

Using a basis of some vector space, we can typically map these 'abstract' vectors into more practical objects such as column vectors. For example we can typically convert the following superposition of say a spin-1 system composed of three distinguishable states $\{|\uparrow\rangle, |0\rangle, |\downarrow\rangle\}$ (read 'spin-up', 'spin-zero', 'spin-down') into the following:

$$|\uparrow\rangle \mapsto \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle \mapsto \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |0\rangle \mapsto \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

And have our arbitrary system state $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle + \gamma|0\rangle$ be represented as the column vector:

$$|\psi\rangle \mapsto \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

Operators and Observables

An operator is a linear function that maps an elemnet of some vector to another element of that vector space. In a finite dimensional vector space, similar to what we have done to represent states in a hilbert space with a column vector,

we can associate these operators as matrices that can then be acted on these column vectors in order to form another vector [1] (cite axler linear algebra)

Operators in quantum mechanics come in different forms with different purposes. We outline two relevant ones: unitary operators associated with the time evolution of the system and so called observables associated with measurement outcomes of a certain quantum particle.

A unitary operator is an operator that preserves the norm of the state (in mathematics this is typically referred to as an isometry). As a consequence of this property, many important corollaries soon follow towards characterizing these unitary operators. For some examples, one can prove that the eigenvalues of any unitary operator must lie along the complex unit circle, show that the determinant of a unitary is 1, show that for any arbitray orthonormal basis of some hilbert space, the set of the image of all these basis members under the operator (say, if $\{|\phi_1\rangle, \dots\}$ is a set of orthonormal bases, then $\{U|\phi_1\rangle, \dots\}$ is the image set under the operator U) is also an orthonormal basis, and so on.

One of the main postulates of quantum mechanics (cite mike and ike) is that the time evolution of the system must be unitary. Say that at some reference time $t = 0$ the state is $|\psi_0\rangle$. Then at some later time t the state of the system will then be

$$|\psi_t\rangle = U(t)|\psi_0\rangle$$

Where U must be some unitary operator that depends on time. The motive for making this an axiom for quantum theory has some sense to it. We require the state to be normalized, which is satisfied by unitarity of the operator.

In quantum computing, much of the circuit diagrams essentially describe the time evolution of the system as gates are subsequently applied one by one. To this we don't typically use time a lot in the same sense that in classical mechanics we describe the position of the particle by a continuum of time. We just say that 'the state of the system right after applying this gate is that' and so on and forth.

Another type of operator that is of common use are observables. An observable of a certain quantity (say, the postion of the particle, the spin-z component of a fermion, etc.) is often described by a hermitian operator. The eigenvalues of a hermitian operator are typically associated with the measurement obtained from observing the eigenstate corresponding to the eigenvalue. To provide brevity, in quantum computing, most measurements are done by using the pauli σ_z operators, whose eigenvectors are the computational basis members $|0\rangle$ and $|1\rangle$ with eigenvalues 1 and -1 respectively. When we measure 1 on the system, that means that our qubit has collapsed into a $|0\rangle$ state.

An observable of particular interest is the energy observable, commonly referred to as the Hamiltonian of a system. The historical nature of why we decide to call the energy observable the Hamiltonian comes the Hamiltonian formulation of classical mechanics, in which the equations of motion are usually derived from the Hamiltonian of the system, where in most natural cases can be considered as the classical energy expression. Of most interest to physicists are

the eigenvalues of the Hamiltonian, commonly referred to as the energy levels of the system. (Do a search in which why finding ground states and energy levels are important)

One of the main postulates of quantum mechanics assert that the time evolution of the state must be unitary. Operators, mathematically speaking (cite Axler Linear Algebra), are linear functions acting on members on a vector space that take a vector and map it onto another vector in that same vector space. We can

Variational Quantum Algorithms

Today's quantum computers are noisy. The term used by the modern literature is *Noisy Intermediate-Scale Quantum* devices, often abbreviated as NISQ devices. Although time will have to wait until fault-tolerant quantum computing devices have come into the full utility scale, that doesn't mean that NISQ devices are useless. One class of algorithms and problems that have found themselves to be of current practical use are variational quantum algorithms, VQA for short. We focus our breadth here on VQAs that are characterized by hybrid classical and quantum processes, in which quantum computers are used for state preparation and measurement that will then be used by classical optimization techniques that then tweak these parameters for quantum devices.

There are a wide variety of VQAs that fall under this shoulder; one class of problems is commonly referred to as the Variational Quantum Eigensolver, which seeks to estimate and find the ground-state energy of the Hamiltonian operator of some given physical system of interest. Its uses are quite popular in quantum chemistry and in condensed matter physics, in which conducting surfaces and molecular bondings are often modelled as a fermionic Hamiltonian that can then be mapped into a qubit via mathematical transformations. (citation needed). Another class of algorithms that fall under the VQA scheme are commonly referred to as Quantum Approximate Optimization Algorithms, in which classical optimization problems are translated into a quantum algorithm to then be solved similarly in some fashion. Applications of this are more mathematical, such as max-cut problems [3] [4] This paper focuses on the variational quantum eigensolver

Variational Quantum Eigensolver

The Variational Quantum Eigensolver has several components: cost function, ansatz circuit and the classical optimizer. We provide descriptions of each process.

Cost Functions: Typical cost functions in a VQE are of the form

$$C(\vec{\theta}) = \langle \psi_{\vec{\theta}} | H | \psi_{\vec{\theta}} \rangle$$

Where $|\psi_{\vec{\theta}}\rangle$ is a prepared 'guess' state prepared by some unitary operation $U_{\vec{\theta}}$ often referred to as the ansatz circuit. What makes VQE useful for finding

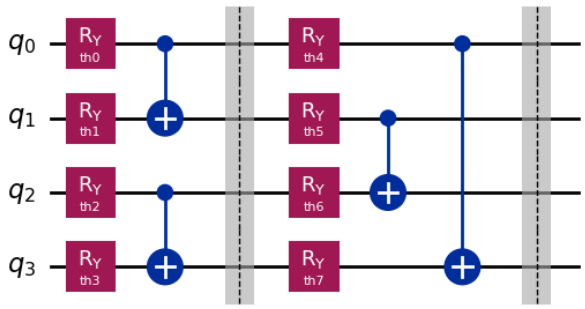
the low ground states is that for any state $|\psi\rangle$, the expectation value of the Hamiltonian will always be greater than the ground energy; that is:

$$C(\vec{\theta}) \geq E_1$$

Where $\{E_1, E_2, \ldots, E_N\}$ are the eigenvalues or energies of the Hamiltonian listed in increasing order. In order to prove this (I haven't proven it yet)

Ansatz Circuits: The ansatz referred in the VQA is a unitary circuit parameterized by some set of real parameters $\vec{\theta}$ that are tweaked by the classical parameter. An ideal ansatze circuit should be one such that the state associated with the minimum optimization value is within its range. This is determined by the gates used within the ansatze, which are rotation gates and some two qubit interaction gates that produce some entanglement within the system, CNOT being an example.

The choice of ansatz depends on the specific VQA problem at hand. Some ansatzes are better than others depending on the problem at hand. One typical example of an ansatze used in VQE is what is commonly called a local-2 circuit. This consists of a series of k layers attached to the quantum circuit one at a time, in which each layer consists of a sublayer consisting of rotation gates across the system and a series of entangling gates among local sites. A figure of a one layer circuit is shown below:



Barren Plateaus One common issue seen in the development of VQAs and optimization is the issue of barren plateaus. The cost function $C : \mathbb{R}^n \to \mathbb{R}$ describes an $n-dimensional$ surface (is it proper to call it manifold) that may have a complicated landscape. In most cases of deep parameterized quantum circuits, it is often the case that the parameter vector reaches a region of flat curvature, in which the cost function gradient vanishes but doesn't converge to an extremum point. ()

Classical Optimizer The output of the expectation value expression shown above is then inputted into a classical optimizer which then tweaks the variables of the expression in order to produce a minimal value via multiple iterations of the expectation value.

Using these components, the step of the algorithm and program are as follows:

1. *Initialization*: Set up the state into a known reference state either by using the ansatze state or by preparation via some circuit that precedes the ansatz. For the example that will ensue, before applying the ansatz circuit, we initialize the qubit state to be an alternating sequence of ones and zeros ($|\psi_0\rangle = |0101\ldots\rangle$. Using the ansatz along with a set of initial parameters initiated at random increases potential risk of landing in a barren plateau [5]

2. *calculation of expectation value* Apply the ansatz circuit with initial parameters $\vec{\theta_0}$ onto the state. We then calculate the expectation value of the operator and use it as a starting point for the optimizer

3. optimization of parameters the optimization routine then repeats the above steps with new guesses of $\vec{\theta}_{\text{opt}}$, the optimal parameter that minimizes the cost function.

Culiminary Example: Transverse Field Ising Model

Running the tests on the ising model, what we need:

1. Compare the runtime of using the VQE method and the straight diagonalization method on the ising hamiltonian for $N \in [2, 10]$. This will be one of our plots: on the x-axis will be the size of the system and on the y-axis will be the time scaling. An optional parameter is to add a best fit curve to the expression

2. We will be using two backends for running the VQE. One of them uses a fake model of an actual quantum computer and the other uses a simulator backend. We will compare the convergence of the VQE algorithm with the atual analytical value. For this, we will fix h and j. For each N, we will run the algorithm for some sample size n and obtain a list containing all of the convergence values of the optimization. We will then form a box plot . This will be gathered into one box plot

3. This is optional. Stick to one simulator and fix h, j and N. We will generate one plot in which we will compare the optimization methods (this could be a gradient desccent, COBYLA, and others) available in Scipy's optimize library. The plot will have on the x-axis the amount of iterations of the optimization algorithm and on the y-axis we will have the value of the cost function per iteration. We can also have a horizontal line that signifies the analytical ground-state energy.

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:

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

Where σ^z, σ^x are the Pauli matrices and the first sum is over adjacent qubit pairs. The lower script indicates the site location at which to apply the operator (σ_1^x on a two-qubit system corresponds to $\sigma^x \otimes \mathbb{I}$) As an example to get the feel of what this looks like, consider an $N = 3$ system of qubits, then our Hamiltonian will be:

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

Because the dimension of the hilbert space increases exponentially with the amount of qubits involved in the system, any method of diagonalization of such matrix will soon be limited by both the space that it takes to store such a large amount of numbers and the runtime it takes to diagonalize $N \times N$ matrices. Better and efficient methods need to be found in order to scale the qubit size up to utility scale, say more than 20 qubits.

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 for comparison:

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

Where

$$\mathcal{E}(m) = \int_0^{\frac{\pi}{2}} \sqrt{1 - m^2\sin^2(\theta)}\mathrm{d}\theta$$

Is the complete Elliptic integral of the second kind [2]

Analysis of Results

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.

References

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