

Fidelity of Kane's Binary Gate

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Chapter 1

Computers meet Quantum Mechanics

1.1 Introduction

The physics of information and computation has been a recognized discipline for several decades. This is not surprising. Information is, after all, encoded in the state of a physical system. Our abilities to compute and process information depend directly on the physics of the system. A computation is something that can be carried out on an actual physically realizable device. Hence the study of information and computation is linked to the study of the underlying physical process. From the perspective of developing state-of-the-art computing technology, study of the principles of physics and material science is essential. From a more abstract and theoretical point of view, there have been noteworthy milestones in our understanding of how physics constrains our ability to use and manipulate information e.g. Landauer's Principle, Reversible Computation, Explanation of Maxwell's Daemon, etc.

1.2 Quantum Information Theory

The concepts of information theory underlying modern methods of computing are essentially classical. However, a better understanding of the laws of quantum mechanics has revealed fundamentally new ways of information processing. Even during the early days of quantum mechanics, it was probably clear that classical theories of information would need revision from the viewpoint of quantum laws.

- **Random Processes** Quantum mechanics is non deterministic. For example, the radioactive decay of a source is described by a truly ran-

dom Poisson process. However, deterministic classical dynamics has no place for true randomness.

- **Non-disruptive Measurements** In quantum theory, non commuting observables A, B cannot simultaneously have precisely defined values. Performing a measurement of A will necessarily influence the outcome of a subsequent measurement of B. Thus the act of acquiring information about a physical system inevitably disturbs the state of the system. Classical physics has no such restrictions.
- **No Cloning Theorem** Quantum theory does not allow for the possibility for cloning of the state of a system. If it were possible to make multiple copies of a system, it would be possible to measure the quantum clone without disturbing the original system, thereby violating the above principle.

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The laws of quantum mechanics also influenced our notions of information in far deeper ways. John Bell showed that the predictions of quantum mechanics cannot be reproduced by any local hidden variable theory. Bell showed that by means of entanglement, quantum mechanics invariably stores information between the correlations of physical systems. A lot of interest has developed in the study of quantum information theory since the 1980's. Benet, Vazirani, et al have been among the pioneers in this field. A number of results in classical information theory have found their generalizations in quantum information theory. The principles of quantum information theory were also put to use in the related fields of quantum computation, teleportation and cryptography. Feynmann [1], et al are credited with the foundations of quantum computation. However, in spite of the fundamentally different and unusual properties of quantum information theory, the world was caught off guard when Peter Shor proposed his now famous quantum algorithm to factorize numbers efficiently [3]. This was to set the trend for quantum information theory and it's related fields from the mid 90's onward.

1.3 Computation

Modern methods of computing are essentially based on classical physics. However, as discussed above a better understanding of the laws of quantum mechanics has revealed fundamentally new ways of information processing. Based on these new ideas, a quantum computer uses a two level quantum system for a qubit - the quantum analog of the classical bit. Unlike it's classical counterpart, a qubit can simultaneously be in a superposition of

it's base states $|0\rangle$ and $|1\rangle$. This allows a quantum computer to perform parallel computation far more naturally than a classical computer. It has also been observed [1] that a classical computer can simulate a quantum system only with exponential slowdown in the size of the system. These concepts lead people to believe that certain problems can be solved far more efficiently using a quantum computer [2]. Interest in quantum computers increased dramatically following the publication of quantum algorithms for prime factorization [3] and exhaustive search[4]. From a completely different viewpoint, a technological viewpoint, Moore's empirical law predicts that the amount of information stored on a chip doubles every 18 months. This rapid decrease in size of classical bits has forced us to take cognizance of quantum effects even in classical information processing. Thus, in a sense, quantum computing has become a necessity.

1.4 Physical Implementation of a Quantum Computer

The above sections outlined the theoretical progress made by quantum computation and quantum information theory. With the publication of the factorization algorithm in 1994 [3], the true potential of a quantum computer was understood. The search for a physically realizable model of a quantum computer assumed new importance. However, interactions with the environment in any realistic model make it is extremely difficult to perform computations through coherent manipulations of qubits. The discovery of error correcting codes[6] allows a quantum computer to function in spite of some degree of decoherence and hence may make quantum computers an experimental reality someday. Yet, bringing the time scales of decoherence into the error correcting range has also proved to be a daunting task.

The hardware for a quantum computer needs to meet some stringent specifications in its ability to store and manipulate quantum information.

- **Storage of Information:** The hardware would need to be able to store quantum information in qubits sufficiently long to perform the computation
- **Logic Gates** The physics of the quantum device should make it possible to manipulate the quantum states of single qubits. It should also allow for interactions between two adjacent qubits in order to perform some non trivial binary gate.

- **Minimal Interaction with Environment** In order to minimize the effects of decoherence, it is important that our qubits be well isolated from the environment.
- **Measurement** It should ultimately be possible to measure the final state of the qubits and thus obtain the result of a computation.

We will very briefly mention some classic schemes for quantum computation that have been proposed.

1.4.1 Ion Trap

This model for quantum computation was proposed by Ignacio Cirac and Peter Zoller [7] and has been pursued by Dave Wineland's group at the National Institute for Standards and Technology (NIST), among others. This model uses single ions held in a Paul trap as qubits. The ground state of the ion $|g\rangle$ is interpreted as the qubit state $|0\rangle$, while the long-lived excited state $|e\rangle$ is the qubit state $|1\rangle$. It is easy to read out the states of the ions by performing a measurement that projects onto the $|e\rangle, |g\rangle$ basis. A laser is tuned to a transition from the state $|g\rangle$ to a short-lived excited state $|e'\rangle$. When this laser illuminates the ions, each qubit with the value $|0\rangle$ absorbs and reemits the laser light, so that it fluoresces. Qubits with the value $|1\rangle$ remain dark. Single qubit gates are performed by addressing individual ions with a laser light of frequency ω , which induces transition between the $|0\rangle$ and $|1\rangle$ states. Mutual coulomb repulsion between ions keeps them sufficiently far enough away to be able to address each atom individually with the laser pulse. The coulombic interactions between ions creates a spectrum of coupled normal modes of vibrations for the trapped ions. This effect can be exploited to perform binary gates in the ion trap quantum computer. One big drawback of the ion trap computer is that it is an intrinsically slow device. The speed of the computer is ultimately limited by the energy-time uncertainty relation.

1.4.2 NMR

Recently another model for quantum computation, NMR Quantum Computing has been proposed [9]. Nuclear spins in a particular molecule represent the qubits of computation. The spin states $|\uparrow\rangle$ and $|\downarrow\rangle$ in the presence of a global magnetic field represent the qubit states $|1\rangle$ and $|0\rangle$. Single qubit states are manipulated by applying a global magnetic field rotating at a frequency ω , in resonance with the particular qubit to manipulate. Dipole dipole interactions between adjacent qubits cause the energy splitting between the $|\uparrow\rangle$,

$|\downarrow\rangle$ states of a qubit to depend on the quantum state of neighboring qubits.
Hence conditional dynamics is possible, allowing for two qubit interactions.

Chapter 2

Quantum Computation in Solid State

As discussed in the previous chapter, numerous schemes for the implementation of quantum computers have been proposed. Ion traps [7] and NMR [9] have been the more notable among them. However, scaling these schemes to more than ten qubits has not been possible due to exponential increase in decoherence with the number of qubits. Recently a lot of interest has been generated in the implementation of a quantum computer in the solid state. By proposing such a scheme, one hopes to make use of the tremendous technological progress made in solid state in the past few decades. One also hopes to mimic the success of the classical computer in this field. Bruce Kane presents a scheme for implementing a quantum computer on an array of nuclear spins located on donors in silicon, the semiconductor used in most conventional computer electronics [8]. Logical operations and measurements can in principle be performed independently and in parallel on each spin in the array. We will discuss specific electronic devices for the manipulation and measurement of nuclear spins as proposed by Kane. The fabrication of these devices will require significant advances in the rapidly moving field of nanotechnology. Although it will be difficult to scale Kane's device to large sizes, a silicon based quantum computer is in a unique position to benefit from the resource and ingenuity being directed towards making conventional electronics of ever smaller size and greater complexity.

2.1 Kane's Quantum Computer

Kane's proposal of building a quantum computer consists of embedding ^{31}P impurities in a Si semiconductor host. There is a global magnetic field

$B \approx 2 \text{ Tesla}$ along the z direction. This magnetic field splits the nuclear levels of the ^{31}P spin $\frac{1}{2}$ nuclei giving us the qubits for our computer. The presence of the one valence electron of each donor impurity is vital to the implementation of single as well as binary gates. A rotating magnetic field B_{ac} , with variable frequency, also needs to be applied in the xy plane to implement the single qubit gate. In addition to the above, two voltage gates, A & J are also needed. The A gates are placed right above the donor atoms so as to control the wavefunction of the associated valence electrons. The J gates are placed between two donor atoms and are used to manipulate the interaction between valence electrons of two adjacent donor atoms. The computer operates at very low temperatures, in the order of 100mK in order to minimize decoherence due to thermal fluctuations.

2.1.1 Logic Gates

A quantum computer operates by making unitary reversible transformations on a series of qubits. A particular gate consists of some such unitary operations of a number of qubits. A 'universal gate' is one which can be used to build any computing network. It has been shown that almost any two-qubit gate is universal [12]. Thus any model of a quantum computer should be able to specify how to do unitary single qubit operations and a non-trivial two-qubit gate. Kane's model of the computer proposes to satisfy these objectives by the precise control and variation of three external parameters.

- A gates control the strength of the hyperfine interactions and hence the resonance frequency of the nuclear spins beneath them.
- The globally defined magnetic field B_{ac} rotates at a variable resonant frequency allowing us to flip nuclear spins.
- J gates between the donors turn on and off electron mediated coupling between nuclear spins.

The hyperfine interaction [13] between the valence electron and nucleus of each donor atom gives us local control over each individual qubit. This interaction changes the split in the energy levels of the ^{31}P nuclei. The strength of the interaction depends on the probability amplitude of the wavefunction of valence electron at the nucleus. By changing the voltage on the A gate, the electron wavefunction can be pulled away from the nucleus under the gate and towards the barrier, thereby reducing the probability amplitude of the electronic wavefunction at the nucleus. The energy split between the two levels of the nucleus is thus changed making its resonant frequency different

from the other nuclei. Now we apply the globally defined rotating magnetic pulse B_{ac} at the resonant frequency of this particular qubit, allowing us to flip only this particular qubit. In this way, one can perform single qubit gates.

Executing a two qubit operation is not quite as simple. In this model, information is stored in the spins of the ^{31}P nuclei. In order to perform a non-trivial binary gate interaction between neighbouring nuclei is essential. However, the physics of the model does not permit such an interaction. Kane proposes to perform the gate using electron mediated interactions between the nuclei.

Due to the hyperfine interaction between a nucleus and its valence electron it becomes possible to couple nuclear spin states to certain electron spin states. The spin exchange interaction between two adjacent electrons can then be used to effectively establish an interaction between the corresponding nuclei. This interaction between adjacent electrons depends on the overlap of their wavefunction and thus can be controlled via the J voltage gate. By biasing the J voltage gate positively, we increase overlap and hence the strength of the interaction. By biasing it negatively we can decrease the overlap and effectively decouple the electrons from each other. For the purpose of simplicity, we will assume that by biasing the A voltage gate we can arbitrarily set the strength of the hyperfine interaction between individual nuclei and electrons to any non-negative value. In the real physical model, the hyperfine interaction has a certain maximum strength when the A voltage gate is neutral. The strength of this interaction can then only be reduced by biasing the gate positively, but can never be zero. It is through the use of the A and J voltage gates that we can control the interactions between the four particles and effectively achieve a non trivial binary gate. We will discuss the physics of this interaction in further detail in the next section.

2.2 Kane's Two Qubit Gate

As mentioned earlier, a non-trivial two qubit gate in Kane's model is executed via electron mediated nuclear coupling. The Hamiltonian of the interactions of these four particles, namely $n1$, $e1$, $n2$, $e2$, is given by

$$\mathbf{H}(A, J) = \begin{cases} \frac{1}{2}\omega_n\sigma_z^{n1} & + A\sigma^{\vec{n}1}\sigma^{\vec{e}1} & + \frac{1}{2}\omega_e\sigma_z^{e1} \\ & + J\sigma^{\vec{e}1}\sigma^{\vec{e}2} \\ +\frac{1}{2}\omega_n\sigma_z^{n2} & + A\sigma^{\vec{n}2}\sigma^{\vec{e}2} & + \frac{1}{2}\omega_e\sigma_z^{e2} \end{cases} \quad (2.1)$$

Here, the $\sigma^{\vec{n}i}$ & $\sigma^{\vec{e}i}$ denote the Pauli spin vectors of the i^{th} nucleus and electron, $i = 1, 2$. The binary gate can be carried out by varying the J voltage gate which affects the overlap of adjacent electron clouds and thus

affects the J term in the above Hamiltonian. The value of A above has to be non-zero to enable the nuclear spin states to couple to electron spin states.

Let us denote the electron spin states by $|\uparrow\rangle, |\downarrow\rangle$ and the nuclear states by $|1\rangle, |0\rangle$. Thus the state $|\uparrow\downarrow 10\rangle$ corresponds to the electron and nucleus of the first qubit being in the 'up' state while the electron and nucleus of the second qubit are in the 'down' state. Kane's proposal for a binary gate consists of performing a swap between the nuclei states. Hence, executing the gate results in the state $|10\rangle$ being converted to the state $|01\rangle$. Since the electrons are not part of our qubits, we do not care about what their states are, as long as they are not entangled with the nuclear states at the end of the gate.

It can be seen that by turning the J gate and the A gate on, our qubit states 'mix' with electron states. Though this 'mixing' is essential for the execution of the gate, we would ideally like to return to pure qubit states at the end of the execution of the binary gate. Kane resolves this difficulty by turning the A and J gates on adiabatically. We thus start our system in product states of the nuclei and electrons and slowly turn on the A and J gates. After allowing the appropriate phase differences to accumulate between the different eigenvectors of the system we adiabatically turn the J and A voltage gates off. Hence, as per the adiabatic theorem, we return to the original (uncoupled) nuclear and electron states we started out with, albeit with phase differences. The phase differences allow us to perform a non-trivial binary gate. In particular, we are able to swap the nuclear states of adjacent nuclei.

2.3 The Swap Gate

As mentioned in section(2.1), the computer operates at very low temperature in the range of milikelvins. Thus, for large values of B , like 2 Tesla, the energy difference between the electron spin states is large enough, so that they are 'mostly' in the $|\downarrow\downarrow\rangle$ state when $A = 0$ and $J = 0$. Hence, the execution of a swap gate, involves the transformation of the state $|\downarrow\downarrow 10\rangle$ to the state $|\downarrow\downarrow 01\rangle$. These states belong to a 4×4 eigenspace, \mathcal{E}_s , of the hamiltonian \mathbf{H} independent of A and J . We can focus our attention on the appropriate 4 sub-matrix of the hamiltonian. Denote it by $\mathbf{H}_s(A, J)$. In the basis $\{|\uparrow\downarrow 00\rangle, |\downarrow\uparrow 00\rangle, |\downarrow\downarrow 10\rangle, |\downarrow\downarrow 01\rangle\}$, $\mathbf{H}_s(A, J)$ can be written as,

$$\mathbf{H}_s(A, J) = \begin{bmatrix} -\omega_n - J & 2J & 2A & 0 \\ 2J & -\omega_n - J & 0 & 2A \\ 2A & 0 & -\omega_e + J & 0 \\ 0 & 2A & 0 & -\omega_e + J \end{bmatrix} \quad (2.2)$$

For given values of A and J denote the eigenvectors and eigenvalues of the sub-matrix by:

$$\begin{aligned} |n_+(A, J)\rangle &: \lambda_{n_+}(A, J) \\ |ne_-(A, J)\rangle &: \lambda_{ne_-}(A, J) \\ |en_-(A, J)\rangle &: \lambda_{en_-}(A, J) \\ |e_+(A, J)\rangle &: \lambda_{e_+}(A, J) \end{aligned} \quad (2.3)$$

where, the eigenstates and eigenvalues are 'smooth' functions of A, J . The use of such a 'complicated' notation will be explained shortly.

2.3.1 Qualitative Analysis of Eigenspace \mathcal{E}_f

We will first attempt to qualitatively understand the nature of the eigenvectors and eigenvalues of $\mathbf{H}(A, J)$. Consider first an initial Hamiltonian of the system of two electrons and two nuclei, obtained by setting $A = 0$ in Eq.(2.1).

$$\therefore \mathbf{H}(0, J) = \begin{cases} \frac{1}{2}\omega_n\sigma_z^{n_1} & + \frac{1}{2}\omega_e\sigma_z^{e_1} \\ & + J\vec{\sigma}_1\vec{\sigma}_2 \\ +\frac{1}{2}\omega_n\sigma_z^{n_2} & + \frac{1}{2}\omega_e\sigma_z^{e_2} \end{cases} \quad (2.4)$$

In this case, there is no coupling between nuclear and electron spins. The eigenvectors of the entire 16×16 Hamiltonian are easily obtained. In particular, eigenvectors of the 4×4 sub-matrix $\mathbf{H}_s(0, J)$ are given by:

$$\begin{aligned} |n_+(0, j)\rangle &= |\downarrow\downarrow\rangle \otimes |10 + 01\rangle \\ |ne_-(0, j)\rangle &= |\downarrow\downarrow\rangle \otimes |10 - 01\rangle \\ |en_-(0, j)\rangle &= |\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle \\ |e_+(0, j)\rangle &= |\uparrow\downarrow + \downarrow\uparrow\rangle \otimes |00\rangle \end{aligned} \quad (2.5)$$

The eigenvalues of these states are

$$\lambda_{n_+(0,J)} = -\omega_e + J \quad (2.6)$$

$$\lambda_{ne_-(0,J)} = -\omega_e + J \quad (2.7)$$

$$\lambda_{en_-(0,J)} = -\omega_n - 3J \quad (2.8)$$

$$\lambda_{e_+(0,J)} = -\omega_n + J \quad (2.9)$$

We are now in a position to explain the notation in Eq.(2.3). Subscripts '+' or '-' denote states which form a symmetric or antisymmetric superposition of spin states respectively, when $A = J = 0$. The first letter denotes whether the nuclei or the electrons are in such that particular superposition. The presence of a second letter for the 2nd and 3rd eigenstates will be explained shortly.

Since the eigenstates of $\mathbf{H}_s(A, J)$ given by Eq.(2.3) are 'smooth' functions of A and J , the adiabatic theorem states that the initial eigenstates of $\mathbf{H}_s(0, J)$, given by Eq.(2.5), will evolve into the eigenstates given by eq.(2.3) as A, J are varied adiabatically. A quick note should be made at this point regarding the uniqueness of the initial eigenstates of $\mathbf{H}_s(0, J)$. Since the states $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$ and $|\downarrow\downarrow\rangle \otimes |10 + 01\rangle$ are degenerate, any linear combination is also an eigenstate of $\mathbf{H}_s(0, J)$ and hence a potential candidate for $|n_+(0, j)\rangle$ and $|ne_-(0, j)\rangle$ (of course we would have to change notation then). However, if for some value of A and J , $\lambda_{n_+}(A, J) \neq \lambda_{ne_-}(A, J)$, an arbitrary linear combination will not be able to satisfy the 'smoothness' condition of the eigenvectors. Hence it is important to pick the 'right' eigenvectors for $|n_+(0, j)\rangle$ and $|ne_-(0, j)\rangle$ from the two dimensional eigensubspace spanned by $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$ and $|\downarrow\downarrow\rangle \otimes |10 + 01\rangle$. Though we have not rigorously proved it yet, eq.(2.5) is the right choice.

The above eigenvectors are independent of J . Their eigenvalues, however, do depend on J and are plotted in fig.(2.3.1).

For the sake of clarity, the eigenvalues of the degenerate states $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$ and $|\downarrow\downarrow\rangle \otimes |10 + 01\rangle$ have been slightly displaced with respect to each other in the diagram. As the value of A is increased adiabatically, the terms $A\sigma^{\vec{n}_1}\sigma^{\vec{e}_1}$ and $A\sigma^{\vec{n}_2}\sigma^{\vec{e}_2}$ are introduced in the hamiltonian. Considering the following equation,

$$\sigma^{\vec{n}}\sigma^{\vec{e}} = 2\sigma_+^e\sigma_-^n + 2\sigma_-^e\sigma_+^n + \sigma_z^e\sigma_z^n$$

where,

$$\sigma_+ = \sigma_x + i\sigma_y$$

$$\sigma_- = \sigma_x - i\sigma_y$$

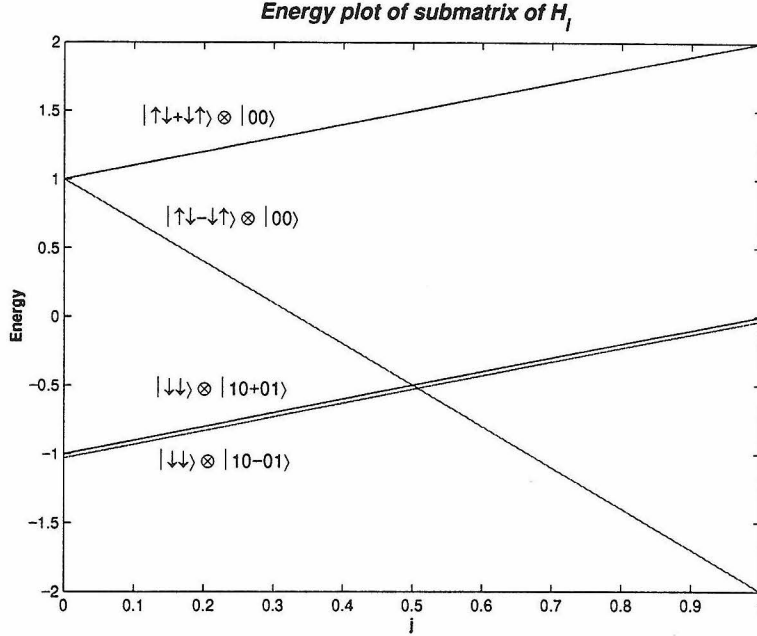


Figure 2.1: Energy Spectrum of \mathcal{E}_f with $A = 0$

The terms $A\sigma^{\vec{n}_1}\sigma^{\vec{e}_1}$ and $A\sigma^{\vec{n}_2}\sigma^{\vec{e}_2}$ couple states in which electron and nuclear spin states have been exchanged. Now we see the advantage of writing the eigenvectors of $\mathbf{H}_s(0, J)$ as $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$ and $|\downarrow\downarrow\rangle \otimes |10 + 01\rangle$ since they couple to the states $|\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle$ and $|\uparrow\downarrow + \downarrow\uparrow\rangle \otimes |00\rangle$ respectively. From Fig.(2.3.1) the states of the same color couple together to form new orthogonal states which are eigenstates of $\mathbf{H}_s(A, J)$.

For the states $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$ and $|\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle$ eigenvalues of the unperturbed hamiltonian ($A = 0$) cross at $2 * J = \frac{\omega_e - \omega_n}{2}$. Hence in the presence of coupling, these levels anti cross each other. Also the relative mixing of the two states changes as J changes due to the J dependence in their unperturbed eigenvalue difference. That is to say that the eigenkets $|ne_-(A, J)\rangle$ and $|en_-(A, J)\rangle$ are J dependent. For small values of A and far below the point of anti-crossing, $|ne_-(A, J)\rangle$ and $|en_-(A, J)\rangle$ are 'mostly' in the states $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$ and $|\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle$. (Hence our notation is still justified). As we go beyond the point of anti-crossing, the eigenket $|ne_-(A, J)\rangle$ flops into the state 'mostly' $|\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle$, while the eigenket $|en_-(A, J)\rangle$ flops into the state 'mostly' $|\downarrow\downarrow\rangle \otimes |10 - 01\rangle$. This explains the presence of the second letter in our notation.

However, for the states $|\downarrow\downarrow\rangle \otimes |10 + 01\rangle$ and $|\uparrow\downarrow + \downarrow\uparrow\rangle \otimes |00\rangle$, the difference in unperturbed ($A = 0$) eigenvalues is independent of J . Hence the

eigenvectors $|n_+(A, J)\rangle$ and $|e_+(A, J)\rangle$ are also independent of J . It is noteworthy that as a result of this property, these two eigenkets are invulnerable to 'damage' due to non-adiabatic variations in J .

2.3.2 Quantitative Analysis of \mathcal{E}_f

From the qualitative understanding obtained above, we write the hamiltonian $\mathbf{H}_s(A, J)$ in the basis $\left\{ \frac{|\uparrow\downarrow+\downarrow\uparrow\rangle\otimes|00\rangle}{\sqrt{2}}, \frac{|\uparrow\downarrow-\downarrow\uparrow\rangle\otimes|00\rangle}{\sqrt{2}}, \frac{|\downarrow\downarrow\rangle\otimes|10-01\rangle}{\sqrt{2}}, \frac{|\downarrow\downarrow\rangle\otimes|10+01\rangle}{\sqrt{2}} \right\}$

In this basis, the hamiltonian can be written as:

$$\mathbf{H}_s(A, J) = \begin{bmatrix} -\omega_n + J & 0 & 0 & 2A \\ 0 & -\omega_n - 3J & 2A & 0 \\ 0 & 2A & -\omega_e + J & 0 \\ 2A & 0 & 0 & -\omega_e + J \end{bmatrix} \quad (2.10)$$

It is now trivial to diagonalize this submatrix and obtain the exact eigenvectors and eigenvalues.

The 4 eigenvectors of the above system are given by

$$|n_+(A, J)\rangle = \cos \frac{\theta_+}{2} |\downarrow\downarrow\rangle \otimes |10 + 01\rangle - \sin \frac{\theta_+}{2} |\uparrow\downarrow + \downarrow\uparrow\rangle \otimes |00\rangle \quad (2.11)$$

$$|ne_-(A, J)\rangle = \cos \frac{\theta_-}{2} |\downarrow\downarrow\rangle \otimes |10 - 01\rangle - \sin \frac{\theta_-}{2} |\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle \quad (2.12)$$

$$|en_-(A, J)\rangle = \sin \frac{\theta_-}{2} |\downarrow\downarrow\rangle \otimes |10 - 01\rangle + \cos \frac{\theta_-}{2} |\uparrow\downarrow - \downarrow\uparrow\rangle \otimes |00\rangle \quad (2.13)$$

$$|e_+(A, J)\rangle = \cos \frac{\theta_+}{2} |\downarrow\downarrow\rangle \otimes |10 + 01\rangle + \sin \frac{\theta_+}{2} |\uparrow\downarrow + \downarrow\uparrow\rangle \otimes |00\rangle \quad (2.14)$$

where,

$$\theta_+(A) = \arctan \frac{2A}{\omega_e - \omega_n} \quad (2.15)$$

$$\theta_-(A, J) = \arctan \frac{2A}{\omega_e - \omega_n - 4J} \quad (2.16)$$

$$0 \leq \theta_+, \theta_- < \pi$$

As expected, θ_+ is a function of A alone.

The corresponding eigenvalues are given by

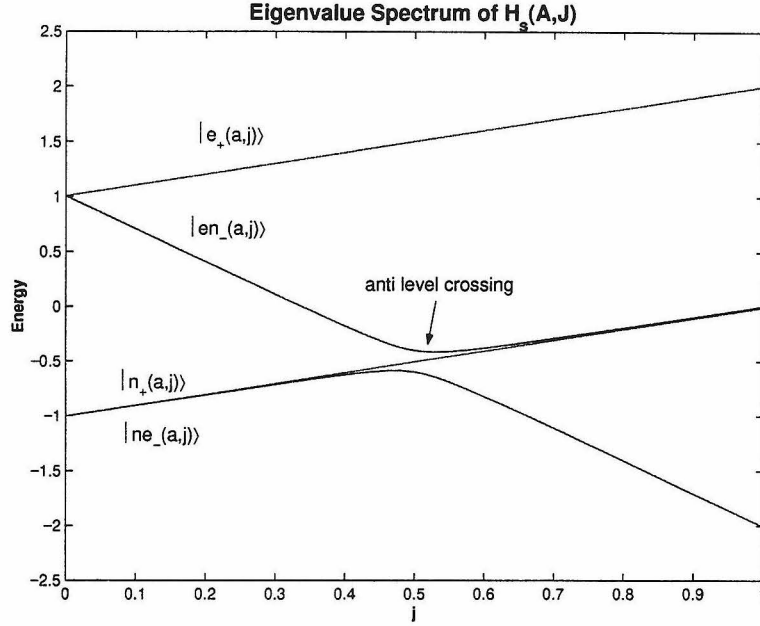


Figure 2.2: Energy Spectrum for \mathcal{E}_f with $A \neq 0$

$$\begin{aligned}\lambda_{n_+(A, J)} &= -\left(\frac{\omega_e + \omega_n}{2}\right) + J - \sqrt{\left(\frac{\omega_e - \omega_n}{2}\right)^2 + (2A)^2} \\ \lambda_{ne_-(A, J)} &= -\left(\frac{\omega_e + \omega_n}{2}\right) - J - \sqrt{\left(\left(\frac{\omega_e - \omega_n}{2}\right) - 2J\right)^2 + (2A)^2} \\ \lambda_{en_-(A, J)} &= -\left(\frac{\omega_e + \omega_n}{2}\right) - J + \sqrt{\left(\left(\frac{\omega_e - \omega_n}{2}\right) - 2J\right)^2 + (2A)^2} \\ \lambda_{e_+(A, J)} &= -\left(\frac{\omega_e + \omega_n}{2}\right) + J + \sqrt{\left(\frac{\omega_e - \omega_n}{2}\right)^2 + (2A)^2}\end{aligned}$$

It is easy to see that the eigenkets and eigenvalues satisfy the 'smoothness' condition and eq(2.5). Fig(2.3.2) is an energy spectrum of the eigenkets as a function of J . A fixed small value of A has been chosen to show the various features talked of qualitatively early.

2.3.3 Ideal Swap Gate

As stated before, the quantum state of the system starts out as $|\downarrow\downarrow 10\rangle$. We propose to adiabatically turn on and then off the *values* (something different might need to be done with the physical voltage gates that determine the values) of A, J so as to swap nuclear states. Thus after a time τ , we would ideally like to have evolved to the quantum state $|\downarrow\downarrow 01\rangle$. We will work within the adiabatic approximation and hence ignore the error due to the finiteness of τ . Let,

$$\phi_{n_+}(t) = \int_0^t \lambda_{n_+}(A(t), J(t)) dt \quad (2.17)$$

$$\phi_{ne_-}(t) = \int_0^t \lambda_{ne_-}(A(t), J(t)) dt \quad (2.18)$$

$$\phi_{en_-}(t) = \int_0^t \lambda_{en_-}(A(t), J(t)) dt \quad (2.19)$$

$$\phi_{e_+}(t) = \int_0^t \lambda_{e_+}(A(t), J(t)) dt \quad (2.20)$$

Let, τ be such that

$$\phi_{n_+}(\tau) - \phi_{ne_-}(\tau) = \pi \quad (2.21)$$

Since, $\lambda_{n_+}(A(t), J(t))$ and $\lambda_{ne_-}(A(t), J(t))$ are finite functions, this is always possible. Let $U(t, 0)$ be the evolutionary operator for the execution of the gate. Hence by the adiabatic theorem,

$$U(t, 0) |n_+\rangle(0, 0) = e^{\phi_{n_+}(t)} |n_+(A(t), J(t))\rangle \quad (2.22)$$

$$U(t, 0) |n_+\rangle(0, 0) = e^{\phi_{n_+}(t)} |n_+(A(t), J(t))\rangle \quad (2.23)$$

$$U(t, 0) |n_+\rangle(0, 0) = e^{\phi_{n_+}(t)} |n_+(A(t), J(t))\rangle \quad (2.24)$$

$$U(t, 0) |n_+\rangle(0, 0) = e^{\phi_{n_+}(t)} |n_+(A(t), J(t))\rangle \quad (2.25)$$

As, required, let the state of the system at a time t be $\psi(t)$. \therefore as per our initial conditions,

$$\psi(0) = |\downarrow\downarrow 10\rangle \quad (2.26)$$

Thus, we have

$$\begin{aligned}
\psi(\tau) &= U(\tau, 0)\psi(0) \\
&= U(\tau, 0) |\downarrow\downarrow 10\rangle \\
&= U(\tau, 0) \left(\frac{|\downarrow\downarrow\rangle \otimes |10 + 01\rangle}{2} + \frac{|\downarrow\downarrow\rangle \otimes |10 - 01\rangle}{2} \right) \\
&= U(\tau, 0) \left(\frac{|n_+(0, 0)\rangle}{\sqrt{2}} + \frac{|ne_-(0, 0)\rangle}{\sqrt{2}} \right)
\end{aligned}$$

Using Eq.(2.22) for the evolution of the quantum system,

$$\begin{aligned}
\psi(\tau) &= \frac{1}{\sqrt{2}} \{ e^{i\phi_{n_+}(\tau)} |n_+(A(\tau), J(\tau))\rangle e^{i\phi_{ne_-}(\tau)} |ne_-(A(\tau), J(\tau))\rangle \} \\
&= \frac{1}{\sqrt{2}} \{ e^{i\phi_{n_+}(\tau)} |n_+(0, 0)\rangle + e^{i\phi_{ne_-}(\tau)} |ne_-(0, 0)\rangle \} \\
&= \frac{e^{i\phi_{n_+}(\tau)}}{\sqrt{2}} \{ |n_+(0, 0)\rangle + e^{i\phi_{ne_-}(\tau) - \phi_{n_+}(\tau)} |ne_-(0, 0)\rangle \} \\
&= \frac{1}{\sqrt{2}} \{ |n_+(0, 0)\rangle + e^{i\phi_{ne_-}(\tau) - \phi_{n_+}(\tau)} |ne_-(0, 0)\rangle \} \\
&= \frac{1}{\sqrt{2}} \{ |n_+(0, 0)\rangle + e^{-i\pi} |ne_-(0, 0)\rangle \} \\
&= \frac{1}{\sqrt{2}} \{ |n_+(0, 0)\rangle - |ne_-(0, 0)\rangle \} \\
&= \frac{|\downarrow\downarrow\rangle \otimes |10 + 01\rangle}{2} - \frac{|\downarrow\downarrow\rangle \otimes |10 - 01\rangle}{2} \\
&= |\downarrow\downarrow 01\rangle
\end{aligned}$$

We have carried out the above calculation, within the limit of the adiabatic approximation. Clearly, there is an error due to the finite size of τ . It would be worthwhile to study the appropriate way in which to change A, J in order to minimize this error given a fixed execution time τ .

Another source of error in the above idealized gate analysis is decoherence. In general, nuclear spins are very robust to spin decoherence, while electron spins are comparatively far more vulnerable. This was the essential motivation behind using the nuclear spins as qubits. However, the electrons do participate in the gate and the effect of electron decoherence might be the limiting factor in this scheme for computation. We shall now study the effect of decoherence on the fidelity of the swap gate.

Chapter 3

Decoherence

Decoherence is the biggest hurdle in the way of building a working model of a quantum computer. It is a daunting task to sufficiently isolate the quantum computer from the environment in order to carry out coherent calculations on qubits. The merits of any quantum computer are in its ability to perform many computations within the time scales of decoherence. We will first define the concept of decoherence and then consider its effects on the swap gate described in the earlier chapter.

3.1 What is decoherence?

A quantum system is generally in a superposition of its base states. Let us consider a quantum register of L qubits as our quantum system. Let

$$|\Psi(t)\rangle = \sum_{i=0}^{2^L-1} a_i(t) |i\rangle \quad (3.1)$$

be the general state of the register. Here i , in its binary decomposition, represents a base state in the 2^L dimensional Hilbert Space of the register. The value of the k^{th} binary digit of i denotes the state of the k^{th} qubit of the register. The density matrix of any quantum state $|\Psi(t)\rangle$ is an operator given by $\rho(t) = |\Psi(t)\rangle \langle\Psi(t)|$ and can be represented as,

$$(\rho(t)) = \sum_{i,j=0}^{2^L-1} a_i(t) a_j^*(t) |i\rangle \langle j| \quad (3.2)$$

or in matrix notation as,

$$\rho = \begin{pmatrix} a_1 a_1^* & a_1 a_2^* & \dots & a_1 a_j^* & \dots \\ a_2 a_1^* & a_2 a_2^* & \dots & a_2 a_j^* & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots \\ a_i a_1^* & a_i a_2^* & \dots & a_i a_j^* & \dots \\ \vdots & \vdots & \ddots & \vdots & \ddots \end{pmatrix}$$

The off-diagonal elements are the coherence terms, while the diagonal elements are called populations. The coherence terms quantify the degree of the interference and entanglement of the quantum system. In general, interactions with the environment cause these terms to decay. As a result, the quantum system essentially ends up as a probabilistic mixture of its base states. All entanglement and superposition is destroyed. This phenomenon is called decoherence. In the case of a quantum computer, decoherence essentially limits the power of the computer to that of a classical one. In the next section we will specifically talk about decoherence for a single qubit interacting with an environmental heat bath. The example is analytically solvable and gives a good idea of the mechanisms of decoherence.

3.2 Decoherence in a Single Qubit

This model of decoherence was analyzed by Palma, Ekert, Souminen[10] for a single qubit. Consider a qubit interacting with a heat bath in thermal equilibrium at temperature T . The initial density matrix of the system, i.e. density matrix of qubit + environment, is assumed to be in a product state.

$$\varrho(0) = \rho(0) \otimes \prod_{\mathbf{k}} R_{\mathbf{k}T} \quad (3.3)$$

Here $R_{\mathbf{k}T}$ is the usual thermal density matrix of the $\vec{\mathbf{k}}$ mode of the field. The summation is carried out over discrete field modes and will be later on extended to the case of continuum of field modes.

The Hamiltonian of interaction between environment and qubit is equivalent to the one introduced by Unruh[11],

$$\mathbf{H} = \frac{1}{2} \sigma_z \omega + \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \nu_{\mathbf{k}} + \sum_{\mathbf{k}} \sigma_z (g_{\mathbf{k}} a_{\mathbf{k}}^\dagger + g_{\mathbf{k}}^* a_{\mathbf{k}}) \quad (3.4)$$

where the $a_{\mathbf{k}}^\dagger$ and the $a_{\mathbf{k}}$ operators stand for the annihilation and creation operators of the $\vec{\mathbf{k}}$ mode of the field. The Hamiltonian above has the particular advantage of being exactly solvable, thus allowing us to study and

understand in detail the mechanism of decoherence of a single qubit. One must note that this Hamiltonian allows for no energy exchange between the environment and the qubit. As a result, the populations of the reduced density matrix of the qubit remain unchanged in time. This is not a serious defect in the model as the populations decay on a far slower time scale than the coherence terms and can be treated as constant to a good approximation.

On calculating the evolution operator in the interaction picture, one sees that it causes entanglement to occur between the qubit and the environment, though we started off initially with product states. As time proceeds, the overlap between the different field states, with which the qubit becomes entangled, decreases. Since the off-diagonal elements in the reduced density matrix are proportional to this overlap, they decay in time. One can rigorously calculate the above terms to show the diminishing value of the off-diagonal elements in the reduced density matrix of the qubit.

Let $\rho(t)$ denote the reduced density matrix of the qubit at a time t , where

$$\rho_{ij}(t) = \langle i | Tr_E \varrho(t) | j \rangle \quad (3.5)$$

Here Tr_E denotes the trace over the environment of the density matrix of whole system (qubit + environment) - $\varrho(t)$. The above considerations then give us $\rho_{11}(t) = \rho_{11}(0)$ and $\rho_{00}(t) = \rho_{00}(0)$, i.e. the populations do not change over time. Also, for the coherence terms we get,

$$\rho_{10}(t) = e^{-\Gamma(t)} \rho_{10}(0). \quad (3.6)$$

$\Gamma(t)$ can be evaluated as (putting Boltzmann constant k_B as unity and transforming to a continuum of field modes),

$$\begin{aligned} \Gamma(t) &\propto \int d\mathbf{k} |g_{\mathbf{k}}|^2 \coth \frac{\nu_{\mathbf{k}}}{2T} \frac{1 - \cos \nu_{\mathbf{k}} t}{\nu_{\mathbf{k}}^2} \\ &\propto \int d\nu \frac{dk}{d\nu} G(\nu) |g(\nu)|^2 (1 + 2\langle n(\nu) \rangle_T) \frac{1 - \cos \nu t}{\nu^2} \end{aligned} \quad (3.7)$$

where $G(\nu)$ is the density of modes at a frequency ν , $\langle n(\nu) \rangle_T = e^{-\frac{\nu}{2T}} \csc \frac{\nu}{2T}$ is the average number of field excitations at temperature T and $\frac{dk}{d\nu}$ is the dispersion relation.

We note at this point, that $G(\nu)|g(\nu)|^2$ is in general characterized by a cutoff frequency which depends on the particular problem at hand. For example, if the environment is a phonon bath, the cutoff frequency could be the Debye frequency. Hence, depending on the no. of dimensions of our field and the cutoff frequency, we can model $G(\nu)|g(\nu)|^2 \propto \nu^n e^{-\frac{\nu}{\nu_c}}$ where n depends on the dimension of the field and ν_c is the cutoff frequency.

From Eq.3.7, we can thus identify three time regimes over which the characteristics of the decoherence varies:

- quite regime for $t < \nu_c^{-1}$, where decoherence essentially does not take place
- a quantum regime, for $\nu_c^{-1} < t < T^{-1}$, where the main cause of decoherence is the quantum fluctuations of the vacuum state of the field modes
- a thermal regime, for $t > T^{-1}$, where thermal fluctuations are responsible for the loss of coherence

Explicit formulae for the value of $\Gamma(t)$ can be evaluated for the case of one dimension and three dimensions for all three of the above regimes.

3.3 Master Equation

It is often possible to describe the evolution of a density matrix, at least to a good approximation, by a differential equation. This equation, the master equation will be our next topic. It is not obvious that it is possible to describe the evolution of a density matrix by means of a single differential equation. As a matter of fact, this is only possible if the quantum system is 'Markovian', or in other words, local in time. In the case that our quantum system is not closed, there is an exchange of information between system and environment. This is called an open system. An open system is dissipative because information can flow from the system to the reservoir. But that means that information can also flow back from reservoir to system, resulting in non-Markovian fluctuations of the system, i.e. fluctuations which depend on the state of the system at an earlier time. Except in the case of coherent unitary evolution, these fluctuations are unavoidable and an exact Markovian description of quantum dynamics is impossible. Yet in many contexts, it is possible to say that the correlation time of the fluctuations are much smaller than the time scale of the evolution that we want to follow. Thus the reservoir 'forgets' the state of the system within a time short enough so as to not bother our 'coarse' evolution of the system. In this realm it is possible to use the Markovian approximation and hence a master equation approach to open system. We will use this approach to analyze decoherence in Kane's quantum computer.

3.4 Decoherence in Kane's Binary Gate

Kane's quantum computer uses the robust nuclear spins for information storage and computation. However, conditional dynamics between the gates is mediated by electron spins, which are highly susceptible to dephasing due to environmental interactions. We believe that this electron mediated coupling will be the Achilles' heel of the computer. We would thus like to study the evolution of the system allowing for electron spin interactions with the environment as in section(3.2). However, we do not care about the exact nature of environment electron interaction (except that it causes dephasing). Hence, we will assume that our system is Markovian and resort to the master equation approach as outlined in *An Open Systems Approach to Quantum Optics* by Howard Carmichael.

Let the density matrix for two qubit system at a time t be given by $\rho(t)$. The master equation determining the evolution of this density matrix for pure dephasing of electrons is given by

$$\dot{\rho} = -i(\mathbf{H}(t), \rho(t)) - \gamma_1 (\rho(t) - \sigma_z^{e1} \rho(t) \sigma_z^{e1}) - \gamma_2 (\rho(t) - \sigma_z^{e2} \rho(t) \sigma_z^{e2}) \quad (3.8)$$

Here $\mathbf{H}(t)$ is determined by the values of A, J at the time t .

As before we want to focus on the particular eigenspace of \mathbf{H} containing the states $|10\rangle$ and $|01\rangle$. σ_z^{e1} and σ_z^{e2} also maintain the structure of the eigenspaces of \mathbf{H} , i.e. they do not contain terms that mix the different eigensubspaces of the hamiltonian. As a result, if we were to start out our density matrix within the relevant subspace, Eq.(3.8) would ensure that it stays within this subspace. Hence it makes sense to talk of a master equation for only the subspace we are interested in, namely the eigenspace space given by $\mathcal{E}_s = \{|\downarrow\downarrow 10\rangle, |\downarrow\downarrow 01\rangle, |\uparrow\downarrow 00\rangle, |\downarrow\uparrow 00\rangle\}$. Let, $\rho_s(t)$ be the density matrix of \mathcal{E}_s at a time t . Let H_s be as defined by Eq.(2.2). Let σ_z^{e2} and σ_z^{e1} be the restrictions acting on the appropriate subspace. Thus the master equation can be written as

$$\dot{\rho}_s = -i(\mathbf{H}_s(t), \rho_s(t)) - \gamma_1 (\rho_s(t) - \sigma_z^{e1} \rho_s(t) \sigma_z^{e1}) - \gamma_2 (\rho_s(t) - \sigma_z^{e2} \rho_s(t) \sigma_z^{e2}) \quad (3.9)$$

It is not easy to obtain an analytical solution of this equation even for the simplified initial conditions of Eq.(2.26). We thus resort to a numerical simulation. In addition, we would like to focus on the decoherence aspect of the error. Hence we assume perfect adiabaticity. We thus turn on A, J to a specified value in a time short enough to ignore the phase collected by the

eigenvectors and decoherence effects. Since we assume perfect adiabaticity, the speed with which we do this does not matter. We then leave A, J at the specified values and allow the quantum system to evolve to collect the necessary phase difference of π as per Eq.(2.21), the ideal gating time. (Note that for different values of A, J the time required to collect the phase π is different and hence the system is exposed to decoherence for different times.) During this period we numerical simulate the evolution of the system using the master equation (3.9). We then calculate the fidelity of the resulting density operator compared to the ideal quantum state of the system in the absence of decoherence. A plot of fidelity for different values of A, J will give us an idea of the feasibility of the quantum computer.

The ideal state of the system is given by

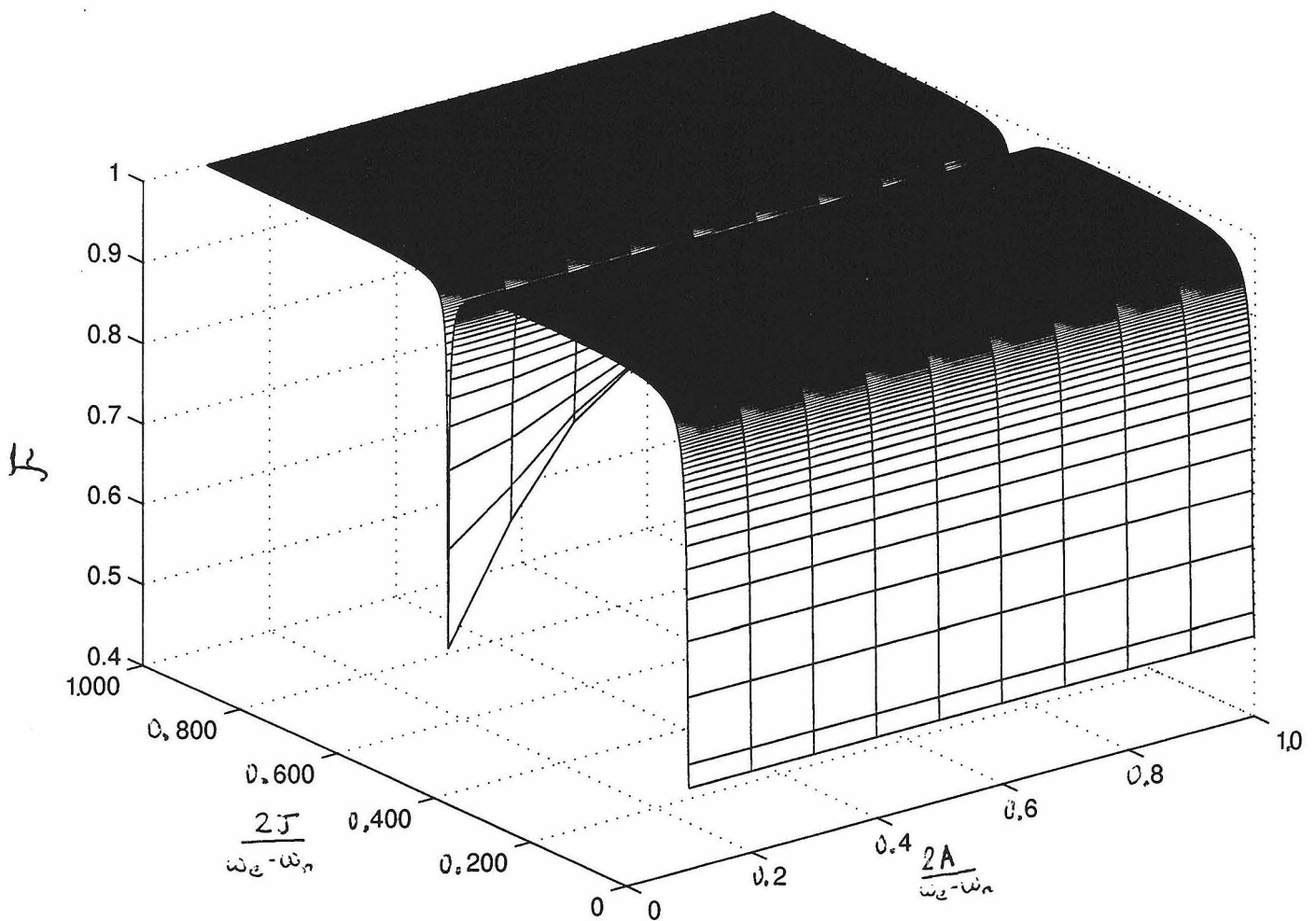
$$|\psi(\tau)\rangle = |n_+(A, J) - |ne_-(A, J)\rangle \quad (3.10)$$

Thus the fidelity of the density operator is defined by,

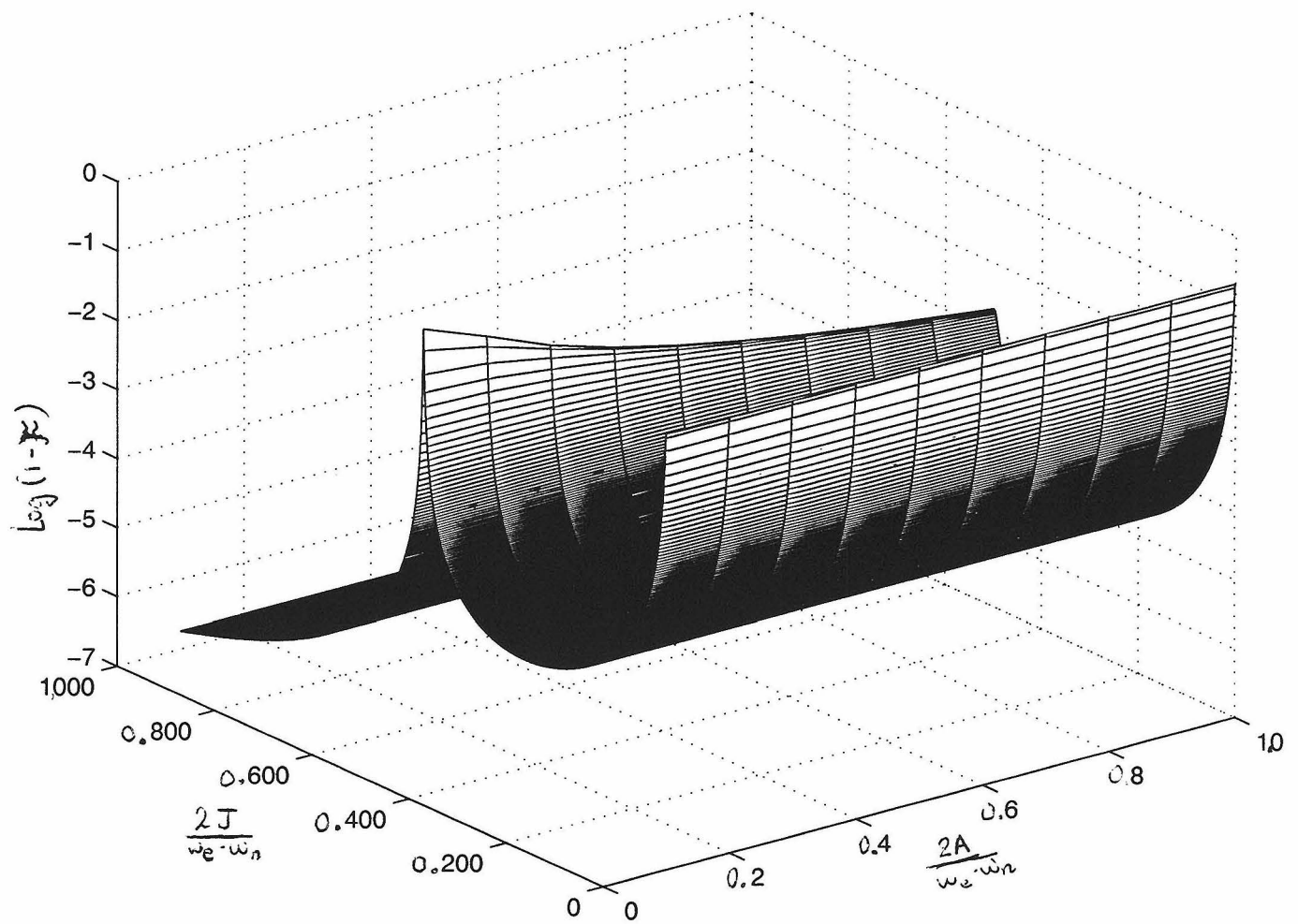
$$\mathcal{F} = \langle \psi(\tau) | \rho_s(\tau) | \psi(\tau) \rangle \quad (3.11)$$

The plot on the following page shows \mathcal{F} for different values of A, J . A plot of $\log(1 - \mathcal{F})$ is also included to better view the features. It can be seen that the fidelity improves for larger values of A, J . However, for values of J larger than $\frac{\omega_e - \omega_n}{4}$ it is necessary to cross the level crossing and the decoherence at this point is very large. The adiabatic approximation will also be important in crossing this point as the difference in energy levels is particularly small. Thus it becomes important to cross the level crossing slowly to minimize adiabatic damage, and yet fast enough to minimize damage due to decoherence.

Fidelity of Kane's Two Qubit Gate



PLOT OF $\log(1 - F(A, J))$



Chapter 4

Results, Conclusions and Acknowledgements

4.1 Conclusions

One of the salient points of Kane's quantum computer was the use of robust nuclear spins to store information, but the use of fast electrons to do the binary gate. It was hoped that in this process we would gain on decoherence time scales but be able to do the gate longer. However, from our numerical simulation, the fidelity of the binary gate improves as we increase the values of A and J . By increasing these values, we are flopping more and more into the electron states from the nuclear states. In other words, though possible decoherence is high for a model using the electron spins as qubits, the swap gate can be carried out fast enough to improve on decoherence as compared to Kane's computer. However, this result should not be taken too seriously. After all, the robustness of the nuclear spins wins over electron spins specially while **storing** information is concerned, which is not tested while calculating the fidelity of the swap gate. Thought a model using electron spins won out as far as swap gate fidelity was concerned, Kane's computer might still outperform in a quantum circuit which takes place over a long enough time period. Learning from the experience that fidelity of the swap gate improves the more we are in the nuclear states, it might be instructive to cross the level crossing and completely swap over to electron states in order to do the gate. However, as noted earlier, the point of level crossing seems to be a troublesome feature, not just from decoherence point of view, but also from adiabaticity. Hence this might not be a valid option. Lastly, it seems unlikely that Kane's model can be scaled up to the size envisaged by Preskill in its present stage. However, building a small prototype might allow us to perform

maybe it can
be pulled out
of the figures

24

In verbal report a numerical
figure of error accumulation,
0.02, was given which I
don't find in this manuscript.

If it is far above Preskill's

small calculations on a few qubits.

4.2 Future Considerations

We have studied only one particular model for decoherence in Kane's computer. There are even other sources of error besides decoherence. Adiabaticity is one such source. In order to obtain a phase difference of Π there are many ways to vary the values of A and J over time. The existence of a particular 'path' in (A, J) space which minimizes the error due to non-adiabaticity is quite plausible. The fidelity calculations done above as A, J are varied along this path would give a good upper bound to the fidelity of the swap gate. Other sources of error like those due to noise in the Voltage gates, etc. can also be studied.

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← Same
as (12)!

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