Quantum entanglement, initialization and readout of nuclear spin qubits with an electric current

by

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B.Sc., University of Western Ontario, 2009

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ABSTRACT

The ability to control the evolution of quantum systems would open the door to a new world of information processing. Nuclear spin qubits in the solid state offer the longest coherence times, of the order of a few seconds, however their initialization, readout and coupling are yet to be demonstrated. This thesis addresses the physical manipulation of nuclear spin qubits with a classical electric current. Our main result is the development of a mechanism that provides high contrast initialization and readout of nuclear spin qubits using their interaction with conduction electrons.

However, we also show that conduction electrons can not be used to entangle nuclear spin qubits without destroying the nuclear spin qubit coherence. We show

this by demonstrating that the quality factor of a Ruderman-Kittel-Kasuya-Yosida (RKKY) gate is always low for electron as well as nuclear spin qubits.

In conclusion, we establish the viability of a quantum computer architecture based on nuclear spins that relies on conduction electrons for quantum read-out and initialization. For coherent entanglement, we argue that the usual direct exchange interaction is still the best option.

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May g-d bless and keep you always, may your wishes all come true, may you always do for other and let others do for you, may you build a ladder to the stars and climb on every rung, may you stay forever young.

May you grow up to be righteous, may you grow up to be true, may you always know the truth and see the light surrounding you, may you always be courageous stand right and be strong and may you stay forever young.

May your hands be busy, may your feet always be swift, may you have a strong foundation when the winds change shift, may your heart always be joyful, may your song always be sung, may you stay forever young.

Bob Dylan

DEDICATION

This thesis is dedicated with love to my parents.

Chapter 1

Introduction

Expanding computational capability to the atomic scale requires the establishment of control in a quantum world. The evolution of quantum systems may be exceeding complex and impossible to predict do to a multitude of accessible outcomes. There exist very few systems for which a definite knowledge of their evolution is understood. The alignment of an electron or nuclear spin state with a globally applied magnetic field is one of these systems. The expectation value of this particle spin is a measurable magnetization that has only two stable configurations, aligned with or against the applied field. The nuclear spin state is intentionally chosen due to its extended coherence in a spin-less substrate. Specifically, a phosphorus donor's nuclear spin state in a silicon substrate may be coherent for many seconds.

This thesis will attempt to establish the requirements of realizable control of the nuclear spin states for the purpose of performing quantum computation. The hope is that this may be accomplished through interactions between the donors and an applied electric current. A two dimensional electron gas (2DEG) is exploited to conduct electrons over the donors to establish control through spin-spin interactions. A simple diagram of this design is presented here.

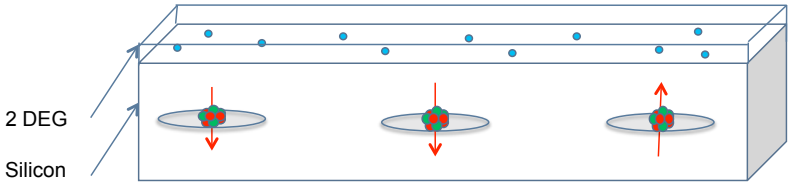


Figure 1.1: 2DEG current for quantum control

As a conduction electron encounters a donor, a spin dependent scattering process occurs, which may offer a means of sustainable control. Before beginning an exploration of how one might actually accomplish this goal it is important to determine what forms of control are required for quantum computation. Here is presented a brief introduction to the theory and terminology of quantum computing and its potential benefits.

1.1 Introduction to Quantum Computing

The power of quantum computation is based in the inherently random nature of the quantum scale world. There exists a dichotomy in quantum theory between an observed and unobserved system which asserts an unobserved system may simultaneously occupy many states. Only upon measurement a system is forced into one of the possible observable outcomes. This fundamental uncertainty does not allow the unobserved computational bits to be expressed in finite terms but rather they must be expressed in terms of a superposition of states. An understanding which leads many to refer to quantum bits simply as 'qubits' (a notation carried throughout the following work). At first glance this result would seem to limit computational abilities, as all information being stored is lost once one simply stops "looking". The implicit beauty of quantum computing is in its exploitation of this nature to not only perform operation but shape nature to its advantage. It turns out that it is in these suppositional states where quantum computers are most valuable as they can

simultaneously represent all outcomes of a specific computation. This is an effect from quantum physics where an experiment will travel down all possible paths, simultaneously, to reach a final result. The end process of measurement destroys this superposition of states and forces each qubit into only one of the allowed observable outcomes.

The consequence is that any computational algorithm does not need to proceed sequentially through all possible outcomes to pick out the desired result. All outcomes can be simultaneously accessible while the desired result may be selected out as the most likely measurement. This is true not only for individual qubits, an extensive array of qubits may be evolved into an entangled state. A state were the orientation of one qubit is essentially dependent on that of its neighbour. Entanglement provides a means of manipulating the evolution of many qubits. A quantum system, when unobserved, is represented as superposition of all allowed state vectors in Hilbert space. The result of observation then is dependent on the probability amplitude of each state, a dependence that is subject to manipulation. The system, progressed through unitary operation, can ensure the desired result acquires the highest probability amplitude, thus becomes the most likely measurement.

To perform computation any quantum computing architecture must have a technique to initialize an array of qubits with a known state, say

$$|010\ldots01> . \tag{1.1}$$

The qubits states may then be evolved with unitary operations to produce a superposition of states:

$$U_1U_2\ldots U_N|010\ldots01> \rightarrow \sum_n a_n|n> . \tag{1.2}$$

Here n is the label for the eigenstate and N the number of unitary operations. As

introduced above the superposition states, simultaneously, represent all possible arrangements of the qubits. An example is presented here for a three qubit array which is evolved into an entangled state, shown by an arrow. The result is a superposition state including all possible arrangements:

$$|010> \rightarrow \alpha_1|000> +\alpha_2|100> +\alpha_3|010> +\alpha_4|001> + \\ \alpha_5|110> +\alpha_6|011> +\alpha_7|101> +\alpha_8|111> . \tag{1.3}$$

The system may be evolved such that the state amplitude, $|a_n|^2$, for obtaining the desired result is optimized upon measurement:

$$\sum_n a_n|n> \rightarrow measurement \rightarrow |100\ldots01> . \tag{1.4}$$

This style of state evolution is at the heart of quantum computation. The theory and implementation of a quantum computer deals not only with the physical limitations of the quantum scale world but also with the difficulty of writing appropriate quantum algorithms. Classical gates have no familiar equivalent in the quantum world and their role must be played by state evolution subject to a Hamiltonian.

In quantum mechanics the time evolution of a state is given by the Schrödinger equation:

$$i\frac{d}{dt}|\Psi> = H(t)|\Psi> . \tag{1.5}$$

Or equivalently in terms of a linear combination of unitary operators:

$$|\Psi(t_2)> = U_1U_2\ldots U_N|\Psi(t_1)> . \tag{1.6}$$

Here t_2 is a time label that is set to be greater than t_1. This opens the door for novel approaches to computation, allowing for engineering of a linear series of unitary

gates or of the Hamiltonian itself. Quantum computation is a relatively new field but advances over the past few decades have been considerable. A short introduction to the progression of the ideas that have led to the state of quantum computing currently may serve to entice and give context to the architecture at the foundation of this thesis.

1.2 Quick History of Quantum Computing

In modern computing energy dissipation sets a upper limit to the number of operations allowed per unit time. Systems evolved by quantum operations naturally do not dissipate much energy due to the fact that reversibility is a crucial requirement of unitary operators in quantum mechanics, in order to preserve space and time reversal symmetry. This idea led Paul Benioff to first examine the possibilities of using quantum systems to perform operation[5]. Jointly Richard Feynman theorized that due to the inability of classical computing machines to reproduce quantum nature a computer governed by quantum mechanics may be the only means of modelling the quantum world[9]. He, at the same time, proposed the open question of wether a quantum computer may be more efficient at solving other open problems.

Though theoretical interest had been established is was not until David Deutsch first demonstrated the universal three qubit quantum gate, in 1989[8], that quantum computation was understood to be possible. Beyond expounding the possibility of computation on the quantum scale Deutsch began to develop the basic ideas required to exploit superposition. He showed that if classical gates could be replaced by unitary operations a functional quantum computer could in theory be built.

Widespread interest in quantum computing was firmly established in 1994 when Peter Shor, furthering initial work by Daniel Simon, created the first quantum al-

gorithm that could perform the factorization of large numbers. His algorithms for factorization and the discrete logarithm were significantly faster than their classical counterparts[22][24]. This discovery was of intrinsic value because factorization and the discrete logarithm serve as a key components for cryptographic algorithms in modern day transfer of sensitive information. This is solely due to the amount of time required for classical computing machines to perform factorization (or discrete logarithms). Shor showed that a computer governed by quantum mechanics, and the resulting superposition of states, would have the ability to factor large numbers in a time proportional to the length of the number squared, L^2, when compared to the exponential dependence, e^L, of classical computers this was a tremendous discovery.

Research began everywhere as groups started to tackle the seemingly insurmountable task of actually building a real quantum computer. The first simplification of the physical requirements came in 1995 when a collective effort of Adriano Barenco, Charles Bennett, Peter Shor et. al. demonstrated that the two qubit control-NOT gate along with single qubit rotations were sufficient to form a universal gate[4]. This is a considerably easier task then performing operation over a large array of qubits simultaneously.

The persistent concerns of error correction in quantum systems were finally put to rest by Peter Shor in 1995 [23]. He demonstrated that quantum computing is indeed possible with gate error, or information transport error, through programming specific types of redundancy.

The daunting task of physical implementation still had not yet begun to take shape. Over the course of the next few years a plethora of creative architectures were developed. The two most exciting of which were put forward in 1998, the first by a collaboration of Daniel Loss and David P. DiVincenzo[17] and the second by Bruce Kane[13].

The Loss-DiVincenzo proposal was formulated to make use of quantum dots as the functional qubits. Quantum dots are formed by subjecting a 2-Dimensional Electron Gas (2DEG) to electric fields, forming depletion zones which act to confine the electrons. Gates are then used to select the number of electrons allowed into each quantum dot, any odd number of electrons would form an uneven spin state. Ideally each quantum dot would contain one electron, forming a spin 1/2 system, a perfect implementation for the qubit.

The Kane architecture [13], based on similar foundation as that presented within the following work, relies on a donors' nuclear spin state physically situated within a silicon substrate to provide a realization of the qubit. Silicon offers an ideal substrate as it is used extensively in modern chip fabrication.

1.3 Quantum Bits (Qubits)

Quantum computing maintains the two state bit system of classical computing, presented however in a slightly novel way. The finite means by which one defines classical bits does not exist in the quantum world as superposition is one of the dominant features of quantum computation. The qubit state must be defined in terms of a superposition of states subject to normalization constraints:

$$|\Psi >= \alpha|0 > +\beta|1 > . \tag{1.7}$$

Mathematically the state is a complex vector in the two-dimensional Hilbert space, the states $|0>$ and $|1>$ form an orthogonal basis within this space. Upon measurement the system is forced into the state $|0>$ or $|1>$ where the probability of measurement is, respectively, $|\alpha|^2$ and $|\beta|^2$. The foundation of quantum computing lies in the manipulation of these probability amplitudes.

A more revealing representation of the qubit can be found by treating the state vector in the Bloch sphere. Where the qubit is defined in three dimensions with a length of 1, due to normalization, the two observable states are defined along the z axis, think of a nuclear spin aligned with or against a global field, as shown below [18].

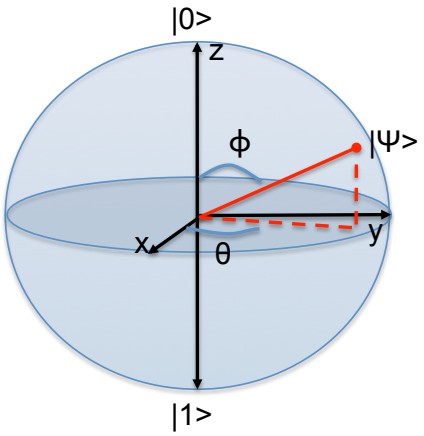


Figure 1.2: Qubit in Bloch Sphere

In this framework it is convenient to redefine the state-vector $|\Psi>$, now given by

$$|\Psi>= cos(\frac{\phi}{2})|0> +e^{i\theta}sin(\frac{\phi}{2})|1> . \tag{1.8}$$

This maintains the required normalization and offers a clear, semi-physical, view of the qubit state. When measured the system jumps into either observable state with a probability dependent on the projection of the vector $|\Psi>$ to the z axis. At all other times the qubit may take any orientation, which corresponds to any angle within the Bloch sphere. This could lead one to think that the qubit could potentially hold an infinite amount of information as there is a infinite number of possible orientations for the state vector. Measurement, however, destroys this superposition and though the state vector may take any position it may only be observed in two. A string of N qubits would then provide N individual pieces of measurable information while

providing a Hilbert space of 2^N dimensions.

1.4 Quantum Gates

The ability to perform selective rotations of the state-vectors within the Bloch sphere would allow for optimization of the probability for measuring a specific outcome. Selective rotations are the analogue of the gates familiar in classical computing as they provide a means by which manipulation of quantum information is possible. Single qubit rotations along with the two qubit control-NOT gate allow for truly universal computation. Any viable quantum computing architecture must posses the ability to perform these state evolutions.

The gates provide a means by which a state may be evolved to ensure that the required result of measurement will have the highest probability of occurrence. Though the final measurement only depends on which of the two possibilities is most likely all intermediate steps play a crucial role in determining the outcome. In this way quantum computing is essentially analogue in that it relies on a continuum of positions which must be exactly evolved to produce the desired outcome. The process of evolution in the quantum system demands unitary evolution operators to preserve the correct normalization and reversibility. One example of such a unitary operator, an interaction common to all proposals presented within this text, is the spin-spin exchange interaction.

1.4.1 Introduction to Exchange Interactions

The theoretical roots of the exchange interaction rest in symmetry arguments centred on type of particle under examination. The qubits, herein discussed, are fermions and fermion particles are described by completely anti-symmetric wavefunctions. This is

due to the fact that no two fermion particles can occupy the same quantum state, otherwise known as the Pauli exclusion principle. Therefore when two fermions interact their overall wave-function must change sign during simultaneous exchange of the the orbital and spin wave-functions. To better see how this results in the exchange interaction one must begin with the Schrödinger equation for an electron pair under the Coulomb potential,

$$H\Psi = (\frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + V(r_1, r_2))\Psi = E\Psi. \tag{1.9}$$

Where ∇ is the momentum operator, r_1 and r_2 are to position of electron 1 and 2 respectively. The spin components of the two-electron wavefunction Ψ can be decomposed into any of $|\uparrow\uparrow>$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow> - |\downarrow\uparrow>)$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow> + |\downarrow\uparrow>)$ and $|\downarrow\downarrow>$. In the presence of an applied magnetic field, in the z-direction, the electron spin will align with or against the applied field, the spin states will have definite total spin, S, and spin in the z-direction, S_z, shown here.

State	S	S_z
$\frac{1}{\sqrt{2}}(\|\uparrow\downarrow> - \|\downarrow\uparrow>)$	0	0
$\|\uparrow\uparrow>$	1	1
$\frac{1}{\sqrt{2}}(\|\uparrow\downarrow> + \|\downarrow\uparrow>)$	1	0
$\|\downarrow\downarrow>$	1	-1

Table 1.1: Two electron spin states

Again the Pauli exclusion principle dictates that the overall wavefunction must change sign under simultaneous exchange of spin and space co-ordinates. As the singlet spin state, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow> - |\downarrow\uparrow>)$, is antisymmetric under spin swap. It must be

paired thus with the symmetric spatial wavefunction. The opposite is true for the triplet spin states, $|\uparrow\uparrow>$, $\frac{1}{\sqrt{2}}(|\uparrow\downarrow> + |\downarrow\uparrow>)$, $|\downarrow\downarrow>$, which are symmetric under spin exchange and require a spatial dependence that is anti-symmetric. There is therefore a strict correlation between the spatial wave-function and the spin states.

What determines the physical orientation of the spins is the ground state energy, that is which energy state $E_{singlet}$ or $E_{triplet}$ is lowest. The Heitler-London approach relies of the difference between the two possible energies, $E_{singlet}$ - $E_{triplet}$, to categorize the "Exchange Interaction" between two spins[3]:

$$J_{exc} = E_s - E_t = \frac{<\Psi_s|H|\Psi_s>}{<\Psi_s|\Psi_s>} - \frac{<\Psi_t|H|\Psi_t>}{<\Psi_t|\Psi_t>}. \tag{1.10}$$

Werner Heisenberg established a convenient Hamiltonian for expressing the tendency of the spins states, for a two electron system, to align in preference to a singlet or triplet orientation. He was able to characterize the interaction in terms of the singlet-triplet energy splitting [3].

To begin it is important to note that the spin operator for the system can be expressed as

$$\hat{S}^2 = (\hat{S}_1 + \hat{S}_2)^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1 \cdot \hat{S}_2. \tag{1.11}$$

Each individual spin operator will satisfy $S_{1,2}^2|\Psi >= \frac{1}{2}(\frac{1}{2}+1)|\Psi >= \frac{3}{4}|\Psi >$ because the eigenvalue of the spin operator is $S(S+1)$. This then gives

$$(S_1 + S_2)^2 = \frac{3}{2} + 2S_1 \cdot S_2. \tag{1.12}$$

Note that the operator $S_1 \cdot S_2$ has an eigenvalue of $\frac{-3}{4}$ in the singlet case and $\frac{1}{4}$ in the triplet.

Consequently the Hamiltonian for the two spin system is given by

$$H_{exc} = \frac{1}{4}(E_s + 3E_t) - (E_s - E_t)S_1 \cdot S_2. \tag{1.13}$$

Redefining the zero energy mark, therefore omitting the $\frac{1}{4}(E_s + 3E_t)$ term gives the final form of the Heisenberg Hamiltonian:

$$H_{exc} = -(E_s - E_t)S_1 \cdot S_2 = -J_{exc}S_1 \cdot S_2. \tag{1.14}$$

Through this Heisenberg has established the framework under which all the proposals introduced in the thesis operate. Whether the qubits be donor nuclear spins, donor electron spins or a single electron in a quantum dot the basis of their mutual interaction is one form of exchange interaction.

1.4.2 Single Qubit Gates

The ability to manipulate individual spin-states, or qubits, is a fundamental requirement of quantum computing. Single qubit flip gates represent an analogue to the classical NOT gates. Beyond that, specific rotations about set axes are vital to the creation of the universal CNOT gate. Here is presented a brief depiction of the how the single qubit flip gate can be expressed in terms of a unitary matrix. Defining the spin component wave-vector as

$$|\Psi >= \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{1.15}$$

The swap operator may be expressed as

$$Swap = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{1.16}$$

The process of flipping the qubit orientation is shown here

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} |\Psi> = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} (\alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix}) = \beta \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \alpha \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{1.17}$$

Single qubit gates in the architecture put forward here are produced through the application of oscillating magnetic fields perpendicular to the nuclear spin orientation. The resonance frequency of a donor's nuclear spin state is tuned through the hyperfine interaction. This allows individual addressing of the spins by changing the hyperfine interaction. The derivation of the Nuclear Magnetic Resonance and Electron Spin Resonance is provided in detail within appendix A.1. However, single qubit rotations are not sufficient for universal quantum computation.

1.4.3 Two Qubit Gates

The analogue of the universal gates familiar to classical computing are formed through single qubit rotations and two-qubit gates. The exchange interaction applied sequentially with single qubit rotations can be shown capable of constructing the universal control-NOT gate [18]. From above, a general exchange interaction may be expressed as

$$H_{exc} = -J_{exc} S_1 \cdot S_2.$$

The exact form of J_{exc} pertinent to our proposal will be left now in favour of a full derivation presented later, for now this simple definition is all that is required. The

time evolution operator subject to the exchange interaction is then given by

$$e^{-i\frac{i}{\hbar}J_{exc}tS_1\cdot S_2}. \tag{1.18}$$

This can be simplified by the substitution:

$$\tilde{J} = \frac{1}{\hbar}\int_{t_0}^{t} J_{exc}(t)\,dt. \tag{1.19}$$

The swap operation, exchanging one qubit's orientation with its neighbour's, is formed when $\tilde{J} = \pi$, demonstrated in appendix A.2:

$$U_{swap} = e^{-i\pi S_1\cdot S_2} = e^{-i\frac{\pi}{4}}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{1.20}$$

Note - The 4 x 4 matrix is written in the basis of $|00>, |01>, |10>, |11>$, that is each row and column is indexed by a state. Each gate will induce an extra phase transition, here $e^{-i\frac{\pi}{4}}$ that will cause the qubits to become out of phase with their neighbours and must be counteracted.

The production of the universal control-NOT gate requires sequential steps of single qubits rotations, entanglement and further rotations. The first step to creating the control-NOT gate requires the formation of the square root of swap gate. Although the swap gate is very useful to move qubits it, however, does not create the necessary

entanglement resulting from the square root of swap gate, with $\tilde{J} = \frac{\pi}{2}$:

$$U_{\sqrt{SWAP}} = e^{-i\frac{\pi}{2}S_1 \cdot S_2} = \frac{e^{-i\frac{\pi}{8}}}{\sqrt{2}} \begin{bmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & e^{i\frac{\pi}{4}} & e^{-i\frac{\pi}{4}} & 0 \\ 0 & e^{-i\frac{\pi}{4}} & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & \sqrt{2} \end{bmatrix}. \tag{1.21}$$

The next step is to construct the control-Z gate, which performs a rotation of the qubits through π radians in the Bloch sphere. Two applications of the square-root of swap gate and three single qubit rotations form the control-Z gate:

$$U_{CZ} = e^{i\frac{3\pi}{2}S_{1z}} e^{i\frac{\pi}{2}S_{2z}} S e^{i\pi S_{1z}} S = e^{i\frac{\pi}{4}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{1.22}$$

Which may finally be employed in the formation of the control-NOT gate, constructed through two single qubit rotations and the control-Z gate:

$$U_{CNOT} = e^{i\frac{\pi}{2}S_{2y}} U_{CZ} e^{i\frac{\pi}{2}S_{2y}} = e^{i\frac{\pi}{4}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{1.23}$$

This clearly demonstrates the constitution of the control-NOT gate for electron qubits through the exchange interaction. The operations presented above lay the foundation of quantum computation and any viable architecture must be able to produce all the required operations forming the control-NOT gate. Measurement, on the other hand, requires that the qubits be sampled individually so that the measurement of

one qubits' state cannot affect the state of its neighbour. Quantum computation then requires an architecture that allows for entanglement and measurement to run concurrently. Here is provided the circuit diagrams for the preceding gate operations:

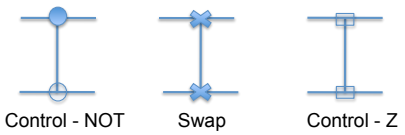


Figure 1.3: Gate Operations

As introduced above the role of the qubit in the architecture presented within this thesis is played by the nuclear spin. The theory of complete qubit control with an applied electric current must demonstrate an ability to readout qubit states and produce a two qubit exchange interaction to perform operation.

1.5 The DiVincenzo Requirements for Quantum Computation[17]

Over the course of the introductory remarks certain criteria, whether they be technical or theoretical, have been established. To be considered a viable means of performing quantum computation the theory presented herein must be able to met all the requirement of computation.

1) A quantum computer must have well defined qubits.

The system which forms the foundation of any quantum computing architecture must be easily distinguishable. This requires that there be two finite states which upon measurement the system is forced into. The states should be as easy to differentiate from one another as possible to allow simple measurement.

2) Qubits must be stable enough to allow multiple operations.

Computation and measurement takes time, no matter how well defined a system

may be, so qubit coherence is a major concern of design. Developing elegant algorithms for computation can help reduce the number of steps to produce a required result but regardless many thousand operations are sometimes required. The longer the coherence the better the machine in any case. The coherence of a qubit is commonly defined in terms of a "quality factor" that is a measure of the relative stability of a qubit in terms of operational speed. Explicitly the quality factor is defined as the operations allowed on an individual qubit while it remains coherent. The lower limit set by most quantum computing algorithms requires approximately 10^3 operations to be performed during the period of qubit coherence [18].

3) Any quantum computer must have the ability to be set into any state of choice.

Possibly the most important attribute required for successful computation is an ability to initialize a set of qubits. Without definite knowledge of the initial state there would be no means of correctly producing a desired result. This is due to the fact that quantum computation functions by taking a known state and evolving it according to a predetermined set of unitary operations. The result being to evolve the system such that the desired outcome is the most probable measurement. Without clear knowledge of the initial conditions the rest of the problem is undefined.

4) Qubits must be measurable to obtain the desired information.

Determining the outcome of operation is crucial, clearly, but remains one of the most difficult requirements to meet due to the small scale of quantum computation. There are proposals for sampling individual spin states based on single electron conductance, spin dependent scattering and single electron transistors (SET's) but none have demonstrated real scalability. Beyond simply being able to perform measurement, precise control over the time and length of measurement is paramount. This is due to the nature of quantum mechanics, namely that measurement destroys the

superposition of states. If the timing and length of measurement are not exact the required information will simply be lost.

5) A set of universal gates must be operational, that is have a functional form within the computer.

The key constituents which form the universal control-NOT gate are the ability to perform single qubit rotations about all axes and two qubit operations. Mechanisms, therefore, must exist to achieve these requirements. Two-qubit operations are the only means of producing entanglement and as such form the basis of computation.

These are requirements of any developed architecture to be considered a viable quantum computing model. Conduction electrons, to establish a true universal means of quantum control, must demonstrate an ability to met these requirements. The remainder of this thesis will serve to directly address these concerns.

Chapter 2

The effect of a Current on Qubit Coherence

2.1 The Effect of Conduction Electrons on the Donor Electron Spin

The scattering of conduction electrons off of donor impurities, in the limit of few impurities, can be reduced to the scattering effect of a single donor. The form of the potential is that of a direct exchange interaction that exists between the conduction and localized (donor) electron spins. This interaction induces spin transitions in the donor electron spin state. As the scattering event must preserve total spin the only spin transitions available are spin flip-flops. The rate of overall spin transition is given by $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$, where $(\Gamma_{\Uparrow})$ is the transition rate of a donor's spin up electron to a spin down electron state and $(\Gamma_{\Downarrow})$ is the converse.

A result from the requirement of overall spin conservation is that conduction electron spin transitions may only occur if they are paired with a donor electron

transition. The exchange scattering Hamiltonian is given by [12]

$$H_{ce} = \sum_{kk'} J_{eff} S_i \cdot S_{ce}. \tag{2.1}$$

Where i is the donor label, k the conduction electron momentum pre-scattering, k' post scattering, and

$$S_i \cdot S_{ce} = S_{ze}S_{zi} + S_{xe}S_{xi} + S_{ye}S_{yi} = S_{ze}S_{zi} + S_{e+}S_{i-} + S_{e-}S_{i+}. \tag{2.2}$$

Which may be rewritten replacing the conduction electron transitions with the corresponding creation and annihilation operators. In this model the interacting potential is then explicitly given by

$$H_{ce} = J_{eff} \sum_{k,k'} (S_- c^\dagger_{k'\uparrow} c_{k\downarrow} + S_+ c^\dagger_{k'\downarrow} c_{k\uparrow} + S_z (c^\dagger_{k'\uparrow} c_{k\uparrow} + c^\dagger_{k'\downarrow} c_{k\downarrow})). \tag{2.3}$$

Where $c^+_{k\sigma}$ and $c_{k\sigma}$ are the creation and annihilation operators, respectively, for a conduction electron with momentum k and spin $\sigma = \Uparrow, \Downarrow$. $S_\pm = S_x \pm iS_y$ are spin raising and lowering operators for the donor electron with J_{eff} being the exchange strength. Each transition rate may be determined by using Fermi's Golden Rule,

$$\Gamma_\Uparrow = \frac{2\pi}{\hbar} \sum_{k,k'} J^2_{eff} | < f | S_- c^\dagger_{k'\uparrow} c_{k\downarrow} | i > |^2 \delta(\epsilon_i - \epsilon_f). \tag{2.4}$$

The initial state is given by $|i> = |FS> | \Uparrow>$ with energy $\epsilon_i = \frac{g_e \mu_e B}{2} + E_{FS}$ where B is the applied field and $|FS>$ is the eigenstate for the Fermi sea. The final state is given as $|f> = |FS + \begin{matrix} ek' \uparrow \\ hk \downarrow \end{matrix} > | \Downarrow>$ with energy $\epsilon_f = -\frac{g_e \mu_e B}{2} + E_{FS} + \epsilon_{k'\uparrow} - \epsilon_{k\downarrow}$. Here $\epsilon_{k\uparrow}$ is the energy of the conduction electron with momentum k, same for $\epsilon_{k'\uparrow}$ but for a hole. The full derivation of ($\Gamma_\Uparrow$) is presented within appendix A.4, only the final

result is important here and is given by

$$\Gamma_{\Uparrow} = \frac{2\pi}{\hbar}|J_{eff}|^2\nu^2 g_e\mu_e B(1 + f_{Bose}(g_e\mu_e B)). \tag{2.5}$$

Here ν is the density of states per unit energy given as $\frac{m^*L^2}{2\pi\hbar^2}$, where m* is the electron's effective mass and L^2 is the area of the 2DEG. It is interesting to note the dependence on the Bose distribution, where $f_{Bose} = \frac{1}{e^{\frac{\epsilon}{kT}}-1}$. The transition of a spin down donor electron to a spin up requires the production of an electron-hole pair in the Fermi sea, see appendix A.4 for further details. The electron-hole pair apparently behaves as though they form one Bosonic particle. The transition rate therefore depends on the population of electron-hole pairs within the Fermi sea.

Likewise the transition rate $\Gamma_{\Downarrow}$ for a spin down donor electron to flip to a spin up is found in the same manner, only with $B \to -B$, giving

$$\Gamma_{\Downarrow} = \frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B f_{Bose}(g_e\mu_e B). \tag{2.6}$$

The addition of these two results gives the overall transition rate as

$$\frac{1}{T_1^e} = (\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) = \frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B coth(\frac{g_e\mu_e B}{2k_B T}). \tag{2.7}$$

This indicates that the choice of a nuclear spin qubit may have been ideal as conduction electrons would destroy any coherence in an electron spin qubit. It is not clear from this result what effect the donor's electron spin transitions will have on the nuclear spin state.

The effective exchange strength J_{eff} can be obtained after summing all orders of perturbation theory. The result is a universal expression that depends only on the

Kondo temperature T_K [10] [12]:

$$|J_{eff}\nu|^2 = (\pi^2 + \frac{4}{3}|ln(\frac{T}{T_K})|^2)^{-1}. \tag{2.8}$$

The physical description of Kondo theory is that of exchange screening. The conduction electrons tend to orient themselves to screen out the spin of the donor atom. The transition rate will vary greatly depending on the regime in which it is operating. For a donor is silicon[7]:

$$k_B T_K = \sqrt{(\epsilon_d + U - \epsilon_F)(\epsilon_F - \epsilon_{sb})(J_{eff}\nu)}e^{-\frac{1}{J_{eff}\nu}} \approx \sqrt{23 J_{eff}\nu}e^{-\frac{1}{J_{eff}\nu}} \tag{2.9}$$

Where ϵ_d is the energy associated with the internal energy of the donor, minus the valence electron , ϵ_{sb} is the sub-band energy, U is the mutual coulomb repulsion between the donors, the energy required to bring the donor into close proximity. ϵ_F is the Fermi energy, $\nu = \frac{m^*}{\hbar^2}\frac{L^2}{2\pi}$, k_F the Fermi wave-vector and r the separation between the donors. The thermal length scale of a conduction electron is given by

$$l_T = \nu_F \frac{\hbar}{k_B T}, \tag{2.10}$$

where the conduction electron velocity is given by $\nu_F = \frac{2\epsilon_F}{k_F \hbar}$.

Eq. (2.7) describes the spin transition rate for the donor electron when $T > T_K$. When $T < T_K$, the donor spin will undergo non-exponential decay with time scale $\frac{k_B T_K}{\hbar}$, that is the time scale for the formation of the Kondo singlet [2]. This result comes from adding all orders of perturbation theory using Wilson's renormalization method [12]. The conduction electrons form a screening "bubble" , called a Kondo singlet, surrounding the donor impurity:

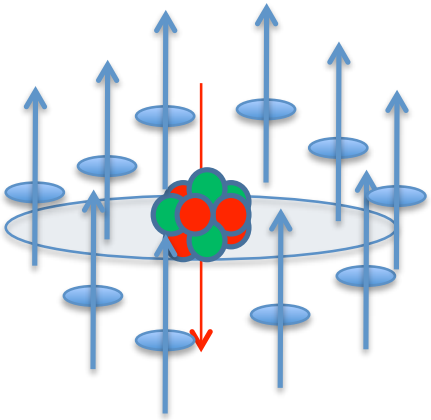


Figure 2.1: Kondo Screening

This effect adds a decay to the electron spin polarization with a rate of $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) \approx \frac{k_B T_K}{\hbar}$. When $T > T_K$ and $2K_BT > B_e$ the hyperbolic cotangent in Eq. (2.7) may be expanded to get

$$(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) = \frac{2\pi}{\hbar}|J_{eff}\nu|^2(2k_BT). \tag{2.11}$$

When $2K_BT << g_e\mu_eB$ the hyperbolic cotangent term in Eq. (2.7) tends to unity and the transition rate is given by

$$(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) = \frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_eB. \tag{2.12}$$

The summed result being a description of the donor electron spin transitions as an outcome of interaction with a conduction electron sea.

2.2 Nuclear Spin Qubit Coherence

So now that it is clear from the preceding section that conduction electrons will induce spin transitions in the donor's electron spin state it time to determine what effect this will have on the donor's nuclear spin state. To examine this issue we must first identify

what connection there is between the donor's electron and nuclear spin states. The exploration of this issue begins with the Hamiltonian defining the interaction between the donors' electron and nuclear spins with the applied field:

$$H = g_e\vec{\mu_e}B \cdot \vec{S} - g_n\vec{\mu_n}B \cdot \vec{I} + A\vec{S} \cdot \vec{I}. \tag{2.13}$$

Where g_e and g_n are the g-factors for the electron and nuclear spins respectively. μ_e and μ_n are the magnetic moments of the electron and nuclear spins and B the applied magnetic field. The electron and nuclear spins, with spin matrices S and I respectively, are connected through the hyperfine interaction with strength A. Adding the effects of the conduction electrons the interaction Hamiltonian takes the following form

$$H = g_e\vec{\mu_e}B \cdot \vec{S} - g_n\vec{\mu_n}B \cdot \vec{I} + A\vec{S} \cdot \vec{I} + H_{environment}. \tag{2.14}$$

Where the $H_{environment}$ term contains the interaction between the conduction electrons and the donor. The spin matrices $\vec{S}$ and $\vec{I}$ may be expressed in terms of Pauli matrices:

$$\vec{S} = \frac{1}{2}\vec{\sigma}, \tag{2.15}$$

$$\vec{I} = \frac{1}{2}\vec{\tau}. \tag{2.16}$$

With these substitutions in mind the ground state Hamiltonian, Eq. (2.13), may be rewritten with $B_e = g_e\mu_e B$ and $B_n = g_n\mu_n B$ as

$$H_0 = \frac{1}{2}\vec{B_e} \cdot \vec{\sigma} - \frac{1}{2}\vec{B_n} \cdot \vec{\tau} + \frac{A}{4}\vec{\sigma} \cdot \vec{\tau}. \tag{2.17}$$

When $T > T_K$ the electron spin polarization does decay exponentially towards its thermal equilibrium. The dominant effect of the conduction electrons is the produc-

tion of spin transitions. Therefore the effect of the conduction electron sea may be traced out in favour of decay terms dependent on $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ and $(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})$. The time evolution of the density matrix is then given by [20]

$$\frac{d\hat{\rho}}{dt} = -i[H_0, \hat{\rho}] + \frac{1}{4}(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(\sigma_1\hat{\rho}\sigma_1 + \sigma_2\hat{\rho}\sigma_2 + \sigma_3\hat{\rho}\sigma_3 - 3\hat{\rho}) - \frac{1}{4}(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})\sigma_3. \quad (2.18)$$

Where the density matrix for electron and nuclear spin can be written as

$$\hat{\rho}(t) = \frac{1}{4}[\mathbb{1}_{4x4} + \sum_{(i,j)\neq(0,0)} \eta_{ij}(t)\sigma_i \otimes \tau_j]. \quad (2.19)$$

η_{ij} represents a fifteen dimensional generalized Bloch vector. It is convenient to not only speak in terms of the spin states but also the magnetization that results from the expectation value of the electron and nuclear spin states, defined as

$$2 < \vec{S} >= \vec{M}_S = \begin{cases} \eta_{10} \\ \eta_{20} \\ \eta_{30} \end{cases} \quad (2.20)$$

$$2 < \vec{I} >= \vec{M}_I = \begin{cases} \eta_{01} \\ \eta_{02} \\ \eta_{03} \end{cases} \quad (2.21)$$

$$\eta_{00} = \sigma_0 = \tau_0 = \mathbb{1}_{2x2} \quad (2.22)$$

M_S and M_I are the electronic and nuclear spin magnetization respectively. The full derivation of the electron and nuclear spin dynamics is provided in appendix A.4. The results which are important to the current discussion are presented here. The

electron spin dynamics are found to be governed by

$$< \dot{\vec{S}} >= (\vec{B}_e \times < \vec{S} >) - A < \vec{S} \times \vec{I} > -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) < \vec{S} > -(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})\hat{z}. \quad (2.23)$$

While the nuclear spin evolves according to

$$< \dot{\vec{I}} >= -(\vec{B}_N \times < \vec{I} >) + A < \vec{S} \times \vec{I} > . \quad (2.24)$$

And evolution of their joint dot product is given by

$$< \dot{\vec{S}}\vec{I} >= B_e \hat{z} \times < \vec{S}\vec{I} > + B_n < \vec{S}\vec{I} > \times \hat{z} + \frac{A}{4}(\vec{S} - \vec{I}) \cdot \epsilon - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) < \vec{S}\vec{I} > . \quad (2.25)$$

Here $< \vec{S}\vec{I} >$ is the outer product of the donor electron and nuclear spin states, ϵ is the Levi-Civita tensor, defined as ϵ_{xyz}, and $\hat{z}$ is the direction of the globally applied magnetic field.

Solving these equations for the time evolution of the spin states allows the identification of their respective decay rates. The coherence of the electron and nuclear spins is defined by two decay rates. The first $\frac{1}{T_1}$ is the rate of decay for the spin orientation aligned with or against the global magnetic field field. The second $\frac{1}{T_2}$ is the rate of perpendicular magnetization (or phase) decay. Each decay rate will have two varieties: one for the donor electron spin and another for the donor nuclear spin.

As expected from Section 2.1 the decay of the donor electron spin will be dominated by the $-(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) < S >$ term found in Eq. (2.23). This also happens to be true for the perpendicular components of the electron spin, demonstrated after transforming to a rotating reference frame. Therefore $\frac{1}{T_1^e}$ and $\frac{1}{T_2^e}$ are given by

$$\frac{1}{T_1^e} = \frac{1}{T_2^e} = (\Gamma_{\Uparrow} + \Gamma_{\Downarrow}). \quad (2.26)$$

Within the current discussion, as these equation are all inter-connected, the importance of these transition rates is limited to their effect on the donor's nuclear spin state. The dynamics of the nuclear magnetization must be solved by transforming to a rotating reference frame and substituting the results for the electron spin dynamics, the details of which are presented in appendix A.4. The results of this examination are presented here.

The time dependence of the parallel components of the nuclear spin magnetization is given by

$$M_{I\|}(t) = (M_{I\|}(0) - p_e)e^{-\frac{A}{2}\frac{A(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{((\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2+(B_e+B_n)^2+\frac{A^2}{2})}t} + p_e. \tag{2.27}$$

With

$$p_e = \frac{(\Gamma_{\Downarrow} - \Gamma_{\Uparrow})}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}. \tag{2.28}$$

The consequence of which clearly shows the parallel nuclear spin magnetization decays according to $\frac{A}{2}\frac{A(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{((\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2+(B_e+B_n)^2+\frac{A^2}{2})}$. So after some simplification $\frac{1}{T_1^n}$ is given by

$$\frac{1}{T_1^n} = \frac{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{1 + 2(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{A})^2 + 2(\frac{B'}{A})^2}. \tag{2.29}$$

Where $B' = B_e + B_n$.

The time dependence of the perpendicular components of the nuclear spin magnetization is given by

$$\begin{aligned} M'_{I\perp} = &\frac{\frac{A}{4}(V'_{\perp}(t=0) - S'_{\perp}(t=0)) - \frac{1}{2}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})} e^{-(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})t} \\ &+ e^{-(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})t} \end{aligned} \tag{2.30}$$

The examination of which clearly shows a decay proportionally to

$$(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2}); \tag{2.31}$$

and

$$(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2}). \tag{2.32}$$

When $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) >> A$ then

$$\frac{\frac{A}{4}(V'_{\perp}(t=0)-S'_{\perp}(t=0))-\frac{1}{2}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})} << 1. \tag{2.33}$$

The first term will then play a significantly smaller role than the second and its effect, therefore, will be negligible. The decay of the perpendicular magnetization may then be characterized exclusively by this second term:

$$\frac{1}{T_2^n} = (\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2}). \tag{2.34}$$

When $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) << A$ the square-root in both terms will become complex. A complex component results in coherent oscillations so it will have no effect on the decay rate and both terms will decay according to

$$\frac{1}{T_2^n} = \frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{2}. \tag{2.35}$$

There also exists a direct interaction between the conduction electron sea and the nuclear spin qubit known as the Korringa mechanism of nuclear spin relaxation. This interaction tends to orient the nuclear spin qubit into thermal equilibrium with the conduction electron sea. However, this interaction is quite weak for a low density of conduction electrons, and we can show that it will take a few minutes to flip the donor

nuclear spin. We calculated the Korringa rate for the phosphorus donor in the silicon transistor. We obtained $(1/T_1^n)_{\text{Korringa}} < 10^{-3}s^{-1}$ for $R/z0 > 2$ at low temperature (T < 10 K). Hence, at times shorter than a few minutes we may neglect this direct interaction between the donor and the electron gas.

2.3 Decay Times by Regime

In the limit where $B > A >> (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ the decay time for the parallel component of the nuclear spin is given by

$$\frac{1}{T_1^n} = (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(2(\frac{A}{B})^2). \tag{2.36}$$

Where the nuclear spin relaxation is predominately independent from the electron relaxation. The decay of the nuclear spin in the case when $A >> (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ again is given by

$$\frac{1}{T_2^n} = \frac{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{2}. \tag{2.37}$$

This indicates that in the limit of $A >> (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$, that is when the hyperfine coupling is far stronger than the electron transition the donor nuclear spin relaxation, $\frac{1}{T_2^n}$, effectively follows the electron spin relaxation.

When $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}), B >> A$ the parallel component of the nuclear spin magnetization relaxation is

$$\frac{1}{T_1^n} = \frac{A^2}{2(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}. \tag{2.38}$$

For the perpendicular magnetization dependence the term $(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) - \sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2 - A^2}}{2})$ tends to zero. To find the real solution the $(\sqrt{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 - A^2})$ term must be ex-

panded giving

$$\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}=(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})(1+\frac{1}{2}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}+\dots). \tag{2.39}$$

Keeping terms up to $\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}$ allows the determination of the perpendicular magnetization decay time for the nuclear spin sates given by

$$\frac{1}{T_2^n}=(\frac{1}{4}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}). \tag{2.40}$$

Where in both cases the nuclear spin state has a decay dependence inversely proportional to the electron spin transition rate. This signals a transition to a regime where the donor nuclear spin no longer follows the electron spin relaxation, a regime of motional narrowing. These expressions set the limits of read-out, initialization and operation within this quantum computing architecture. Whether they constitute working limits or preclude conduction electrons as an option for quantum control has yet to be established. Moving forward these coherence limits will play a crucial role and it will be helpful to stop now and give some true physical examples of these decay rates.

2.4 Sample Decay Calculation for the Donor Electron Spin

The physical parameters that most truly represent a phosphorus nuclear spin qubit in a silicon substrate with an applied magnetic field are given by:

k_B - Boltzmann Constant	$1.38062 \times 10^{-16} ergK^{-1}$
T - Temperature	$0.1 - 5K$
μ_e - Magnetic Moment (Electron)	$9.2848 \times 10^{-21} ergG^{-1}$
g_e - g-factor (Electron)	2.002
B - Applied magnetic field	1×10^4G
A - Hyperfine coupling	120 MHz
1 erg	$6.24150974 \times 10^{11}$ eV
$\hbar$	$4.13567 \times 10^{15} eV \cdot S$

Table 2.1: Physical Parameters for Coherence Calculations

To start it is important to determine an approximate value for $J_{eff}\nu$ in order to solve for the electron and nuclear spin decay times. The temperature dependent conduction electron spin-flip scattering rate, within the Suhl-Nagaoka approximation, is given by [10]:

$$\frac{1}{T_1^{ce}} = (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})_{ce} = \frac{1}{2\pi\hbar\nu} \frac{\pi^2 S(S+1)}{\pi^2 S(S+1) + (ln(\frac{T}{T_K}))^2}. \tag{2.41}$$

Where again S is the spin operator, here assuming $S = \frac{1}{2}$, T is the temperature in Kelvin and T_K is the Kondo temperature. This then provides a means of relating the J_{eff} to the Kondo temperature through the decay rate for the donor electron. When $2k_BT > g_e\mu_eB$ then $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ for the conduction electrons, found like $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ for the donor electron by performing Fermi's Golden Rule, becomes

$$(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})_{ce} = \frac{2\pi}{\hbar\nu} |J_{eff}\nu|^2. \tag{2.42}$$

Assuming $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \approx (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})_{ce}$ gives

$$|J_{eff}\nu|^2 = (\frac{1}{\pi^2} + \frac{4}{3}(ln(\frac{T}{T_k}))^2)^{-1}. \tag{2.43}$$

Note that $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})_{ce}$ is maximum when it approaches the resonant frequency of the donor electron, this occurs when $T \approx 10T_K$. Assuming $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \approx (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})_{ce} \approx B$ in the limit of $B >> A$ the spin relaxation for the donor electron is given by

$$\frac{1}{T_1^e} = \frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B coth(\frac{g_e\mu_e B}{2k_B T}). \tag{2.44}$$

Which may be simplified in the limit of $g\mu B >> 2k_B T$ where $\frac{1}{T_1^e}$ becomes

$$\frac{1}{T_1^e} = \frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B. \tag{2.45}$$

In the regime of maximum $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ the decay time of the electron spin is given by

$$T_1^e \approx 0.04ns \tag{2.46}$$

2.5 Sample Decay Calculation for the Donor Nuclear Spin

T_1^n is the characteristic decay time to parallel spin polarization of the donor nucleus. In the limit of $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \approx B >> A$

$$\frac{1}{T_1^n} = \frac{A^2}{4\frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B coth(\frac{g_e\mu_e B}{2k_B T})}. \tag{2.47}$$

Which again in the regime of maximum $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})$ and when $g\mu B >> 2k_BT$ the decay of the nuclear spin is

$$T_1^n \approx 1\mu s \tag{2.48}$$

This represents a regime where the conduction electrons have a large effect on the donor nuclear spin state. This may offer a means of fast initialization as T_1^n represents the characteristic decay time for the donor to reach thermal equilibrium, the ground state.

Chapter 3

Qubit Readout and Initialization

3.1 Qubit Readout through Electrically Detected Magnetic Resonance (EDMR)

Any computer system cannot function without an ability to readout the results of an operation. Quantum computing is no different as there must be some means of reading out the information stored within the qubits. As introduced above this work relies on nuclear spins to serve as the functional qubits. As we now show it is theoretically possible to measure individual nuclear spin states in semiconductors provided the electron spin resonance can be detected. Conventional magnetic resonance detection requires the presence of at least 10^{12} spins [25]. In order to detect one spin, we must use a much more sensitive method. Electrically detected magnetic resonance (EDMR) [26] [27] consists in running a current on top of the donor impurity. The current resulting from the donor's presence is spin-dependent according to[7]

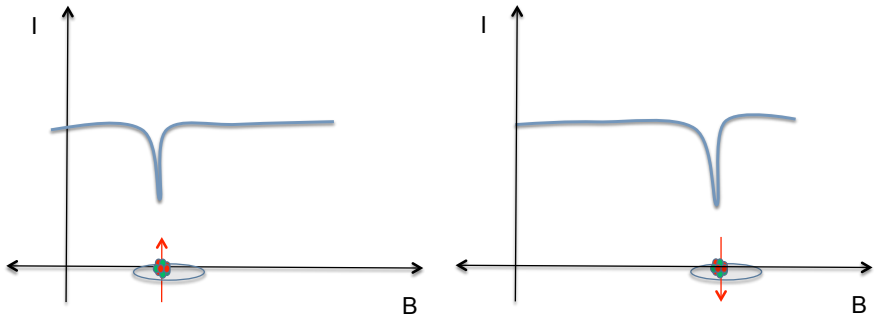
$$I = I_0(1 + \alpha p_{ce} p_i). \tag{3.1}$$

Where p_{ce} is the polarization of the conduction electrons and p_i the polarization of the donor electron. The donor electron polarization can be manipulated through the application of a perpendicular oscillating magnetic field, of frequency $\Omega_{\perp}$, at resonance, creating an equally populated spin state. The result is p_i drops effectively to zero. This then drops the device current by $\alpha p_{ce} p_i$.

The resonant frequency of a donor electron is intrinsically connected to the donor's nuclear spin state through the hyperfine interaction. Therefore current measurements as a function of applied magnetic field offer a means of identifying a donors electron resonant frequency and through association the nuclear spin state [21]. The overall interaction of an individual donor with a globally applied magnetic field is given by

$$H = g_e \vec{\mu_e} B \cdot \vec{S} - g_n \vec{\mu_n} B \cdot \vec{I} + A\vec{S} \cdot \vec{I}. \tag{3.2}$$

Where g_e and g_n are the gryomagnetic ratios for the electron and nuclear spins, respectively, and μ_e and μ_n their Bohr magnetons. The orientation of the donors nuclear spin changes the resonant frequency. When the nuclear spin is aligned with the applied field the resonant frequency is $\omega_+ \approx \frac{(g_e \mu_e B - \frac{A}{2})}{\hbar}$ when aligned against $\omega_- \approx \frac{(g_e \mu_e B + \frac{A}{2})}{\hbar}$. This is shown in Fig. 3.1 below, where the two resonant frequencies are separated by the hyperfine constant A.



(a) Donor nuclear spin up (b) Donor nuclear spin down

Figure 3.1: Donor nuclear spin readout using Electrically Detected Magnetic Resonance [21]

However, it is not clear that this read-out scheme is possible. EDMR read-out of nuclear spin states can only be achieved if the time to detect EDMR is less than T_1^n, the nuclear spin flip rate, and longer than T_2^n, the time required for the nuclear spin wave function to collapse into one of the outcome states.

3.2 Operating Regime of EDMR

In Chapter 2 conduction electrons were shown to induce spin transitions in the donor electron spin states, the rate of transition was given as $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})$. The question where EDMR is concerned is what effect the electron spin flips will have on the nuclear spin states. In other words we need to determine if the donor nuclear spin is coherent long enough to allow measurement. In the limit of $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) << A$ we found

$$\frac{1}{T_1^n} = \frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{2(\frac{B'}{A})^2}, \tag{3.3}$$

$$\frac{1}{T_2^n} = \frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{2}. \tag{3.4}$$

Where $B' = B_e + B_n$.

As introduced above EDMR functions by irradiating a donor with a oscillating magnetic field perpendicular to the globally applied magnetic field. When the oscillating field comes into resonance with the donor electronic spin state a decrease in current, ΔI_{EDMR}, will be observed. This will only occur if the donor spin polarization is saturated to zero, $p_i \to 0$. The condition for this to happen is that $\Omega_\perp \geq (\Gamma_\Uparrow + \Gamma_\Downarrow)$. If this was not the case than the effect of the resonant field will be masked by the transitions induced by the conduction electrons. As shown in [7], EDMR is optimized when $\Omega_\perp = (\Gamma_\Uparrow + \Gamma_\Downarrow)$. As a side note, it is also crucial that $A > \frac{1}{T_1^n} = \Omega_\perp$, that is, that the separation between the two EDMR peaks, A, be greater that the electron spin line-width, $\frac{1}{T_1^n}$.

In terms of the Kondo temperature the optimum resonance condition $\Omega_{perp} = (\Gamma_\Uparrow + \Gamma_\Downarrow)$ occurs when

$$ln(\frac{T}{T_K}) = \sqrt{2\pi \frac{B}{p_e B_\perp}}. \tag{3.5}$$

Here the donor spin polarization $p_i = \frac{(\Gamma_\Uparrow - \Gamma_\Downarrow)}{(\Gamma_\Uparrow + \Gamma_\Downarrow)} = tanh(\frac{g_e \mu_e B}{2k_B T})$ and the conduction electron polarization is $p_{ce} = \frac{g_e \mu_e B}{(\epsilon_F - \epsilon_{sb})}$ (where ϵ_F is the Fermi energy and ϵ_{sb} the subband energy). This regime requires low Kondo temperature and from here on is referred to as the "weak" coupling regime. Here is presented the band diagrams for the donor (ϕ) and conduction electron (ψ) wavefunctions:

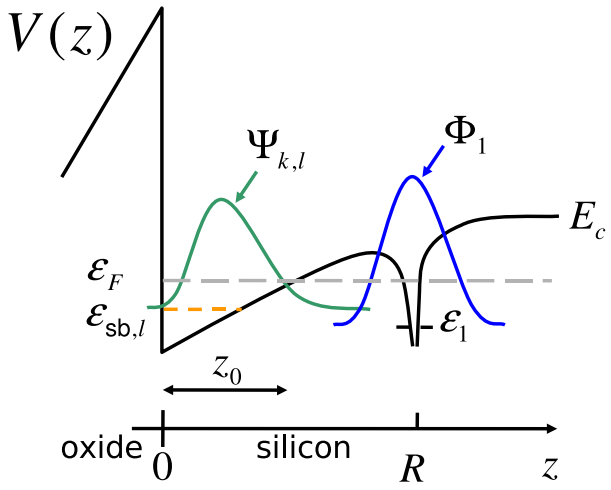


Figure 3.2: Band Diagram for Donor and Conduction Electron Wavefunctions

In order for this to be possible $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})$ must be significantly lower than B, which only occurs when the donor is separated from the 2DEG by a large distance, resulting is a low transition rate. When $B = 1T$ and $B_{\perp} = 0.3T$ the weak coupling regime requires $ln(\frac{T}{T_K}) \approx 500$. We recall that the minimum EDMR read-out time is given by T_2^n, because the nuclear spin must collapse into one of the outcome states for the read-out to occur. As a result, the maximum read-out contrast is given by $e^{(-\frac{T_2^n}{T_1^n})}$.

With $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) \approx \Omega_{\perp} << A$

$$\frac{T_2^n}{T_1^n} = \frac{\Omega_{\perp}}{2}(\frac{(\frac{B'}{A})^2}{\Omega_{\perp}}) = (\frac{B'}{A})^2. \tag{3.6}$$

Hence when $B >> A$ the maximum contrast is given by

$$e^{-\frac{T_2^n}{T_1^n}} = e^{-(\frac{A}{B'})^2} \approx 1. \tag{3.7}$$

In reality, we expect that the time it takes to detect the EDMR of a single donor, t_{EDMR}, will be much larger than T_2^n. The longest allowable time for readout is set

by T_1^n, armed with this limit it is possible to define a minimum sensitivity criterion for EDMR. The sensitivity of EDMR is critically dependent on change in current caused by one donor moving from being in resonance to off, ΔI_{EDMR}. An important concern is the shot noise associated with running a current over a donor. Due to the discreteness of the electron charge, a current can not have a fixed value; rather it will have a range of values subject to a Poisson distribution. The noise associated with this spread in current values is called the shot noise and ΔI_{EDMR} can only be measured if it is greater than this shot noise, ΔI_{shot}. The shot noise represents the minimum possible noise associated with EDMR. This noise could be reduced if the measurement time was of the order of a few minutes but the qubit decoherence forbids that[16]. The minimum contrast of the shot noise with the applied current is given by

$$(\frac{\Delta I}{I})_{shot} = \frac{1}{\sqrt{N(t_{EDMR})}}. \tag{3.8}$$

Where $N(t_{EDMR})$ is the number of electrons that pass through the device and in the lower sensitivity limit of $t_{EDMR} = T_1^n$ we get

$$N(t_{EDMR}) = \frac{IT_1^n}{e}. \tag{3.9}$$

Where e is the charge of an electron and I is the device current. Using Eqs. (3.5) and (3.12) we get the the sensitivity criterion for nuclear spin read-out:

$$(\frac{\Delta I}{I})_{EDMR} > \sqrt{\frac{e\Omega_\perp}{2I}}(\frac{A}{B'}). \tag{3.10}$$

For $I = 1\mu A$, $B_\perp = 0.3G$ and $B = 1T$:

$$(\frac{\Delta I}{I})_{EDMR} \geq 3 \times 10^{-6}. \tag{3.11}$$

This result demonstrates that so long as an EDMR device can measure current drops larger than $(3 \times 10^{-6})IA$ the nuclear spin coherence is long enough to allow measurement. This lower bound was derived under the assumption that the shot noise dominates over other noise sources. Because I and T_1^n are somewhat low, the shot noise is quite large, and is expected to dominate in many devices. However, when other sources of noise are important, we must add them to the right hand side of Eq. (3.14). In any case, we emphasize that the shot noise bound given by Eq. (3.14) is unsurmountable and therefore represents a true physical limit.

3.3 Qubit Initialization

The results for T_1^n, the decay time of the parallel magnetization, suggests a novel approach to the process of qubit initialization. The spin transition rate will be maximum if $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ can be tuned to be approximately equal to the energy splitting between the spin up and spin down electron $\approx B'$. This provides a means of optimizing T_1^n in order to do a fast transfer of electron spin polarization p_i into the nuclear spin polarization, so that $p_n = p_i$ will be much higher than its thermal equilibrium value. This is a convenient means of quantum control whereby the spin transfer of the conduction electron sea is capable of aligning all nuclear spins in their ground state, aligned with the applied field.

From Eq. (3.5), the minimum T_1^n requires the condition $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \approx g_e \mu B/\hbar$. In terms of the Kondo temperature this can be achieved when

$$ln(\frac{T}{T_K}) \approx \sqrt{\frac{2\pi}{|p_i|}}, \tag{3.12}$$

or when $T \approx 10T_K$ requiring $p_i = 1$. This is labelled the "strong" coupling regime as it requires a small donor-2DEG separation to optimize the transition rate ensuring

$(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \approx B'$. In this strong coupling regime T_1^n is given by

$$\frac{1}{T_1^n} = \frac{A^2}{4B'}. \tag{3.13}$$

For a phosphorus donor in silicon, $A = 120MHz$ and $B' = 28GHz$ when $B = 1T$, leading to qubit initialization times, T_1^n, of the order of $1\mu s$. When compared to the 1 ms times usually associated with NMR this represents a considerable improvement.

3.4 Tuning between Readout and Initialization

The idea is to electrically tune the system between the weak coupling regime required for EDMR and the strong coupling regime for initialization. This is possible because the Kondo temperature is dependent upon the overlap between the conduction electron sea and the donor's electronic wavefunction, an overlap that is subject to manipulation through electric fields. It is possible to draw the the electrons in the 2DEG closer to the edge thereby increasing the electron donor separation and the Kondo temperature. One could conversely widen the 2DEG with electric leads situated above the donors.

Here is presented a plot of the Kondo temperature as a function of donor depth:

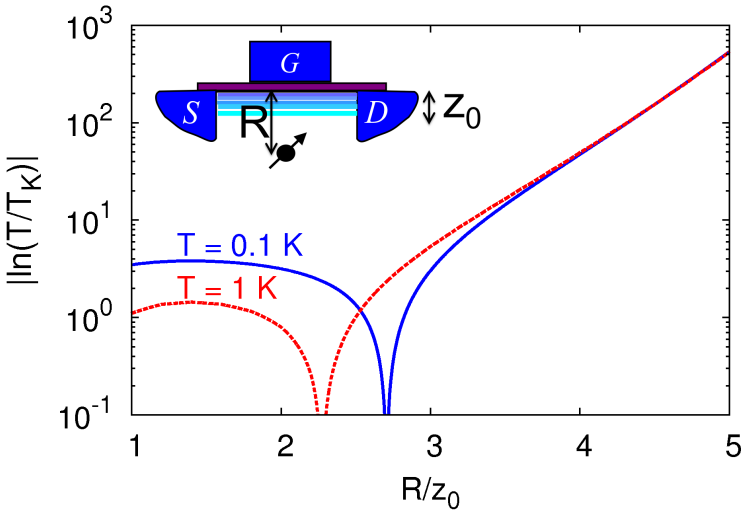


Figure 3.3: Kondo Temperature as a Function of Electron Depth

This figure demonstrates how a donor impurity implanted in a silicon accumulation field effect transistor (inset) can be tuned into and out of the Kondo regime using a top gate voltage. z_0 here represents the thickness of the 2DEG and R the depth of the donor. The 2DEG width is controllable from $z_0 = 30 - 100\mathring{A}$. A donor can then be tuned from the strong coupling regime, where $\frac{R}{z_0} = 3$, to the weak coupling regime, where $\frac{R}{z_0} = 5$. The outcome is an all electric integrated readout and initialization design with conduction electrons.

Chapter 4

The RKKY Quantum Gate

Having established the use of conduction electrons to read-out and initialize nuclear spin qubits the hope is now that conductions electrons may be shown to facilitate the coupling operation. An interaction between localized spins mediated through conduction electrons was first described by Ruderman, Kittel, Katsuya and Yoshida and the interaction bears their name, often abbreviated as the RKKY interaction. This form of interaction is possible because the scattering of conduction electrons is spin dependent. When a conduction electron scatters off the first donor its outgoing state is intrinsically connected to the electronic spin state of the first donor. This conduction electron then scatters off of the second donor, in another spin dependent scattering process. By this manner the information contained within the first scattering event plays a crucial role in the outcome of the second. The result is an interaction between the electron spin states of the two donors.

4.1 The RKKY Interaction

A simple introduction to how the RKKY interaction functions is to treat the scattering of a conduction electron off two donors in second order perturbation theory. This will

serve to give the basic ideas that underlie this interaction. As introduced in Chapters 2 and 3 there exists a direct exchange interaction when a conduction electron and a donor's valence electron interact. The scattering of the conduction electron conserves the overall spin of the two electron system. The two scattering events that may occur between a donor and a conduction electron either preserve their original spin states or induce a spin flip-flop (or spin-exchange) An example then of an operation performed by the RKKY interaction would be to perform a spin flip-flop operation on two donor electrons.

The interaction Hamiltonian is defined as the sum of the ground state plus interaction terms in perturbation theory $H = H_0 + V$ where $V = H^1_{exc} + H^2_{exc}$. The first order term gives rise to exchange scattering and the second order term results in the RKKY Interaction which is of interest here[14]. The transmission matrix, in the Born approximation, may be expressed as

$$T = V + V\frac{1}{E - H_0 + i\epsilon}V + V\frac{1}{E - H_0 + i\epsilon'}V\frac{1}{E - H_0 + i\epsilon}V + \ldots. \tag{4.1}$$

The RKKY interaction, in this approximation, is then given by

$$H^{e-e}_{RKKY} =< FG|H^1_{exc}\frac{1}{E - H_0 + i\epsilon'}H^2_{exc}|FG > . \tag{4.2}$$

The ground state wavefunction is taken as

$$|FG >= \Pi_{k<k_F}c^+_k|0 >, \tag{4.3}$$

where k_F is the Fermi wave vector and c^+_k the creation operator for a donor electron with momentum k. The exchange interaction between a conduction and donor

electron is given by

$$H^i_{exc} = \frac{1}{2}\sum_{kk'} e^{i(k-k')\bar{x}} J^c_{kk'} S_i \cdot S_{ce}. \tag{4.4}$$

The labels k through k"' in the following work refer to donor electron momentum (all $< k_F$), the 'e' label refers to the conduction electrons and the 'i' label refers to donor i. Here J_c is the exchange strength between the conduction electron and the donor. Again note:

$$S_i \cdot S_{ce} = S_{ze}S_{zi} + S_{xe}S_{xi} + S_{ye}S_{yi} = S_{ze}S_{zi} + S_{e+}S_{i-} + S_{e-}S_{i+}. \tag{4.5}$$

Where S_{i+} acts to flip a spin down electron to a spin up for donor i, S_{i-} the converse. In this framework the effect of the S_{e+} and S_{e-} terms is to destroy, c_k, or create, c^+_k, a valence electron as the scattering process must conserve total spin. This is due to the fact that in order to flip a conduction electron from say a spin down to spin up a donor electron must flip from a spin up to a spin dow to preserve the overall spin. It is exactly this requirement that during each scattering process the total spin must be conserved that results in a electron spin interaction between the two donors.

It would be needlessly complicated to solve all terms simultaneously. Here the contributing factors which result in a $S_{1+}S_{2-}$ operation between the two donors will be examined. The remaining results being determined through comparison. Replacing the conduction electron operators with their corresponding effects on the donor electron gives:

$$H^1_{exc} = \frac{1}{2}\sum_{kk'} e^{i(k-k')\bar{x}} J^{c_1}_{kk'} (S_{1+} c^+_{k'\downarrow} c_{k\uparrow}), \tag{4.6}$$

$$H^2_{exc} = \frac{1}{2}\sum_{k''k'''} e^{i(k''-k''')\bar{x}} J^{c_2}_{k''k'''} (S_{2-} c^+_{k'''\downarrow} c_{k''\uparrow}). \tag{4.7}$$

Substituting these scattering relations into Eg.(4.2) above gives:

$$H^{e-e}_{RKKY} = \frac{1}{4} < FG| \sum_{kk'} e^{i(k-k')\bar{x_1}} J^{c_1}_{kk'} (S_{1+} c^{+}_{k'\downarrow} c_{k\uparrow}) \frac{1}{E - H_0 + i\epsilon}$$
$$\sum_{k''k'''} e^{i(k''-k''')\bar{x_2}} J^{c_2}_{k''k'''} (S_{2-} c^{+}_{k'''\downarrow} c_{k''\uparrow}) |FG > + c.c. \tag{4.8}$$

Which may be simplified to:

$$H^{e-e}_{RKKY} = \frac{1}{4} \sum_{kk'} \sum_{k''k'''} e^{i(k-k')\bar{x_1}} e^{i(k''-k''')\bar{x_2}} J^{c_1}_{kk'} J^{c_2}_{k''k'''}$$
$$< FG| c^{+}_{k'\downarrow} c_{k\uparrow} \frac{1}{E - H_0 + i\epsilon} c^{+}_{k'''\downarrow} c_{k''\uparrow} |FG > (S_{1+} S_{2-}) + c.c. \tag{4.9}$$

It is important to take note of the effect of the conduction electron operator on the donor ground state:

$$< FG| c^{+}_{k'\downarrow} c_{k\uparrow} \frac{1}{E - H_0 + i\epsilon} c^{+}_{k'''\downarrow} c_{k''\uparrow} |FG > = < \begin{matrix} ek'' \uparrow \\ hk' \downarrow \end{matrix} | \frac{1}{E - H_0 + i\epsilon} | \begin{matrix} ek''' \uparrow \\ hk \downarrow \end{matrix} > . \tag{4.10}$$

Creating an electron "e" and hole "h" in the ground state wavefunction. The next step is to evaluate the expectation value which gives:

$$< \begin{matrix} ek'' \uparrow \\ hk' \downarrow \end{matrix} | \frac{1}{E - H_0 + i\epsilon} | \begin{matrix} ek''' \uparrow \\ hk \downarrow \end{matrix} > = \frac{\delta_{k'',k'''} \delta_{k',k}}{E - H_0 + i\epsilon'}. \tag{4.11}$$

For the $S_{1+}S_{2-}$ term, the donor-donor interaction which results from a second order conduction electron scattering process is given by

$$H^{e-e}_{RKKY} = \frac{1}{2} \sum_{kk'} e^{i(k'-k)(\bar{x_1}-\bar{x_2})} J^{c_1}_{kk'} J^{c_2}_{k'k} \frac{1}{E_{k'} - E_k + i\epsilon'} (S_{1+} S_{2-}) + c.c. \tag{4.12}$$

This shows clearly how two successive electron scattering events can result in a spin

dependent donor-donor interaction. The full treatment of this scattering process in presented in appendix A.5. We note that ϵ' is the relaxation rate for each conduction electron; in our model this is zero, so the RKKY interaction will be evaluated in the limit $\epsilon' -> 0$. The resulting donor-donor interaction including all terms is found to be

$$H^{e-e}_{RKKY} = J^{e-e}_{RKKY}(S_1 \cdot S_2). \tag{4.13}$$

Where J^{e-e}_{RKKY} is given by

$$J^{e-e}_{RKKY} = -\frac{m * J_c^2}{(8\pi)\hbar^2}\frac{k_F^2 L^4}{2}\frac{sin(2k_F\bar{x})}{(2k_F\bar{x})^2}. \tag{4.14}$$

Where L^2 is the area of the 2DEG (we note that L^4 will drop out of Eq. (4.14) since $J_c \propto \frac{1}{L^2}$), m^* the effective mass of the electron, k_F the fermi wave-vector and k_0 the valley minima. The calculation of the individual interaction strengths J_c^1 and J_c^2 is presented in appendix A.7.

The RKKY expression, Eq. (4.14), is valid when the distance between donors is less than the length scale associated to the thermal coherence of the electron, $l_T = \nu_F \frac{\hbar}{k_B T}$. When the distance between donors is larger than the thermal coherence length of the conduction electrons the information obtained by the first donor would be lost by the time the conduction electron reaches the second donor. Though conduction electrons may establish an interaction between the donors this does not ensure coherent coupling. In the next section we will address the question of whether the RKKY interaction can couple two qubits without degrading their coherence.

4.2 Quality Factor for J^{e-e}_{RKKY} the Electron-Spin Quantum Gate

In order to identify the applicability of the RKKY interaction in quantum computing we will compute the quality factor for a quantum gate based on the RKKY interaction. The quality factor for a quantum gate is given by the ratio of the decoherence time to the gating time [18]. In other words it gives the number of operations that the gate can execute before decoherence takes place. In this section, we calculate the quality factor for a RKKY gate that couples electron spins; in the next section we compute the quality factor for the RKKY nuclear spin quantum gate. For a donor electron the period of coherence for the parallel magnetization is equal to period of phase coherence, thats is $T^e_1 \approx T^e_2$. When $T > T_K$ and $2k_BT > B_e$

$$\frac{1}{T^e_1} = \frac{2\pi}{\hbar}(\pi^2 + \frac{4}{3}|ln(\frac{T}{T_K})^2)^{-1}(2k_BT). \tag{4.15}$$

The quality factor for the RKKY interaction is given by

$$Q^{e-e}_{RKKY} = \frac{\frac{J_{RKKY}}{\pi\hbar}}{\frac{1}{T^e_1}}. \tag{4.16}$$

So, neglecting the oscillatory term in J_{RKKY} the quality factor may be given by

$$Q^{e-e}_{RKKY} = \frac{\frac{\pi\epsilon_F|J\nu_d|^2}{(2k_Fr)^2\pi\hbar}}{(\pi^2 + \frac{4}{3}|ln(\frac{T}{T_K})^2)^{-1}(2k_BT)}. \tag{4.17}$$

Which after some simplification becomes

$$Q^{e-e}_{RKKY} = \frac{1}{4\pi}\frac{\epsilon_F}{k_BT}\frac{1}{(2k_Fr)^2}(\pi^2|J\nu_d|^2 + \frac{4}{3}(|J\nu_d|ln(\frac{T}{T_K}))^2) = (\frac{l_{e-e}}{r})^2 \tag{4.18}$$

where l_{e-e} is the length scale for the coherence of the RKKY interaction, in this limit, see Eq. (2.9)

$$|J\nu_d| ln(\frac{T}{T_K}) \approx |J\nu_d|(\frac{1}{|J\nu_d}| + ln(\frac{k_B T}{\sqrt{23 J_{eff}\nu}})) \tag{4.19}$$

Which is ≈ 1 because $k_B T$ is small due to the low operating temperature. This gives

$$l_{e-e} = \sqrt{(\frac{1}{4\pi}\frac{\epsilon_F}{k_B T}(1 + \pi^2 |J\nu_d|^2))}\frac{1}{2k_F}. \tag{4.20}$$

Since $|J\nu_d| < 1$:

$$l_{e-e} \approx \sqrt{\frac{1}{4\pi}\frac{\epsilon_F}{k_B T}}\frac{1}{2k_F}. \tag{4.21}$$

When $T < T_K$

$$\frac{1}{T_1^e} = \Gamma_{Kondo} = \frac{k_B T_K}{\hbar}. \tag{4.22}$$

The quality factor is then given by

$$Q_{RKKY}^{e-e} = \frac{\frac{\pi\epsilon_F |J\nu_d|^2}{\hbar(2k_F r)^2}}{\frac{k_B T_K}{\hbar}}. \tag{4.23}$$

Which is equivalent to

$$Q_{RKKY}^{e-e} = \frac{\epsilon_F}{k_B T_K}\frac{|J\nu_d|^2}{(2k_F r)^2} = (\frac{l_{e-e}}{r})^2. \tag{4.24}$$

Since $|J\nu_d| < 1$:

$$l_{e-e} \approx \sqrt{\frac{\epsilon_F}{k_B T}}\frac{1}{2k_F}. \tag{4.25}$$

This is very close to the coherence length for the limit when $T > T_K$ except for a factor of 1/4. When $T \approx T_K = 5K$, $\epsilon_F \approx 0.1meV$, $k_B T = 0.43meV$ and $(2k_F)^{-1} = 2 \times 10^2 \mathring{A}$ then

$$l_{e-e}^{T>T_K} \approx l_{e-e}^{T<T_K} \approx 1 \times 10^2 \mathring{A}. \tag{4.26}$$

Unfortunately this length scale is less than ideal. Quantum error correction requires quality factors of at least 10^3, so the electron spin qubits would need to be separated by only a few Angstroms. In addition, at a few angstroms the direct exchange interaction between the donors will dominate any effects of the RKKY interaction.

4.3 Nuclear Spin Interaction

We now take a step back and determine the effective interaction between two donor nuclear spins when a general exchange interaction persists between their electron states. The Hamiltonian for such an interaction may be expressed in terms of the ground state, H_0, with a perturbative potential, V:

$$H_0 = J\vec{S_1} \cdot \vec{S_2} + B_e(S_{1z} + S_{2z}) - B_n(I_{1z} + I_{2z}). \tag{4.27}$$

Where the specific form of perturbation here is the two respective hyperfine interactions:

$$V = A((\vec{S_1} \cdot \vec{I_1}) + (\vec{S_2} \cdot \vec{I_2})). \tag{4.28}$$

Here S is the electron spin operator, I the nuclear spin operator, $B_e = g_e\mu_e B$, $B_n = g_n\mu_n B$ and J is a general exchange energy between the two donors.

The eigenstates of the ground state hamiltonian, with the associated eigenvalues are given by:

Eigenstate	Eigenvalue
$\|\tau_1\tau_2> \|s>$	$E^0 = -\frac{3}{4}J - B_n(\frac{\tau_1+\tau_2}{2})$
$\|\tau_1\tau_2> \|\Uparrow\Uparrow>$	$E^0 = \frac{1}{4}J - B_n(\frac{\tau_1+\tau_2}{2}) + B_e$
$\|\tau_1\tau_2> \|t_0$	$E^0 = \frac{1}{4}J - B_n(\frac{\tau_1+\tau_2}{2})$
$\|\tau_1\tau_2> \|\Downarrow\Downarrow>$	$E^0 = \frac{1}{4}J - B_n(\frac{\tau_1+\tau_2}{2}) - B_e$

Table 4.1: Eigenstates of the ground state Hamiltonian for a pair of donor impurities

Where τ_1, τ_2 represent the donor's nuclear spin states, while the double arrows represent the electronic spin states. The singlet electron state is given as $|s>= \frac{1}{\sqrt{2}}(|\Uparrow\Downarrow> - |\Downarrow\Uparrow>)$ and the entangled triplet state is given as $|t_0>= \frac{1}{\sqrt{2}}(|\Uparrow\Downarrow> + |\Downarrow\Uparrow>)$. To find the effective Hamiltonian between the nuclear spin states second order degenerate perturbation theory in V is used, giving

$$< \tau_1\tau_2|H_{eff}|\tau_1'\tau_2' >= \sum_{\alpha=\Downarrow\Downarrow,S,t_0,\Uparrow\Uparrow} p_\alpha \sum_{\tau_1''\tau_2''\beta}{}' \frac{< \tau_1\tau_2\alpha|V|\tau_1''\tau_2''\beta >< \tau_1''\tau_2''\beta|V|\tau_1'\tau_2'\alpha >}{(E^0_{\tau_1\tau_2\alpha} - E^0_{\tau_1''\tau_2''\beta}) \pm i\Gamma_\beta}. \tag{4.29}$$

Here the states labelled by β represent the intermediary states for the interaction. The interaction is therefore limited principally by the lifetime of the intermediate states which is given in the $\frac{1}{\pm i\Gamma_\beta}$ terms. The $\sum'$ terms exclude states where $|\tau_1''\tau_2''\beta>$ will have equal energy to $|\tau_1\tau_2\alpha>$. p_{alpha} is the occupation probability of conduction electrons with a particular state α. It is assumed here that the electrons are in a mixed density matrix state. Eq. (4.29) then becomes:

$$H_{eff} = A^2 \sum_\alpha p_\alpha \sum_{\tau_1''\tau_2''\beta}{}' \frac{((\vec{I_1})_{\tau_1\tau_1''}\delta_{\tau_2\tau_2''} \cdot (\vec{S_1})_{\alpha\beta} + (\vec{I_2})_{\tau_2\tau_2''}\delta_{\tau_1\tau_1''} \cdot (\vec{S_2})_{\alpha\beta})(\vec{I_1})_{\tau_1''\tau_1'}\delta_{\tau_2''\tau_2'}}{(E^0_{\tau_1\tau_2\alpha} - E^0_{\tau_1''\tau_2''\beta}) \pm i\Gamma_\beta}$$
$$\cdot ((\vec{S_1})_{\alpha\beta} + (\vec{I_2})_{\tau_2''\tau_2'}\delta_{\tau_1''\tau_1'} \cdot (\vec{S}_{2\beta\alpha})). \tag{4.30}$$

Combining terms, while requiring the result to be Hermitian, gives rise to

$$H_{eff} = A^2 \sum_{\alpha} p_{\alpha} (\sum_{\beta} (\frac{\vec{I}_{1\tau_1\tau_1'} \cdot \vec{S}_{1\alpha\beta} \vec{I}_{2\tau_2\tau_2'} \vec{S}_{2\beta\alpha}}{(E^0_{\tau_1\tau_2\alpha} - E^0_{\tau_1'\tau_2\beta}) + i\Gamma_{\beta}} + \frac{\vec{I}_{2\tau_2\tau_2'} \cdot \vec{S}_{2\alpha\beta} \vec{I}_{1\tau_1\tau_1'} \vec{S}_{1\beta\alpha}}{(E^0_{\tau_1\tau_2\alpha} - E^0_{\tau_1\tau_2'\beta}) - i\Gamma_{\beta}} + ...). \quad (4.31)$$

Where .... equals terms like $(\vec{I}_1\vec{I}_1 + \vec{I}_2\vec{I}_2) = I_z^2$ which only add a global phase. Performing the sum over all possible intermediate states β gives

$$H_{eff} = A^2 \sum_{\alpha} p_{\alpha} ((\vec{I}_1)_{\tau_1\tau_1'} \cdot [(\sum_{\beta} \frac{< \alpha|\vec{S}_1|\beta >< \beta|\vec{S}_2|\alpha >}{(E^0_{\tau_1\tau_2\alpha} - E^0_{\tau_1'\tau_2\beta}) + i\Gamma_{\beta}})] \cdot (\vec{I}_2)_{\tau_2\tau_2'} + ...). \quad (4.32)$$

Using $\alpha =\Uparrow\Uparrow$, $\Downarrow\Downarrow$, s, and t_0. The combined result for the donor-donor nuclear spin interaction is

$$H_{eff} = \frac{A^2}{32}((p_e(1-2p_e)\frac{J - B - i\Gamma_{\beta}}{(J-B)^2 + \Gamma_{\beta}^2} - p_e(1+2p_e)\frac{J + B + i\Gamma_{\beta}}{(J+B)^2 + \Gamma_{\beta}^2} + 2p_e\frac{2(B + i\Gamma_{\beta})}{B^2 + \Gamma_{\beta}^2})I_{1+}I_{2-} + h.c.). \quad (4.33)$$

Which is valid when $J \neq \pm B$ so that none of the denominators go to zero.

It is possible to create an interaction of the form $J^{n-n}I_1 \cdot I_2$ by applying single qubit rotations to change

$$e^{iJ'_{n-n'}(I_{1+}I_{2-} + I_{1-}I_{2+})} \rightarrow e^{iJ'_{n-n'}(I_{1z}I_{2z})}. \quad (4.34)$$

Then performing the H_{eff} operation twice while rotating one application would give

$$(I_{1+}I_{2-} + I_{1-}I_{2+})R^{2*}_{\hat{x}}(\frac{\pi}{2})R^{1*}_{\hat{x}}(\frac{\pi}{2})R^{2*}_{\hat{y}}(\frac{\pi}{2})R^{1*}_{\hat{y}}(\frac{\pi}{2})(I_{1+}I_{2-} + I_{1-}I_{2+})R^{1}_{\hat{y}}(\frac{\pi}{2})R^{2}_{\hat{y}}(\frac{\pi}{2})R^{1}_{\hat{x}}(\frac{\pi}{2})R^{2}_{\hat{x}}(\frac{\pi}{2}) = I_1 \cdot I_2. \quad (4.35)$$

A general exchange interaction is therefore capable of producing a donor-donor nuclear spin exchange interaction. The critical remaining question is what quality factor is this interaction going to have.

4.4 Quality Factor for J^{n-n} the Nuclear-Spin Quantum Gate

We now compute the quality factor for the nuclear spin qubit RKKY quantum gate. J and B are controllable and may take any value so there are various regimes in which H_{eff} may operate and all must be examined to determine if one may be ideal. The first regime is that when B dominates. There are two possible cases in this regime, namely when $B >> \Gamma_\beta >> J$ or when $B >> J >> \Gamma_\beta$. In the regime of large magnetic field H_{eff} may be simplified to

$$H_{eff} = \frac{1}{4}(\frac{A}{B})^2 J p_e^2 (\frac{I_{1+}I_{2-}}{2} + h.c.). \tag{4.36}$$

In the limit when $\Gamma_\beta << A$:

$$\frac{1}{T_2^n} = \frac{\Gamma_\beta}{2}. \tag{4.37}$$

The quality factor for the phase coherence is then given by

$$Q_{n-n} = \frac{1}{\pi}\frac{\frac{1}{4}(\frac{A}{B})^2 J p_e^2}{\frac{\Gamma_\beta}{2}} = \frac{1}{2}(\frac{A}{B})^2 p_e^2 Q_{e-e} << Q_{e-e}. \tag{4.38}$$

Where Q_{e-e} is the quality factor for the electron spin qubit gate. Therefore Q_{n-n} can never be large in this regime. When $B >> \Gamma_\beta >> J$ both Q_{e-e} and Q_{n-n} are also bad. When $\Gamma_\beta >> A$

$$\frac{1}{T_2^n} = \frac{A^2}{4\Gamma_\beta}. \tag{4.39}$$

The quality factor is then given as

$$Q_{n-n} = \frac{1}{\pi}\frac{\frac{1}{4}(\frac{A}{B})^2 J p_e^2}{\frac{A^2}{4\Gamma_\beta}} = (\frac{\Gamma_\beta}{B})^2 p_e^2 Q_{e-e} << Q_{e-e}. \tag{4.40}$$

Which is small in all cases.

In the second regime, that of large J, $J >> B >> \Gamma_\beta$ or $J >> \Gamma_\beta >> B$ H_{eff} may be simplified to

$$H_{eff} = -\frac{1}{8}(\frac{A^2}{J})p_e^2(\frac{I_{1+}I_{2-}}{2} + h.c.). \tag{4.41}$$

When $\Gamma_\beta << A$ the quality factor for the phase coherence is

$$Q_{n-n} = \frac{1}{\pi}\frac{\frac{1}{8}(\frac{A^2}{J})p_e^2}{\frac{\Gamma_\beta}{2}} = \frac{1}{4}(\frac{A}{J})^2 p_e^2 Q_{e-e} << Q_{e-e}. \tag{4.42}$$

Which is small in all cases. When $\Gamma_\beta >> A$ the quality factor is

$$Q_{n-n} = \frac{1}{\pi}\frac{\frac{1}{8}(\frac{A^2}{J})p_e^2}{\frac{A^2}{4\Gamma_\beta}} = \frac{1}{2}(\frac{\Gamma_\beta}{J})^2 p_e^2 Q_{e-e} << Q_{e-e}. \tag{4.43}$$

Which again is small in all cases.

Putting all this together, because of the intermediate state decay it is clear no matter what regime you are in the quality factor for the phase coherence is less that Q_{e-e}. This is of serious concern as the de-phasing of the qubits will cause loss of information during the process of operation. This demonstrates a critical limit on any possible attempt of performing operation with the RKKY interaction. The final requirement we were treating was a capability to perform operation. The hope was that conduction electrons would be capable of mediating a exchange interaction between the donors known as the RKKY interaction. This, however, is simply not possible. Any attempt at formulating a working quantum computing design, therefore, cannot rely on the RKKY interaction for coupling.

Chapter 5

An attempt to design a Quantum Computer

It is now time to look back in an attempt to formulate a quantum computing design. As coupling must be achieved thought the direct exchange interaction and readout/ initialization though 2DEG interactions both can not operate in the same regime. Two distinct design regimes are therefore presented here.

5.1 Readout and Initialization Regime

The design for readout and initialization requires a 2DEG situated above the donors to act as a conduit to ensure the conduction and donor electrons interact, in sufficient strength. The necessary tuning for readout and initialization can be accomplished by adjusting the thickness of the 2DEG with at top gate to switch between the weak and strong regimes.

We need to apply an external magnetic field in order to generate donor Zeeman splitting and a 2DEG spin polarization. To avoid Landau levels in the 2DEG, the magnetic field has to be applied along the 2DEG plane.

A figure depicting a possible design for performing readout and initializations is presented below.

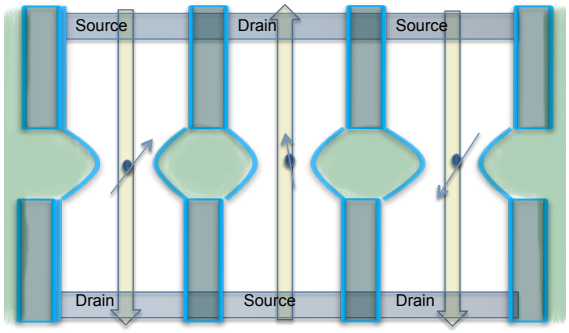


Figure 5.1: Top view of the proposed device for Qubit Readout and Initialization

Here the 2DEG formation gates produce a potential which confines the electrons to the two-dimensional electron gas, represented by the areas shown in white. Gates situated above the 2DEG induce a voltage from source to drain causing a current to flow. Additional gates situated above the 2DEG provide a means of depleting the electron density in specific areas, shown in green, confining the current to a path that transits over one specific donor. Presented next is a side view of the same design.

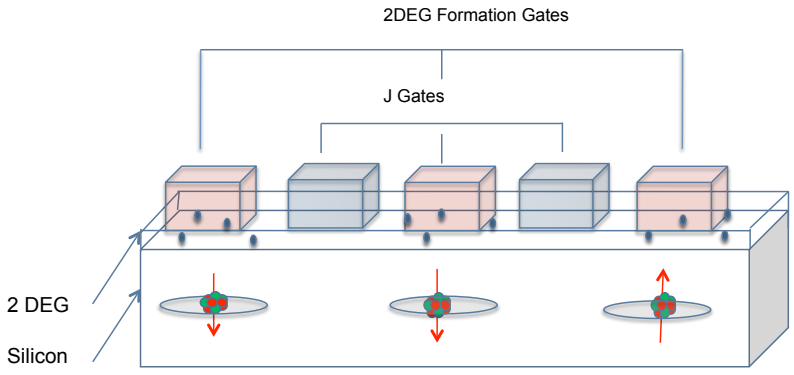


Figure 5.2: Electric readout and Initialization

The donor separation gates, J gates, ensure that no two donors interact through direct exchange during the period of measurement. The J gates also guarantee the applied current can only interact with a single donor; preventing coupling through

the RKKY interaction. Individual addressability of qubits can be achieved with a global applied field because a current is used for readout. It is therefore possible to pick qubits for measurement by running a current over them.

5.2 Coupling Regime

Two qubit coupling must be done by depleting the 2DEG with a top gate and using a J gate to induce the direct exchange interaction, shown in white [13]. The quality factor can be extremely large due to the very long nuclear spin coherence times when the donor is not overlapping with a 2DEG. This is because when the current is turned off, we hope that the qubit coherence will be similar to coherence measurements of a few seconds found by Morton et. al. [1]. While the coherence measurement of a nuclear spin qubit situated with an EDMR device has never been done we do hope this would be the case if the Si/Si_2O_3 interface is passivated [6]. Here is a figure showing a possible design accomplishing this requirement:

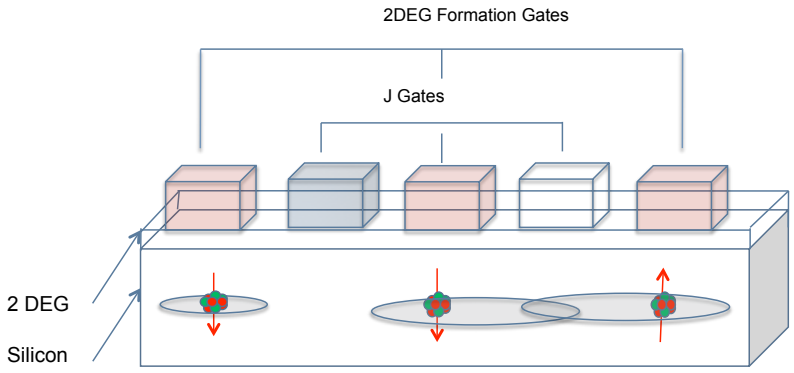


Figure 5.3: Coupling through Direct Exchange

The J gates, if tuned precisely, may be used to induce the direct exchange interaction between two donors without inducing a 2DEG. This would entail a double usage in the usual J gates to deplete the 2DEG and promote the direct exchange. Device modelling would need to be done to determine the exact operating regime but

in theory it seems plausible. The ability of performing individual single qubit rotations is an integral part of universal gate operation. NMR is a convenient means of performing single qubit rotations. An external oscillating magnetic field can be used to rotate the spin states of individual donor nuclei. To achieve this with individual qubit addressability we suggest the use of the micro-magnet technology developed by Pioro-Ladriére et. al. [19].

5.3 The DiVincenzo Requirements Revisited

For any quantum computing architecture to be viable it must meet all the DiVincenzo requirements introduced in chapter one.

1) A quantum computer must have well defined qubits.

The most stable qubits are formed by a donor's nuclear spin state aligned with or against a global field. The resulting two state system is as easy to distinguish as any quantum system may be. As silicon can be engineered almost entirely in its spin zero state it offers an ideal substrate for a spin based qubits.

2) Qubits must be stable enough to allow multiple operations.

When not interacting with the 2DEG, both the donor electron and nuclear spins have extremely long coherence times [1]. During the process of EDMR conduction electron will be present within the 2DEG in this case we showed that so long as the EDMR sensitivity is above the lower limit set by the shot noise detection is indeed possible.

3) Any quantum computer must have the ability to be set into any state of choice.

Chapter 2 established the use of conduction electrons in the strong coupling regime to perform fast initialization of nuclear spin qubits.

4) Qubits must be measurable to obtain the desired information.

Single spin measurements are possible through the use of electrically detected magnetic resonance (EDMR)[7]. The current over a donor can be measured as a function of applied perpendicular magnetic field. When the applied field is in resonance with the donor electron spin the current will decrease due to an increase in the scattering cross-section. The orientation of the donor's nuclear spin will alter the resonant frequency of the donor electron spin. Based on the applied field that demonstrates a decrease in measured current the donor spin orientation may be identified. This scheme uses the donor electron as a method to read-out the donor nuclear spin.

5) A set of universal gates must be operational, that is have a functional form within the computer.

Single qubit rotations can be performed through Nuclear Magnetic Resonance (NMR). This is achieved by applying an oscillating magnetic field perpendicular to the nuclear spin orientation.

The ability to take a quantum state, one qubit or two, and evolve it to any other state constitutes the major requirement of quantum computation. Any architecture must demonstrate the ability to achieve this requirement. The direct exchange interaction (with the 2DEG-donor overlap turned off) possess a great quality factor and as such would constitute an ideal realization of coupling.

Chapter 6

Conclusions

The objective of this work was to fully explore an architecture for silicon-based quantum computing that uses conduction electrons for quantum control of donor impurity nuclear spins. Our hope was that conduction electrons would provide all the required control for universal quantum computation, initialization and readout.

Our first task was to understand the effect conduction electrons had on the donor electron and nuclear spin dynamics. The results of this interaction tends to draw the donor electrons into thermal equilibrium with the conduction electron sea. The relaxation rate of the nuclear spin was not known to follow the electron's or act independently. When the hyperfine coupling, A, is greater than the transition rate for donor electron spin $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$, we got $\frac{1}{T_2^n} \approx \frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}{2}$ and $\frac{1}{T_1^n} \approx \frac{1}{2}(\frac{A}{g_e\mu_e B})^2(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$. In the opposite limit when the hyperfine coupling is much smaller than the transition rate we got instead $\frac{1}{T_1^n} \approx \frac{2}{T_2^n} \approx \frac{A^2}{2(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}$. In the former regime we see that the nuclear spin coherence tends to follow the electron's, while in latter regime the nuclear spin is approximately decoupled from the electron, signalling motional narrowing behaviour. Therefore, the nuclear spin dynamics are critically dependent on the electron spin dynamics. When $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \approx g_e\mu_e B/\hbar$, $\frac{1}{T_1^n}$ is maximized. This offered a convenient

means of fast qubit initialization.

The next task was to establish a means of coupling donors with an electric current. A current will couple donors through the RKKY interaction, however we showed that it also destroys qubit coherence. In other words, the quality factor (the number of two-qubit quantum operations before decoherence takes place) was really poor. This was a disappointment as conduction electrons failed to mediate two-qubit operations. Therefore we proposed the use of a mixed architecture whereby conduction electrons are used for readout/ initialization and the donor-donor direct exchange interaction is used for coupling. So long as an interaction between the donors and the 2DEG is turned off, the direct exchange between donors can provide a high quality factor [13].

The most important result of this work was the establishment of the criteria for quantum readout through conduction electron scattering. We were able to identify the effects of conduction electrons on the nuclear spin qubit coherence and determined the regime for optimal qubit initialization with an electric current. We were also able to place a limit on the minimum required sensitivity for the readout of single nuclear spin qubits with EDMR.

In conclusion the exploration into the use of conduction electrons for quantum control produced some interesting results. Single nuclear spin qubit readout was shown to be possible with initialization times far faster than conventional NMR. Therefore, we established a quantum computer architecture based on nuclear spins that relies on conduction electrons for quantum read-out and initialization. For coherent entanglement, however, we argue that the usual direct exchange interaction is the best option.

Appendix A

Appendix

A.1 NMR and ESR

An introduction to the theory of spin resonance will serve to describe the function of performing individual spin rotations and add further context to understanding the dynamics of atomic spin states. The dynamics of spin state under the influence of an applied magnetic field is given by the Landau-Lifshitz-Gilbert equation, the derivation of which is shown here.

Starting with the time evolution of density operator subject to the applied magnetic field hamiltonian:

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}]. \tag{A.1}$$

Where the ground state Hamiltonian is given by

$$\hat{H} = \frac{g\mu_B}{2}(\hat{\sigma} \cdot \vec{B}). \tag{A.2}$$

With

$$\rho = \frac{1}{2}(\mathbb{1} + \vec{M} \cdot \hat{\sigma}). \tag{A.3}$$

Putting this all together gives

$$\frac{1}{2}\frac{d\vec{M}}{dt}\cdot\hat{\sigma} = \frac{g\mu_B}{4i\hbar}[B\cdot\hat{\sigma}, \vec{M}\cdot\hat{\sigma}]. \tag{A.4}$$

Taking note that

$$\begin{aligned}[B_i\sigma_i, M_i\sigma_i] &= B_iM_j[\sigma_i,\sigma_j] \\ &= 2i\epsilon_{ijk}\sigma_kB_iM_j \\ &= 2i(\vec{B}\times\vec{M})\cdot\hat{\sigma}. \end{aligned} \tag{A.5}$$

Results in

$$\frac{dM}{dt} = \gamma B(t)\times M. \tag{A.6}$$

Where $\gamma = \frac{g\mu}{\hbar}$. Assuming the spins are polarized in the $\hat{z}$ direction, the applied magnetic fields is given by

$$B = -B_\perp(cos(\omega t)\hat{x} + sin(\omega t)\hat{y}) + B_0\hat{z}. \tag{A.7}$$

Plugging this into the Landau-Lifshitz-Gilbert equation gives;

$$\frac{\partial M_x}{\partial t} = -\omega_0M_y - \omega_\perp sin(\omega t)M_z, \tag{A.8}$$

$$\frac{\partial M_y}{\partial t} = \omega_0M_x + \omega_\perp cos(\omega t)M_z \tag{A.9}$$

and

$$\frac{\partial M_z}{\partial t} = \omega_\perp sin(\omega t)M_x - \omega_\perp cos(\omega t)M_y. \tag{A.10}$$

Moving to a rotating reference frame the magnetization equations are then given by;

$$M_x = M'_x cos(\omega t) + M'_y sin(\omega t), \tag{A.11}$$

$$M_y = M'_x sin(\omega t) - M'_y cos(\omega t), \tag{A.12}$$

$$M_z = M'_z. \tag{A.13}$$

Putting this all together gives

$$\begin{aligned} \frac{\partial M_x}{\partial t} &= \frac{\partial M'_x}{\partial t} cos(\omega t) - \omega M'_x sin(\omega t) + \frac{\partial M'_y}{\partial t} sin(\omega t) + \omega M'_y cos(\omega t) \\ &= -\omega_0 (M'_x sin(\omega t) - M'_y cos(\omega t)) - \omega_\perp cos(\omega t) M'_z. \end{aligned} \tag{A.14}$$

Collecting terms in cosine gives

$$\frac{\partial M'_x}{\partial t} = (\omega_0 - \omega) M'_y. \tag{A.15}$$

Collecting terms in sine gives

$$\frac{\partial M'_y}{\partial t} = (\omega_0 - \omega) M'_x - \omega_\perp M'_z, \tag{A.16}$$

$$\frac{\partial M'_z}{\partial t} = \omega_\perp M'_y. \tag{A.17}$$

These equations are equivalent to

$$\frac{\partial M'}{\partial t} = (\omega') M'. \tag{A.18}$$

Where $\omega' = \omega_\perp \hat{x} + (\omega_0 - \omega)\hat{z}$. When $\omega_0 = \omega$ then $(\omega_0 - \omega) = 0$ and $\omega' = \omega_\perp \hat{x}$ allowing for spin flips.

A.2 The Swap and Square-root of Swap Gates

The two qubit swap gate may be expressed as

$$e^{\frac{-i}{\hbar}J_{n-n}I_1\cdot I_2 t}|\uparrow\downarrow>=|\downarrow\uparrow> . \tag{A.19}$$

It is useful to redefine the wavefunctions in terms of the singlet and triplet wavefunctions as they are eigen-kets of the $I_1 \cdot I_2$ operator;

$$|\uparrow\downarrow>=(|S>+|t_0>), \tag{A.20}$$

$$|\downarrow\uparrow>=(-|S>+|t_0>). \tag{A.21}$$

Where $|S>$ is the singlet state $(\frac{1}{\sqrt{2}}|\uparrow\downarrow> -\frac{1}{\sqrt{2}}|\downarrow\uparrow>)$ and $|t_0>$ is the spin zero triplet state $(\frac{1}{\sqrt{2}}|\uparrow\downarrow> +\frac{1}{\sqrt{2}}|\downarrow\uparrow>)$. The eigenvalues are of the $I_1 \cdot I_2$ operator are;

$$I_1 \cdot I_2|S>=(-\frac{3}{4})|S>, \tag{A.22}$$

$$I_1 \cdot I_2|t_0>=(\frac{1}{4})|t_0> . \tag{A.23}$$

Putting this together gives

$$e^{\frac{-i}{\hbar}J_{n-n}t\frac{-3}{4}}|S>+e^{\frac{-i}{\hbar}J_{n-n}t\frac{1}{4}}|t_0>)=(-|S>+|t_0>). \tag{A.24}$$

Factoring out $e^{\frac{-i}{\hbar}J_{RKKY}t\frac{1}{4}}$ gives

$$e^{\frac{-i}{\hbar}J_{n-n}t\frac{1}{4}}(e^{\frac{-i}{\hbar}J_{n-n}}|S>+|t_0>). \tag{A.25}$$

So if $\frac{J_{n-n}}{\hbar}t = \pi$ then $e^{\frac{-i}{\hbar}J_{n-n}t} = -1$ This requires that the time of interaction be precisely to $t = \frac{\hbar\pi}{J_{n-n}}$ and then the two-qubit swap operation can be performed. The swap gate alone cannot perform the required operations as it does not act to entangle the qubits. This is where square root of swap gate is important as it does entangle the qubits. It can be shown that entanglement is accomplished when $J_{n-n}t = \frac{\pi}{2}$:

$$e^{-i\frac{\pi}{8}}(e^{i\frac{\pi}{2}}|S> + |t_0>). \tag{A.26}$$

Which is equivalent to

$$e^{-i\frac{\pi}{8}}(i|S> + |t_0>). \tag{A.27}$$

Substituting the spin wavefunction for $|S>$ and $|t_0>$ gives

$$e^{-i\frac{\pi}{8}}(i(\frac{1}{\sqrt{2}}|\uparrow\downarrow> - \frac{1}{\sqrt{2}}|\downarrow\uparrow>) + (\frac{1}{\sqrt{2}}|\uparrow\downarrow> + \frac{1}{\sqrt{2}}|\downarrow\uparrow>)). \tag{A.28}$$

The result seems clearly to be an entangled state.

A.3 Derivation of the Donor Electron Transition Rate $(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$

The interacting potential is explicitly given by

$$H_{ce} = J_{eff}\sum_{k,k'}(S_- c^{\dagger}_{k'\uparrow}c_{k\downarrow} + S_+ c^{\dagger}_{k'\downarrow}c_{k\uparrow} + S_z(c^{\dagger}_{k'\uparrow}c_{k\uparrow} + c^{\dagger}_{k'\downarrow}c_{k\downarrow}). \tag{A.29}$$

Each transition rate may individually be determined by exploiting Fermi's Golden Rule, given for ($\Gamma_{\Uparrow}$):

$$\Gamma_{\Uparrow} = \frac{2\pi}{\hbar} < \sum_{k,k'} J_{eff}^2 | < f|S_- c_{k'\uparrow}^\dagger c_{k\downarrow}|i > |^2 \delta(\epsilon_i - \epsilon_f) > . \tag{A.30}$$

The initial state is given as $|i>=|FS>|\Uparrow>$ with energy $\epsilon_i = \frac{g_e \mu_e B}{2} + E_{FS}$ where $|FS>$ is the state for the Fermi sea. The final state is given as $|f>=|FS + \overset{ek'\uparrow}{hk\downarrow}>$ $|\Downarrow>$ with energy $\epsilon_f = -\frac{g_e \mu_e B}{2} + E_{FS} + \epsilon_{k'\uparrow} - \epsilon_{k\downarrow}$. The final state may be written by identifying the fact that

$$|f>=|FS + \overset{ek'\uparrow}{hk\downarrow}>|\Downarrow>= c_{k'\uparrow}^\dagger c_{k\downarrow}|FS>|\Downarrow> . \tag{A.31}$$

Then

$$< f|S_- c_{k'\uparrow}^\dagger c_{k\downarrow}|i >=<\Downarrow |S_-| \Uparrow>< FS|c_{k\downarrow}^\dagger c_{k'\uparrow} c_{k'\uparrow}^\dagger c_{k\downarrow}|FS> . \tag{A.32}$$

The creation/annihilation commutation relations are given by

$$[c_{k\downarrow}^\dagger, c_{k'\uparrow}] = 0. \tag{A.33}$$

The same holds for all variations were the operators are not acting upon the same states. When they are acting on the same states the commutation relation is given by

$$[c_{k\uparrow}^\dagger, c_{k'\uparrow}] = 1. \tag{A.34}$$

This allows expectation value to be expressed as

$$< f|S_- c_{k'\uparrow}^\dagger c_{k\downarrow}|i >=<\Downarrow |S_-| \Uparrow>< FS|(c_{k\downarrow}^\dagger c_{k\downarrow})(1 - c_{k'\uparrow}^\dagger c_{k'\uparrow})|FS> . \tag{A.35}$$

Where

$$c^{\dagger}_{k\downarrow}c_{k\downarrow} = \eta_{k\downarrow}; \tag{A.36}$$

$$c^{\dagger}_{k'\uparrow}c_{k'\uparrow} = \eta_{k'\uparrow}. \tag{A.37}$$

ν is either 1 if the state is filled or 0 if it is vacant and is therefore equal to its own square. This gives

$$< \eta_{k\downarrow}(1-\eta_{k'\uparrow})\delta(\epsilon_i - \epsilon_f >= f(\epsilon_{k\downarrow})(1-f(\epsilon_{k'\uparrow}))\delta(g_e\mu_e B + \epsilon_{k'\uparrow} - \epsilon_{k\downarrow}). \tag{A.38}$$

Where the Fermi distribution $f(\epsilon)$ is given by

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon-\epsilon_f)}+1}. \tag{A.39}$$

So the transition rate of a spin down donor electron to a spin up becomes

$$\Gamma_{\Uparrow} = \frac{2\pi}{\hbar}\sum_{k,k'} J^2_{eff} f(\epsilon_{k\downarrow})(1-f(\epsilon_{k'\uparrow}))\delta(g_e\mu_e B + \epsilon_{k'\uparrow} - \epsilon_{k\downarrow}). \tag{A.40}$$

Performing an analytic continuation taking $\sum_k \rightarrow \nu\int d\epsilon$ and $\sum_{k'} \rightarrow \nu\int d\epsilon'$, where the energy density of the 2DEG is $\nu = \frac{L^2}{2\pi}\frac{m*}{\hbar^2}$, gives

$$\Gamma_{\Uparrow} = \frac{2\pi}{\hbar}\int_0^{\infty} d\epsilon \int_0^{\infty} d\epsilon' |\nu J_{eff}|^2 f(\epsilon)(1-f(\epsilon'))\delta(g_e\mu_e B + \epsilon' - \epsilon). \tag{A.41}$$

Evaluating the delta function:

$$\Gamma_{\Uparrow} = \frac{2\pi}{\hbar}\int_0^{\infty} d\epsilon |\nu J_{eff}|^2 f(\epsilon)(1-f(\epsilon - g_e\mu_e B)). \tag{A.42}$$

Changing variables to $x = \beta(\epsilon - \epsilon_f) - \frac{\beta}{2}g_e\mu_e B$ and extending integration to x from

$(-\infty, \infty)$ while redefining $\beta g_e \mu_e B = \tilde{B}$ gives

$$Gamma_{\Uparrow} = \frac{2\pi}{\hbar}|\nu J_{eff}|^2 \frac{1}{\beta}\int_{-\infty}^{\infty} dx(\frac{1}{e^{x+\frac{\tilde{B}}{2}}+1})(1-\frac{1}{e^{x-\frac{\tilde{B}}{2}}+1}). \tag{A.43}$$

It is convenient to rearrange this to

$$Gamma_{\Uparrow} = \frac{2\pi}{\hbar}|\nu J_c|^2 \frac{1}{\beta}[\int_{-\infty}^{\infty} dx(\frac{1}{e^{x+\frac{\tilde{B}}{2}}+1}) - \int_{-\infty}^{\infty} dx(\frac{e^{-\frac{\tilde{B}}{2}}}{e^x+e^{-\frac{\tilde{B}}{2}}})(\frac{e^{\frac{\tilde{B}}{2}}}{e^x+e^{\frac{\tilde{B}}{2}}})]. \tag{A.44}$$

Making use of the fact that $\frac{1}{ab} = \frac{1}{b-a}(\frac{1}{a}-\frac{1}{b})$ the terms within the brackets $[\dots]$ can be rearranged again to give

$$[\dots] = \int_{-\infty}^{\infty} dx(\frac{1}{e^{x+\frac{\tilde{B}}{2}}+1}) - \frac{1}{e^{\frac{\tilde{B}}{2}}-e^{-\frac{\tilde{B}}{2}}}\int_{-\infty}^{\infty} dx(\frac{1}{e^x+e^{-\frac{\tilde{B}}{2}}} - \frac{1}{e^x+e^{\frac{\tilde{B}}{2}}}). \tag{A.45}$$

Which could alternatively be written:

$$[\dots] = \lim_{\Lambda\to\infty}\int_{-\Lambda}^{\Lambda} dx(\frac{1}{e^{x+\frac{\tilde{B}}{2}}+1}) - \frac{1}{sinh(\frac{\tilde{B}}{2})}(e^{\frac{\tilde{B}}{2}}\int_{-\Lambda}^{\Lambda} dx\frac{1}{e^{x+\frac{\tilde{b}}{2}}+1} - e^{-\frac{\tilde{B}}{2}}\int_{-\Lambda}^{\Lambda} dx\frac{1}{e^{x-\frac{\tilde{b}}{2}}+1}). \tag{A.46}$$

Where

$$\int_{-\Lambda}^{\Lambda} dx(\frac{1}{e^{x+\frac{\tilde{B}}{2}}+1}) = \lim_{\Lambda\to\infty} ln(\frac{e^{\Lambda+\frac{\tilde{B}}{2}}+1}{e^{-\Lambda+\frac{\tilde{B}}{2}}+1}) \to (\Lambda+\frac{\tilde{B}}{2}). \tag{A.47}$$

This then gives

$$[\dots] = (\Lambda+\frac{\tilde{B}}{2}) - \frac{1}{2sinh(\frac{\tilde{B}}{2})}(2sinh(\frac{\tilde{B}}{2})\Lambda + \tilde{B}cosh(\frac{B}{2})). \tag{A.48}$$

Which after some cancelation equals

$$\frac{\tilde{B}}{2}(1-\frac{cosh(\frac{\tilde{B}}{2})}{sinh(\frac{\tilde{B}}{2})}). \tag{A.49}$$

Which may be rewritten as

$$\frac{\tilde{B}}{2}(1-\frac{e^{\frac{\tilde{B}}{2}}+e^{-\frac{\tilde{B}}{2}}}{e^{\frac{\tilde{B}}{2}}-e^{-\frac{\tilde{B}}{2}}})=\tilde{B}(\frac{e^{\frac{\tilde{B}}{2}}}{e^{\frac{\tilde{B}}{2}}-e^{-\frac{\tilde{B}}{2}}})=\tilde{B}\frac{1}{1-e^{-\tilde{B}}}. \tag{A.50}$$

Putting this all together results in

$$[\dots]=\tilde{B}(1+\frac{1}{e^{\tilde{B}}-1})=\tilde{B}(1+f_{Bose}(\tilde{B})). \tag{A.51}$$

The transition rate $\Gamma_{\Uparrow}$ is then given by

$$\Gamma_{\Uparrow}=\frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B(1+f_{Bose}(g_e\mu_e B)). \tag{A.52}$$

$\Gamma_{\Downarrow}$ is found through the same procedure, however, with $B\rightarrow -B$:

$$\Gamma_{\Downarrow}=\frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B(f_{Bose}(g_e\mu_e B)). \tag{A.53}$$

FInally putting this two results together gives

$$(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})=\frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B(1+\frac{2}{e^{\tilde{B}}-1}). \tag{A.54}$$

Where

$$(1+\frac{2}{e^{\tilde{B}}-1})=\frac{e^{\tilde{B}}-1+2}{e^{\tilde{B}}-1}=\frac{1+e^{\tilde{B}}}{e^{\tilde{B}}-1}=\frac{e^{\frac{\tilde{B}}{2}}+e^{-\frac{\tilde{B}}{2}}}{e^{\frac{\tilde{B}}{2}}-e^{-\frac{\tilde{B}}{2}}}=coth(\frac{\tilde{B}}{2}). \tag{A.55}$$

The final result is

$$(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})=\frac{2\pi}{\hbar}|J_{eff}\nu|^2 g_e\mu_e B coth(\frac{g_e\mu_e B}{2k_B T}). \tag{A.56}$$

A.4 Decoherence Derivation

Here a full derivation of the electron and nuclear spin dependancies is developed. With this in mind the density matrix may be rewritten as

$$\hat{\rho}(t) = \frac{1}{4}[\mathbb{1}_{4x4} + (\vec{M}_S \cdot \vec{\sigma}) \otimes \tau_0 + \sigma_0 \otimes (\vec{M}_I \cdot \vec{\tau}) + \sum_{(i\neq 0, j\neq 0)} \eta_{ij}(t)\sigma_i \otimes \tau_j]. \tag{A.57}$$

An accurate description of decoherence is only possible through an examination of the time evolution of the density matrix broken into its composite parts. The final term from above can be simplified by noting

$$(\sigma_1\hat{\rho}\sigma_1 + \sigma_2\hat{\rho}\sigma_2 + \sigma_3\hat{\rho}\sigma_3 - 3\hat{\rho}) = -\sum_{i\neq 0} \eta_{ij}(\hat{\sigma}_i \otimes \hat{\tau}_j) = -(\vec{M}_S \cdot \vec{\sigma}) \otimes \tau_0 - \vec{\sigma} \cdot \vec{N} \cdot \vec{\tau}. \tag{A.58}$$

The next step is to simplify the commutator relation:

$$[H_0, \hat{\rho}] = \frac{1}{4}[\underbrace{\frac{1}{2}\vec{B}_e \cdot \vec{\sigma}}_{1} - \underbrace{\frac{1}{2}\vec{B}_n \cdot \vec{\tau}}_{2} + \underbrace{\frac{A}{4}\vec{\sigma} \cdot \vec{\tau}}_{3}, \sum_{(i,j)\neq(0,0)} \eta_{ij}(t)\sigma_i \otimes \tau_j]. \tag{A.59}$$

The result for the commutation relation for term 1 is that

$$[\frac{1}{2}\vec{B}_e \cdot \vec{\sigma}, \sum_{(i,j)\neq(0,0)} \eta_{ij}(t)\sigma_i \otimes \tau_j] = \frac{1}{4}i((\vec{B}_e \times \vec{M}_S) \cdot \vec{\sigma} \otimes \tau_0 + \vec{\sigma} \cdot (\vec{B}_e \times (\vec{N} \cdot \vec{\tau}))). \tag{A.60}$$

Where $\vec{N} = \eta_{ij}\hat{e}_i\hat{e}_j$. Similarly the result for the commutation relation for terms 2 is

$$[\frac{1}{2}\vec{B}_n \cdot \vec{\tau}, \sum_{(i,j)\neq(0,0)} \eta_{ij}(t)\sigma_i \otimes \tau_j] = -\frac{1}{4}i(\sigma_0 \otimes (\vec{B}_n \times \vec{M}_I) \cdot \vec{\tau} + \vec{\tau} \cdot (\vec{B}_n \times (\vec{\sigma} \cdot \vec{N}))). \tag{A.61}$$

The more difficult contribution comes from term 3 and is found to be

$$[\frac{A}{4}\vec{\sigma}\cdot\vec{\tau}, \sum_{(i,j)\neq(0,0)} \eta_{ij}(t)\sigma_i\otimes\tau_j] = \frac{A}{8}i((\vec{M}_S\times\vec{\sigma})\cdot\vec{\tau}+\vec{\sigma}\cdot(\vec{M}_I\times\vec{\tau})+(\vec{\sigma}\times\vec{\tau})\cdot(\vec{N}\cdot\vec{\tau})-(\vec{\sigma}\cdot\vec{N})\cdot(\vec{\sigma}\times\vec{\tau})). \tag{A.62}$$

Substituting these expressions gives

$$\frac{d\hat{\rho}}{dt} = \frac{1}{4}(\vec{M}_S\cdot\vec{\sigma})\otimes\tau_0 + \frac{1}{4}\sigma_0\otimes(\vec{M}_I\cdot\vec{\tau}) + \frac{1}{4}\vec{\sigma}\cdot\vec{N}\cdot\vec{\tau}. \tag{A.63}$$

After collecting all the simplified terms for the right hand side:

$$\begin{aligned}\frac{d\hat{\rho}}{dt} &= \frac{1}{4}((\vec{B}_e\times\vec{M}_S)\cdot\vec{\sigma}\otimes\tau_0 + \vec{\sigma}\cdot(\vec{B}_e\times(\vec{N}\cdot\vec{\tau}))) - \frac{1}{4}(\sigma_0\otimes(\vec{B}_n\times\vec{M}_I)\cdot\vec{\tau}+\vec{\tau}\cdot(\vec{B}_n\times(\vec{\sigma}\cdot\vec{N})))\\ &+ \frac{A}{8}((\vec{M}_S\times\vec{\sigma})\cdot\vec{\tau}+\vec{\sigma}\cdot(\vec{M}_I\times\vec{\tau})+(\vec{\sigma}\times\vec{\tau})\cdot(\vec{N}\cdot\vec{\tau})-(\vec{\sigma}\cdot\vec{N})\cdot(\vec{\sigma}\times\vec{\tau}))\\ &- \frac{1}{4}(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})((\vec{M}_S\cdot\vec{\sigma})\otimes\tau_0-\vec{\sigma}\cdot\vec{N}\cdot\vec{\tau}) - \frac{1}{4}(\Gamma_{\Uparrow}-\Gamma_{\Downarrow})(\sigma_3\otimes\tau_0).\end{aligned} \tag{A.64}$$

Using the orthogonality relation

$$Tr((\sigma_i\otimes\tau_j)\cdot(\sigma_k\otimes\tau_l)) = Tr(\sigma_i\sigma_k)Tr(\tau_j\tau_l) = \delta_{ik}\delta_{jl}. \tag{A.65}$$

It is possible to trace out all the unwanted terms in order to determine the decoherence of the qubits. The time evolution of the electron magnetizations is found by taking

$$Tr((\vec{\sigma}\otimes\tau_0\cdot LHS) = Tr((\vec{\sigma}\otimes\tau_0\cdot RHS). \tag{A.66}$$

Where LHS and RHS are the left and right hand of the Eq. (A.64) respectively. The result for the electron magnetization is found to be

$$<\dot{S}> = (\vec{B}_e\times<S>) - A<S\times I> -(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})<S> -(\Gamma_{\Uparrow}-\Gamma_{\Downarrow})\hat{z}. \tag{A.67}$$

Where $< S \times I >= \frac{1}{2} < \vec{\sigma} \times \vec{\tau} >= \epsilon_{\gamma\alpha\beta} N_{\alpha\beta}$, with α and β running from 1 to 3. The time evolution of the nuclear magnetization can be found by applying

$$Tr((\sigma_0 \otimes \vec{\tau} \cdot LHS) = Tr((\sigma_0 \otimes \vec{\tau} \cdot RHS). \tag{A.68}$$

Which gives

$$< \dot{I} > = -(\vec{B}_N \times < I > + A < S \times I > . \tag{A.69}$$

The connection term between the electron and nuclear spins states, $N_{\alpha\beta}$, can be found by applying

$$Tr((\sigma_\alpha \otimes \tau_\beta) \cdot LHS) = Tr((\sigma_\alpha \otimes \tau_\beta) \cdot RHS). \tag{A.70}$$

Resulting in

$$\dot{N}_{\alpha\beta} = \hat{e}_\alpha \cdot (\vec{B}_e \times (\vec{N} \cdot \hat{e}_\beta)) + ((\hat{e}_\alpha \cdot \vec{N}) \times \vec{B}_n) \cdot \hat{e}_\beta + \frac{A}{2}(\hat{e}_\alpha \cdot (\hat{e}_\beta \times \vec{M}_S) + \hat{e}_\alpha \cdot (\vec{M}_I \times \hat{e}_\beta)) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) N_{\alpha\beta}. \tag{A.71}$$

Which alternatively may be written as

$$< \dot{S}I > = B_e \hat{z} \times < SI > + B_n < SI > \times \hat{z} + \frac{A}{4}(S - I)\dot{\epsilon} - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) < SI > . \tag{A.72}$$

Where ϵ is the Levi-Civita tensor. Multiplying both sides by $\epsilon_{\gamma\alpha\beta}$ gives

$$\dot{\vec{v}}_N = -(\vec{B}_e + \vec{B}_n) Tr(\vec{N}) + \vec{B}_n \cdot \vec{N} + \vec{N} \cdot \vec{B}_e + A(\vec{M}_S - \vec{M}_I) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) \vec{v}_N. \tag{A.73}$$

In the case of no ESR or NMR then $\vec{B}_e \parallel \vec{B}_n \parallel \hat{z}$ and we can rewrite the previous equations:

$$\vec{M}_S = \vec{M}_{S\perp} + \vec{M}_{S\parallel}, \tag{A.74}$$

$$\vec{M}_I = \vec{M}_{I\perp} + \vec{M}_{I\parallel}. \tag{A.75}$$

Where $\vec{M}_{S\parallel} = \vec{M}_S \cdot \hat{z}$, etc. With the use of the following definitions it is possible to simplify these equations into a series of solvable inter-dependent differential equations:

$$d_s = N_{11} + N_{22}, \tag{A.76}$$

$$d_a = N_{11} - N_{22}; \tag{A.77}$$

$$d_\parallel = N_{33}, \tag{A.78}$$

$$v_\parallel = N_{12} - N_{21}; \tag{A.79}$$

$$\vec{v}_\perp = (N_{23} - N_{32})\hat{x} + (N_{31} - N_{13})\hat{y}, \tag{A.80}$$

$$s_\parallel = (N_{12} + N_{21}); \tag{A.81}$$

$$\vec{s}_\perp = (N_{23} + N_{32})\hat{x} - (N_{31} + N_{13})\hat{y}. \tag{A.82}$$

This then results in the following series of differential equations:

$$\dot{M}_{S\parallel} = -\frac{A}{2} Re(v_\parallel + id_s) - (\Gamma_\Uparrow + \Gamma_\Downarrow) M_{S\parallel} - (\Gamma_\Uparrow - \Gamma_\Downarrow), \tag{A.83}$$

$$\dot{M}_{I\parallel} = \frac{A}{2} Re(v_\parallel + id_s); \tag{A.84}$$

$$\dot{(v_\parallel + id_s)} = -((\Gamma_\Uparrow + \Gamma_\Downarrow) - i(B_e + B_n))(v_\parallel + id_s) + A(M_{S\parallel} - M_{I\parallel}). \tag{A.85}$$

The next four may be used to solve for the perpendicular magnetization:

$$\dot{\vec{M}}_{S\perp} = B_e \hat{z} \times \vec{M}_{S\perp} - \frac{A}{2}\vec{v}_\perp - (\Gamma_\Uparrow + \Gamma_\Downarrow)\vec{M}_{S\perp}, \tag{A.86}$$

or rewritten as,

$$\dot{\vec{M}}_{S\perp} = B_e \hat{z} \times \vec{M}_{S\perp} - \frac{A}{4}((\vec{v}_\perp + \vec{s}_\perp) + (\vec{v}_\perp - \vec{s}_\perp)) - (\Gamma_\Uparrow + \Gamma_\Downarrow)\vec{M}_{S\perp}; \tag{A.87}$$

$$\dot{\vec{M}}_{I\perp} = -B_n\hat{z} \times \vec{M}_{I\perp} + \frac{A}{2}\vec{v}_\perp, \tag{A.88}$$

or rewritten as,

$$\dot{\vec{M}}_{I\perp} = -B_n\hat{z} \times \vec{M}_{I\perp} + \frac{A}{4}((\vec{v}_\perp + \vec{s}_\perp) + (\vec{v}_\perp - \vec{s}_\perp)); \tag{A.89}$$

$$(\vec{v}_\perp \dot{+} \vec{s}_\perp) = B_e\hat{z} \times (\vec{v}_\perp + \vec{s}_\perp) - (\Gamma_\Uparrow + \Gamma_\Downarrow)(\vec{v}_\perp + \vec{s}_\perp) + A(M_{S\perp} - M_{I\perp}), \tag{A.90}$$

$$(\vec{v}_\perp \dot{-} \vec{s}_\perp) = -B_n\hat{z} \times (\vec{v}_\perp - \vec{s}_\perp) - (\Gamma_\Uparrow + \Gamma_\Downarrow)(\vec{v}_\perp - \vec{s}_\perp) + A(M_{S\perp} - M_{I\perp}); \tag{A.91}$$

lastly,

$$(s_\parallel \dot{+} id_a) = -((\Gamma_\Uparrow + \Gamma_\Downarrow) - i(B_e - B_n))(s_\parallel + id_a), \tag{A.92}$$

$$\dot{d}_\parallel = -(\Gamma_\Uparrow + \Gamma_\Downarrow)d_\parallel. \tag{A.93}$$

Which may be readily integrated to show that both decay as $e^{-(\Gamma_\Uparrow+\Gamma_\Downarrow)t}$. These equations may be used to solve for the time evolution of the nuclear spin magnetization:

$$\dot{M}_{S\parallel} = -\frac{A}{2}Re(v_\parallel + id_s) - (\Gamma_\Uparrow + \Gamma_\Downarrow)M_{S\parallel} - (\Gamma_\Uparrow - \Gamma_\Downarrow). \tag{A.94}$$

Due to the presence of the $-(\Gamma_\Uparrow + \Gamma_\Downarrow)M_{S\parallel}$ which will cause the $\dot{M}_{S\parallel}$ term to decay according to $(\Gamma_\Uparrow+\Gamma_\Downarrow)$ so it may be assumed that after an appreciable time $\dot{M}_{S\parallel}$ tends to zero. This then gives

$$0 = -\frac{A}{2}Re(v_\parallel + id_s) - (\Gamma_\Uparrow + \Gamma_\Downarrow)M_{S\parallel} - (\Gamma_\Uparrow - \Gamma_\Downarrow). \tag{A.95}$$

Rearranging for $M_{S\parallel}$ then gives

$$M_{S\parallel} = -\frac{A}{2(\Gamma_\Uparrow + \Gamma_\Downarrow)}Re(v_\parallel + id_s) - \frac{(\Gamma_\Uparrow - \Gamma_\Downarrow)}{(\Gamma_\Uparrow + \Gamma_\Downarrow)}. \tag{A.96}$$

The next step is the treatment of Eq (A.85):

$$(v_{\parallel} \dot{+} id_s) = -((\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) - i(B_e + B_n))(v_{\parallel} + id_s) + A(M_{S\parallel} - M_{I\parallel}). \tag{A.97}$$

Due to the presence of the term $-((\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) - i(B_e + B_n))(v_{\parallel} + id_s)$ will cause the $(v_{\parallel} + id_s)$ term to decay according to $((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})$ so it may be assumed again that after an appreciable time $(v_{\parallel} \dot{+} id_s)$ tends to zero, giving

$$0 = -((\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) - i(B_e + B_n))(v_{\parallel} + id_s) + A(M_{S\parallel} - M_{I\parallel}). \tag{A.98}$$

Rearranging for $(v_{\parallel} + id_s)$ then gives

$$(v_{\parallel} + id_s) = \frac{A}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) - i(B_e + B_n))}(M_{S\parallel} - M_{I\parallel}). \tag{A.99}$$

Multiplying the right hand side by $\frac{((\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+i(B_e+B_n))}{((\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+i(B_e+B_n))}$ gives

$$(v_{\parallel} + id_s) = \frac{A((\Gamma_{\Uparrow} + \Gamma_{\Downarrow}) + i(B_e + B_n))}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 + (B_e + B_n)^2)}(M_{S\parallel} - M_{I\parallel}). \tag{A.100}$$

The real part of $(v_{\parallel} + id_s)$ is then given by

$$Re(v_{\parallel} + id_s) = \frac{A(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 + (B_e + B_n)^2)}(M_{S\parallel} - M_{I\parallel}). \tag{A.101}$$

Substituting the result for $M_{S\parallel}$ then gives

$$Re(v_{\parallel}+id_s) = \frac{A(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 + (B_e + B_n)^2)}(\frac{A}{2(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}Re(v_{\parallel}+id_s) - \frac{(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})} - M_{I\parallel}). \tag{A.102}$$

Which can be rearranged to

$$Re(v_{\parallel} + id_s) = \frac{A(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 + (B_e + B_n)^2 + \frac{A^2}{2})}(-M_{I\parallel} - \frac{(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}). \tag{A.103}$$

This can then be substituted in Eq. (A.84) to solve for $M_{I\parallel}$:

$$\dot{M_{I\parallel}} = \frac{A}{2}\frac{A(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 + (B_e + B_n)^2 + \frac{A^2}{2})}(-M_{I\parallel} - \frac{(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}). \tag{A.104}$$

Solving for $M_{I\parallel}$ gives

$$M_{I\parallel}(t) = (M_{I\parallel}(0) + \frac{(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})})e^{-\frac{A}{2}\frac{A(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}{((\Gamma_{\Uparrow} + \Gamma_{\Downarrow})^2 + (B_e + B_n)^2 + \frac{A^2}{2})}t} - \frac{(\Gamma_{\Uparrow} - \Gamma_{\Downarrow})}{(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})}. \tag{A.105}$$

The next step is to use the perpendicular equations equations to solve for the perpendicular dependence of the nuclear magnetization. The first step is to transform these equation into a rotating reference frame to remove the cross product terms. The following transformations are used:

$$M_{Sx} = M'_{Sx}cos(B_e t) + M'_{Sy}sin(B_e t), \tag{A.106}$$

$$M_{Sy} = M'_{Sx}sin(B_e t) - M'_{Sy}cos(B_e t); \tag{A.107}$$

$$(V_x + S_x) = (V'_x + S'_x)cos(B_e t) + (V'_y + S'_y)sin(B_e t), \tag{A.108}$$

$$(V_y + S_y) = (V'_x + S'_x)sin(B_e t) - (V'_y + S'_y)cos(B_e t); \tag{A.109}$$

$$(V_x - S_x) = (V'_x - S'_x)cos(B_n t) - (V'_y - S'_y)sin(B_n t), \tag{A.110}$$

$$(V_y - S_y) = -(V'_x - S'_x)sin(B_n t) - (V'_y - S'_y)cos(B_n t); \tag{A.111}$$

$$M_{Ix} = M'_{Ix}cos(B_n t) - M'_{Iy}sin(B_n t), \tag{A.112}$$

$$M_{Iy} = -M'_{Ix}sin(B_nt) - M'_{Iy}cos(B_nt). \tag{A.113}$$

The time evolution of the perpendicular electron spin magnetization expressed in terms of this new co-ordinate system, after some cancellation, is given by

$$\begin{aligned}\dot{M'}_{Sx}cos(B_et) + \dot{M'}_{Sy}sin(B_et) = -\frac{A}{4}((V'_x + S'_x)cos(B_et) + (V'_y + S'_y)sin(B_et)+ \\ (V'_x - S'_x)cos(B_nt) - (V'_y - S'_y)sin(B_nt))- \\ (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(M'_{Sx}cos(B_et) + M'_{Sy}sin(B_et)).\end{aligned} \tag{A.114}$$

Which may be simplified by substituting

$$cos(B_nt) \rightarrow (cos((B_n - B_e)t)cos(B_et) - sin((B_n - B_e)t)sin(B_et)); \tag{A.115}$$

$$sin(B_nt) \rightarrow (sin((B_n - B_e)t)cos(B_et) - cos((B_n - B_e)t)sin(B_et)). \tag{A.116}$$

Collecting terms in $cos(B_et)$:

$$\dot{M'}_{Sx} = -\frac{A}{4}((V'_x - S'_x)cos((B_n - B_e)t) + (V'_y - S'_y)sin((B_n - B_e)t) + (V'_x + S'_x)) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})M'_{Sx}. \tag{A.117}$$

Then cancelling the highly oscillatory $cos((B_n - B_e)t)$ and $sin((B_n - B_e)t)$ terms:

$$\dot{M'}_{Sx} = -\frac{A}{4}(V'_x + S'_x) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})M'_{Sx}. \tag{A.118}$$

Collecting terms in $sin(B_et)$:

$$\dot{M'}_{Sy} = -\frac{A}{4}(-(V'_x - S'_x)sin((B_n - B_e)t) + (V'_y - S'_y)cos((B_n - B_e)t) + (V'_y + S'_y)) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})M'_{Sy}. \tag{A.119}$$

Then cancelling the highly oscillatory $sin((B_n - B_e)t)$ and $cos((B_n - B_e)t)$ terms:

$$\dot{M'}_{Sy} = -\frac{A}{4}(V'_y + S'_y) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})M'_{Sy}. \tag{A.120}$$

The time evolution of the perpendicular magnetization of the electron spin is then given by

$$\dot{M'}_{S\perp} = -\frac{A}{4}(V'_\perp + S'_\perp) - (\Gamma_{\Uparrow} + \Gamma_{\Downarrow})M'_{S\perp}. \tag{A.121}$$

The time evolution of the $(\vec{v}_\perp + \vec{s}_\perp)$ term expressed in terms of this new co-ordinate system, after some cancellation, is given by

$$\begin{aligned}(\dot{v'_x + s'_x})cos(B_e t) + (\dot{v'_y + s'_y})sin(B_e t) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})((V'_x + S'_x)cos(B_e t) + (V'_y + S'_y)sin(B_e t)) + \\ A(M'_{Sx}cos(B_e t) + M'_{Sy}sin(B_e t) + \\ M'_{Ix}cos(B_n t) - M'_{Iy}sin(B_n t)).\end{aligned} \tag{A.122}$$

Again substituting

$$cos(B_n t) \rightarrow (cos((B_n - B_e)t)cos(B_e t) - sin((B_n - B_e)t)sin(B_e t)); \tag{A.123}$$

$$sin(B_n t) \rightarrow (sin((B_n - B_e)t)cos(B_e t) - cos((B_n - B_e)t)sin(B_e t)). \tag{A.124}$$

Collecting terms in $cos(B_e t)$:

$$(\dot{v'_x + s'_x}) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_x + S'_x) + A(M'_{Sx} + M'_{Ix}cos((B_e - B_n)t) - M'_{Iy}sin((B_e - B_n)t)). \tag{A.125}$$

Then cancelling the highly oscillatory $cos((B_n - B_e)t)$ and $sin((B_n - B_e)t)$ terms:

$$(\dot{v'_x + s'_x}) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_x + S'_x) + A(M'_{Sx}). \tag{A.126}$$

Collecting terms in $sin(B_e t)$:

$$(v'_y \dot{+} s'_y) = -(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})(V'_y+S'_y)+A(M'_{Sy}+M'_{Ix}sin((B_e-B_n)t)-M'_{Iy}cos((B_e-B_n)t)). \tag{A.127}$$

Then cancelling the highly oscillatory $sin((B_n - B_e)t)$ and $cos((B_n - B_e)t)$ terms:

$$(v'_y \dot{+} s'_y) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_y + S'_y) + A(M'_{Sy}). \tag{A.128}$$

The time evolution of the $(\vec{v}_\perp + \vec{s}_\perp)$ term is then given by

$$(v'_\perp \dot{+} s'_\perp) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_\perp + S'_\perp) + A(M'_{S\perp}). \tag{A.129}$$

The time evolution of the $(\vec{v}_\perp - \vec{s}_\perp)$ term expressed in terms of this new co-ordinate system, after some cancellation, is given by

$$\begin{aligned}(v'_x \dot{-} s'_x)cos(B_n t) - (v'_y \dot{-} s'_y)sin(B_n t) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})((V'_x - S'_x)cos(B_n t) - (V'_y - S'_y)sin(B_n t))+ \\ A(M'_{Sx}cos(B_e t) + M'_{Sy}sin(B_e t)- \\ M'_{Ix}cos(B_n t) + M'_{Iy}sin(B_n t)).\end{aligned} \tag{A.130}$$

Then substituting

$$cos(B_e t) \rightarrow (cos((B_e - B_n)t)cos(Bt) - sin((B_e - B_n)t)sin(B_n t)); \tag{A.131}$$

$$sin(B_e t) \rightarrow (sin((B_e - B_n)t)cos(B_e t) - cos((B_e - B_n)t)sin(B_n t)). \tag{A.132}$$

Collecting terms in $cos(B_n t)$:

$$(\dot{v'_x - s'_x}) = -(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})(V'_x - S'_x)+A(M'_{Sx}cos((B_e - B_n)t)+M'_{Sy}sin((B_e - B_n)t)+M'_{Ix}). \tag{A.133}$$

Then cancelling the highly oscillatory $cos((B_e - B_n)t)$ and $sin((B_e - B_n)t)$ terms:

$$(\dot{v'_x - s'_x}) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_x - S'_x) - A(M'_{Ix}). \tag{A.134}$$

Collecting terms in $sin(B_n t)$:

$$-(\dot{v'_y - s'_y}) = (\Gamma_{\Uparrow}+\Gamma_{\Downarrow})(V'_y - S'_y)+A(-M'_{Sx}sin((B_e - B_n)t)-M'_{Sy}cos((B_e - B_n)t)+M'_{Iy}). \tag{A.135}$$

Then cancelling the highly oscillatory $sin((B_e - B_n)t)$ and $cos((B_e - B_n)t)$ terms:

$$(\dot{v'_y - s'_y}) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_y - S'_y) - A(M'_{Iy}). \tag{A.136}$$

The time evolution of the $(\vec{v}_{\perp} - \vec{s}_{\perp})$ term is given by

$$(\dot{v'_{\perp} - s'_{\perp}}) = -(\Gamma_{\Uparrow} + \Gamma_{\Downarrow})(V'_{\perp} - S'_{\perp}) - A(M'_{I\perp}). \tag{A.137}$$

The time evolution of the perpendicular nuclear spin magnetization expressed in terms of this new co-ordinate system, after some cancellation, is given by

$$\dot{M'}_{Ix}cos(B_n t) - \dot{M'}_{Iy}sin(B_n t) = \frac{A}{4}((V'_x + S'_x)cos(B_e t) + (V'_y + S'_y)sin(B_e t)+ (V'_x - S'_x)cos(B_n t) - (V'_y - S'_y)sin(B_n t)). \tag{A.138}$$

Then substituting:

$$cos(B_e t) \rightarrow (cos((B_e - B_n)t)cos(Bt) - sin((B_e - B_n)t)sin(B_n t)); \tag{A.139}$$

$$sin(B_e t) \rightarrow (sin((B_e - B_n)t)cos(B_e t) - cos((B_e - B_n)t)sin(B_n t)). \tag{A.140}$$

Collecting terms in $cos(B_n t)$:

$$\dot{M'}_{Ix} = \frac{A}{4}((V'_x + S'_x)cos((B_e - B_n)t) + (V'_y + S'_y)sin((B_e - B_n)t) + (V'_x - S'_x)). \tag{A.141}$$

Then cancelling the highly oscillatory $cos((B_e - B_n)t)$ and $sin((B_e - B_n)t)$ terms gives

$$\dot{M'}_{Ix} cos(B_n t) = \frac{A}{4}(V'_x - S'_x). \tag{A.142}$$

Collecting terms in $sin(B_n t)$:

$$-\dot{M'}_{Iy} = \frac{A}{4}(-(V'_x + S'_x)sin((B_e - B_n)t) - (V'_y + S'_y)cos((B_e - B_n)t) - (V'_y - S'_y)). \tag{A.143}$$

Then cancelling the highly oscillatory $cos((B_e - B_n)t)$ and $sin((B_e - B_n)t)$ terms gives

$$\dot{M'}_{Iy} = \frac{A}{4}(V'_y - S'_y). \tag{A.144}$$

The time evolution of the perpendicular nuclear spin magnetization is given by

$$\dot{M'}_{I\perp} = \frac{A}{4}(V'_\perp - S'_\perp). \tag{A.145}$$

The $(\Gamma_\Uparrow + \Gamma_\Downarrow)M'_{S\perp}$ term of equation for the perpendicular donor spin magnetization ensures that the spin will decay to equilibrium quickly when $(\Gamma_\Uparrow + \Gamma_\Downarrow)$ is large. The equation of true concern here is nuclear spin dependencies as qubit information is

stored in the nuclear spin state. The first step to find the solution for the perpendicular nuclear magnetization is to take the derivative of Eq. (A.145), giving

$$\ddot{M'}_{I\perp} = \frac{A}{4}(\dot{V'_\perp} - \dot{S'_\perp}). \tag{A.146}$$

Substituting Eq. (A.121) into this gives

$$\ddot{M'}_{I\perp} = \frac{A}{4}(-(\Gamma_\Uparrow + \Gamma_\Downarrow)(V'_\perp - S'_\perp) - A(M'_{I\perp})). \tag{A.147}$$

Substituting equation Eq. (A.145) back into this gives

$$\ddot{M'}_{I\perp} = -(\Gamma_\Uparrow + \Gamma_\Downarrow)\dot{M'}_{I\perp} - \frac{A^2}{4}(M'_{I\perp})). \tag{A.148}$$

Subject to the following constraint;

$$\dot{M'}_{I\perp}(t=0) = \frac{A}{4}(V'_\perp(t=0) - S'_\perp(t=0)). \tag{A.149}$$

Assuming a solution of the form;

$$M'_{I\perp} \propto e^{-\alpha t}. \tag{A.150}$$

Which when substituted into the previous result gives

$$\alpha^2 - (\Gamma_\Uparrow + \Gamma_\Downarrow)\alpha + \frac{A^2}{4} = 0. \tag{A.151}$$

Solving for α gives

$$\alpha = \frac{(\Gamma_\Uparrow + \Gamma_\Downarrow) \pm \sqrt{(\Gamma_\Uparrow + \Gamma_\Downarrow)^2 - A^2}}{2}. \tag{A.152}$$

$M'_{I\perp}$ can then be expressed as

$$M'_{I\perp} = c_0 e^{-(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})t} + c_1 e^{-(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})t}. \tag{A.153}$$

Which is subject to the constraint of Eq. (A.149), giving

$$\frac{A}{4}(V'_{\perp}(t=0) - S'_{\perp}(t=0)) = c_0(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})+ \tag{A.154}$$

$$c_1(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2}). \tag{A.155}$$

In the limit of $(\Gamma_{\Uparrow}+\Gamma_{\Downarrow}) >> A$;

$$(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2}) = (\Gamma_{\Uparrow}+\Gamma_{\Downarrow}), \tag{A.156}$$

$$(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2}) = \frac{1}{2}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}. \tag{A.157}$$

When setting

$$c_1 = 1, \tag{A.158}$$

We get

$$c_0 = \frac{\frac{A}{4}(V'_{\perp}(t=0) - S'_{\perp}(t=0)) - \frac{1}{2}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})}. \tag{A.159}$$

The final result for the perpendicular magnetization of the nuclear spin state is then

$$M'_{I\perp} = \frac{\frac{A}{4}(V'_{\perp}(t=0) - S'_{\perp}(t=0)) - \frac{1}{2}\frac{A^2}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2}}{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})} e^{-(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})+\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})t}$$

$$+ e^{-(\frac{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})-\sqrt{(\Gamma_{\Uparrow}+\Gamma_{\Downarrow})^2-A^2}}{2})t}. \tag{A.160}$$

A.5 Derivation of the RKKY Interaction in 2nd Order Born Approximation

The transmission matrix, in the Born approximation, may be expressed as

$$T = V + V\frac{1}{E - H_0 + i\epsilon}V + V\frac{1}{E - H_0 + i\epsilon'}V\frac{1}{E - H_0 + i\epsilon}V + \ldots. \tag{A.161}$$

The RKKY interaction is then given by

$$H^{e-e}_{RKKY} =< FG|H^1_{exc}\frac{1}{E - H_0 + i\epsilon'}H^2_{exc}|FG > . \tag{A.162}$$

Where the ground state wavefunction is taken as

$$|FG >= \Pi_{k<k_F}c^+_k|0 > . \tag{A.163}$$

Where;

$$H^i_{exc} = \frac{1}{2}\sum_{kk'} e^{i(k-k')\bar{x}}J^c_{kk'}S_i \cdot S_e. \tag{A.164}$$

The labels k through k"' refer to donor electron wave-vectors (all $< k_F$), the 'e' label refers to the conduction electrons and the 'i' label refers to donor electron i. - note:

$$S_i \cdot S_{ce} = S_{ze}S_{zi} + S_{xe}S_{xi} + S_{ye}S_{yi} = S_{ze}S_{zi} + S_{e+}S_{i-} + S_{e-}S_{i+}. \tag{A.165}$$

The scattering of a conduction electron off a donor atom is dominated by a virtual scattering process. A process by which a conduction electron forms a doubly occupied ground state with the donor electron. In this framework the effect of the S_{e+} and S_{e-} terms is to create or destroy a valence electron within the overall donor wavefunction. It would be needlessly complicated to solve all terms simultaneously. Here the

contributing factors which result in the $S_{1+}S_{2-}$ term will be examined in detail with the remaining results being determined through comparison.

In this case

$$H^1_{exc} = \frac{1}{2}\sum_{kk'} e^{i(k-k')\bar{x}} J^{c_1}_{kk'}(S_{1+}c^+_{k'\downarrow}c_{k\uparrow}); \tag{A.166}$$

$$H^2_{exc} = \frac{1}{2}\sum_{k''k'''} e^{i(k''-k''')\bar{x}} J^{c_2}_{k''k'''}(S_{2-}c^+_{k'''\downarrow}c_{k''\uparrow}). \tag{A.167}$$

Substituting these relation into equation into H^{e-e}_{RKKY} above gives

$$\begin{aligned} H^{e-e}_{RKKY} = \frac{1}{4} < FG| \sum_{kk'} e^{i(k-k')\bar{x_1}} J^{c_1}_{kk'}(S_{1+}c^+_{k'\downarrow}c_{k\uparrow}) \frac{1}{E - H_0 + i\epsilon'} \\ \sum_{k''k'''} e^{i(k''-k''')\bar{x_2}} J^{c_2}_{k''k'''}(S_{2-}c^+_{k'''\downarrow}c_{k''\uparrow})|FG> + c.c. \end{aligned} \tag{A.168}$$

Which may be simplified to

$$\begin{aligned} H^{e-e}_{RKKY} = \frac{1}{4}\sum_{kk'}\sum_{k''k'''} e^{i(k-k')\bar{x_1}} e^{i(k''-k''')\bar{x_2}} J^{c_1}_{kk'} J^{c_2}_{k''k'''} \\ < FG|c^+_{k'\downarrow}c_{k\uparrow}\frac{1}{E - H_0 + i\epsilon}c^+_{k'''\downarrow}c_{k''\uparrow}|FG> (S_{1+}S_{2-}) + c.c. \end{aligned} \tag{A.169}$$

It is important to note that

$$< FG|c^+_{k'\downarrow}c_{k\uparrow}\frac{1}{E - H_0 + i\epsilon}c^+_{k'''\downarrow}c_{k''\uparrow}|FG> = < \begin{matrix} ek'' \uparrow \\ hk' \downarrow \end{matrix} |\frac{1}{E - H_0 + i\epsilon}| \begin{matrix} ek''' \uparrow \\ hk \downarrow \end{matrix} > . \tag{A.170}$$

Where

$$< \begin{matrix} ek'' \uparrow \\ hk' \downarrow \end{matrix} |\frac{1}{E - H_0 + i\epsilon}| \begin{matrix} ek''' \uparrow \\ hk \downarrow \end{matrix} > = \frac{\delta_{k'',k'''}\delta_{k',k}}{E - H_0 + i\epsilon'}. \tag{A.171}$$

Here 'e' represents and electron and 'h' represents a hole. This then gives

$$H^{e-e}_{RKKY} = \frac{1}{2}\sum_{kk'} e^{i(k'-k)(\bar{x_1}-\bar{x_2})} J^{c1}_{kk'} J^{c2}_{k'k} \frac{1}{E_{k'} - E_k + i\epsilon'} (S_{1+} S_{2-}) + c.c. \tag{A.172}$$

Adding all the other terms to the result for H_{RKKY} gives

$$H^{e-e}_{RKKY} = \frac{1}{2}\sum_{kk'} \frac{e^{i(k'-k)(\bar{x_1}-\bar{x_2})} J^{c1}_{kk'} J^{c2}_{k'k}}{E_{k'} - E_k + i\epsilon'} (S_1 \cdot S_2). \tag{A.173}$$

Where

$$J^{e-e}_{RKKY} = \frac{1}{2}\sum_{kk'} \frac{e^{i(k'-k)(\bar{x_1}-\bar{x_2})} J^{c1}_{kk'} J^{c2}_{k'k}}{E_{k'} - E_k + i\epsilon'}. \tag{A.174}$$

Here $E_k = \frac{k^2}{2m*}$ and assuming equal $J^{c1}_{kk'}$ and $J^{c2}_{k'k}$ J^{e-e}_{RKKY} becomes

$$J^{e-e}_{RKKY} = \frac{m*}{\hbar^2}\sum_{kk'} \frac{e^{i(k'-k)(\bar{x_1}-\bar{x_2})} J^{c1}_{kk'} J^{c2}_{k'k}}{k'^2 - k^2 + i\epsilon'}. \tag{A.175}$$

To solve for J^{e-e}_{RKKY}, within the 2 dimensional case of a 2DEG, a continuum of states must be assumed, giving

$$\sum_k = \int \frac{1}{(2\pi)^2} \mathrm{d}k^2. \tag{A.176}$$

Then J^{e-e}_{RKKY} becomes

$$J^{e-e}_{RKKY} = \frac{m * J_c^2}{(2\pi)^4 \hbar^2} \int_0^{kf}\int_0^{2\pi}\int_0^{kf}\int_0^{2\pi} \frac{e^{ik\bar{x_1}cos(\theta)} e^{ik'\bar{x_2}cos(\theta')}}{k'^2 - k^2 + i\epsilon'} \mathrm{d}\theta \mathrm{d}k \mathrm{d}\theta' \mathrm{d}k'. \tag{A.177}$$

Where $cos(\theta)$ is the angle between the wave-vector k and the position vector $\bar{x}$, likewise for k' and θ'. Switching to polar coordinates J_{RKKY} is given by

$$J^{e-e}_{RKKY} = \frac{m * J_c^2}{(2\pi)^4 \hbar^2} \int_0^{k_F} \mathrm{d}k k \int_0^{2\pi} \mathrm{d}\theta e^{-ik\bar{x}cos(\theta)} \int_0^{k_F} \mathrm{d}k' k' \int_0^{2\pi} \mathrm{d}\theta' e^{-ik'\bar{x}cos(\theta')} \frac{-1}{(k' + k_p)(k' - k_p)}. \tag{A.178}$$

With $k_p = k + \frac{i\epsilon'}{2k}$. -note [28];

$$\int_0^{2\pi} \mathrm{d}\theta e^{-ik\bar{x}cos(\theta)} = 2\pi J_0(k\bar{x}). \tag{A.179}$$

J^{e-e}_{RKKY} is then given by

$$J^{e-e}_{RKKY} = \frac{m * J_c^2}{(2\pi)^4\hbar^2} \int_0^{k_F} \mathrm{d}k k J_0(k\bar{x})(-2\pi) \int_0^{\infty} \mathrm{d}k' \frac{k' J_0(k'\bar{x})}{(k'+k_p)(k'-k_p)}. \tag{A.180}$$

The Bessel function J_0 may be expressed in terms of the Henkel functions given by [28]

$$J_0(k'\bar{x}) = \frac{H_0^1(k'\bar{x}) + H_0^2(k'\bar{x})}{2}. \tag{A.181}$$

The integral over k' then becomes

$$-(\frac{2\pi}{2}) \int_{-\infty}^{\infty} \mathrm{d}k' \frac{\frac{H_0^1(k'\bar{x})+H_0^2(k'\bar{x})}{2}}{(k'+k_p)(k'-k_p)} = -\frac{\pi}{2}(\int_{-\infty}^{\infty} \mathrm{d}k' \frac{\frac{H_0^1(k'\bar{x})}{2}}{(k'+k_p)(k'-k_p)} + \int_{-\infty}^{\infty} \mathrm{d}k' \frac{\frac{H_0^2(k'\bar{x})}{2}}{(k'+k_p)(k'-k_p)} \tag{A.182}$$

$$= -(\frac{\pi}{2})(2\pi i \frac{H_0^1((k_p\bar{x})}{2} - 2\pi i \frac{H_0^2((k_p\bar{x})}{2}) \tag{A.183}$$

$$= \pi^2 \frac{H_0^1((k_p\bar{x}) - H_0^2((k_p\bar{x})}{2i} \tag{A.184}$$

$$= \pi^2 N_0(k_p\bar{x}). \tag{A.185}$$

After substituting this back in J_{RKKY} in the limit of $\epsilon \to 0$ we get

$$J^{e-e}_{RKKY} = \frac{\pi^2 m * J_c^2}{(2\pi)^3\hbar^2} \int_0^{k_F} \mathrm{d}k k J_0(k\bar{x}) N_0(k\bar{x}). \tag{A.186}$$

-note [28]

$$\int \mathrm{d}y y J_0(ay) N_0(ay) = \frac{y^2}{2}(J_0(ay)N_0(ay) + J_1(ay)N_1(ay)). \tag{A.187}$$

Assuming $k_F\bar{x} > 0.5$

$$\frac{y^2}{2}(J_0(ay)N_0(ay) + J_1(ay)N_1(ay)) = -\frac{sin(2ay)}{(2ay)^2}. \tag{A.188}$$

FInally J^{e-e}_{RKKY} is found to be

$$J^{e-e}_{RKKY} = -\frac{m * J_c^2}{(8\pi)\hbar^2}\frac{k_F^2 A^2}{2}\frac{sin(2k_F\bar{x})}{(2k_F\bar{x})^2}. \tag{A.189}$$

Where

$$H^{e-e}_{RKKY} = J^{e-e}_{RKKY}(S_1 \cdot S_2). \tag{A.190}$$

A is the area of the 2DEG (cancelled later by results for J_c), m^* the effective mass of the electron, k_F the fermi wave-vector and k_0 the valley minima. All that remains is a calculation of the individual interaction strengths J_c^1 and J_c^2 which is presented in appendix A.7.

A.6 Effective Interaction Between Nuclear Spins

The capability of an electron mediated interaction to cause an effective interaction between donor nuclei is most readily demonstrated through degenerate perturbation theory. The hamiltonian may be expressed in terms of the ground state dependence, H_0 with a perturbative potential, V:

$$H_0 = J\vec{S}_1 \cdot \vec{S}_2 + B_e(S_{1z} + S_{2z}) - B_n(I_{1z} + I_{2z}). \tag{A.191}$$

Where

$$V = A((\vec{S}_1 \cdot \vec{I}_1) + (\vec{S}_2 \cdot \vec{I}_2)). \tag{A.192}$$

Here S is the electron spin operator, I the nuclear spin operator, $B_e = g_e\mu_e B$, $B_n = g_n\mu_n B$ and J the electron interaction strength between the two donors. In this result J may be the direct donor exchange interaction presented by Bruce can or the RKKY interaction described earlier in this paper. The eigenstates of the ground state hamiltonian, with the associated eigenvalues are given by:

Eigenstate	Eigenvalue
$\|\tau_1\tau_2> \|s>$	$E^0 = -\frac{3}{4}J - B_n(\frac{\tau_1+\tau_2}{2})$
$\|\tau_1\tau_2> \|\Uparrow\Uparrow>$	$E^0 = \frac{1}{4}J - B_n(\frac{\tau_1+\tau_2}{2}) + B_e$
$\|\tau_1\tau_2> \|t_0$	$E^0 = E^0 = \frac{1}{4}J - B_n(\frac{\tau_1+\tau_2}{2})$
$\|\tau_1\tau_2> \|\Downarrow\Downarrow>$	$E^0 = \frac{1}{4}J - B_n(\frac{\tau_1+\tau_2}{2}) - B_e$

Table A.1: Eigenstates of the ground state Hamiltonian

The τ_1, τ_2 states represent the donor, 1 or 2, nuclear spin states, while the double arrows represent the electronic spin states. The singlet electron state $|s>= \frac{1}{\sqrt{2}}(|\Uparrow\Downarrow> - |\Downarrow\Uparrow>$ and the middle energy triplet state $|t_0>= \frac{1}{\sqrt{2}}(|\Uparrow\Downarrow> + |\Downarrow\Uparrow>$. To find the effective Hamiltonian between the nuclear spin states second order degenerate perturbation theory in V is used:

$$<\tau_1\tau_2|H_{eff}|\tau_1'\tau_2'>= \sum_{\alpha=\Downarrow\Downarrow,S,t_0,\Uparrow\Uparrow} p_\alpha \sum_{\tau_1''\tau_2''\beta}{}' \frac{<\tau_1\tau_2\alpha|V|\tau_1''\tau_2''\beta><\tau_1''\tau_2''\beta|V|\tau_1'\tau_2'\alpha>}{(E^0_{\tau_1\tau_2\alpha} - E^0_{\tau_1''\tau_2''\beta}) \pm i\Gamma_\beta}. \tag{A.193}$$

Here the states labelled by β represent the intermediary states for the interaction. The interaction is therefore limited principally by the lifetime of the intermediate states which is given in the $\frac{1}{\pm i\Gamma}$ terms. The $\sum'$ terms exclude states where$|\tau_1''\tau_2''\beta>$ which have equal energy to $|\tau_1\tau_2\alpha>$. p_{alpha} is the density of conduction electrons with a particular state α. It is assumed here that the electrons are in a mixed density matrix state and that the decay time for the electrons Γ_e is far less that the time of

interaction. The effective nuclear spin interaction is then found to be

$$H_{eff} = A^2 \sum_{\alpha} p_\alpha \sum_{\tau_1'' \tau_2'' \beta}{}' \frac{((\vec{I_1})_{\tau_1 \tau_1''} \delta_{\tau_2 \tau_2''} \cdot (\vec{S_1})_{\alpha\beta} + (\vec{I_2})_{\tau_2 \tau_2''} \delta_{\tau_1 \tau_1''} \cdot (\vec{S_2})_{\alpha\beta})(\vec{I_1})_{\tau_1'' \tau_1'} \delta_{\tau_2'' \tau_2'}}{(E^0_{\tau_1 \tau_2 \alpha} - E^0_{\tau_1'' \tau_2'' \beta}) \pm i\Gamma_\beta}$$
$$\cdot ((\vec{S_1})_{\alpha\beta} + (\vec{I_2})_{\tau_2'' \tau_2'} \delta_{\tau_1'' \tau_1'} \cdot (\vec{S}_{2\beta\alpha})). \tag{A.194}$$

Combining terms, while requiring the result to Hermitian, gives rise to

$$H_{eff} = A^2 \sum_{\alpha} p_\alpha (\sum_{\beta} (\frac{\vec{I}_{1\tau_1 \tau_1'} \cdot \vec{S}_{1\alpha\beta} \vec{I}_{2\tau_2 \tau_2'} \vec{S}_{2\beta\alpha}}{(E^0_{\tau_1 \tau_2 \alpha} - E^0_{\tau_1' \tau_2 \beta}) + i\Gamma_\beta} + \frac{\vec{I}_{2\tau_2 \tau_2'} \cdot \vec{S}_{2\alpha\beta} \vec{I}_{1\tau_1 \tau_1'} \vec{S}_{1\beta\alpha}}{(E^0_{\tau_1 \tau_2 \alpha} - E^0_{\tau_1 \tau_2' \beta}) - i\Gamma_\beta} + ...). \tag{A.195}$$

Where .... = terms like $(\vec{I_1}\vec{I_1} + \vec{I_2}\vec{I_2}) = I_z^2$ and only add a global phase. Performing the sum over all possible intermediate states β gives

$$H_{eff} = A^2 \sum_{\alpha} p_\alpha ((\vec{I_1})_{\tau_1 \tau_1'} \cdot [(\sum_{\beta} \frac{< \alpha | \vec{S_1} | \beta >< \beta | \vec{S_2} | \alpha >}{(E^0_{\tau_1 \tau_2 \alpha} - E^0_{\tau_1' \tau_2 \beta}) + i\Gamma_\beta})] \cdot (\vec{I_2})_{\tau_2 \tau_2'} + ...). \tag{A.196}$$

Where ... is the same as the first term with the labels 1 and 2 interchanged and with a $-i\Gamma_\beta$. For the time being Γ_β will simply be written as Γ. It is most convenient to proceed with the remainder of this calculation part parts. When $\alpha = \Downarrow\Downarrow$ and $\beta = \Downarrow\Downarrow$, $\Uparrow\Uparrow$ then

$$[\cdot] = \frac{<\Downarrow\Downarrow | \vec{S_1} | s >< s | \vec{S_2} | \Downarrow\Downarrow>}{J - \frac{B_n}{2}(\tau_1 - \tau_1') - B_e + i\Gamma} + \frac{<\Downarrow\Downarrow | \vec{S_1} | t_0 >< t_0 | \vec{S_2} | \Downarrow\Downarrow>}{-B_e - \frac{B_n}{2}(\tau_1 - \tau_1') + i\Gamma}. \tag{A.197}$$

Where $\beta = |s>, |t_0>$. S_1 only operates on donor one, and the opposite being true for S_2. This allows a simplification to

$$[\cdot] = \frac{-\frac{1}{2} <\Downarrow | \vec{S_1} | \Uparrow><\Uparrow | \vec{S_2} | \Downarrow>}{J - \frac{B_n}{2}(\tau_1 - \tau_1') - B_e + i\Gamma} + \frac{\frac{1}{2} <\Downarrow | \vec{S_1} | \Uparrow><\Uparrow | \vec{S_2} | \Downarrow>}{-B_e - \frac{B_n}{2}(\tau_1 - \tau_1') + i\Gamma}. \tag{A.198}$$

It is important to take note that

$$<\Downarrow |\vec{S_1}| \Uparrow>= \frac{1}{2}(\hat{x} + i\hat{y}); \tag{A.199}$$

$$<\Uparrow |\vec{S_2}| \Downarrow>= \frac{1}{2}(\hat{x} - i\hat{y}). \tag{A.200}$$

When $\tau_1 = \tau_1' + 2$

$$H_{eff}^{\Downarrow\Downarrow} = p_{\Downarrow\Downarrow}\frac{A^2}{8}(-\frac{I_{1+}I_{2-}}{J - B_n - B_e + i\Gamma} + \frac{I_{1-}I_{2+}}{-B_n - B_e + i\Gamma}) + h.c. \tag{A.201}$$

When $\alpha = S$ and $\beta =\Downarrow\Downarrow, \Uparrow\Uparrow$ then

$$[\cdot] = \frac{< S|\vec{S_1}| \Uparrow\Uparrow><\Uparrow\Uparrow |\vec{S_2}|S >}{-J - \frac{B_n}{2}(\tau_1 - \tau_1') - B_e + i\Gamma} + \frac{< S|\vec{S_1}| \Downarrow\Downarrow><\Downarrow\Downarrow |\vec{S_2}|S >}{-J + B_e + \frac{B_n}{2}(\tau_1 - \tau_1') + i\Gamma} + \frac{< S|\vec{S_1}|t_0 >< t_0|\vec{S_2}|S >}{-J + i\Gamma}. \tag{A.202}$$

Taking note that

$$< S|\vec{S_1}| \Uparrow\Uparrow>= -\frac{1}{\sqrt{2}}\frac{1}{2}(\hat{x} + i\hat{y}); \tag{A.203}$$

$$< S|\vec{S_1}| \Downarrow\Downarrow>= \frac{1}{\sqrt{2}}\frac{1}{2}(\hat{x} - i\hat{y}), \tag{A.204}$$

$$< S|\vec{S_1}|t_0 >= \frac{1}{2}\hat{z}; \tag{A.205}$$

$$< t_0|\vec{S_1}|S >= -\frac{1}{2}\hat{z}. \tag{A.206}$$

Again when $\tau_1 = \tau_1' + 2$

$$H_{eff}^{S} = -\frac{A^2}{8}p_S(\frac{I_{1+}I_{2-}}{-J - B_n - B_e + i\Gamma} + \frac{I_{1-}I_{2+}}{-J + B_n + B_e + i\Gamma}) - \frac{A^2}{4}\frac{I_{1z}I_{2z}}{-J + i\Gamma} + h.c. \tag{A.207}$$

When $\alpha = t_0$ and $\beta = \Downarrow\Downarrow, \Uparrow\Uparrow$ then

$$[\cdot] = \frac{< t_0|\vec{S_1}| \Uparrow\Uparrow><\Uparrow\Uparrow |\vec{S_2}|t_0 >}{-\frac{B_n}{2}(\tau_1 - \tau_1') - B_e + i\Gamma} + \frac{< t_0|\vec{S_1}| \Downarrow\Downarrow><\Downarrow\Downarrow |\vec{S_2}|t_0 >}{+B_e + \frac{B_n}{2}(\tau_1 - \tau_1') + i\Gamma} + \frac{< t_0|\vec{S_1}|S >< S|\vec{S_2}|t_0 >}{J + i\Gamma}. \tag{A.208}$$

Which gives

$$H_{eff}^{t_0} = -\frac{A^2}{8} p_{t_0} \left(\frac{I_{1+}I_{2-}}{-B_n - B_e + i\Gamma} + \frac{I_{1-}I_{2+}}{+B_n + B_e + i\Gamma}\right) - \frac{A^2}{4}\frac{I_{1z}I_{2z}}{J + i\Gamma} + h.c. \tag{A.209}$$

When $\alpha = \Uparrow\Uparrow$ and $\beta = \Downarrow\Downarrow, \Uparrow\Uparrow$ then

$$[\cdot] = \frac{<\Uparrow\Uparrow |\vec{S_1}|S >< S|\vec{S_2}| \Uparrow\Uparrow>}{J + \frac{B_n}{2}(\tau_1 - \tau_1') + B_e + i\Gamma} + \frac{<\Uparrow\Uparrow |\vec{S_1}|t_0 >< t_0|\vec{S_2}| \Uparrow\Uparrow>}{B_e + \frac{B_n}{2}(\tau_1 - \tau_1') + i\Gamma}. \tag{A.210}$$

Which gives

$$H_{eff}^{\Uparrow\Uparrow} = p_{\Uparrow\Uparrow}\frac{A^2}{8}\left(-\frac{I_{1+}I_{2-}}{J + B_n + B_e + i\Gamma} + \frac{I_{1-}I_{2+}}{+B_n + B_e + i\Gamma}\right) + h.c. \tag{A.211}$$

Putting all the preceding results together gives

$$\begin{aligned}
H_{eff} = p_{\Downarrow\Downarrow}\frac{A^2}{8}((&\frac{-1}{J-B_e-B_n+i\Gamma}+\frac{1}{-B_e-B_n+i\Gamma})I_{1+}I_{2-}\\
&+(\frac{-1}{J-B_e-B_n-i\Gamma}+\frac{1}{-B_e-B_n-i\Gamma})I_{1-}I_{2+})\\
&+p_{\Uparrow\Uparrow}\frac{A^2}{8}((\frac{-1}{J+B_e+B_n-i\Gamma}+\frac{1}{B_e+B_n-i\Gamma})I_{1+}I_{2-}\\
&+(\frac{-1}{J+B_e+B_{n+i\Gamma}}+\frac{1}{B_e+B_n+i\Gamma})I_{1-}I_{2+})\\
&-p_S\frac{A^2}{8}((\frac{1}{-J-B_e-B_n+i\Gamma}+\frac{1}{-J+B_e+B_n-i\Gamma})I_{1+}I_{2-}\\
&+(\frac{1}{-J-B_e-B_n-i\Gamma}+\frac{1}{-J+B_e+B_n+i\Gamma})I_{1-}I_{2+}\\
&+2(\frac{1}{-J+i\Gamma}+\frac{1}{-J-i\Gamma})I_{1z}I_{2z})\\
p_{t_0}\frac{A^2}{8}((&\frac{1}{-B_e-B_n+i\Gamma}+\frac{1}{B_e+B_n-i\Gamma})I_{1+}I_{2-}\\
&+(\frac{1}{-B_e-B_n-i\Gamma}+\frac{1}{B_e+B_n+i\Gamma})I_{1-}I_{2+}\\
&-2(\frac{1}{J+i\Gamma}+\frac{J-i\Gamma}{)}I_{1z}I_{2z}).
\end{aligned} \tag{A.212}$$

Again assuming $t >> \Gamma_e^{-1}$ allows the redefinition of the population functions

$$p_{\Downarrow\Downarrow} = p_{\Downarrow}p_{\Downarrow} = \frac{1-2p_e+p_e^2}{4}; \tag{A.213}$$

$$p_{\Uparrow\Uparrow} = p_{\Uparrow}p_{\Uparrow} = \frac{1+2p_e+p_e^2}{4}, \tag{A.214}$$

$$p_S = p_{\Uparrow}p_{\Downarrow} = \frac{1-p_e^2}{4}; \tag{A.215}$$

$$p_{t_0} = p_{\Uparrow}p_{\Downarrow} = \frac{1-p_e^2}{4}. \tag{A.216}$$

Which after their substitution and some simplification, setting $B = B_e + B_n$, gives

$$H_{eff} = \frac{A^2}{32} p_e ((\frac{J - B - i\Gamma}{(J-B)^2 + \Gamma^2} - \frac{J + B + i\Gamma}{(J+B)^2 + \Gamma^2} + \frac{2(B + i\Gamma)}{B^2 + \Gamma^2}) I_{1+} I_{2-} + h.c) + \frac{A^2}{32} p_e^2 ((-\frac{2(J - B - i\Gamma)}{(J-B)^2 + \Gamma^2} - \frac{2(J + B + i\Gamma)}{(J+B)^2 + \Gamma^2)} I_{1+} I_{2-} + h.c.). \quad \text{(A.217)}$$

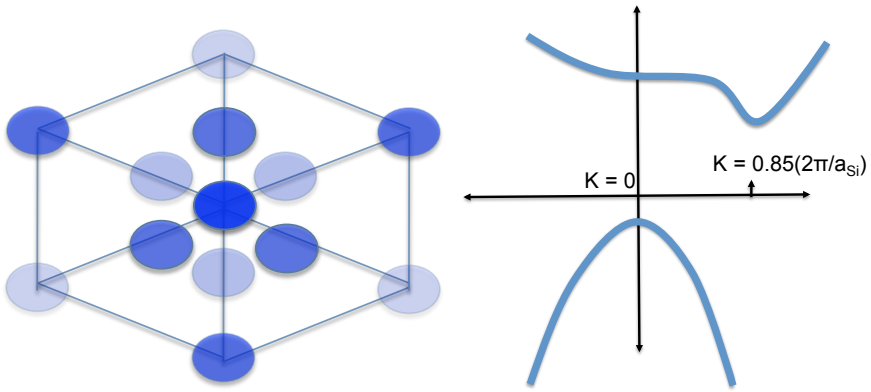
Which may finally be simplified to give

$$H_{eff} = \frac{A^2}{32} ((p_e(1-2p_e) \frac{J - B - i\Gamma_\beta}{(J-B)^2 + \Gamma_\beta^2} - P_e(1+2P_e) \frac{J + B + i\Gamma_\beta}{(J+B)^2 + \Gamma_\beta^2} + 2p_e \frac{2(B + i\Gamma_\beta)}{B^2 + \Gamma_\beta^2}) I_{1+} I_{2-} + h.c.). \quad \text{(A.218)}$$

Which is valid when none of the denominators equal zero.

A.7 Valley Degeneracy of Silicon

Silicon has a six-fold degeneracy along the $< 100 >$ planes. This results in a distorted band structure with a minima located about 85 percent of the way between the centre and the boundary of the Brillouin zone. A rough diagram showing a diamond unit cell is presented to give and idea of the symmetry along with a band diagram depicting the effects of this degeneracy .



(a) Symmetry of the Diamond Lattice (b) Band Structure of Silicon

Figure A.1: Valley Degeneracy

The degeneracy of silicon must be incorporated into this architecture to identify any prevalent effects it may have.

A.7.1 Valley Degeneracy in the Direct Exchange Interaction

Kane's proposal employed the Herring-Flicker exchange formula[11] for two hydrogen centres to estimate the exchange energy between the donors. Donors in silicon, however, are not simply hydrogenic and valley degeneracy plays a major role in their behaviour. Silicon naturally arranges itself a diamond lattice structure which possesses a six-fold symmetry. This symmetry distorts the band structure producing a degenerate minima located along the $< 100 >$ directions about 85 percent of the way between the centre and the boundary of the Brillouin zone. The interference between the 6-fold degenerate states results in oscillations on the few angstroms scale. This severely limit the physical implementation of the Kane model due to the realistic difficulty associated with positioning atoms on the angstrom scale. This can been seen when the interference between the 6 degenerate wavefunctions is added to the Herring-Flicker model.

The Herring-Flicker approximation to hydrogenic centres for the Kane model gives the following exchange strength formula[13]:

$$J_0 = \frac{1.6}{4}\frac{e^2}{\epsilon a_B}(\frac{r}{a_B})^{\frac{5}{2}}e^{\frac{-2r}{a_B}}. \tag{A.219}$$

Where $r = \sqrt{(X_1 - X_2)^2 + (Y_1 - Y_2)^2 + (Z_1 - Z_2)^2}$ and $X_i, Y_i and Z_i$ are the positions of donor i. Belita Koiller showed that this approximation was not sufficient to reproduce the true degenerate nature of silicon [15]. Using the Heitler-London approach Koiller showed that the exchange interaction actually took the form of

$$J \approx J_0 \sum_{\mu}(cos(k_0 \cdot r_\mu))^2. \tag{A.220}$$

As k_0 is very large the direct donor-donor exchange interaction will oscillate quickly with separation r . When plotted as a function of donor separation this new feature gave the following result:

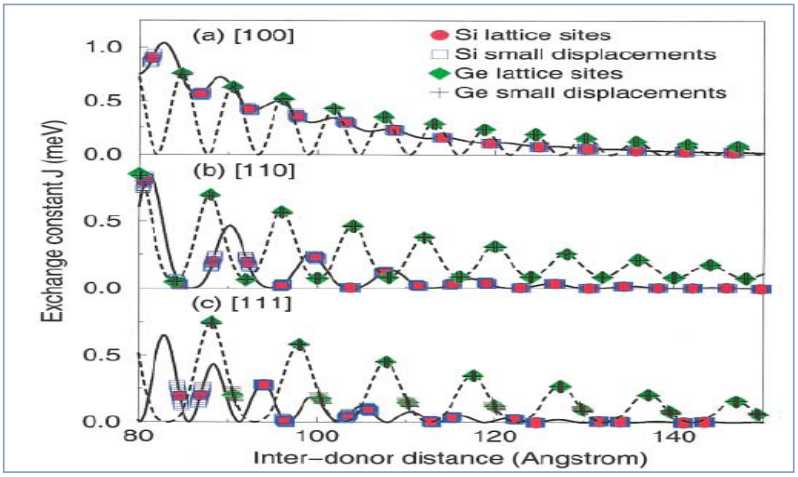


Figure A.2: Valley Degeneracy and the Direct Exchange Interaction[15]

It is clearly evident from this result that the interference between the valley minima will severely limit any attempt to physically construct a computer based on the

Kane architecture. It is not possible, yet, to place donors with angstrom precision. To be readily constructed this architecture must be altered in favour of an interaction that does not result in these critical oscillations.

A.7.2 Valley Degenerate Effects for the RKKY Interaction

The effects of valley degeneracy for the RKKY interaction are considered within the results for J^{e-e}_{RKKY} given by

$$J^{e-e}_{RKKY} = -\frac{m * J_c^2}{(8\pi)\hbar^2}\frac{k_F^2 A^2}{2}\frac{sin(2k_F\bar{x})}{(2k_F\bar{x})^2}.$$

Specifically within the interaction strength term J_c. The electron interaction strength may be defined in terms of the difference between triplet, overall spin 1, and singlet, overall spin 0, scattering amplitudes. J^{e-e}_{RKKY} is measure of the tendency of electron spins to align themselves in a singlet or triplet state. This is again due to the same symmetry arguments presented in chapter 1 when discussing the development of the exchange interaction. It is evident then that the strength of the RKKY interaction, besides depending on physical parameters such as donor depth and 2DEG electron density, will depend on the energy difference between the singlet and triplet states themselves. It is within this dependence on the singlet-triplet energy splitting where the valley degenerate effect are dominant.

Using the Heitler-London approximation the expressions for the triplet and singlet scattering amplitudes may be defined explicitly as

$$J_c = A^T - A^S. \tag{A.221}$$

As all scattering avenues allowed for the triplet case are also available to the singlet

case all terms cancel except the ground state singlet scattering amplitude given by

$$J_c = -\frac{< \Psi^S_{k'\mu'}|H|\Phi\Phi >< \Phi\Phi|H|\Psi^s_{k\mu} >}{\epsilon_d - \epsilon_F + U}. \tag{A.222}$$

Where Ψ is the conduction electron wave-function and Φ the donors valence electron wave-function. The Pauli exclusion principle dictates that the total wavefunction of the two electrons must change sign under simultaneous exchange of both space and spin co-ordinates. If this were not the case two interacting particles could simultaneously occupy the same energy in the same space which is forbidden. The singlet electron spin arrangement, given as $|\uparrow\downarrow> - |\downarrow\uparrow>$, changes sign under exchange of the spins states. This then demands that the combined conduction-donor electron spatial wave-function must be symmetrical under co-ordinate exchange. The donor spatial wave-function is then given by

$$|\Psi^s_k >= \frac{1}{\sqrt{2}}(|\Psi_k > |\Phi > + |\Phi > |\Psi_k >). \tag{A.223}$$

Is is assumed the energy of the donor atoms are roughly given by

$$H|\Phi\Phi > \simeq (2\epsilon_d + U - 2\epsilon_F)|\Phi\Phi > . \tag{A.224}$$

Where ϵ_d is the energy associated with the internal energy of the donor, minus the valence electron. ϵ_f is the energy of the valence electron which assumed to be approximately at the fermi energy, that is almost a free conduction electron. U is the mutual coulomb repulsion between the donors, the energy required to bring the donor into close proximity. When these results are substituted back into the equation for J_c we get

$$J_c = \frac{2(2\epsilon_d + U - 2\epsilon_f)^2}{\epsilon_d + U - \epsilon_F} < \Psi_{k'\mu'}|\Phi >< \Phi|\Psi_{k\mu} > . \tag{A.225}$$

In the case when the conduction electrons are confined within in a 2DEG the six-fold degeneracy is broken. Due to the confinement in the $\hat{z}$ direction the minima located along direction are shifted to a lower energy. This is due to the reflections that persist of the top and bottom of the 2DEG, $e^{ik_0x_{\hat{z}}}$ and $e^{-ik_0x_{\hat{z}}}$ which may be characterized by a sine and cosine term. The resulting conduction electron wave-functions are then given by

$$|\Psi_{k1}>=\sqrt{2}\phi(z)Cos[k_0z]\frac{e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}_\perp}}{\sqrt{A}}; \tag{A.226}$$

$$|\Psi_{k2}>=\sqrt{2}\phi(z)Sin[k_0z]\frac{e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}_\perp}}{\sqrt{A}}. \tag{A.227}$$

Where k_0 is the valley minima wave-vector with $\phi(z)$ being the envelope wave-function for the conduction electron confined to the 2DEG, taken to be

$$\phi(z)=\sqrt{\frac{3}{2z_0}}(\frac{z}{z_0})e^{-\frac{1}{2}(\frac{z}{z_0})^{\frac{3}{2}}}. \tag{A.228}$$

The donor wave-function Φ may then be expressed as

$$|\Phi>=\frac{e^{-\frac{r^i}{a_0}}}{\sqrt{\pi a_0^3}}\frac{1}{\sqrt{6}}\sum_{\mu=1}^{6}e^{i\vec{\boldsymbol{k}}_\mu(\vec{\boldsymbol{x}}-Z_i\hat{\boldsymbol{z}})}. \tag{A.229}$$

Where the $e^{-\frac{r^i}{a_0}}$ term confines the valence electron propagation term $e^{i\vec{\boldsymbol{k}}_\mu(\vec{\boldsymbol{x}}-Z_i\hat{\boldsymbol{z}})}$ to the donor. The co-ordinate r^i is given by

$$r^i=\sqrt{x^2+y^2+(z-Z_i)^2}. \tag{A.230}$$

Where Z_i is the donor's depth and i the donor number, i.e. 1 or 2. After substituting

these expressions back into J_c the expectation value is given by

$$< \Psi_{k1}|\Phi_1 >= \int \frac{\frac{1}{\sqrt{3}}\phi(z)e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}_\perp}}{\sqrt{A}} \frac{e^{\frac{-1}{a_0}\sqrt{x^2+y^2+(z-Z_1)^2}}}{\sqrt{\pi a_0^3}} \mathrm{d}x^3 (Cos(k_0 r_i)); \tag{A.231}$$

$$< \Psi_{k2}|\Phi_1 >= \int \frac{\frac{1}{\sqrt{3}}\phi(z)e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}_\perp}}{\sqrt{A}} \frac{e^{\frac{-1}{a_0}\sqrt{x^2+y^2+(z-Z_1)^2}}}{\sqrt{\pi a_0^3}} \mathrm{d}x^3 (Sin(k_0 r_i)). \tag{A.232}$$

Redefining

$$S_k = \int \frac{\frac{1}{\sqrt{3}}\phi(z)e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{x}}_\perp}}{\sqrt{A}} \frac{e^{\frac{-1}{a_0}\sqrt{x^2+y^2+(z-Z_1)^2}}}{\sqrt{\pi a_0^3}} \mathrm{d}x^3; \tag{A.233}$$

$$S_{\mu=1} = Cos(k_0 Z_i), \tag{A.234}$$

$$S_{\mu=2} = Sin(k_0 Z_i). \tag{A.235}$$

The resulting final dependence of J_c can at last be expressed as

$$Jc^i = \frac{2(2\epsilon_d + U - 2\epsilon_F)^2}{\epsilon_d + U - \epsilon_F} \frac{1}{\sqrt{3}} \sum_{\mu\mu'} |S_k^i|^2 S_\mu^i S_{\mu'}^i. \tag{A.236}$$

Where:

$$\sum_{\mu\mu'} S_\mu^1 S_{\mu'}^1 S_\mu^2 S_{\mu'}^2 = (Cos(k_0 Z_1)Cos(k_0 Z_2) + Sin(k_0 Z_1)Sin(k_0 Z_2))^2 = (Cos(k_0(Z_1 - Z_2)))^2. \tag{A.237}$$

This gives the final form of J_c:

$$Jc^i = \frac{2(2\epsilon_d + U - 2\epsilon_F)^2}{\epsilon_d + U - \epsilon_F} \frac{1}{\sqrt{3}} |S_k^i|^2 (Cos(k_0(Z_1 - Z_2)))^2. \tag{A.238}$$

As in the direct exchange interaction valley degeneracy play an important role in the determination of the interaction strength. The results of this section show the culminating effect of this valley degeneracy. The use of electrons situated in a 2DEG to mediate the RKKY interaction breaks the six-fold symmetry of the silicon lattice

structure. The final result is only two-fold degenerate in terms of the donor depths.

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