A Non-Adiabatic Controlled Not Gate for the Kane Solid State Quantum Computer

C. Wellard†, L.C.L. Hollenberg‡∗ and H.C. Pauli∗.

† School of Physics, University of Melbourne, 3010, AUSTRALIA.
‡ Max-Planck-Institut für Kernphysik, Heidelberg D69029, GERMANY.

The method of iterated resolvents is used to obtain an effective Hamiltonian for neighbouring qubits in the Kane solid state quantum computer. In contrast to the adiabatic gate processes inherent in the Kane proposal we show that free evolution of the qubit-qubit system, as generated by this effective Hamiltonian, combined with single qubit operations, is sufficient to produce a controlled-NOT (c-NOT) gate. Thus the usual set of universal gates can be obtained on the Kane quantum computer without the need for adiabatic switching of the controllable parameters as prescribed by Kane [1]. Both the fidelity and gate time of this non-adiabatic c-NOT gate are determined by numerical simulation.
In the Kane proposal for a solid state quantum computer a series of spin $\frac{1}{2}$ $^{31}\text{P}$ nuclei in a silicon substrate are used as qubits [1]. The interaction between these qubits is mediated by valence electrons weakly bound to the nuclei, such that at energies much lower than these electrons binding energy the system Hamiltonian is given by

$$H = \mu_B B(\sigma_{1e}^+ + \sigma_{2e}^+) - g_n \mu_n B(\sigma_{1n}^z + \sigma_{2n}^z) + A_1 \vec{\sigma}_{1e} \cdot \vec{\sigma}_{1n} + A_2 \vec{\sigma}_{2e} \cdot \vec{\sigma}_{2n} + J \vec{\sigma}_{1e} \cdot \vec{\sigma}_{2e}. \quad (1)$$

The interaction strengths $A_1$, $A_2$ as well as $J$ are controllable by means of voltage biases applied to “A” and “J” gates respectively [1,2]. In the case where $J = 0$, the energy splitting between the electron spin states is approximately 1600 times larger than the splitting of the nuclear states. Thus at temperatures low compared to these energy splittings the nuclear spin states, in the electron ground state, can be manipulated without significantly altering the electron states. This gives a basis in which quantum computation can be performed, the reduced Hilbert space of the electron ground state. The quantum computing basis is then:

$$|\downarrow \downarrow 00\rangle, |\downarrow \downarrow 01\rangle, |\downarrow \downarrow 10\rangle, |\downarrow \downarrow 11\rangle. \quad (2)$$

Here $|\downarrow\rangle$ denotes an electron in the spin down state and $|0\rangle, |1\rangle$ denote a nucleus in the spin up and down state respectively. The electron spin down state remains the ground state as long as $J < \frac{\mu B}{2}$, although the energy difference between this state and the odd superposition of electrons reduces as $J$ increases, thus in operating our quantum computer we want to keep $J$ below this limit.

A requirement of a universal quantum computer is that it be able to implement a universal set of gates. One such universal set comprises of the set of single qubit rotations and the controlled-NOT (c-NOT) gate [3,4]. The currently proposed implementation of the c-NOT in the Kane quantum computer relies on an adiabatic switching on of the $A$ and $J$ couplings to produce a unique energy splitting between states which can then be swapped using a Rabi type flipping induced by a transverse...
magnetic field rotating at a frequency such that it is in resonance with the desired transition \([1,2]\). This adiabatic switching process has been studied in detail \([11]\) and can produce a c-NOT gate with an error of \(\epsilon \approx 10^{-5}\) in a time \(t_{c-NOT} = 26\mu s\). In this article we introduce a c-NOT gate that does not rely on adiabatic switching. We derive an effective Hamiltonian that describes the interaction of the qubits in the subspace of the electron ground state using the method of iterated resolvents. This effective Hamiltonian is then used to derive a c-NOT gate that relies only on the evolution of the qubits that it generates, in combination with the single qubit operations. We then use this fact to argue that the family of gates consisting of the free evolution of neighbouring qubits for pre determined times, is a suitable alternative to the adiabatically constructed c-NOT gate for use in the implementation of quantum algorithms.

**II. THE EFFECTIVE HAMILTONIAN**

To understand the dynamics of the qubits in the computational subspace, it is useful to calculate an effective Hamiltonian that describes the action of Eq (1) in this reduced bases. To do this we use the method of iterated resolvents \([7]\), which has been used successfully to calculate effective Hamiltonians in reduced bases in QCD. The method of iterated resolvents involves the systematic reduction of the dimension of the system to that of the subspace of interest. In this case a reduction of the full \(16 \times 16\) system Hamiltonian, \(H_{16}\), to a \(4 \times 4\) effective Hamiltonian, \(H_4\).

We begin by writing the eigenvalue problem for the complete Hamiltonian

\[
\sum_{j=1}^{16} \langle i | H_{16} | j \rangle \langle j | \Psi \rangle = E \langle i | \Psi \rangle.
\]  

Let us divide the rows and columns of \(H_{16}\) into separate subspaces, take the first 15 rows to be the first subspace, call it \(P\), and the remaining subspace we call \(Q\). Thus Eq(3) can be expressed as

\[
\sum_{j=1}^{15} \langle i | H_{16} | j \rangle \langle j | \Psi \rangle + \langle i | H_{16} | 16 \rangle \langle 16 | \Psi \rangle = E \langle i | \Psi \rangle,
\]  

which can be written in the block matrix form
\begin{align*}
\langle P|H_{16}|P\rangle\langle P|\Psi\rangle + \langle P|H_{16}|Q\rangle\langle Q|\Psi\rangle &= E\langle P|\Psi\rangle, \quad (5) \\
\langle Q|H_{16}|P\rangle\langle P|\Psi\rangle + \langle Q|H_{16}|Q\rangle\langle Q|\Psi\rangle &= E\langle Q|\Psi\rangle. \quad (6)
\end{align*}

Because the eigenvalue $E$ is in general unknown, it is replaced with a free parameter $\omega$ to be determined later. Thus if the matrix $\langle Q|\omega - H_{16}|Q\rangle$ can be inverted, the Q space wave function can be expressed in terms of the P space wave function.

\begin{align*}
\langle Q|\Psi(\omega)\rangle &= G_Q(\omega)\langle Q|H_{16}|P\rangle\langle P|\Psi\rangle, \quad (7)
\end{align*}

where we have written the resolvent

\begin{align*}
G_Q(\omega) &= \frac{1}{\langle Q|\omega - H_{16}|Q\rangle}. \quad (8)
\end{align*}

Substituting Eq(7) into Eq(6) gives

\begin{align*}
\langle P|H_{15}(\omega)|P\rangle\langle P|\Psi(\omega)\rangle &= E(\omega)\langle P|\Psi(\omega)\rangle, \quad (9)
\end{align*}

which defines an eigenvalue equation in the P space

\begin{align*}
\langle P|H_{15}(\omega)|P\rangle\langle P|\Psi(\omega)\rangle &= E(\omega)\langle P|\Psi(\omega)\rangle, \quad (10)
\end{align*}

which in turn defines for an effective 15 Hamiltonian in the P space

\begin{align*}
H_{15}(\omega) &= H_{16} + H_{16}|Q\rangle G_Q(\omega)\langle Q|H_{16}. \quad (11)
\end{align*}

The method of iterated resolvents calls for this procedure to be repeated until an effective $4 \times 4$ Hamiltonian for the computational sub-space is produced. Finally it is necessary to solve the fixed point equation $\langle 4|H_4(\omega)|4\rangle = w$. This equation produces many solutions, the correct one to choose is the one that yields an eigenspectrum for $H_4$ that is as close as possible to the four lowest eigenvalues of the complete Hamiltonian. This procedure was completed numerically for parameters similar to those used in the adiabatic gate $A_1 = A_2 = 1.683$ and $J = 600$ in units of $g_n\mu_n B$.

This yielded an effective Hamiltonian of the form

\begin{align*}
H_{\text{eff}} &= \Delta(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + \Theta\sigma_1^z\sigma_2^z + \Lambda(\sigma_1^z + \sigma_2^z) + \Gamma, \quad (12)
\end{align*}

where it is understood that the subscripts denote the first and second nucleus.

The values of the parameters were $\Delta = 2.3723 \times 10^{-3}$, $\Theta = -1.4645 \times 10^{-5}$, $\Lambda = 2.6871$, $\Gamma = 5.3578$. 

4
III. CONSTRUCTING A C-NOT GATE

The generator of the c-NOT operator, $U_{c\text{-NOT}} = \exp[-iG]$, is given by

$$G = \frac{\pi}{4}(1 - \sigma_1^z - \sigma_2^z + \sigma_1^z\sigma_2^z).$$  \hspace{1cm} (13)

All the terms on the right hand side commute, and so the c-NOT operator can be written as

$$U_{c\text{-NOT}} = \exp\left[-\frac{i\pi}{4}\right]\exp\left[i\frac{\pi}{4}\sigma_1^z\right]\exp\left[i\frac{\pi}{4}\sigma_2^z\right]\exp\left[-\frac{i\pi}{4}\sigma_1^z\sigma_2^z\right].$$  \hspace{1cm} (14)

Here, reading from left to right, the first factor just represents a phase factor, this is unimportant as all that is required is a c-NOT operation up to an overall phase. The second factor is a $\sigma^z$ rotation, this can be realized by a combination of the single particle rotations common to NMR theory [5,10].

$$\exp\left[i\frac{\pi}{4}\sigma^z\right] = \exp\left[i\frac{\pi}{4}\sigma^x\right]\exp\left[-i\frac{\pi}{4}\sigma^y\right]\exp\left[-i\frac{\pi}{4}\sigma^z\right].$$  \hspace{1cm} (15)

The third factor is just another standard single particle operation. The fourth factor requires a combination of pulses to give the required evolution. Given an effective Hamiltonian of the form Eq(12) we can use standard refocusing techniques standard to construct this evolution of the qubit-qubit system. The c-number factor in the effective Hamiltonian commutes with all other terms and simply leads to an overall phase in the evolution, it can thus be ignored in the calculations and included at the end. Our first step then is to refocus out the Zeeman evolution of the nuclei, using rf pulses targeted at both nuclei simultaneously:

$$\exp\left[i\frac{\pi}{2}(\sigma_1^x + \sigma_2^x)\right]\exp\left[-\frac{it}{4\hbar}(H_{\text{eff}} - \Gamma)\right] \times \exp\left[-\frac{i\pi}{2}(\sigma_1^x + \sigma_2^x)\right]\exp\left[-\frac{it}{4\hbar}(H_{\text{eff}} - \Gamma)\right]$$

$$= \exp\left[-\frac{it}{2\hbar}(\Delta(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + \Theta\sigma_1^z\sigma_2^z)\right].$$  \hspace{1cm} (16)

The next step is to refocus out the $\sigma_1^y\sigma_2^y$ and $\sigma_1^z\sigma_2^z$ parts of the evolution:

$$\exp\left[i\frac{\pi}{2}\sigma_1^x\right]\exp\left[-\frac{it}{2\hbar}(\Delta(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + \Theta\sigma_1^z\sigma_2^z)\right] \times$$

$$\exp\left[-\frac{i\pi}{2}\sigma_1^x\right]\exp\left[-\frac{it}{2\hbar}(\Delta(\sigma_1^x\sigma_2^x + \sigma_1^y\sigma_2^y) + \Theta\sigma_1^z\sigma_2^z)\right]$$

$$= \exp\left[-\frac{it}{\hbar}\Delta\sigma_1^x\sigma_2^x\right].$$  \hspace{1cm} (17)
Again targeting the first spin only, we can obtain
\[
\exp\left[\frac{i\pi}{4} \sigma^y_1\right] \exp\left[-\frac{it}{\hbar} \Delta \sigma^x_1 \sigma^x_2\right] \exp\left[-\frac{i\pi}{4} \sigma^y_1\right] = \exp\left[-\frac{it}{\hbar} \Delta \sigma^x_1 \sigma^x_2\right];
\]
this evolution for a time \( t = \pi \hbar/(4\Delta) \) gives the required operator in Eq (14). Substituting these pulses into Eq(14) we find that the c-NOT operation can be written as,
\[
U_{c-NOT} = \exp\left[-\frac{i\pi}{4} \left(1 - \frac{\Gamma}{\Delta}\right)\right] \exp\left[\frac{i\pi}{4} \sigma^x_1\right] \exp\left[-\frac{i\pi}{4} \sigma^y_1\right] \exp\left[-\frac{it}{\hbar} \Delta \sigma^x_1 \sigma^x_2\right] \times \exp\left[\frac{i\pi}{4} \sigma^x_2\right] \exp\left[\frac{i\pi}{4} \sigma^y_1\right] \exp\left[\frac{i\pi}{2} (\sigma^x_1 + \sigma^x_2)\right] \times \exp\left[\frac{i\pi}{2} \frac{\pi \hbar}{16\Delta}\right] \exp\left[-\frac{i\pi}{2} (\sigma^x_1 + \sigma^x_2)\right] \exp\left[-\frac{i\pi}{4} \sigma^y_1\right] \times \exp\left[-\frac{i\pi}{2} \frac{\pi \hbar}{16\Delta}\right] \exp\left[-\frac{i\pi}{4} \sigma^y_1\right] \times \exp\left[-\frac{i\pi}{2} \frac{\pi \hbar}{16\Delta}\right] \exp\left[-\frac{i\pi}{4} \sigma^y_1\right],
\]
where \( F[t] = \exp\left[i\pi t H_{eff}/\hbar\right] \) denotes free evolution generated by \( H_{eff} \) over a time \( t \). The first term is simply a phase correction, it cannot be implemented physically but tells us by what overall phase the composite operator must be corrected to produce exact c-NOT evolution.

**IV. GATE TIME AND FIDELITY**

It is first necessary to check that Eq(12) does give an accurate description of the two qubit effective Hamiltonian. This was done by numerically solving the Schrödinger equation for the time development of the entire electron-nuclear system using the Hamiltonian Eq(1) over a time of several microseconds, and comparing the evolution of the qubits to that predicted by the effective Hamiltonian over the same period. It was found that final states agreed with an error probability of \( 10^{-5} \).

Let us now calculate the time this non-adiabatic gate takes to execute, using similar values for the operating parameters to those prescribed for the adiabatic c-NOT gate. The construction requires that the system evolves freely for a total time \( t = \pi/(4\Delta) \approx 3\mu s \). In addition to this free evolution, we also have the single particle rotations, the time scale of which is set by the time it takes to implement a π rotation, \( \tau \approx 22\mu s \). The combination of single particle operations necessary for
this implementation takes a total of $t \approx 77 \mu s$ to execute, taking the total gate time to $t_{\text{c-NOT}} \approx 80 \mu s$, compared with $26 \mu s$ for the adiabatic implementation.

This gate was simulated numerically and it was found that the operation is indeed that of a c-NOT gate, with an error probability of $\epsilon = 4 \times 10^{-4}$. This is slightly outside current estimates of the error tolerance of a QC using error correcting codes, which vary between $\epsilon < 10^{-6} - 10^{-4}$ [9,8,12]. These error tolerances, most authors admit, are probably pessimistic, and are based on some very general assumptions about the type of error process and the architecture of the computer. It is possible that by tailoring an error correcting code to a specific problem, the error tolerance may be more forgiving and the error probability of this gate may fit well within the new bound.

The problem still remains however, that this non-adiabatic c-NOT gate is both slower, and of lower fidelity than the adiabatic implementation. Both these facts can in part, be attributed to the large number of single qubit operations performed in the c-NOT implementation. Note that the period of “free evolution” required to implement the c-NOT gate is only about $3 \mu s$. During this free evolution is the only time that there can possibly be information flow between the two qubits, in contrast to the adiabatic case in which information flow occurs over the entire gate time of $26 \mu s$. With this in mind, we can consider free evolution for this time to be an elementary two-qubit gate that is capable of transferring the same quantity of quantum information between two qubits as is a c-NOT gate, in just over 10% of the time. It therefore seems reasonable to speculate that it would be possible to recast any large scale quantum algorithm, into a series of single qubit rotations, and two-qubit “free evolutions” without the need to explicitly construct a c-NOT gate, and that this recipe for constructing the algorithm may be faster than one which relies on an explicit adiabatic implementation of the c-NOT gate, for the Kane quantum computer.
V. ACKNOWLEDGEMENTS

CJW would like to acknowledge the support of an Australian Postgraduate Award, a Melbourne University Postgraduate Abroad Scholarship and the Max-Planck-Institut für Kernphysik. LCLH wishes to thank the Alexander Von Humboldt foundation and the Max-Planck-Institut für Kernphysik.
