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May 7th, 2024

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Dear Griffith's Publishing,

The following is a short excerpt from my in-progress textbook, **Applications of Quantum Computers to Optimization Problems**. Quantum optimization is a field which will revolutionize many industries, and desperately needs to be further explored.

From my time in academia, it is clear there is a massive disjoint between physicists and computer scientists, specifically surrounding quantum computers. Not enough literature exists surrounding advanced topics in the field. Those with understanding typically comprehend either the physical or algorithmic side of systems. More advanced material needs to be created without baseline levels of understanding, so that individuals outside of their specified area can understand the entire field.

Claims have been made towards virtual laboratories, improved financial models, and other lofty goals for quantum systems. These will not be achievable unless physicists and computer scientists work together hand in hand. This piece serves as an introduction to quantum optimization for those without rigorous experience in algorithmic development or physical systems. Hopefully it will allow the idea to be exposed to a greater array of individuals, further publicizing an idea which could help revolutionize the next few decades.

I am currently in the progress of creating a manuscript for this piece. It should be finished before the end of the summer. If you have an interest in pursuing this idea with me as a publishing partner, you can reach me by mail, email, phone, or any method you'd prefer. Let me know, I look forward to your response.

Best,
Jonah Sachs

Applications of Quantum Computers to Optimization Problems

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May 7 2024

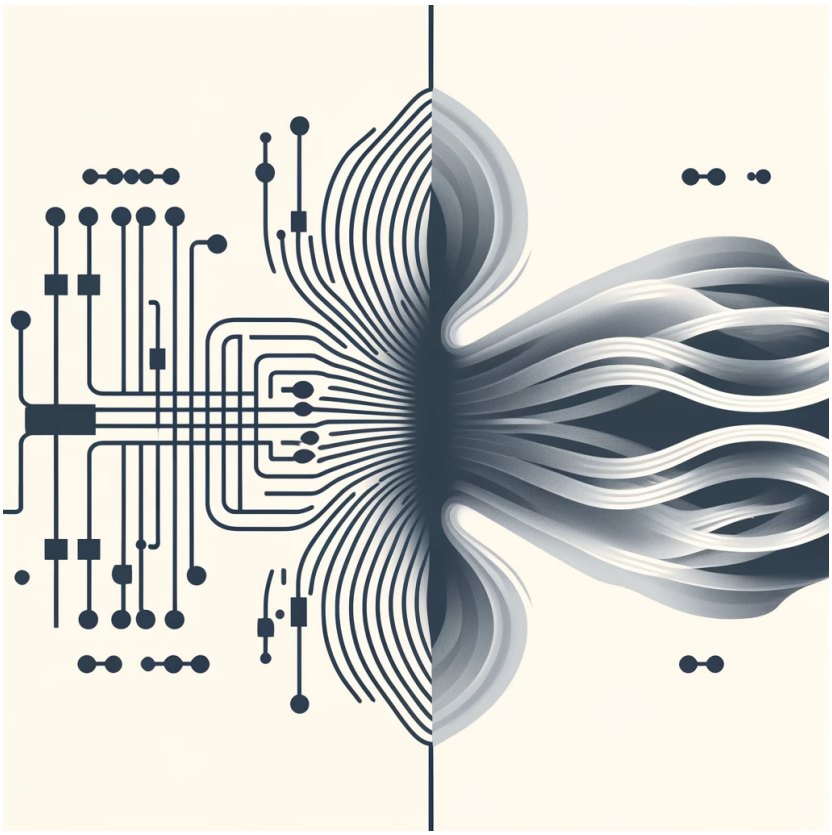

Figure 1: An illustrative comparison between gate based quantum computers (L) and more fluid adiabatic systems (R). Generated using DALL-E 2

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1 Abstract

Quantum "weirdness" creates mathematical advantage in certain types of computer science problems for quantum systems over classical systems. Given the hardware for quantum systems is scaled large enough, quantum systems can outpace classical systems for many extremely profitable problem types. A widely cited example is optimization problems. Two quantum methods will be investigated, one discrete method (VQE) and one continuous method (adiabatic systems). These procedures operate very differently, but both utilize quantum mechanics for optimization-based problem-solving. The complexity of both will also be compared, and an analysis will be made on the future of the quantum optimization industry.

2 Methodology

This paper is intended as an introduction to quantum mechanics and optimization procedures. No prior knowledge about quantum systems is assumed, but some underlying STEM/engineering background is assumed. The problem types were chosen to illustrate different areas of quantum problems. The Infinite Potential Well is a relatively simple example which is always presented early on in quantum mechanics courses. The Max Cut Problem is an extremely famous selection from the optimization family, and can be decomposed into a variety of other popular problem types. Optimization problems are also well known to those outside of computer science, and are widely applicable to other engineering fields. A chemical model was not illustrated, as the details would have been much too intense.

The methodology of this paper shifted from a direct comparison of these two optimization systems to an introduction of both, with a light comparison also included. This was done in an attempt to illuminate the field to those who may not have experience with it, as the methods for quantum optimization are not widely known, but could be useful to a variety of engineers and scientists now and in the near-future.

3 Classical Mechanics

Suppose we have mass m, which is restrained to exclusively move along the x-axis. It is subject to some external force $F(x,t)$. For a problem of this nature, classical mechanics can be applied to achieve a solution for x(t). We can apply Newton's Second Law: $F = ma$, where a is the acceleration (a = $\frac{d^2x}{dt^2}$). In a problem of this form, we can also define the velocity (v = $\frac{dx}{dt}$), the momentum (p = mv), and the kinetic energy (T=$\frac{1}{2}mv^2$).

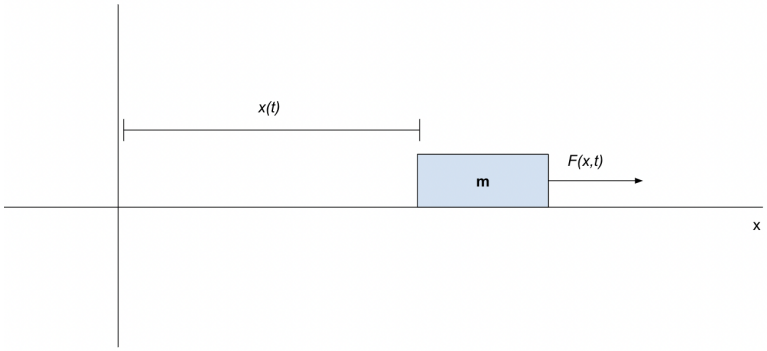

Figure 2: A mass m constrained on the x-axis under a time-dependent force.

Given this force is conservative, we can assume the following relation, where V is the potential energy of the system: $F = -\frac{\partial V}{\partial x}$. Newton's Second Law thus simplifies to a solvable differential equation which will provide a general solution for our system. Applying initial conditions to (1) will provide a closed-form expression for x(t). [4]

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x} \tag{1}$$

4 Quantum Weirdness

In quantum mechanics, our approach is much different. Position cannot be exactly specified, and a closed form solution for x(t) is not achievable. In order to understand this completely, we must consider the quantum principles of superposition and entanglement through the lens of measurement.

4.1 Superposition

First, let's define a quantum state as a general discrete property of a particle. Examples of this can include polarization, spin, or even momentum. Quantum superposition can occur within the state of a single quantum particle. Superposition describes the linear combination of two discrete states, a feat which is remarkable to observe physically. [6]

To further explain superposition, let's consider the Double-Slit Experiment presented in Figure 3. For years, scientists could not determine whether light acted like a wave or a particle. It exhibited wave like properties in experiments and yet it could also be broken down into tiny packets of light (now called photons). The double slit experiment demonstrated the overlap between wave-like and particle-like behaviour.

In the experiment, a light source is shot into two gaps in a metal sheet. The resulting pattern on the back screen can reveal the intermediate behaviour of the

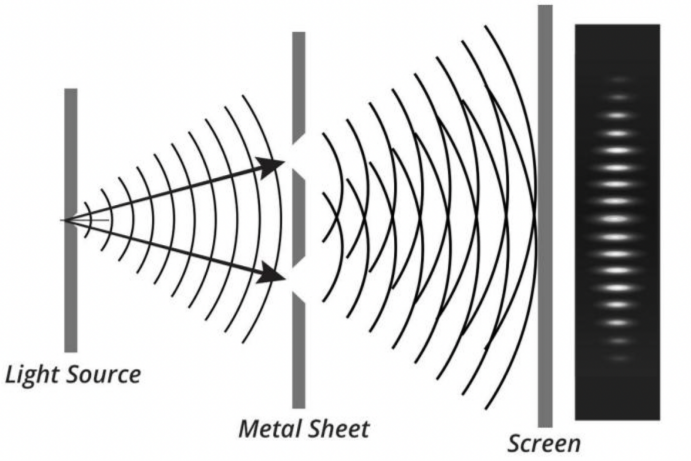

Figure 3: The Double-Slit Experiment [1]

light source. If a diffraction pattern is revealed, like that shown in Figure 3, the light source acted as a wave as it passed through the metal sheet. In order for this to occur, the light had to have passed through two places at once, and then was able to interfere with itself on the other side of the sheet. This multiplicity of state, such as the light's position, is known as a quantum superposition. [1]

But when does the light source exhibit particle-like behaviour? Upon measurement! Practically, an object cannot be in two places at once, or spinning in two different directions. Once we look at the object, or upon measurement, its state **collapses**. This is our way of aligning quantum mechanics with real observations. In the double slit experiment, two distinct stripes will be revealed on the back screen due to this collapse. The light can either pass through one slit, or the other, not both at the same time. Experimental results have revealed that upon closer and closer observation, the diffraction pattern will vanish in lieu of two distinct stripes at the locations of the slits. [7]

4.2 Entanglement

Now let's consider the strangest of the quantum properties, entanglement. Two quantum particles are entangled when one particle's state cannot be described independently of another particle's state. They are intrinsically linked over a possibly infinite distance, a tenet Einstein hated with a passion due to its implications of surpassing the speed of light. [7] An example could involve two spinning particles, which we know have a total spin which adds up to zero. Suppose we separate these particles by infinite distance, and measure one. If the spin is measured to be $\frac{1}{2}$, we immediately know the other particle's spin is $-\frac{1}{2}$.

4.3 Schrodinger's Cat

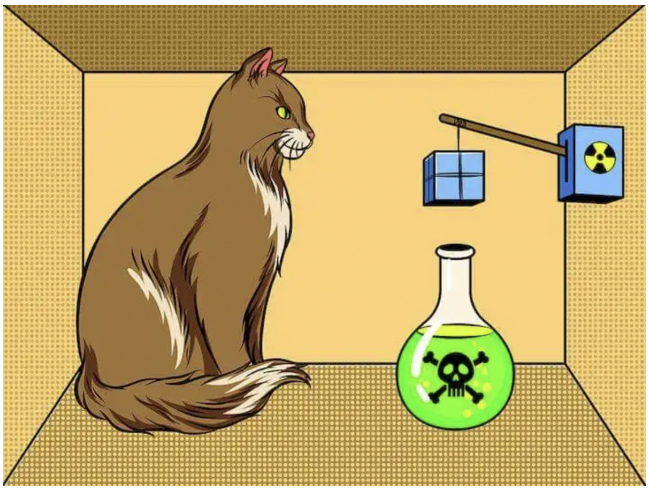

Figure 4: An illustration of the Schrodinger's Cat thought experiment[2]

Both superposition and entanglement are extremely strange to visualize for macroscopic objects. In order to highlight this absurdity, famed physicist Erwin Schrodinger devised a feline-based thought experiment known as Schrodinger's Cat.

The hypothetical situation devised by Schrodinger is presented in Figure 4. He assumed a cat trapped in a box was entangled with a radioactive particle which has the possibility of decay. A Geiger counter is used to detect the radiation which would be released from such a reaction. If it is detected, a switch is flipping releasing poison gas, and the cat is killed.

Now, assume we can't see into the box. Due to superposition of the state of the particle, the particle has simultaneously decayed and not decayed. The cat is both alive and dead. Opening the box, synonymous to measurement, determines the singular state, and the health, of the cat. [8]

This is extremely weird to think about and conceptualize, and yet, these properties are the basis of quantum mechanics. For small objects, quantum mechanics has been thoroughly tested to an extremely rigorous degree. Small particles don't act exactly how Newton and classical physicists thought they should. [9]

4.4 Quantum Computers

Quantum Computers use both of these quantum characteristics to their advantage. Instead of using binary switches, or bits, which operate classical computers, quantum computers utilize qubits. Qubits can be on, off, or in any possible number of superpositions of on and off. This, combined with the shared information contained within entanglement, gives quantum computers mathematical advantage over classical computers for certain operations.[10]

Quantum Computers rely on linear algebra. Each qubit is represented using a 2-entry column vector. A gate is used to perform operations on a qubit. A 1 qubit gate is represented by a 2x2 matrix. General forms for both are provided below.

$$|\psi>= \begin{bmatrix} a \\ b \end{bmatrix} \qquad U = \begin{bmatrix} c & d \\ e & f \end{bmatrix} \tag{2}$$

Through gates applied to qubits, we can form quantum algorithms which produce a desired resultant qubit state. This process is analogous to circuit formation in classical systems. [11] This is known as a gate-based quantum system.

4.5 The Schrodinger Equation

In quantum mechanics, the path of a particle is non-deterministic. Classically, we can solve out for x(t), knowing exactly how a baseball or a moving cart will travel in the presence of outside forces. This is not the case for quantum objects, and we have to model this mathematically. The wave function (ψ) defines the movement of a quantum particle. Squaring the wave function $|\psi(x,t)|^2$ yields the probability of measuring the particle at a specific distance and time. The Schrodinger equation governs the values of the wavefunction and its general form is presented below:

$$H\psi = E\psi \tag{3}$$

Here, H is the Hamiltonian of the system and E are the discrete energy levels. In physics, the Hamiltonian is the total energy of the system ($H = T + V$) and E represents the energy levels a particle can hold. Quantum mechanics gets its name from these **quantized** energy levels. Figure 5 illustrates the discrete energy levels of the Hydrogen atom as an example. Given a Hamiltonian, our goal is to solve for both the energy levels (E) and wavefunctions (ψ). [4]

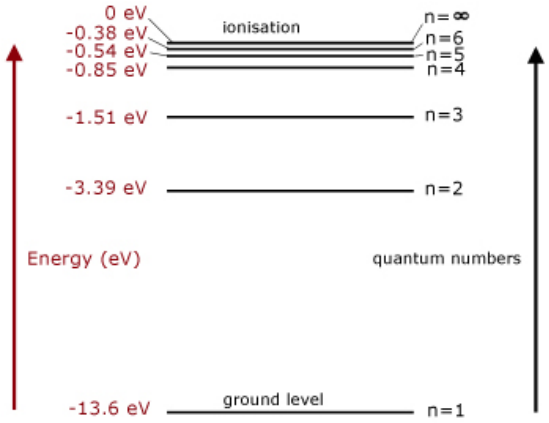

Figure 5: Discrete Energy Levels of the Hydrogen Atom System [3]

For those of you who have taken Linear Algebra, this is simply an eigenvalue equation. E_n are eigenvalues and ψ_n are eigenvectors of H. If you don't remember what these are, you may need a refresher on your matrix abilities. I recommend the cited textbook, which helped me hone my knowledge. [12]

4.6 Quantum Well

This section will provide some elements of a basic quantum mechanics example given in most physics courses. It is included to give some understanding of what the energy levels and wavefunctions of a system represent.

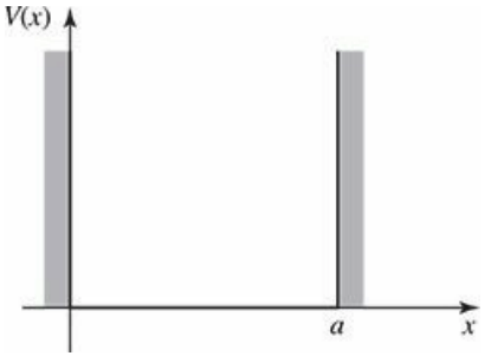

Figure 6: Setup for the Infinite Potential Well [4]

Assume we have a potential (V) energy graph such that a particle is trapped within an Infinite Potential Well is zero. Outside the region, the potential energy is infinite. Figure 6 has been provided as a reference.

Due to this infinite barrier, our particle is guaranteed to stay within the well. Our goal is to find the energy levels and wavefunctions associated with the system. Let us first define our Hamiltonian where $\hbar = 1.05 * 10^{-34} J \cdot s$ is reduced Planck's constant:

$$H(x,p) = T + V(x) = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{4}$$

Plugging into (2), we find the following differential equation for the region inside the well (V=0), included in Equation (5).

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi \tag{5}$$

Which, when solved, provides us with the following general solution:

$$\psi(x) = c_1 cos(kx) + c_2 sin(kx) \tag{6}$$

We can then apply the boundary conditions $\psi(x = 0) = \psi(x = a) = 0$ to determine the value of c_1 and of k. Normalization requires that all probabilities

$|\psi(x,t)|^2$ add up to one. This condition determines the final constant, c_1. The final solutions for the energy values and wavefunctions are provided in Equation (7). [13]

$$E_n = \frac{\hbar^2\pi^2n^2}{2ma^2} \qquad \psi_n = \sqrt{\frac{2}{a}}sin(\frac{n\pi x}{a}) \qquad n = 1, 2, ... \tag{7}$$

Figure 7 visualizes the first 3 wavefunctions ψ_n. Remember, squaring the results is the probability of finding the particle in a specific location. These results are not universal, and are specific to the problem setup.

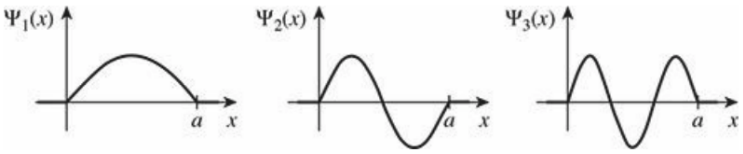

Figure 7: First 3 wavefunctions for the infinite square well [4]

Each wavefunction is associated with a specific energy level. Given Figure 7, a particle with E_1 is most likely to be found towards the center of the well. Differently, a particle with E_2 has zero probability of being found at the center of the well. [13] The wavefunction governs properties of the particle via probabilities, contrary to the definite nature of classical physics.

4.7 Expectation Values

Hamiltonians aren't always as simple as the Infinite Potential Well. They are often extremely complicated. The Hamiltonian for the simplest molecular system, the Hydrogen Molecule, has been provided below.

$$H = -\sum_{i=1}^{N}\frac{1}{2} * \nabla_i^2 - \sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{j>i}\frac{1}{r_{ij}} + \sum_{B>A}\frac{Z_AZ_B}{R_{AB}}$$

Looks like gibberish, right? For molecular systems specifically, the Hamiltonian is often extremely large and complicated. Large molecules are unable to be solved analytically due to the size of the Hamiltonian. There is interest in deriving useful information, such as the lowest energy energy level and wavefunction, without performing a full eigenvalue decomposition. In order to do this, we must introduce the idea of bra-ket notation and of expectation values.

Let $|\psi>$ be a wavefunction, represented by a column vector. $<\psi|$ is its complex conjugate, represented by a row vector. If this doesn't make sense, see [12] for linear algebra prep. In order to find the expectation value of an operator, like the Hamiltonian, we will use the following definition. This aligns with our classical understanding of expectation values according to [14].

$$E(H) = \sum < \psi_n | H | \psi_n > \quad = \sum (p(E_n))(E_n) \tag{8}$$

Given (8), every expectation value is guaranteed to be above the minimum energy level. This is known as the variational principle, included in (9). This states that our returned energy is guaranteed to be an upper bound for the lowest energy state.

$$E(H) \geq \quad < \psi_{min} | H | \psi_{min} > \quad = E_{min} \tag{9}$$

Thus, we can pick a ψ, find its expectation value, rinse, and repeat. Our task is to vary ψ until we find the lowest possible value. If you've studied computer science, this should sound like a very specific type of problem: optimization.

5 Optimization Problems

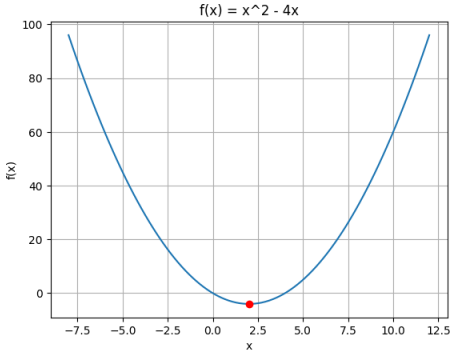

Figure 8: The function $f(x) = x^2 - 4x$, plotted using Python

Optimization problems can take many forms. The simplest examples involve one dimensional cost functions. For example, take the function $f(x) = x^2 - 4x$, presented in Figure 8. To find its extremum (maximum and minimum points), we take the derivative and set it equal to zero: $(\frac{df}{dx} = 2x - 4 = 0)$ and achieve $x = 2$ as the exclusive extrema point. The sign of the concavity, or $\frac{d^2 f}{dx^2}$, can be checked to determine whether the point is a minima or maxima.[15]

For more variables and more complicated cost functions, the situation is not so simple. First, let's consider the already established example, the Infinite Potential Well.

5.1 Variational Principle for Infinite Well

The Hamiltonian for the Infinite Potential Well was established in equation (3). Our process for the variational method is as follows: We can pick guesses for our wavefunction $|\psi>$, and calculate expectation values based upon these guesses. These guesses are guaranteed to be above the lowest energy level. Repeated guesses can yield us an extremely close guess to this energy level. All these solutions will approximately satisfy the Schrodinger equation, and will not yield exact solutions. [4] The steps below declare a guess for the wavefunction (Φ). This was chosen in order to maintain the boundary conditions for Infinite Potential Well. The constant N_1 can be found via normalization, explained in section 2.5. The expectation values are then calculated by integrating across the region from 0 to a.

$$\Phi_1 = N_1 x(a-x) \qquad N_1 = \frac{\sqrt{30}}{a^{\frac{5}{2}}}$$

$$< H >_n = \int_0^a \Phi_n H \Phi_n dx \qquad < H >_1 = \frac{5\hbar^2}{ma^2}$$

From Equation (6), we can find $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$. Creating a direct comparison with our found expectation value, we see the actual energy is below our guess, as it should be.[16]

$$E_1 = \frac{\pi^2}{2}[\frac{\hbar^2}{ma^2}] \approx 4.93[\frac{\hbar^2}{ma^2}] \leq 5[\frac{\hbar^2}{ma^2}]$$

5.2 Max Cut

Many problems based outside of physics can be cast into a Hamiltonian form. Optimization problems are one of the most studied examples. Here, I will consider a small example of the Max Cut problem.

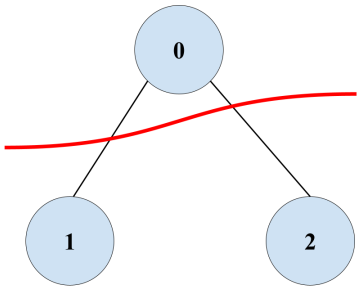

Figure 9: A Three Node, Two Edge Max Cut Problem with Maximal Cut

The Max Cut problem is based around a graph, **G**. This graph is composed of Edges, **E**, and vertices **V**. A cut is a partition of the vertices, or a line drawn

on the graph, splitting **V** into two sets. Typically, edges in **E** can possess edge weights; we will consider all edges to be unweighted with weight 1. For an unweighted graph, the max cut is that which cuts the maximum number of edges in **E**. The graph we are considering is presented in Figure 9. A cut is included; this cut is the maximal cut of the graph.

Assume every node can be represented by z_i and that $z_i \in \{-1, 1\}$. -1 and 1 will be assigned to either of the two sets, and will be given to nodes assigned to either set. Let us consider the product $z_i z_j$. If two nodes are in the same set, $z_i z_j = 1$, and if two nodes are in different sets, $z_i z_j = -1$. Under this definition, if we sum over all edges in **E**, the maximal cut will be the minimum total value of these products. In other words,

$$MaxCut(G) \equiv Minimize \sum_{(i,j)\in E} z_i z_j \tag{10}$$

But where does quantum computing come in? Consider the Pauli gates, presented below:

$$\sigma_Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \sigma_Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_I \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{11}$$

For simplicity, most measurements in quantum computing occur within the Pauli Z basis. What this means is that upon measurement, the state will collapse to one of its two eigenvectors. The eigenvectors of the Pauli Z gate are known as the computational basis, and have been presented below.

$$|0> = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |1> = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{12}$$

The computational basis vectors are each associated with a specific eigenvalue, -1 and 1. Upon measurement in the Z basis, any general state will collapse to one of these two vectors. The outputted expectation value computed with this state will either be 1 or -1: the eigenvalue attached to the specific basis vector. Thus, we can theoretically use measurement in the Z basis to represent possible combinations of -1 and 1 across all of our nodes. The basis vectors $|0>$ and $|1>$ represent node placement in the two distinct sets.

The tensor product allows us to scale this system past one qubit. An example state for the 3-qubit computational basis has been provided. (13) represents a cut which places three nodes into the same set. $|111>$ would represent an identical cut.

$$|0> \otimes |0> \otimes |0> = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{13}$$

With this astute observation about the Pauli Z gate, forming the Hamiltonian for this system becomes extremely simple. Z gates are applied between nodes with an edge. The Identity gate σ_I is applied to nodes with no edge. For our example in Figure 9, the Hamiltonian is as follows.

$$H \equiv (Z \otimes Z \otimes I) + (Z \otimes I \otimes Z) \tag{14}$$

In matrix form, this is written as:

$$H \equiv \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix} \tag{15}$$

We can compute the expectation value of this Hamiltonian given any general vector. Below, I've provided a brute force method, manually going through all possible combinations of the 3-qubit computational basis. The amount of qubits scales with the number of nodes. For larger systems, this method would not be possible, since the number of basis states scales with 2^n.

ψ	$\langle\psi\|H\|\psi\rangle$	ψ	$\langle\psi\|H\|\psi\rangle$
$\|000\rangle$	2	$\|100\rangle$	-2
$\|001\rangle$	0	$\|101\rangle$	0
$\|010\rangle$	0	$\|110\rangle$	0
$\|011\rangle$	-2	$\|111\rangle$	2

We see that two values produce the minimum value, or the max cut. Each has node 0 cut off from node 1 and node 2, representing the cut illustrated in Figure 9. Two solutions exist because 1 and -1 can be assigned to a given set with no difference in interpretation. [14]

5.3 Max Cut on a Quantum Computer

But how would we produce these expectation values on a quantum computer? Setting up the Hamiltonian is easy, and we already provided its form in Equation (14). Our goal is to supply either the state $|011>$ or $|100>$ to this Hamiltonian, which will produce the minimum expectation value.

Every qubit on a quantum computer starts in state $|0>$ by convention. Our goal is to design a circuit U which transforms $|000>$ to either $|011>$ or $|100>$, producing the minimum state. These gates are easy to find, U_1 transforms to $|011>$ and U_2 transforms to $|100>$. We previously introduced the Pauli X gate σ_X, which acts like a classical NOT-gate, flipping the state. We can apply X gates to flip the state, and I gates to imply no effect to easily find the transformation.

$$U_1 = \sigma_I \otimes \sigma_X \otimes \sigma_X \qquad U_2 = \sigma_X \otimes \sigma_I \otimes \sigma_I$$

The problem is, we typically don't know the state we want to transform to for larger systems. For this we utilize a parameterized gate, called an ansatz when used in this form. This gate has a set of inputtable variables which modify the entries of the matrix. When combined with the Hamiltonian, the ansatz can be changed to produce variable expectation values. [17] The entirety of the quantum circuit described, with ansatz and Hamiltonian included, is provided in Figure 10. EfficientSU2 was the parameterized circuit chosen for the ansatz.

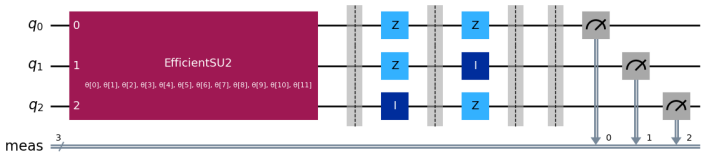

Figure 10: The Quantum Circuit Designed to find the Max Cut

Let's take a step back. Our Hamiltonian is a predefined large matrix which represents our system. By feeding a changing gate into this Hamiltonian (called our ansatz), we can produce a range of expectation values. But what is done with these produced expectation values?

At this point, we hand the keys off to a classical computer. A classical optimizer will be given the inputs to the ansatz and will continually modify them and run expectation values on the quantum system until a minimum point is reached. Through this quantum-classical combination, we can find the minimum

point without evaluating every computational basis state. This mechanism is known as the Variational Quantum Eigensolver (VQE).[14]

5.4 Quantum Optimization

Methods exist similar to VQE; there's actually an entire class of algorithms named Quantum Approximate Optimization Algorithms (QAOAs) which uses gated-based Quantum Computers to solve optimization problems. Solvable problems types can include quantum mechanical problems like the Infinite Potential Well or optimization problems like Max Cut and the famous Graph Coloring Problem. These methods rely on the gate-based model of quantum computing. They can provide runtime speedup over classical optimization algorithms, but in only specific scenarios.

Take VQE as an example. Instead of sorting through 2^n possible solutions, we can model the system on n qubits. This is not always guaranteed to be faster. If our Hamiltonian was an extremely long series of gates, running these could take longer than classical modeling. For VQE specifically, the length of the number of gates needs to be reduced passed a certain threshold. This is extremely important for chemical modeling on quantum systems.[18]

Quantum optimization on gate-based quantum computers is a developing field with problem speedup in various areas depending on Hamiltonian structure. But, it is not the only method for quantum optimization. Adiabatic quantum systems, or their modern equivalent: quantum annealers, dominated quantum optimization long before VQE or other QAOAs.

6 Adiabatic Quantum Computers

The adiabatic theorem was first proposed in the context of quantum computation by Farhi, Goldstone, Gutmann, and Sipser in 2000. [19] The adiabatic theorem's use in science has existed long before that. It is a tool used by physicists, chemists, and engineers alike.

Before applying it to an optimization, I need to describe what an adiabatic process is and how it can be utilized.

6.1 Adiabatic Approximations

Imagine a pendulum, like the one presented in Figure 11. This pendulum lies in a box which is initially still. The pendulum has a period: the time the pendulum takes to return to a specific spot. Let us define this period as the internal time of the system, T_i.

Now assume the box is rotated. The period of this rotation will be defined as T_e. If this rotation is quick, the motion of the pendulum will be chaotic, and extremely hard to predict. Something strange happens when the motion is slow enough. The pendulum continues to oscillate as if it weren't being rotated,

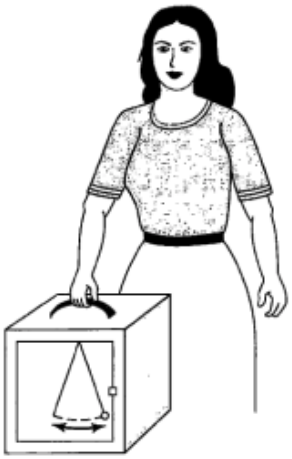

Figure 11: A rotating pendulum within a box[5]

with the plane of rotation slowly shifting. It experiences normal non-rotational behaviour in a rotational frame.

A very slow change in the boundary conditions of a system (in this case the rotation of the box) is an adiabatic process. Adiabatic processes are possible when T_e is much larger than T_i. [5] In layman's terms, the time it takes to create one cycle is much longer externally than the time it takes for an internal cycle. Related, the internal rotational velocity will be much faster than the external rotational velocity.

6.2 Applications to Hamiltonians

Why does this matter, and how do we apply this to our pesky Hamiltonians?

Let $\tilde{H}(s)$ be a Hamiltonian that is evolving with time and is also smooth. Mathematically, this means the Hamiltonian is both continuous and differentiable at every point in time. s is defined as $\frac{t}{T}$, where T is the total time. Using Eq (8), we can define our Hamiltonian as a sum of the eigenvalues and their corresponding probabilities. We write:

$$\tilde{H} = (s) \sum_{j=0}^{n-1} E_j(s)|\psi_j(s)|^2 \quad s = \frac{t}{T} \quad s \in [0,1] \tag{16}$$

Think about this intuitively and this should make sense. An average is just the combination of all possible values multiplied by their probability of occurrence. This definition is exactly identical. [19]

This is the hardest part to explain, but please stick with me. Given the movement is slow enough, or T is large enough, the process is adiabatic and the

internal process will dominate over the external conditions (like in the pendulum earlier). Assume our internal Hamiltonian is well-known, and our external Hamiltonian is the state which we desire to find (the Hamiltonian as we knew it previously). If the evolution is slow enough, the internal conditions are invariant under the influence of the external forces (in a given reference frame). In plainer words, the lack of outside influence can turn a known state into an unknown state, or our desired E_0. Mathematically we can describe this process as follows:

$$H = (1 - s)\tilde{H}_i + s\tilde{H}_e \tag{17}$$

Where $\tilde{H}_i$ is the internal Hamiltonian and $\tilde{H}_e$ is the external Hamiltonian, possessing our unknown state E_0. If $\tilde{H}_e$ is introduced slow enough, an eigenvector/eigenvalue pair for $\tilde{H}_i$ is guaranteed to produce an eigenvector/eigenvalue pair for $\tilde{H}_e$. The only thing left to do is make sure the pair for $\tilde{H}_e$ is the value we desire, the lowest energy state of the system. The process also has to be made slow enough so that it is guaranteed to be adiabatic. [20]

6.3 Conditions for an Adiabatic Process

Earlier, I mentioned that for an adiabatic Hamiltonian process, the internal eigenvector pair is guaranteed to morph into an external eigenvector pair. I never mentioned which one. For an adiabatic process, energy levels must be spaced far enough apart that we are guaranteed to achieve this lowest energy level. Otherwise, we could jump into a higher energy state and not achieve the desired solution. [20]

In addition, the process must be slow enough to guarantee that the procedure is adiabatic. Written in 1961, Messiah describes an estimate for this threshold. We must define Δ(s) as the difference between the first and second energy state for any s. More rigorously:

$$\Delta(s) = E_1(s) - E_0(s) \qquad \Delta = \min_{s\in[0,1]} \Delta(s) \tag{18}$$

We also must define a value Γ which relies on the rate of change of the Hamiltonian. Rigorously, Γ is defined as:

$$\dot{\tilde{H}}(s) = \frac{d}{ds}\tilde{H}(s) \qquad \Gamma^2 = \max_{s\in[0,1]} |[\dot{\tilde{H}}]|^2 \tag{19}$$

With these two expressions, we can define the time limit required for adiabatic conditions:[19]

$$T_e \gg \frac{\Gamma^2}{\Delta^2} \tag{20}$$

This is only a simple example of the conditions required for an adiabatic process. More rigorously proved definitions exists, but they are out of the scope of this study.

6.4 D-Wave

D-Wave is the current leader in Quantum Computing technology involving the adiabatic theorem. They produce quantum annealing computers which approximate adiabatic conditions. The accuracy of these conditions to true adiabatic nature is contentious. [21]

The way they do this is extremely complicated, and involves applying entanglement and voltage biases to specific qubits to form a voltage landscape that returns the desired minimum solution. If you're interested in what this entails, I'll provide literature written by D-Wave.[22] It's extremely interesting, but the physical hardware is well out of the scope of this study.

D-Wave produces a quantum computer much different from other popular quantum systems. Any quantum algorithm cannot be run on D-Wave's quantum annealer, and their setup is specific to optimization problems. Currently D-Wave technology contains over 5000 qubits. This is on par or greater than the level achieved by more universal quantum systems.

D-Wave has hedged all their bets in the optimization game, but who can blame them? The field has proved extremely lucrative. There are applications in finance, chemical modeling, and data storage, among a variety of other fields. Lockheed Martin was reported to have paid over 15 million dollars to acquire a D-Wave system in 2022.[23] Keep in mind, this purchase occurred with the field in its infancy. The price and use cases for optimization problem solvers will only go up as the technology improves.

7 Quantum Advantage

The question then shifts to, will adiabatic quantum systems have a role in the future quantum landscape? As shown earlier, normal quantum computers can also solve optimization problems. Who will dominate the future quantum optimization landscape, and with what type of system?

A 2008 paper in arXiv tried to answer this question. It cited previous studies which have proved that an adiabatic process can be simulated on a normal quantum computing system. By this reduction, they also proved that an adiabatic computation can not have computational power greater than a normal quantum computer. [24] The question then becomes, which will scale quicker in size and total qubit count? Whoever does will end up dominating quantum optimization.

Google and IBM have both released public road-maps that anticipate surpassing 1 million qubits by 2030. [25] D-Wave does not appear as invested in this pursuit. Their most recently released estimates suggest increases in the thousands of qubits, not millions. Despite this, results from optimization problems run on D-Wave have proved extremely promising. Quantum annealers and gate-based quantum computers share a lot of overlapped hardware. It is entirely possible that D-Wave could join the gate-based arena as well.[26]

8 Conclusion

Quantum optimization is a promising field with a variety of use cases in different areas. Optimization is at the center of many Machine Learning and Computer Science developments. In addition, quantum optimization has applications for chemical modeling for future virtual laboratories. It also has the possibility of improving the financial modeling of global economic systems.

Recent studies have shown advantage for D-Wave's optimization procedures over classical systems. Gate-based systems should be able to scale much quicker while being able to gain similar advantage in optimization problems. D-Wave's success only illustrates the possible lucrative nature of this field. More research should be done in understanding the full array of possible use cases for quantum optimization.

Work should also be done producing helpful literature for utilizing these systems. These tools can be extremely useful for a variety of problem types, specifically to those pursuing STEM-based endeavors. Similar to MATLAB or Python, quantum optimization tools should be more widely known and used as helper mechanisms.

Glossary

adiabatic Slow enough external conditions that the internal behaviour of a system dominates, avoiding possible chaotic behaviour.. 15–18

ansatz A parameterized gate representing our wavefunction. The ansatz is varied by the classical optimizer till a minimum point is reached. 14

eigenvalue The scaling factor (value) attached to the eigenvalue equation. In quantum mechanics, the discrete energy levels of the Hamiltonian. E_0, the lowest valued eigenvalue, is our desired solution. 8, 9, 12, 16, 17

eigenvector The vector attached to the eigenvalue equation. Represents a linear transformation in matrix algebra equal to a scaling factor. In Quantum Mechanics, an eigenvector is the wavefunction. When squared, this gives us the probability of a system being in a certain state. 8, 12, 17

entanglement The property describing shared information between two separated objects. In the case of quantum computers: qubits. 4–6, 18

Hamiltonian $H = T + V$: The total energy of the system including Potential and Kinetic Energy Terms. 7–9, 11, 13–17

Infinite Potential Well A toy quantum mechanics example where a particle is constrained between two infinite barriers of potential energy. 3, 8–11, 15

Max Cut A graph-based optimization problem. The solution is the maximal cut of a graph, a physical cut which partitions the nodes into two sets, taking out max edge weights in the process . 3, 11, 15

normalization To gain physical meaning, all probabilities must add up to 1. Normalization skews a wavefunction to adhere to this strict condition. 8, 11

optimization A field of computer science centered around finding the extremum of cost functions of varying complexities. 3, 10, 11, 15, 18, 19

superposition A linear combination of two quantum states. 4–6

V The Potential Energy of a System. How much energy an object could potentially acquire. 4, 8

VQE A gate based method for optimization using both classical and quantum systems. Expectation values are calculated by a quantum computer, and varied by a classical optimizer. 3, 15

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