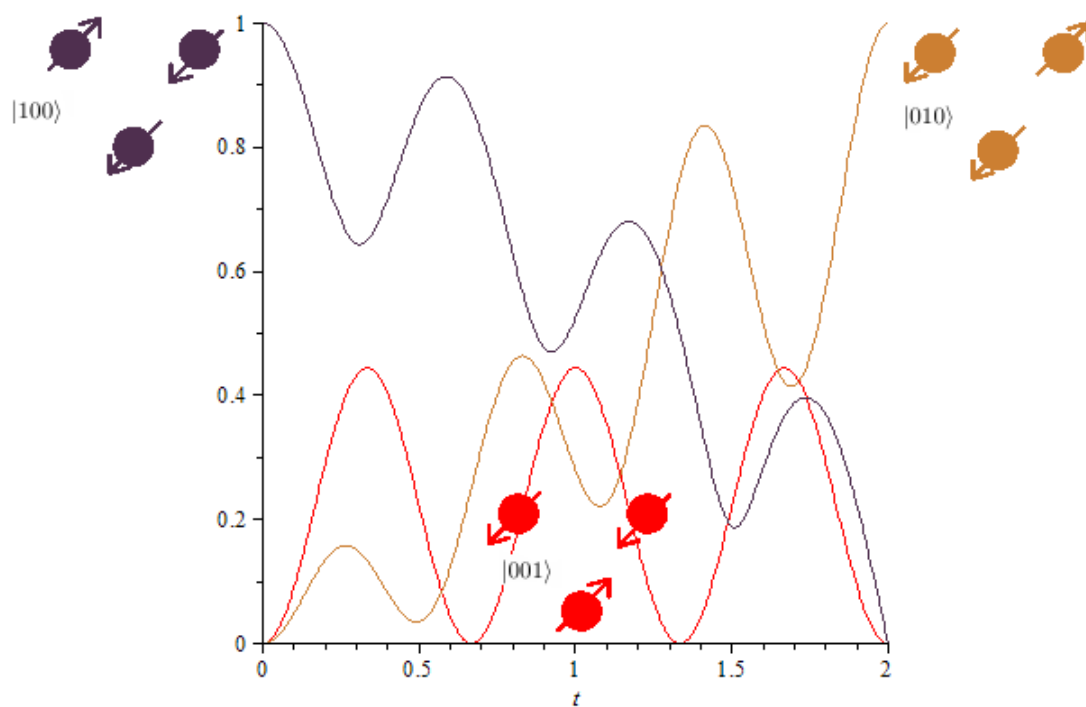


Quantum computation and spin interactions in a molecule

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1 Summary

1.1 English

In this thesis, we will explore the world of the quantum computer, as well as the information theory and quantum mechanics that surround it. In chapter 3, the basics of quantum information theory are examined and developed, establishing the key elements that make up a quantum bit and a quantum gate. Following it is a look into the quantum logic circuit, describing the nature of individual gates and how they operate on qubits and in circuits. Lastly, two fundamental concepts will be explained, the no-cloning theorem which posits that you cannot take a copy of a qubit that you do not know, and quantum error correction, which brilliantly exploits certain limitations of quantum mechanics and information theory, and is vital to the future of quantum computers.

Chapter 4 is a brief foray into the harsher physics that make up the backbone of the quantum computer, which will also give an idea of why they have yet to become a household object. The gates established in chapter 3 will be shown in a physical context, and we will get a notion of the source of the universal 1-qubit gate. We will also look into the physical systems that are currently used for quantum processing.

In chapter 5, a very simple quantum gate is derived from a basic spin Hamiltonian, and is used as a foothold to work on the more complex 3-qubit systems explored in chapter 6. We will explore a pair of regimes which arise from experiments others have done with third-spin coupling systems, and examine the time evolutions of these. What is found is that this coupling allows for an evolution that can be used as a SWAP gate under the correct conditions.

1.2 Danish

I dette bachelorprojekt vil vi undersøge kvantecomputerens verden, samt den informationsteori og kvantemekanik der omhandler den. I kapitel 3 bliver grundpunkterne indenfor kvanteinformationsteori berørt, hvilket etablerer nøgleelementerne bag kvante-bitten og kvante-gaten. Så tager vi et kig på kvantelogikkredsløbet, virken af de individuelle gates og hvordan de påvirker qubits i kredsløbene. Til sidst undersøger vi to fundamentale koncepter, nemlig ingen-kloning teoremet der siger at man umuligt kan kopiere en qubit man ikke kender, samt kvantefejlretning, som på genial vis gør brug af hvad der ellers er begrænsninger fra kvantemekanik og informationsteori til at være et af de elementer der giver kvantecomputeren en fremtid.

Kapitel 4 dykker lidt ned i den tungere fysik der lægger baggrund til kvantecomputeren, og vil også give en idé om hvorfor de stadig ikke er et husstandsobject. De gates der blev etableret i kapitel 3 bliver vist i en fysisk sammenhæng, og vi får en idé om kilden til den universelle 1-qubit gate. Vi tager også et kig på de fysiske systemer hvor man allerede nutildags kan køre nogle kvanteprocesser.

I kapitel 5 udleder vi en meget simpel kvante-gate fra en lille spin-Hamilton, og bruger denne som et fodfæste for at arbejde os ind på mere indviklede 3-qubit systemer der undersøges i kapitel 6. Vi kigger på et par regimer der dukker op fra andres eksperimenter med 3-qubit systemer, og ser på hvordan disse tidsudvikles. Det vil visse sig at denne slags kobling vil, under de rette forhold, føre til en tidsudvikling der kan anvendes som en SWAP-gate.

2 Introduction

The quantum computer is a relatively young, but very interesting subject. In the infancy of the modern computer, a number of physicists and information theory experts began to ponder the

possibility of a computer on a processor of quantized states instead of the more rough mechanical and electronic states of the computers of those days. With the discovery of quantum cryptography, the prospect of data processing seemed closer than ever. The first complete proposal of how such a theoretical device could be designed came from David Deutsch, who in one fell swoop proposed a complete set of operations that would be required[3]. In the following decade, the processing power and capabilities of the quantum computer were explored by the works of Shor, Grover and Steane[1], who invented algorithms and failsafes that would let a theoretical quantum computer perform operations that the laws of physics say a classical computer will never achieve.

Most of the processing power the quantum computer comes from the concept of parallel processing. Since it can operate on superpositions of quantum bits, it is possible for a quantum processor to query every bit simultaneously with a single operation. In contrast to this, a classical computer querying an index has to examine one element at a time. This does not mean that a quantum processor can solve an arbitrarily large problem in a single operation, however. When its output is read, it usually only has a certain probability of being the correct answer. The amount of operations required to get a probability of correctness very close to one is much less than that of a classical computer.

At present, however, the quantum computer is little more than an interesting thought, though progress is being made faster than ever. Scientific institutions entirely dedicated to the further development of quantum computers have emerged in recent years, and the quantum computer is a growing element of the field of nanoscience.

3 Quantum information theory

This section is primarily sourced by [2] and [1]

The quantum computer and its underlying concepts are defined with quantum information theory. This theory is based on another pair of relatively young theories. As its name implies, these are information theory and the theory of quantum mechanics. Information theory introduced a way of looking at the world which led to the creation of the computer, and quantum mechanics introduced several concepts which allow for a radically different approach to information processing, the two most central being the existence of quantum states as superpositions of orthogonal states and the ability of quantum states to become entangled.

In the same way that Alan Turing's proposal of the universal Turing Machine is considered to be the first proposal of the modern computer, the father of the quantum computer is considered to be David Deutsch[3], who suggested that it was theoretically possible to create a universal quantum computer and the specifics of how this would be done. The notion of a quantum computer had been considered in various forms, such as Richard Feynman's suggestion of a machine that could physically emulate the behaviour of any system[4], but Deutsch had concretely stated that a quantum bit (qubit) could be manipulated in any fashion feasible using nothing but operations acting on a single or two qubits. A branch of quantum computation that predates Deutsch' machine is quantum cryptography, which involves sending information encoded in the polarization of photons. Intercepting and measuring these photons will alter them unless the interceptor possesses specific knowledge about the information in them, so the recipient can tell if someone has eavesdropped on them [5]. Without this limitation, an arbitrarily large amount of information could be stored within a single theoretical qubit.

We will discuss decoherence and instability of individual qubits on occasions where they are only the targets of coherent, stable time evolutions. In this scenario, we simply mean that the qubit has time-dependent fluctuations, which means that if it were to be measured, the result would depend on the exact time of measurement. Think of these coherent but undesired time

evolutions as a simplification of potential environmental effects.

3.1 The quantum bit

The quantum bit, commonly abbreviated as qubit or occasionally Qbit, is the basic unit of quantum computation, analogous to the bit of classical computation. It can be symbolized by anything possessing of two orthogonal quantum states, but by far the most common are the polarization of a photon or the spin of an electron or greater system. The state of a qubit is written as a two-dimensional vector; for example, the zero state of an electron would be a spin-down state, which could be expressed as any of

$$|0\rangle = |\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and the corresponding orthogonal spin-up state would be

$$|1\rangle = |\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

For a photon, the zero state could be *r*-polarization and the one state could be *l*-polarization. A spin qubit is used for storage and manipulated within a system, while a photon qubit is used to transmit information.

The basis presented above is commonly referred to as the computational basis, due to its similar nature to the classical bit. More complicated qubits are often described as the superposition of these two, such that a state

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

would be written as $\alpha|0\rangle + \beta|1\rangle$. Another very common basis set has the two states of the computational basis states at equal amplitude but with or without a phase shift. This basis set contains

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

and is usually called the plus/minus basis. From the nature of basis sets arises the important fact that a qubit about which you know nothing is entirely useless. If you do a measurement in the plus/minus basis on a qubit in the computational basis, you have an equal probability of getting the result $|+\rangle$ or $|-\rangle$.

A common shorthand for systems containing multiple qubits would be reducing the tensor product

$$|\alpha\rangle \otimes |\beta\rangle \otimes |\gamma\rangle = |\alpha\beta\gamma\rangle$$

3.2 Quantum gates

As the quantum bit is analogous to the bit, so too is the quantum logic gate (or simply gate) analogous to the classical logic gate. A quantum logic gate is an operator acting on one or several qubits, inducing a unitary time evolution. While theory deals with gates acting on more than two qubits and these are physically possible to design, any logic circuit can be reduced to a series of two-qubit gates and in practice it turns out that these are much simpler to design. A gate needs to be reversible to be meaningful due to the nature of quantum states, as any non-reversible operation will yield a binary result.

3.2.1 The quantum logic circuit

When describing a series of quantum logic gates, it becomes quite cumbersome to describe it as a series of operations, particularly as the amount of qubits involved increases. More advanced operations are instead written as part of a network diagram, analogous to logic circuits used in programming. Figure 1 shows an example of how such a circuit will be described, as well the notation for every gate shown in the following section, while an example of a network diagram will eventually be shown in figure 5.

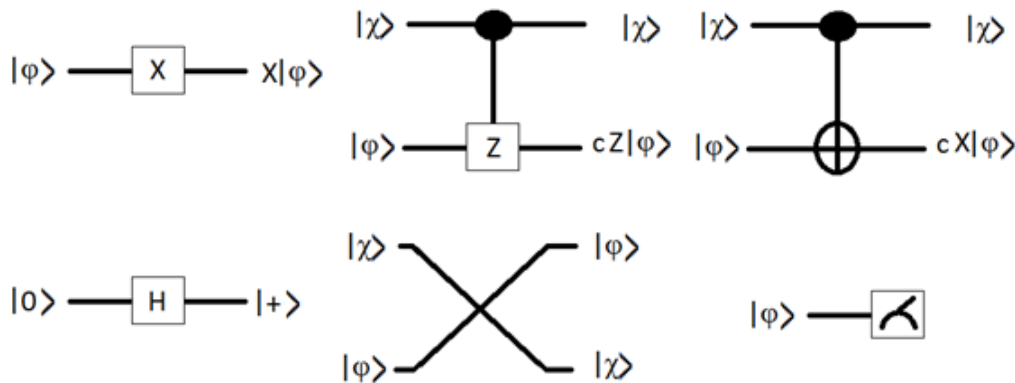


Figure 1: Some common gate identities. From left to right, top: The bit-flip NOT gate, a controlled phase-flip gate, alternate notation for the controlled NOT gate commonly used in handwriting. From left to right at the bottom: the Hadamard gate, a SWAP gate, the measuring operator which yields an output.

3.2.2 Bit- and phase-flip gates

The two simplest operators in quantum information theory are the bit-flip and phase-flip gates. The bit-flip, or simply X , gate working on a qubit $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$ takes it to $X|\varphi\rangle = \beta|0\rangle + \alpha|1\rangle$. Similarly, the phase-flip or Z gate working on a qubit $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$ takes it to $Z|\varphi\rangle = \alpha|0\rangle - \beta|1\rangle$. The Y gate consists of applying both Z and X to a qubit, yielding $Y|\varphi\rangle = \beta|0\rangle - \alpha|1\rangle$ or $Y|\varphi\rangle = -\beta|0\rangle + \alpha|1\rangle$ on our example qubit. The relative internal phase of a qubit is typically a more important quantity than the absolute phase, so by convention, the phase of the zero state is real and positive. A qubit that deviates from this has the further phase alteration outside of the qubit's name, so that the state $\frac{1}{\sqrt{2}}(-|0\rangle + |1\rangle)$ would be $-|-\rangle$. Together with the trivial identity gate 1 (takes $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$ to $1|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$), these gates form the set of Pauli gates. A gate can be represented as either a function as shown earlier, or as a matrix which acts on the vector representation of the qubit. Figure 2 shows the matrix representation of these four gates. Together with the Hadamard and SWAP gates, these comprise the vast majority of gates employed in current quantum algorithms.

3.2.3 The Hadamard gate

The Hadamard transform will take a qubit $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$ and map it to $H|\varphi\rangle = \frac{1}{\sqrt{2}}(\alpha|0\rangle + \alpha|1\rangle + \beta|0\rangle - \beta|1\rangle)$. This notably has the effect of turning the state $|0\rangle$ into the state $|+\rangle$ and vice versa. It also has the same effect on $|1\rangle$ and $|-\rangle$. A Hadamard transform is therefore convenient

$$\begin{array}{cc}
 \text{---} \boxed{1} \text{---} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \text{---} \boxed{X} \text{---} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
 \text{---} \boxed{Y} \text{---} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} & \text{---} \boxed{Z} \text{---} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
 \end{array}$$

Figure 2: The four Pauli gates and their corresponding matrix representations.

for changing the basis states of a system. Further, since the X gate interchanges $|0\rangle$ and $|1\rangle$ while the Z gate interchanges $|-\rangle$ and $|+\rangle$, a Hadamard gate introduces the ability to interchange the two gates, such that an HZH circuit would have the same function as an X gate, and a ZH circuit would have the same effect as an HX circuit. This comes in handy when designing some more complex logic circuits. Figure 3 shows the matrix representation of the Hadamard gate.

3.2.4 The controlled gate

A gate that acts on multiple qubits will typically be one that alters one qubit while using the other as a control. The ubiquitous example is the CNOT gate, which is analogous to the computational XOR gate. If the control qubit is in the state $|1\rangle$, it has the effect of a NOT gate on the affected qubit. If the control qubit is in the state $|0\rangle$, it has the effect of the identity gate. Similarly, there exist controlled phase gates and controlled Y gates. What makes these so different from the controlled logic gates of a computer is that the control qubit can have a value other than 0 or 1. For example, the CNOT gate on a control qubit $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and a target qubit $|0\rangle$ would map them as $CNOT|+\rangle|0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, which is an entangled state. This entangled state is known as a Bell state, named for the physicist John Bell, who famously worked with entangled states and posited that the EPR paradox did not arise from a hole in our understanding of quantum mechanics, and instead from an intrinsic quantum mechanical property.

Acting on the second qubit of the Bell state with each of the four Pauli gates yields four orthogonal two-qubit states, which is known as the Bell basis. An example of a controlled gate is shown in figure 3.

3.2.5 The Toffoli gate

The simplest example of a three-qubit gate would just be a CNOT gate that is controlled by an additional qubit, which is what the Toffoli gate does. Interestingly, the Toffoli gate is a typical example of how it is easier to create a gate using multiple two-qubit gates than a single three-qubit gate, but the Toffoli gate was actually created experimentally in 2008[6], and turned out to be more viable than the alternatives. An example of a more general two-qubit controlled gate and its appearance as a three-qubit gate as well as a series of two-qubit gates is shown in figure 4. Gates requiring an arbitrarily large amount of control qubits can be very easily designed using only Toffoli gates as well as $n - 2$ ancillary control qubits simply called “ancilla.” [2]

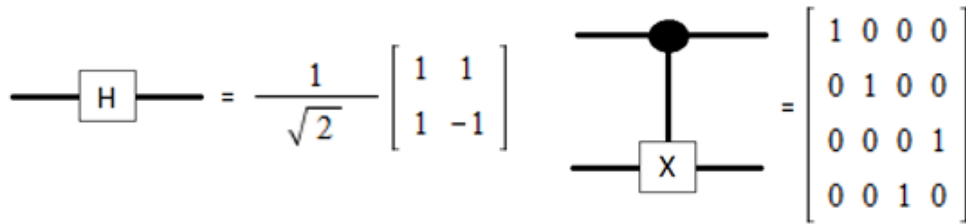


Figure 3: On the left is the matrix representation of the Hadamard gate, which maps a single computational basis state to an equal superposition of the two, and vice versa. On the right is a CNOT gate, where the circle on the top qubit indicates that it acts as a control qubit on the bottom target qubit. The matrix representation of this gate is a 4x4 matrix, as it acts on the tensor product of the two qubits, which is a four-dimensional vector.

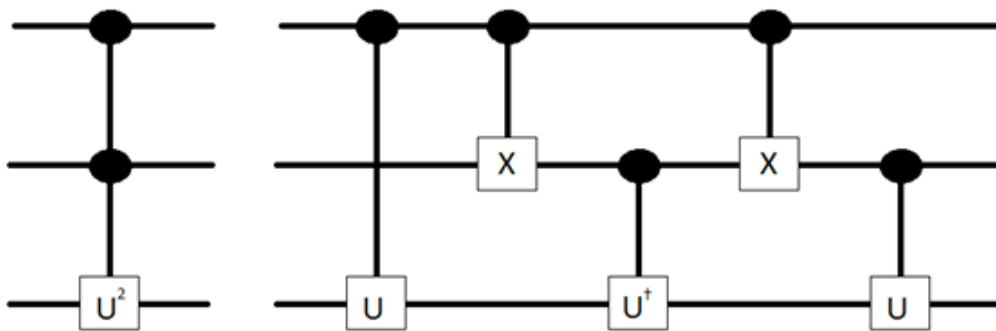


Figure 4: A generalized version of the Toffoli gate, implementing the function U^2 using two control qubits. The single gate on the left is what is commonly shown in a circuit diagram, even if the more complex circuit on the right is shown. Note on the right that if both control qubits are 0, nothing will happen. If one is 1 and the other is 0, the function U will be implemented, but so will its inverse function U^\dagger . If and only if both qubits are 1, U will be implemented twice.

3.2.6 The SWAP gate

The last of the important gates is the SWAP gate, which simply interchanges the state of two qubits.

$$SWAP|\varphi\rangle_1|\chi\rangle_0 = |\chi\rangle_1|\varphi\rangle_0$$

The utility of being able to perform a SWAP function lies in moving states within your system. Due to the no-cloning theorem, you cannot merely copy a state onto a different qubit unless the two are part of the same orthogonal basis. SWAP gates allow you to transmit data throughout a system without knowing the basis of a qubit. This gate has the matrix representation

$$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The SWAP gate is notable in that it can be employed with electronic interactions alone. For this reason, we will examine the SWAP gate in greater detail, attempting to create one ab initio

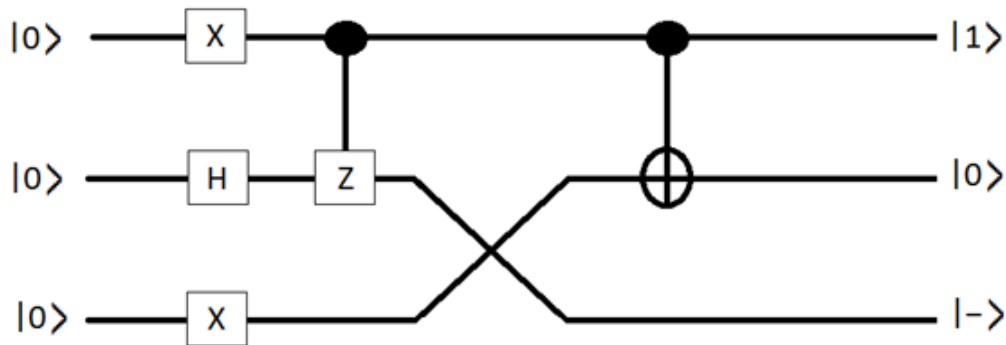


Figure 5: An example of a complete quantum circuit, with the input qubits on the left and their output on the right. The top qubit is flipped from the state 0 to the state 1, and unaltered throughout the time evolution. The middle qubit is moved to the superposition state $+$, and then has its phase flipped to the $-$ state by the controlled phase flip gate. Its state is swapped with the bottom qubit. The bottom qubit is flipped to a 1 state, then flipped back to a 0 state by the controlled NOT gate, as the top qubit is still 1

from a simple electronic Hamiltonian.

3.3 The no-cloning theorem

Another consequence of the requirement that quantum gates must be reversible is that it becomes impossible to simply copy a qubit state onto another. Consider the function $U|\varphi\rangle|0\rangle = |\varphi\rangle|\varphi\rangle$. For the operator U to be universal, it must also hold true that $U|\chi\rangle|0\rangle = |\chi\rangle|\chi\rangle$. However, consider the state $|\sigma\rangle = \frac{1}{\sqrt{2}}(|\chi\rangle + |\varphi\rangle)$, which this operator would map as $U|\sigma\rangle|0\rangle = \frac{1}{\sqrt{2}}(|\varphi\rangle|\varphi\rangle + |\chi\rangle|\chi\rangle)$, which is an entangled state and not two separate qubits. It turns out that it is possible to copy states, but it demands a gate suited to the qubit in question. For example, a CNOT gate will successfully clone either computational basis state.

3.4 Quantum error correction

What may very well be the most incredible phenomenon in quantum computing is that of quantum error correction. The greatest issue plaguing the concept of quantum computation is that quantum information is very fragile and will almost invariably be frequently disturbed by outside sources. Until the discovery of the option of quantum error correction by Peter Shor and Andrew Steane, independent of each other, in 1995, quantum computation was little more than a thought experiment that would be impossible to manifest in reality.

Classical error correction is exceedingly simple in comparison. The scale of an electronic bit is significantly greater than the atomic scale of a qubit, so with the exception of very extreme conditions (such as magnetic memory in a strong magnetic field), a spontaneous error will not occur on stored binary memory. Under conditions where error correction might be necessary, such as the electronic transmission of data, a very simple trick will suffice. Encode each bit redundantly, so that $|0\rangle$ becomes $|000\rangle$ and $|1\rangle$ becomes $|111\rangle$. Then the state of the system is measured frequently enough that the probability of two errors happening between three adjacent bits is negligible, and correct every three-bit sequence that has had a bit flipped by flipping

it back. To reduce the frequency of corrections, one can replace the triple redundancy with a quintuple, septuple or however great a redundancy is required, although this will slow the transmission of data by sheer bulk.

In quantum computing, several significant obstacles appear. As mentioned, even stored memory is quite fragile and may spontaneously interact with its environment to create a new state, but more significantly, one cannot measure qubits to see if they have spontaneously changed. If a qubit needs to be in a specific state, it is possible to measure it in the correct basis and perform the appropriate flip if one gets the wrong orthogonal state, but this would require having each desired state stored as classical information, and in case of the corrected qubit being entangled, the collapse of the wave function will likely alter whatever the qubit was entangled with upon breaking the entanglement. Even if measurement were possible, the no-cloning theorem is also an issue; we need to know the exact state to be able to introduce redundancy in the first place. Lastly, the only error that can happen in a classical system is the bit flip, while qubits struggle with planar rotation and phase changes. Fortunately, solutions to each problem actually exist, the most prevalent of which is fault-tolerant coding.

While you cannot introduce redundancy by cloning a qubit, you can create superposition states, which serve a similar function. The simplest example is a qubit $|\varphi\rangle$ in the state $\alpha|0\rangle + \beta|1\rangle$, alongside two qubits both in the state $|0\rangle$. Applying a CNOT gate with $|\varphi\rangle$ as the control and the $|0\rangle$ qubits as the target will entangle your qubits into the superposition state $\alpha|000\rangle + \beta|111\rangle$. In the trivial case that $|\varphi\rangle$ is a computational basis state, it will simply be copied. This state is functionally equivalent to the triple redundancy, in that a single erroneous qubit can be corrected through majority. Now our main issue is that we still cannot read the state of our qubits without disturbing them. Amazingly, a method exists to learn if something has happened to a qubit without actually learning anything about the state of the qubit itself. In the simplest example, using a state in a superposition over three qubits, and assuming that the only error that could occur is a bit-flip, exactly four correctable states will exist. No qubits being flipped or one of three qubits being flipped. If more than one qubit has been flipped, the redundancy has failed. This requires two ancillary qubits. Figure 6 shows an example of how this error could be faultlessly fixed. The thing to note is that in spite of our control qubits not being in the computational basis state, the CNOT gates will act as either an identity or a NOT gate. If acted on by two unflipped states, the ancillary qubit will be mapped to an entangled state and then immediately unentangled by the next CNOT gate. If acted on by two inverse entangled states, the second state will unentangle it to the $|1\rangle$ state.

Figure 6 only shows the solution for a very basic case, but it can actually be generalized for *any* error given enough ancillary qubits. Imagine that a state $|\varphi\rangle$ is acted upon by an environmental effect $|e\rangle$. This can be generalized as the effect

$$|e\rangle|\varphi\rangle = (|e_1\rangle 1 + |e_X\rangle X + |e_Y\rangle Y + |e_Z\rangle Z)|\varphi\rangle$$

Obviously, you cannot set up a system that accounts for every possible combination of these, but what you can do is set up a system that checks for some correctable errors, entangling the state over more qubits, introducing more ancillary qubits and setting up gates which also examine if phase-flips have occurred. Quantum mechanics tell us that we cannot learn anything about a system without disturbing it, but as mentioned, checking for errors in this way does not actually tell you anything about the system itself. When you perform a measurement on the ancillary qubits you will, however, observe the state of errors in the system, and the state of errors collapses. Whatever the results of our measurement on the error are, the actual error in the system *becomes* that specific error, and correcting the error restores the system. Note that it is possible to collapse into an error that is not within the set of correctable errors, so advanced networks are designed to account for every probable error.

elapsed, the qubits are subjected to a π -pulse which rotates them 180 degrees in the xy -plane. Once the two qubits finish their coupled pulse, they may need an oppositely-directed π -pulse to realign them.

4.2 The ion trap

So far, only two kinds of experimental setup have managed to perform relatively complex computations using 10 or more qubits. One of these is the ion trap. It consists of a number of static and oscillating electric fields which trap a line of ions within the system at high vacuum. A laser beam is split into a large number of beam pairs, with each beam being modulated individually, and each beam pair illuminating a single ion. Modulating the beams then allows you to create any one-qubit gate, while two-qubit gates require qubit coupling, which is possible but not trivial.

4.3 NMR qubits

The other setup which has been used to experiment on many qubits is the NMR bath. The qubits in this case are the nuclear spins of the liquid molecules in the container. One cannot simply use the nuclear spins as qubits, however, as there are far too many and they are packed far too close. The trick to generating NMR qubits is that as long as the spins that are not in use are distributed in a uniform spread of states, their total interaction with the systems used is negligible. Non-unitary operations can then be used to create small pockets of ground state in the vat, with each state acting as a qubit. As the qubits are in NMR, their natural evolution back to the excited states can be neutralized with the spin-echo technique.

4.4 Molecules

Qubits as elements of molecules have been under investigation as long as their rivals, but larger operations have yet to be solved on the scale of NMR and ion trapped qubits. The strength and weakness of molecules as quantum processors is that their qubits are highly localized, which makes them easy to keep track of and manipulate, but also makes coupling and decoupling very difficult. Molecular spin qubits have, however, been the subject of many interesting experiments due to the relative ease of working with them. Examples include coupling the electronic spins with nuclear spins, creating a fairly stable storage method, and the 2- and 3-qubit SWAP gates.

5 Thinking up a 2-qubit gate

5.1 Defining our quantum gate

We have looked at a number of quantum gates and their physical implication already, but being told how they work is one thing. What would be interesting to investigate is if we can also pull off the opposite, deriving a quantum gate from an initial qubit interaction. Let us first examine a very simple Hamiltonian, such as one between two spins coupled by a coupling constant J . [8]

$$H_0 = JS_1 \cdot S_2$$

The operator $S_1 \cdot S_2$ can conveniently be written as $S_1^Z S_2^Z + \frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+)$, which acts on a 4-dimensional vector of spin states. S^Z will flip the sign of a qubit in the state $|1\rangle$ and take it to one half its value, so two S^Z operators will reduce the state by three quarters and flip the sign if the spins are opposite. $S_1^+ S_2^-$ increases the state of one qubit by one and reduces the

other; in the case of individual spins, which only have two states, it can fail to increase or reduce a state and produces no result. As is convention, we assign the down spin to the state $|0\rangle$,

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and the up spin to the state $|1\rangle$,

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

. These are in the computational basis, and the tensor products expressing the total state are given by

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

. The Hamiltonian can then be represented by the matrix

$$H = \frac{J}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

5.2 Time evolution

In a more generalized way, we can look at the state of any qubit superposition

$$|\psi\rangle = \sum_{i=0}^3 c_i |i\rangle$$

whose time evolution is given by $i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle$, which can be expressed as the differential equation

$$i\hbar \dot{c}_i = \sum_j H_{ij} c_j$$

To solve this, we calculate the eigenvalues of our Hamiltonian H .

$$\begin{aligned} 0 &= \det(H - \lambda \mathbf{1}) \\ &= \left(\frac{J}{4} - \lambda\right)^2 \left(-\frac{J}{4} - \lambda\right)^2 - \left(\frac{J}{2}\right)^2 \end{aligned}$$

One doubly degenerate state comes out of the leftmost section, with an eigenvalue $\lambda = \frac{J}{4}$. We find out the remaining states by combining the remaining internal squares, yielding

$$\lambda = \frac{J}{4} \qquad \lambda = -\frac{3J}{4}$$

Our former eigenvalue becomes triply degenerate, and we obtain one singly degenerate eigenvalue. The eigenvectors corresponding to such a set of eigenvalues must be those of the singlet

and triplet states. In the computational basis, these are given as

$$\begin{aligned} |S\rangle &= \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle) = \begin{pmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} & |T_{-1}\rangle &= |00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\ |T_0\rangle &= \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} & |T_1\rangle &= |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \end{aligned}$$

The eigenvalues further give us a period element of the time evolution of these states

$$\begin{aligned} \varepsilon_S &= -3\frac{J}{4} \\ \varepsilon_T &= \frac{J}{4} \\ |\psi(t)\rangle &= c_S e^{-i\varepsilon_S \frac{t}{\hbar}} |S\rangle + c_T e^{-i\varepsilon_T \frac{t}{\hbar}} |T\rangle \end{aligned}$$

Where $n = \{s, T_{-1}, T_0, T_1\}$. We now know the time evolution, but to fully evaluate this system, we also need to know the constants \tilde{c}_n . To properly evaluate these, we need to be able to convert our constants between the computational basis state $|i\rangle$ and the singlet/triplet basis state $|n\rangle$. As the computational basis is diagonal, the basis shift matrix $\langle n|i\rangle$ is simply a matrix with the singlet/triplet states in each row:

$$\langle n|i\rangle = \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

In the initial computational basis, the state $|01\rangle$ takes the form

$$|01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}_i$$

While in the computational basis, it instead takes the form

$$|01\rangle = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}_n$$

We get to observe the time evolution

$$\begin{aligned}
|\psi(t)\rangle &= \frac{1}{\sqrt{2}}(-e^{-i\varepsilon_s \frac{t}{\hbar}}|s\rangle + e^{-i\varepsilon_{T0} \frac{t}{\hbar}}|T_0\rangle) \\
&= \frac{1}{\sqrt{2}}(e^{-iJ\frac{t}{4\hbar}}|T_0\rangle - e^{+i3J\frac{t}{4\hbar}}|s\rangle) \\
&= \frac{1}{\sqrt{2}}e^{-iJ\frac{t}{4\hbar}}(|T_0\rangle - e^{iJ\frac{t}{\hbar}}|s\rangle) \\
\theta &\equiv J\frac{t}{\hbar} \\
|\psi(t)\rangle &= \frac{1}{\sqrt{2}}e^{-i\theta/4}\left(\frac{1}{\sqrt{2}}(|10\rangle + |01\rangle - e^{i\theta}|10\rangle + e^{i\theta}|01\rangle)\right) \\
&= \frac{1}{2}e^{-i\frac{\theta}{4}}((1 - e^{i\theta})|10\rangle + (1 + e^{i\theta})|01\rangle)
\end{aligned}$$

It looks like this Hamiltonian induces Rabi oscillations for certain initial configurations. This means that if we only pulse the coupling over a set duration, it will have the function of a SWAP gate. Since the variable θ also holds the constant J/\hbar , one could physically attach and separate the qubits as a function of time to achieve the same effect. From this we can deduce the probability of being in a given state at any time, by simply squaring the amplitude of each state. Figure 7 shows the probability fluctuations. This coupling also represents a known source of decoherence in quantum computing, namely that qubits are likely to fluctuate between states if any coupling exists. [1]

In the following section, we will explore some more advanced spin interactions.

6 Three-qubit interactions

6.1 Molecules of interest

We will be examining the interactions on two molecules in particular, both of which have experimentally been shown to exhibit cotunneling behavior. The first is polyoxomethalate, a molecule examined by Lehmann and Loss[9], which contains two coupled electron qubits that become entangled and interchange when a third electron qubit is added between them. Another is the cruciform molecule OPE5 recently examined by Jeppe Fock[10], which displays a similar behavior, containing two electron qubits and allowing a third to be coupled to the system to induce a function. Both cases involve a 2-qubit system that is activated by a third qubit. The two molecules in question are shown in figure 8, and the electronic layout of the cruciform molecule is shown in figure 9

These systems also represent two separate regimes. In the polyoxomethalate, the two initial spins are separated and have a weak coupling, while the additional qubit should have a significantly stronger bonding to the other two. Let us call this the isolated regime. On OPE5, the final qubit makes a roughly equilateral triangle with the original two, which causes the three constants to be of similar values. The first two qubits have been shown to exhibit ferromagnetic behavior, which would make their coupling constant negative, however. Let us call this the ferromagnetic regime.

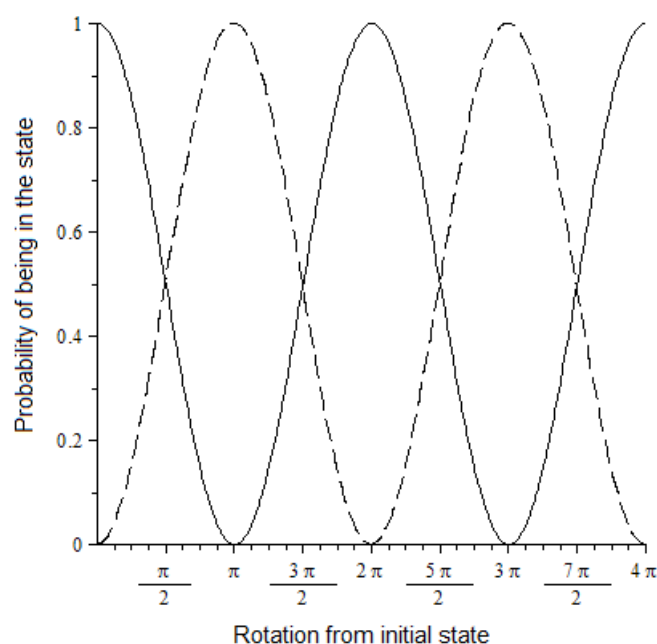


Figure 7: The probability of being in a given state after a certain amount of oscillation, relative to the initial state. To achieve a SWAP operation on this qubit, one selects a coupling time that causes $\theta = \pi$. The solid line represents the initial state, while the dashed line represents this state flipped.

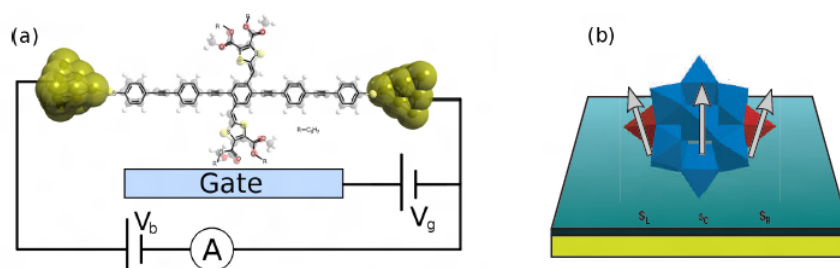


Figure 8: Our molecules of interest. On OPE5, two electronic states of interest appear due to aromatic rings. The third qubit is added with a slight increase of the gate voltage, which attracts a third electron to the system, creating a rough triangle. In polyoxometalate (b), the two qubits are separated by an inert core, but a bias across the core will activate it with an electron.

6.2 Basis sets

We need a basis set to describe our three-spin system. We are combining three spins $1/2$, so we will be able to describe the system with 2^3 states, leading to an 8×8 matrix. The simplest basis would just involve each combination of spins, such that the first state would be $|000\rangle$, followed

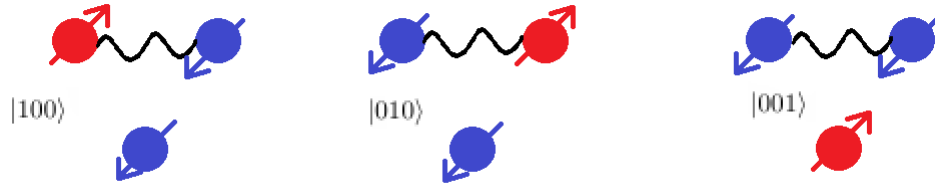


Figure 9: The three potential locations of a spin on a cruciform molecule. The wavy line symbolizes the coupling between the two original qubits.

by $|001\rangle$ and so on. Let us label these numerically:

$$\begin{aligned}
 |\psi_1\rangle &= |000\rangle & |\psi_2\rangle &= |001\rangle \\
 |\psi_3\rangle &= |010\rangle & |\psi_4\rangle &= |100\rangle \\
 |\psi_5\rangle &= |011\rangle & |\psi_6\rangle &= |101\rangle \\
 |\psi_7\rangle &= |110\rangle & |\psi_8\rangle &= |111\rangle
 \end{aligned}$$

Acting on these is the Hamiltonian

$$H_0 = J_{12}\mathbf{S}_1 \cdot \mathbf{S}_2 + J_{13}\mathbf{S}_1 \cdot \mathbf{S}_3 + J_{23}\mathbf{S}_2 \cdot \mathbf{S}_3$$

which is very similar to the one we explored earlier, only a touch more complicated as we now have three spin-spin couplings instead of just one. Since off-diagonal elements will only be produced by the S^+S^- element of H , it is evident that $|\psi_1\rangle$ and $|\psi_8\rangle$ will have no overlap with any other states, and that diagonal states will only appear internally between $|\psi_2\rangle, |\psi_3\rangle$ and $|\psi_4\rangle$, as well as $|\psi_5\rangle, |\psi_6\rangle$ and $|\psi_7\rangle$.

$$\begin{aligned}
 H_0|000\rangle &= \frac{1}{4}(J_{12} + J_{23} + J_{13})|000\rangle \\
 H_0|001\rangle &= \frac{1}{4}(J_{12} - J_{23} - J_{13})|001\rangle + \frac{1}{2}(J_{23}|010\rangle + J_{13}|100\rangle) \\
 H_0|010\rangle &= \frac{1}{4}(-J_{12} + J_{23} - J_{13})|010\rangle + \frac{1}{2}(J_{23}|001\rangle + J_{12}|100\rangle) \\
 H_0|100\rangle &= \frac{1}{4}(-J_{12} - J_{23} + J_{13})|100\rangle + \frac{1}{2}(J_{12}|010\rangle + J_{13}|001\rangle) \\
 H_0|011\rangle &= \frac{1}{4}(-J_{12} - J_{23} + J_{13})|011\rangle + \frac{1}{2}(J_{12}|101\rangle + J_{13}|110\rangle) \\
 H_0|101\rangle &= \frac{1}{4}(-J_{12} + J_{23} - J_{13})|101\rangle + \frac{1}{2}(J_{23}|110\rangle + J_{12}|011\rangle) \\
 H_0|110\rangle &= \frac{1}{4}(J_{12} - J_{23} - J_{13})|110\rangle + \frac{1}{2}(J_{23}|101\rangle + J_{13}|011\rangle) \\
 H_0|111\rangle &= \frac{1}{4}(-1)^2(J_{12} + J_{23} + J_{13})|111\rangle
 \end{aligned}$$

The Hamiltonian matrix $\langle\psi_i|H_0|\psi_j\rangle$ then possesses four different diagonal elements, which

we will rename

$$\begin{aligned} J_0 &= \frac{1}{4}(J_{12} + J_{23} + J_{13}) & J_1 &= \frac{1}{4}(J_{12} - J_{23} - J_{13}) \\ J_2 &= \frac{1}{4}(-J_{12} + J_{23} - J_{13}) & J_3 &= \frac{1}{4}(-J_{12} - J_{23} + J_{13}) \end{aligned}$$

$$\langle \psi_i | H_0 | \psi_j \rangle = \begin{pmatrix} J_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & J_1 & \frac{J_{12}}{2} & \frac{J_{13}}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{J_{12}}{2} & J_2 & \frac{J_{23}}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{J_{13}}{2} & \frac{J_{23}}{2} & J_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & J_3 & \frac{J_{23}}{2} & \frac{J_{13}}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{J_{23}}{2} & J_2 & \frac{J_{13}}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{J_{13}}{2} & \frac{J_{12}}{2} & J_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & J_0 \end{pmatrix}$$

The nature of the molecules of interest inspire a different basis set, however. We know the three-spin interaction possesses the states $|\mathbf{s}; \mathbf{s}^z\rangle$

$$\begin{aligned} |3/2; 3/2\rangle &= |000\rangle & |3/2; 1/2\rangle &= \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle) \\ |3/2; -1/2\rangle &= \frac{1}{\sqrt{3}}(|011\rangle + |101\rangle + |110\rangle) & |3/2; -3/2\rangle &= |111\rangle \\ |1/2; 1/2\rangle &= \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle - |100\rangle) & |1/2; -1/2\rangle &= \frac{1}{\sqrt{3}}(|011\rangle - |101\rangle - |110\rangle) \end{aligned}$$

Which is, of course, not a viable basis set, since we need 8 states, and there is overlap between some of the states. Since both of the molecules of interest have two qubits which are never removed, and we have seen earlier that trouble arises when these are not aligned, the parity of the first two electrons make for a good last parameter. We then get the basis states $|P; \mathbf{s}; \mathbf{s}^z\rangle$

$$\begin{aligned} |\psi_1\rangle &= |1; 3/2; 3/2\rangle = |000\rangle \\ |\psi_2\rangle &= |1; 3/2; 1/2\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle) \\ |\psi_3\rangle &= |1; 3/2; -1/2\rangle = \frac{1}{\sqrt{3}}(|011\rangle + |101\rangle + |110\rangle) \\ |\psi_4\rangle &= |1; 3/2; -3/2\rangle = |111\rangle \\ |\psi_5\rangle &= |1; 1/2; 1/2\rangle = \frac{1}{\sqrt{6}}(2|001\rangle - |010\rangle - |100\rangle) \\ |\psi_6\rangle &= |1; 1/2; -1/2\rangle = \frac{1}{\sqrt{6}}(|011\rangle + |101\rangle - 2|110\rangle) \\ |\psi_7\rangle &= |-1; 1/2; 1/2\rangle = \frac{1}{\sqrt{2}}(|010\rangle - |100\rangle) \\ |\psi_8\rangle &= |-1; 1/2; -1/2\rangle = \frac{1}{\sqrt{2}}(|011\rangle - |101\rangle) \end{aligned}$$

Again, we act on these states with the Hamiltonian H_0 .

$$\begin{aligned}
H_0|1; 3/2; 3/2\rangle &= 1/4(J_{12} + J_{23} + J_{13})|000\rangle \\
H_0|1; 3/2; 1/2\rangle &= \frac{1}{\sqrt{3}}(J_{12}(1/4(|001\rangle - |010\rangle - |100\rangle) + 1/2(|010\rangle + |100\rangle)) \\
&\quad + J_{13}(1/4(-|001\rangle + |010\rangle - |100\rangle) + 1/2(|001\rangle + |100\rangle)) \\
&\quad + J_{23}(1/4(-|001\rangle - |010\rangle + |100\rangle) + 1/2(|010\rangle + |001\rangle)) \\
H_0|1; 3/2; -1/2\rangle &= \frac{1}{\sqrt{3}}(J_{12}(1/4(|110\rangle - |101\rangle - |011\rangle) + 1/2(|101\rangle + |011\rangle)) \\
&\quad + J_{13}(1/4(-|110\rangle + |101\rangle - |011\rangle) + 1/2(|110\rangle + |011\rangle)) \\
&\quad + J_{23}(1/4(-|110\rangle - |101\rangle + |011\rangle) + 1/2(|101\rangle + |110\rangle)) \\
H_0|1; 3/2; -3/2\rangle &= 1/4(J_{12} + J_{23} + J_{13})|111\rangle \\
H_0|1; 1/2; 1/2\rangle &= \frac{1}{\sqrt{6}}(J_{12}(1/4(2|001\rangle + |010\rangle + |100\rangle) + 1/2(-|010\rangle - |100\rangle)) \\
&\quad + J_{13}(1/4(-2|001\rangle - |010\rangle + |100\rangle) + 1/2(2|001\rangle - |100\rangle)) \\
&\quad + J_{23}(1/4(-2|001\rangle + |010\rangle - |100\rangle) + 1/2(2|010\rangle - |001\rangle)) \\
H_0|1; 1/2; -1/2\rangle &= \frac{1}{\sqrt{6}}(J_{12}(1/4(2|110\rangle + |101\rangle + |011\rangle) + 1/2(-|101\rangle - |011\rangle)) \\
&\quad + J_{13}(1/4(-2|110\rangle - |101\rangle + |011\rangle) + 1/2(2|011\rangle - |110\rangle)) \\
&\quad + J_{23}(1/4(-2|110\rangle + |101\rangle - |011\rangle) + 1/2(2|101\rangle - |110\rangle)) \\
H_0|-1; 1/2; -1/2\rangle &= \frac{1}{\sqrt{2}}((J_{12}(1/4(-|010\rangle + |100\rangle) + 1/2(|100\rangle - |010\rangle)) \\
&\quad + J_{13}(1/4(|010\rangle + |100\rangle) + 1/2(-|001\rangle) + 1/4(-|010\rangle - |100\rangle) + 1/2(|001\rangle)) \\
H_0|-1; 1/2; -1/2\rangle &= \frac{1}{\sqrt{2}}(1/4(-|011\rangle + |101\rangle) + 1/2(|011\rangle - |101\rangle)) \\
&\quad + J_{13}(1/4(-|011\rangle - |101\rangle) + 1/2(|110\rangle) + J_{23}(|011\rangle + |101\rangle) + 1/2(-|101\rangle))
\end{aligned}$$

We can already predict that the four $m = 3/2$ states will have no off-diagonal elements, as there is no internal overlap, and the remaining states can't achieve the same angular momentum. Further, of the $\mathbf{s} = \mathbf{1}/2$ elements, only those with the same s^z value will have any overlap.

$$\begin{aligned}
\langle\psi_1|H_0|\psi_1\rangle &= 1/4(J_{12} + J_{13} + J_{23}) & \langle\psi_2|H_0|\psi_2\rangle &= 1/4(J_{12} + J_{13} + J_{23}) \\
\langle\psi_3|H_0|\psi_3\rangle &= 1/4(J_{12} + J_{13} + J_{23}) & \langle\psi_4|H_0|\psi_4\rangle &= 1/4(J_{12} + J_{13} + J_{23}) \\
\langle\psi_5|H_0|\psi_5\rangle &= -1/4(J_{12} + 2J_{13} + 2J_{23}) & \langle\psi_6|H_0|\psi_6\rangle &= -1/4(J_{12} + 2J_{13} + 2J_{23}) \\
\langle\psi_7|H_0|\psi_7\rangle &= 3/4J_{12} & \langle\psi_8|H_0|\psi_8\rangle &= 3/4J_{12} \\
\langle\psi_5|H_0|\psi_7\rangle &= \sqrt{3}/4(J_{13} - J_{23}) & \langle\psi_7|H_0|\psi_5\rangle &= \sqrt{3}/4(J_{13} - J_{23}) \\
\langle\psi_6|H_0|\psi_8\rangle &= \sqrt{3}/4(J_{13} - J_{23}) & \langle\psi_8|H_0|\psi_6\rangle &= \sqrt{3}/4(J_{13} - J_{23})
\end{aligned}$$

Since we only get four distinct values, let's name them before setting up our matrix

$$\begin{aligned}
\varepsilon_{3/2} &= \frac{1}{4}(J_{12} + J_{13} + J_{23}) & \varepsilon_{+,1/2} &= \frac{1}{4}(J_{12} - 2J_{13} - 2J_{23}) \\
\varepsilon_{-,1/2} &= \frac{3}{4}J_{12} & \varepsilon_{od} &= \frac{\sqrt{3}}{4}(J_{13} - J_{23})
\end{aligned}$$

$$H_0 = \begin{pmatrix} \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_{3/2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_{+;1/2} & 0 & \varepsilon_{od} & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_{+;1/2} & 0 & \varepsilon_{od} \\ 0 & 0 & 0 & 0 & \varepsilon_{od} & 0 & \varepsilon_{-;1/2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_{od} & 0 & \varepsilon_{-;1/2} \end{pmatrix}$$

To diagonalize this matrix fully, we can make the assumption that $(J_{13} - J_{23})$, which will eradicate any off-diagonal elements. This a particularly reasonable assumption in the case of polyoxometalate, as the third spin appears exactly in the middle of the other two and the authors of the experiment already make the same assumption[9]. Thus, we have our eigenvectors in the $|P; \mathbf{s}; \mathbf{s}^z\rangle$ basis, and our eigenvalues in the diagonal of the matrix.

The basis shift matrix between the computational and parity bases is given by

$$\langle i|p\rangle = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}$$

6.3 Time evolution

Now, let us examine the time evolution of $|100\rangle$, for example. Since

$$\langle i|p\rangle|100\rangle = \frac{1}{\sqrt{3}}|1; 3/2; 1/2\rangle - \frac{1}{\sqrt{6}}|1; 1/2; 1/2\rangle - \frac{1}{\sqrt{2}}|-1; 1/2; 1/2\rangle$$

it must take the form

$$|\psi(t)\rangle = c_{3/2}e^{-i\varepsilon_{3/2}\frac{t}{\hbar}}|1; 3/2; 1/2\rangle + c_{+;1/2}e^{-i\varepsilon_{+;1/2}\frac{t}{\hbar}}|1; 1/2; 1/2\rangle + c_{-;1/2}e^{-i\varepsilon_{-;1/2}\frac{t}{\hbar}}|-1; 1/2; 1/2\rangle$$

Since we have assumed the couplings of the third spin to be of the same strength, let us rename $J_{12} = J_f$ and $J_{13} = J_{23} = J_s$

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{3}}e^{-i\frac{1}{4}(J_f+2J_s)\frac{t}{\hbar}}|1; 3/2; 1/2\rangle - \frac{1}{-\sqrt{6}}e^{i\frac{1}{4}(J_f-4J_s)\frac{t}{\hbar}}|1; 1/2; 1/2\rangle - \frac{1}{\sqrt{2}}e^{-i\frac{3}{4}J_f\frac{t}{\hbar}}|-1; 1/2; 1/2\rangle \\ &= \frac{1}{3}e^{-i\frac{1}{4}(J_f+2J_s)\frac{t}{\hbar}}(|001\rangle + |010\rangle + |100\rangle) \\ &\quad - \frac{1}{6}e^{-i\frac{1}{4}(J_f-4J_s)\frac{t}{\hbar}}(2|001\rangle - |010\rangle - |100\rangle) \\ &\quad - \frac{1}{2}e^{-i\frac{3}{4}J_f\frac{t}{\hbar}}(|010\rangle - |100\rangle) \\ &= \left(\frac{1}{3}e^{-i\frac{1}{4}(J_f+2J_s)\frac{t}{\hbar}} - \frac{1}{3}e^{-i\frac{1}{4}(J_f-4J_s)\frac{t}{\hbar}}\right)|001\rangle \\ &\quad + \left(\frac{1}{3}e^{-i\frac{1}{4}(J_f+2J_s)\frac{t}{\hbar}} + \frac{1}{6}e^{-i\frac{1}{4}(J_f-4J_s)\frac{t}{\hbar}} - \frac{1}{2}e^{-i\frac{3}{4}J_f\frac{t}{\hbar}}\right)|010\rangle \\ &\quad + \left(\frac{1}{3}e^{-i\frac{1}{4}(J_f+2J_s)\frac{t}{\hbar}} + \frac{1}{6}e^{-i\frac{1}{4}(J_f-4J_s)\frac{t}{\hbar}} + \frac{1}{2}e^{-i\frac{3}{4}J_f\frac{t}{\hbar}}\right)|100\rangle \end{aligned}$$

Let us express the time in terms of $\tau = J_F/h$. One unit of time on the graph represents a time t/τ . For example, if $J_F/h = \frac{1}{10ps}$, one unit of time on a plot of these functions represents 10 picoseconds passing. Instead of approximating a value of J_f , we will instead concentrate on the relationship $\frac{J_s}{J_f}$. Figure 10 shows us that when the third qubit is entirely out of the picture, the system will flip states as fast as $\frac{2\tau}{3}$. If our goal is to create a SWAP gate, we need to compare it to this time scale and induce a flip considerably faster. This is on the assumption that J_f is not altered by the absence or presence of J_s , which is not a fair assumption. In the actual system, J_f is likely considerably smaller.

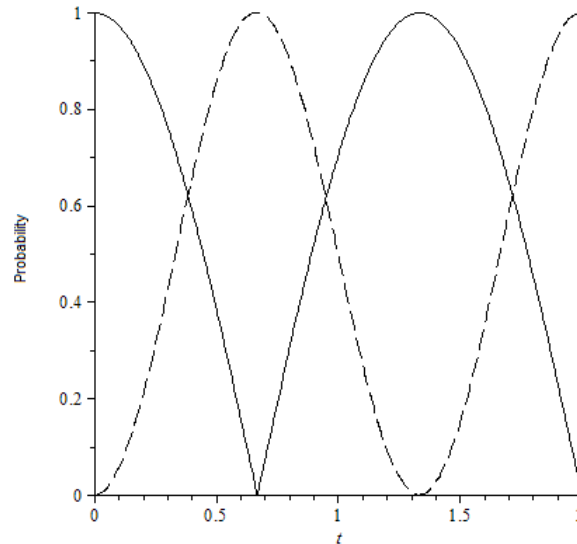


Figure 10: The probability of occupying a given state at the given time when oscillating between $|10\rangle$ and $|01\rangle$. At this point, the third qubit has not been introduced, so it is good that it looks similar to our result from earlier. The sharp spike of the solid line at the bottom is supposed to be curved, but the current build of the program used for the plots has the occasional spiky inclination.

We then examine the results of some coupling ratios. Figure 11 explores the ferromagnetic regime, which allows for a SWAP to happen, while figure 12 shows an asymptotic regime, where the probability of finding anything but the original state never rises above a third. Figure 13 shows a good candidate for an anti-ferromagnetic SWAP gate, which swaps the states quite certainly. Figures 14 and 15 show that if we go too far into the isolated regime, our ability to create a reliable SWAP gate actually starts to taper off.

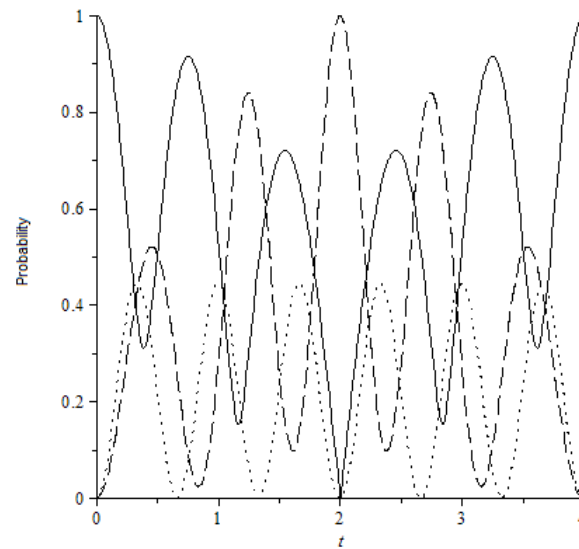


Figure 11: The same probability, occurring in the ferromagnetic regime where $J_s = -J_f$. The solid line represents the initial state, the dashed line is the probability of the state moving to the second qubit, and the dotted line represents the final, coupled qubit stealing the state. Note how the third qubit actually slows the swap, even though it induces faster oscillations

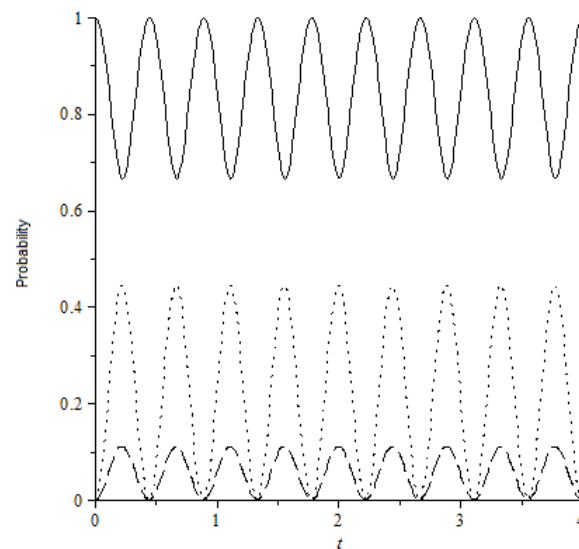


Figure 12: An asymptotic state that occurs when $J_s = 1.5J_f$. The solid line represents the initial state, and the dashed state the probability of being interchanged with the second qubit. Notably, the third qubit (dashed line) is always more likely to take the state than the actual second qubit.

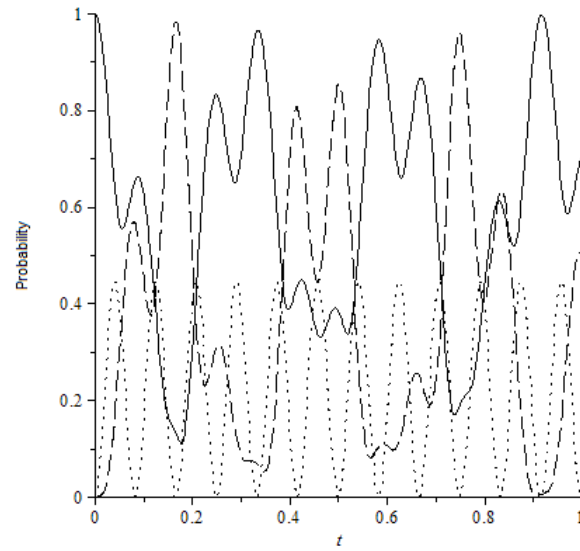


Figure 13: A feasible SWAP gate that occurs when $J_s = 8J_f$. The solid line represents the initial state, the dashed state the probability of being interchanged with the second qubit and the dotted line is the third qubit. The SWAP happens in $.17\tau$, which would be a fairly significant speed-up even if we assume there is an exchange while uncoupled.

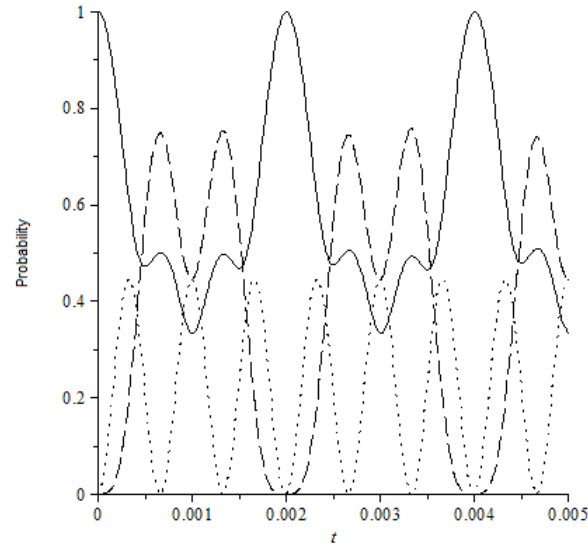


Figure 14: A curious feature of our coupling is that if the central coupling constant is too great, the probability of swapping actually caps off around $.75$. Here, the probability is the dashed line, in the extreme scenario where $J_s = 1000J_f$.

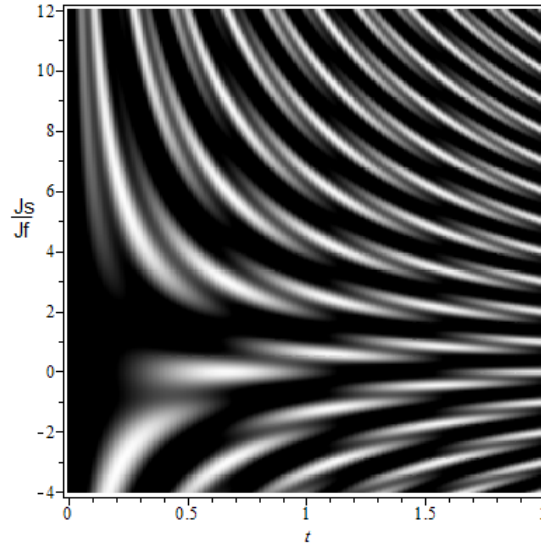


Figure 15: A density matrix showing the probability of swapping the first two qubits, with the white areas being the most probable. Once the ratio between the central and outer coupling becomes much larger than 10, the white areas will begin to taper off. Note the asymptotic line at $\frac{J_s}{J_f} = 1.5$, which is shown in figure 12

6.4 A full three-way interaction

We've made the assumption that our two secondary coupling constants are the same, but this is not necessarily the case for the ferromagnetic, cruciform regime that we are also considering. To consider this, we need to diagonalize the matrix H_0 instead of making the assumption. Since the only non-diagonal elements belong to two similar 2×2 subspaces, this is a fairly simple task.

$$H_0 = \begin{pmatrix} \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_{3/2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_{+,1/2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_{+,1/2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \varepsilon_{-,1/2} - \frac{\varepsilon_{od}^2}{\varepsilon_{+,1/2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \varepsilon_{-,1/2} - \frac{\varepsilon_{od}^2}{\varepsilon_{-,1/2}} & 0 \end{pmatrix}$$

Everything else, such as our basis shift matrix remains the same. Let us examine the time evolution of the state $|100\rangle$

$$|\psi(t)\rangle = \frac{1}{\sqrt{3}} e^{-i\varepsilon_{3/2} \frac{t}{\hbar}} |1; 3/2; 1/2\rangle - \frac{1}{\sqrt{6}} e^{-i\varepsilon_{+,1/2} \frac{t}{\hbar}} |1; 1/2; 1/2\rangle - \frac{1}{\sqrt{2}} e^{-i(\varepsilon_{-,1/2} - \frac{\varepsilon_{od}^2}{\varepsilon_{+,1/2}}) \frac{t}{\hbar}} |-1; 1/2; 1/2\rangle$$

Let's examine our newest constant

$$\begin{aligned}\varepsilon_{-,1/2} - \frac{\varepsilon_{od}^2}{\varepsilon_{+,1/2}} &= \frac{3}{4}J_{12} - \frac{(\frac{\sqrt{3}}{4}(J_{13} - J_{23}))^2}{\frac{1}{4}(J_{12} - 2J_{13} - 2J_{23})} \\ &= \frac{3}{4}J_{12} - \frac{3(J_{13} - J_{23})^2}{\frac{1}{4}(J_{12} - 2J_{13} - 2J_{23})}\end{aligned}$$

$$\begin{aligned}|\psi(t)\rangle &= \frac{1}{\sqrt{3}}e^{-i\frac{1}{4}(J_{12}+J_{13}+J_{23})\frac{t}{\hbar}}|1; 3/2; 1/2\rangle \\ &\quad - \frac{1}{\sqrt{6}}e^{-i\frac{1}{4}(J_{12}-2J_{13}-2J_{23})\frac{t}{\hbar}}|1; 1/2; 1/2\rangle \\ &\quad - \frac{1}{\sqrt{2}}e^{-i(\frac{3}{4}J_{12}-\frac{3(J_{13}-J_{23})^2}{4(J_{12}-2J_{13}-2J_{23})})\frac{t}{\hbar}}|-1; 1/2; 1/2\rangle \\ &= \left(\frac{1}{3}e^{-i\frac{1}{4}(J_{12}+J_{13}+J_{23})\frac{t}{\hbar}} - \frac{1}{3}e^{-i\frac{1}{4}(J_{12}-2J_{13}-2J_{23})\frac{t}{\hbar}}\right)|001\rangle \\ &\quad + \left(\frac{1}{3}e^{-i\frac{1}{4}(J_{12}+J_{13}+J_{23})\frac{t}{\hbar}} + \frac{1}{6}e^{-i\frac{1}{4}(J_{12}-2J_{13}-2J_{23})\frac{t}{\hbar}} - \frac{1}{2}e^{-i(\frac{3}{4}J_{12}-\frac{3(J_{13}-J_{23})^2}{4(J_{12}-2J_{13}-2J_{23})})\frac{t}{\hbar}}\right)|010\rangle \\ &\quad + \left(\frac{1}{3}e^{-i\frac{1}{4}(J_{12}+J_{13}+J_{23})\frac{t}{\hbar}} + \frac{1}{6}e^{-i\frac{1}{4}(J_{12}-2J_{13}-2J_{23})\frac{t}{\hbar}} + \frac{1}{2}e^{-i(\frac{3}{4}J_{12}-\frac{3(J_{13}-J_{23})^2}{4(J_{12}-2J_{13}-2J_{23})})\frac{t}{\hbar}}\right)|100\rangle\end{aligned}$$

If we set the two third-qubit couplings to be equal, we will see the same results we got in the previous section. We will simply examine two cases, one where a single coupling is turned off, as well as one where the two couplings are not equal. Figures 16 and 17 demonstrate that one-sided central coupling will not get in the way of producing a SWAP gate.

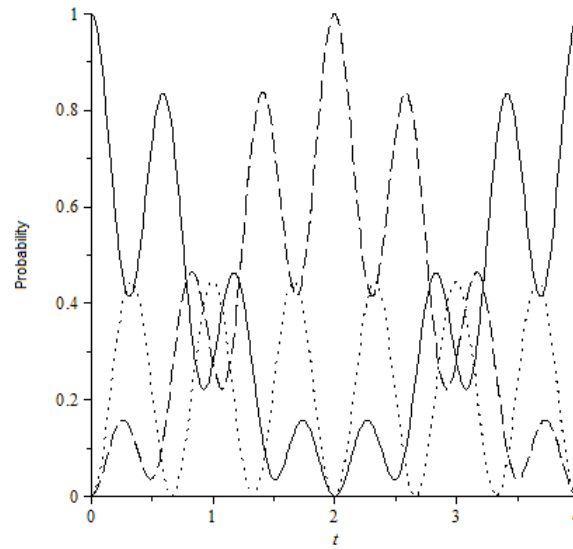


Figure 16: A coupling exchange where $J_{13} = 2J_{12}$ and $J_{23} = 0$. This generates a perfectly viable SWAP gate, and looking at the behavior of the probabilities, it would almost appear as though the initial state is slowly feeding into the swapped state across the third qubit, and reversing once it has been swapped.

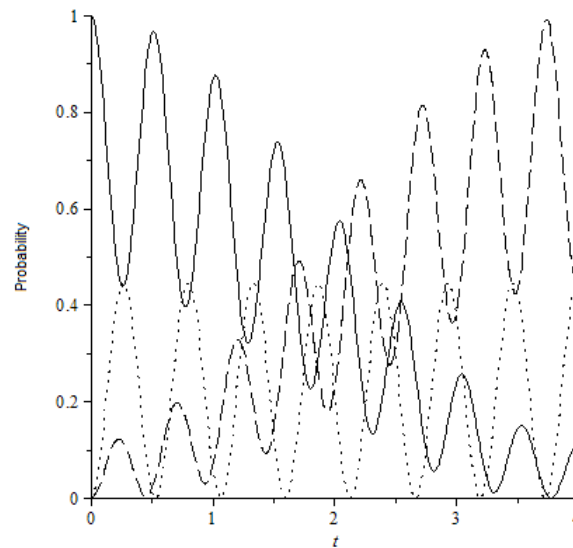


Figure 17: A coupling exchange where $J_{13} = 2J_{12}$ and $J_{23} = \frac{1}{2}J_{12}$. This seems to severely lopsided the function compared to what appears in figure 16, but it does not actually prevent the swap.

7 Concluding remarks

One thing we have shown is that for a time scale relevant to the strength of their coupling, two qubits cannot be stable if they're coupled and unaligned. This is, as mentioned, the biggest weakness of the molecule as a quantum processing element, since most advanced computations require the ability to couple and uncouple qubits without losing them. We did find that it is possible to design a reliable time evolution from base principles with regards to the SWAP gate. Interestingly, we found that while having a stronger coupling between your initial qubits in the disconnected regime was favorable to a weak one, using a significantly stronger coupling would actually be counterproductive.

OPE5 is an interesting molecule as it encourages ferromagnetic coupling, and it seems to have potential as a nanotransistor element, but the ever present coupling between its initial qubits means that it would be difficult to employ as a quantum processing element, though it might have some potential as a storage unit.

Polyoxomethalate is a rare molecular system which does allow the coupling and decoupling of its initial qubit states. It would be interesting to explore how the coupling strength between the two initial qubits is affected by the third, as we have only explored systems where the third qubit is present. Under the proper conditions, polyoxomethalate could be a quantum processing element.

Further research with this subject could include endless variations of input in the derived expressions, perhaps examining the effect of a very small difference between coupling constants, or if all three are on separate orders of magnitude. Many interesting refinements could also be made on the expressions themselves, such as exploring what would happen if the third qubit was being affected by some outside noise.

Further research in the field that would be interesting could be the development of complex quantum gates such as CNOT from base principles, and the examination of molecular systems that do allow for coherent decoupling.

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