Multi-qubit gates protected by adiabaticity and dynamical decoupling applicable to donor qubits in silicon

Wayne M. Witzel, Richard P. Muller, and Malcolm S. Carroll

1 Sandia National Laboratories, New Mexico 87185 USA

We present a strategy for producing multi-qubit gates that promise high fidelity with minimal tuning requirements. Our strategy combines gap protection from the adiabatic theorem with dynamical decoupling in a complementary manner. To avoid degenerate states and maximize the benefit of the gap protection, the scheme is best suited when there are two different kinds of qubits (not mutually resonant). Furthermore, we require a robust operating point in control space where the qubits interact with little sensitivity to noise. This allows us to circumvent a No-Go theorem that prevents block-box dynamically corrected gates [Phys. Rev. A 80, 032314 (2009)]. We show how to apply our strategy to an architecture in Si with P donors where we assume we can shuttle electrons between different donors. Electron spins act as mobile ancillary qubits and P nuclear spins act as long-lived data qubits. This system can have a very robust operating point where the electron spin is bound to a donor in the quadratic Stark shift regime. High fidelity single qubit gates may be performed using well-established global magnetic resonance pulse sequences. Single electron spin preparation and measurement has also been demonstrated. Putting this all together, we present a robust universal gate set for quantum computation.

One of the main challenges in realizing a quantum information processor is the ability to implement high-fidelity entangling operations. It can be relatively easy to control well isolated qubits. Nuclear magnetic resonance (NMR) is well developed for manipulating nuclear spins and decoupling them from their environment [1]. Electron spin resonance (ESR) had also been demonstrated to producing high fidelity gates [2]. Turning interactions between qubits on and off in a controllable manner for a coherent quantum operation remains very challenging. The process of coupling different qubits is often accompanied by an enhanced sensitivity to the environment. When qubits are not isolated, they are vulnerable to noise.

The adiabatic theorem [3] provides remarkably robust operations in the sense that transitions between non-degenerate eigenstates are suppressed. If the Hamiltonian of a quantum system is varied slowly enough, instantaneous eigenstates will be tracked. This effect is to be exploited in an adiabatic quantum computer which is initialized in a ground state that is easy to prepare then adiabatically evolved to a final Hamiltonian whose ground state encodes the solution to a problem [4]. This model of quantum computation is polynomially equivalent to the standard circuit-based model [5]. However, it lacks a threshold theorem [6] that has been established in the circuit model [7, 8]. The holonomic [9] scheme for quantum log  gating provides one strategy to use the adiabatic theorem in the circuit model setting. In that scheme, a qubit is encoded in a degenerate subspace and an adiabatic cycle induces a geometric transformation on the qubit(s). While elegant, it requires the proper setting with a degenerate computational basis and is vulnerable to noise that breaks the degeneracy. In our proposal, we perform an adiabatic process involving two qubits and non-degenerate eigenstates (diabetic energy level crossings are allowed, however). Transition errors are suppressed by the adiabatic theorem, but phase errors must be mitigated using a different mechanism.

The Hahn echo [10] is a simple and effective way to cancel phase errors induced by low-frequency noise and uncertainty. By flipping a qubit midway through it's evolution with an $X$ gate, the effects of an unknown but systematic $Z$ interaction are reversed. The Hahn echo, and a variety of more elaborate sequences or strategies [11–15] for prolonging coherence in the presence of noise or control errors, are very good techniques for storing quantum information. These are known as dynamical decoupling (DD) schemes because they decouple the qubit system from its environment. There also exist analogous strategies called dynamically corrected gates (DCGs) to cancel errors during nontrivial quantum gate operations [16–20]. However, there is an obstacle to producing and applying DCGs. A No-Go theorem proves that a black-box approach can not exist for DCGs as it does for identity gates using DD [17]. DCGs must assume there are relationships between the effects of noise induced under different control settings. In a two-qubit DCG, for example, you would need to vary the interaction between the qubits but maintain consistent or correlated environmental interactions in order to cancel their effects. This presents a problem when interactions are varied by moving the qubits (such as localized electrons in a solid state material) and the environment varies at this length scale.

We circumvent this No-Go theorem by assuming that we have a robust operating point (ROP), a ”sweet spot” in control space where the qubits interact stably with respect to noise. We don’t attempt to correct for errors induced during this ROP time, but we do correct for errors induced in transit (adiabatically) to and from this control space point. This is illustrated schematically in Fig. 1. We will show how this can be accomplished in a generic model in three nested components, prove its
FIG. 1. Control space schematic showing an adiabatic path between isolated qubits and a ROP where the qubits interact. We wish to cancel the phase accumulated during the traversal between these points using dynamical decoupling.

universality, and then discuss the suitability of silicon donor qubits for implementing this scheme.

The first of our nested components is the adiabatic cycle of moving isolated qubits to a ROP, where they interact, and then back. In an ideal limit, adiabatic operations are, by definition, diagonal with respect to instantaneous eigenstate bases. Up to an irrelevant global phase such an operation for two qubits is generically

\[
\begin{pmatrix}
  e^{i\alpha} & 0 & 0 & 0 \\
  0 & e^{i\beta} & 0 & 0 \\
  0 & 0 & e^{i\gamma} & 0 \\
  0 & 0 & 0 & e^{-i(\alpha+\beta+\gamma)}
\end{pmatrix} = \begin{pmatrix} Z_a & Z_b \\ Z_b & Z_a \end{pmatrix} \tag{1}
\]

\[
\begin{pmatrix}
  Z_a \\
  Z_b
\end{pmatrix} = \begin{pmatrix} Z_a & Z_b \\ Z_b & Z_a \end{pmatrix} \begin{pmatrix} \tau \end{pmatrix} = \begin{pmatrix} \tau \end{pmatrix} \tag{2}
\]

\[
Z_a = e^{-i\alpha}, \quad Z_b = e^{-i\beta}, \quad Z_c = e^{-i\gamma},
\]

in the eigenstate basis using a matrix representation (left) or a circuit-model representation (right). Consider the path illustrated in Fig. 1, consisting of three stages: 1) traversing from isolated qubits to the ROP; 2) waiting at the robust operating point; 3) traversing back to isolated qubits. Each is an operation as in Eq. (1) and these operations commute. Generically, we may write the circuit model representation as

\[
\begin{pmatrix}
  Z_a & Z_b & Z_c \\
  Z_b & Z_c & Z_d \\
  Z_c & Z_d & Z_e
\end{pmatrix} \tag{3}
\]

where \( a = a_1 + a_3, \quad b = b_1 + b_3, \quad c = c_1 + c_3, \quad d(\tau) = a_2, \quad e(\tau) = b_2, \quad f(\tau) = c_2 \). We use \( \tau \) to denote the amount of time spent at the second stage, parameterizing this operation in a controlled manner. Somewhat arbitrarily, we will refer to the top rail of Eq. (2) as the ancilla and the bottom rail as the data.

We’d like to cancel out the dependence on \( a, b \) and \( c \), which are vulnerable to uncertainty and low-frequency noise. The remaining \( d(\tau), e(\tau), \) and \( f(\tau) \) dependence are incurred while waiting at the ROP and are therefore presumed to be less susceptible to noise. The second and third components of our procedure are designed for that purpose. In the second component, we cancel out the \( a \) dependence by applying DD to the ancilla qubit in what we will call an “ancilla-refocused double-cycle”. This component has three stages. First, we perform an adiabatic cycle where we set \( \tau \) such that \( f(\tau) = \pi \). Next, we apply a refocusing X gate on the ancilla qubit. Finally, we perform another adiabatic cycle that is the same as the first except we take \( \tau = 0 \). This does not mean we literally must spend no time at the ROP in this second adiabatic cycle, but rather that the difference in the two adiabatic cycles should amount to an extra controlled-Z operation. We can always pad stage 1 and 3 of the adiabatic cycle with ROP time if convenient. To the extent these operations are not ideally realized, there will be noise that is not canceled, but it is instructive to assume idealism in the initial analysis. The net operation of this component is then

\[
\begin{pmatrix}
  Z_a & Z_d \\
  Z_d & Z_e \\
  Z_e & Z_g
\end{pmatrix} = \begin{pmatrix} Z_d & X \\ X & Z_d \end{pmatrix} \tag{4}
\]

where \( g = 2b+c+e \). Notice that, in addition to canceling the \( a \) dependence, we have also made the \( c \) rotation on the data qubit deterministic rather than dependent upon the ancilla state. As far as the ancilla qubit is concerned, it has performed a CPhase operation with the data qubit and the uncertainty has been canceled.

The final, top-level component applies DD in a three stage process as before, but it will involve two different ancilla qubits. In the first stage, we do an ancilla-refocused double-cycle with one ancilla. Next, we perform a refocusing X gate on the data qubit. Finally, we do another ancilla-refocused double-cycle but with a different ancilla. The circuit-model representation is

\[
\begin{pmatrix}
  Z_a & X & Z_g \\
  Z_g & X & Z_a
\end{pmatrix} = \begin{pmatrix} Z_a & X \\ X & Z_a \end{pmatrix} \Rightarrow \begin{pmatrix} X \\
\end{pmatrix} \tag{4}
\]
initialize and measure ancilla qubits. We will show that the ancilla qubits can be used to initialize and prepare data qubits, test as well as mediate entangling interactions between them. Our construction will be a proof-in-principle without concern of the efficiency. First, we will simplify matters by reducing our three-qubit gate to a single CPhase between data and ancilla qubits:

\[ |0\rangle \begin{array}{c} \text{X} \\ \text{X} \end{array} = \begin{array}{c} \text{X} \\ \text{X} \end{array} \Rightarrow \begin{array}{c} \text{X} \\ \text{X} \end{array} \]  

With this CPhase, we can measure a data qubit via

\[ |0\rangle \begin{array}{c} \text{H} \\ \text{H} \\ \text{H} \\ \text{H} \end{array} = |0\rangle \begin{array}{c} \text{H} \\ \text{H} \\ \text{H} \\ \text{H} \end{array} = \begin{array}{c} \text{X} \\ \text{X} \end{array}. \]  

Since this is a non-destructive measurement of the data qubit, we can use it for initialization as well (simply flip the qubit conditional on the measurement outcome). We can mediate a CPhase gate between two data qubits via

\[ |0\rangle \begin{array}{c} \text{H} \\ \text{H} \\ \text{H} \\ \text{H} \end{array} = |0\rangle \begin{array}{c} \text{H} \\ \text{H} \\ \text{H} \\ \text{H} \end{array} = \begin{array}{c} \text{X} \\ \text{X} \end{array}. \]  

where the two bottom rails are data qubits. With these, we have data qubit initialization, measurement, single qubit gates, and CPhase which is a universal set.

We now transition from an abstract to a concrete proposal applied to donor qubits in silicon. We envision a similar layout as the well-known Kane architecture \[21\] in which we have array of P donors in Si and donor electrons are controlled with electrostatic pads from above. Rather than mediating interactions through the exchange coupling of electrons, however, we propose to shuttle individual electrons between donors as proposed in Refs. \[22\] and \[23\], possibly by shuttling the electron along an oxide interface \[24\]. The innovation in our proposal is the use of adiabaticity and DD to cancel uncertainty and low-frequency noise incurred during the shuttling process. We treat the electron spins as ancilla qubits and donor nuclear spins as data qubits and apply our robust multi-qubit gate proposal directly to this system. Single electron spin preparation may be performed via spin-selective tunneling into a single-electron transistor \[25\] \[27\]. Single qubit operations can be performed using global ESR and NMR \[1\] \[2\]. We can implement selective data qubit operations by addressing only donors that are occupied with properly initialized electrons. Universality does not require ancilla gate operations to be selective beyond the shuttling done with local electrostatic controls; the ancilla only need to be able to mediate data qubit interactions selectively (and in parallel). The two-qubit interaction is simply the hyperfine (HF) coupling between an electron and the donor it is occupying.

In order to establish the suitability of our multi-qubit gate strategy to this Si:P system, we must address the following questions. How isolated are the qubits when the interaction is supposed to be off? How robust is the ROP? How adiabatic can we make the shuttling process?

When electrons and nuclei are sufficiently far apart, the dipole interaction is the dominant coupling. When wavefunctions of electrons overlap, the exchange interaction dominates. When the electron wavefunction has considerable amplitude on a phosphorus donor, the contact HF interaction, proportional to the probability density of the electron on the donor, dominates. We’ll assume the dipolar interaction dominates in the regime in which we regard qubits to be isolated. The dipolar Hamiltonian between a pair of spins is

\[ H_D = \frac{\mu_0 \gamma_1 \gamma_2 \hbar^2}{4\pi r^3} \left[ \vec{I}_1 \cdot \vec{r} - 3(\vec{r} \cdot \vec{I}_1)(\vec{r} \cdot \vec{I}_2) \right] \]

where \( \gamma_1 \) and \( \gamma_2 \) are respective gyromagnetic ratios, \( \vec{I}_1 \) and \( \vec{I}_2 \) are respective spin operators, and \( \vec{r} \) is the vector between the spin positions (the sign is unimportant). For the P nuclear spin, \( \gamma_P = 10.8 \times 10^7 / Ts \). For the electron spin, \( \gamma_S = g \mu_B \) where \( g = 2 \) in Si. The left side of Fig. 2 shows approximate dipolar interaction strengths between electron and/or nuclear spins versus distance. Let us suppose the donor qubit separation is 100 nm. Then the unwanted data qubit interaction will be tens of \( \mu \)Hz scale, data and ancilla qubits can interact on the tens of mHz scale (suppressed, as well, by being out-of-resonance in a finite magnetic field), and the ancilla qubits will interact at about 100 Hz. The data qubits are therefore very well isolated when the interaction is off. Ancilla qubits can also be regarded as well isolated if they are only used briefly compared to 10 ms.

Now consider a single electron spin and nuclear spin within the regime of a strong contact HF interaction.
The Hamiltonian is
\[ \hat{H} = B (\gamma_S S^z - \gamma_P I^z) + A(\vec{E}) \cdot \mathbf{S} \]  
where \( S \) and \( I \) are respective electron and nuclear spin operators, \( B \) is the magnetic field applied along \( z \), and \( A \) is the HF interaction that depends upon the electric field. The robust operating point occurs at the quadratic Stark shift regime, where \( A(\vec{E}) \) is maximum and therefore has no linear dependence on \( \vec{E} \). According to calculations in Ref. 25, \( A(\vec{E}) \approx A(0)(1+2.8 \times 10^{-3} E^2) \) for donors deeper than about 15 nm. The right of Fig. 2 plots this sensitivity to electric field noise. Shallower donors may need extra characterization to account for the linear Stark effect but should be similarly robust to electric field noise.

We tested the limits of adiabaticity by simulating this two qubit system with a time-varying contact HF interaction. We used \( B = 100 \) mT, ample for good gap protection. The top of Fig. 3 shows the eigenstate energies as a function to the contact HF strength from zero to its maximum bulk value of 117.5 MHz [29]. There is an energy level crossing that occurs when the interaction is relatively small. There is nothing to split these energy levels in this Hamiltonian. However, these can be split by the anisotropic HF interaction, which is simply the dipolar interaction averaged over the electron wavefunction. This interaction is quite small at a 10 nm scale [Fig. 2], but could be more substantial as the contact HF turns on. The precise amount of energy splitting depends upon specifics in the valley physics and Bloch oscillations. We will assume this crossing is perfectly diabatic and leave this issue for future work.

We simulated the contact-only HF model using \( A(t) = 117.5 \) MHz \times \( \sin(\pi t/T) \) for \( t \in [0, T] \). Consistent with the claims of Ref. 30 that adiabaticity can improve by setting time derivatives of the initial and final Hamiltonian to zero, we find that this yields better performance than a piecewise linear time dependence. The only transition error allowed by this model is a flip-flop between nuclear and electron spin, which is extremely small on the 10 ns shuttle time scale as seen at the bottom of Fig. 3. The tunnel coupling relevant to the shuttle process will probably be a more stringent limitation, but is dependent upon details of the fabrication.

In conclusion, we present a procedure for making robust multi-qubit operations. It produces two CPhase gates between one data qubit and two different ancilla qubits. This is an entangling operation sufficient for universality. It utilizes adiabatic gap protection and dynamical decoupling in complementary ways to make the operation robust against uncertainty and low frequency noise. It can be implemented on a system with two off-resonant species of qubits (to avoid energy level degeneracy) where interactions can be controllably turned on and off between qubits of different species and where there is a robust operating point for each pairwise interaction.

These conditions are well met for a system of P donors in Si, using electron and nuclear spins as the two qubit species.

We acknowledge numerous discussions with intellectual contributions to this work from our diverse, multidisciplinary team of quantum device and architecture experts at Sandia National Laboratories including Nathan Bishop, Robin Blume-Kohout, Anand Ganti, Matthew Grace, N. Tobias Jacobson, Andrew Landahl, Ines Montano, Erik Nielsen, and Kevin Young.

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
[1] L. Vandersypen and I. Chuang, Reviews of Modern Physics 76, 1037 (2005).
[2] J. J. L. Morton, A. M. Tyrnyshkin, A. Ardavan, K. Porfyariskis, S. A. Lyon, and G. A. Briggs, Physical Review Letters 95, 200501 (2005).
[3] T. Kato, Journal of the Physical Society of Japan 5, 435 (1950).
[4] E. Farhi, J. Goldston, G. Gutmann, and M. Sipser, “Quantum computation by adiabatic evolution,” quant-ph/0001106.
[5] D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, SIAM Review 50, 755 (2008).
[6] D. A. Lidar, Physical Review Letters 100, 160506 (2008).
[7] E. Knill, R. Laflamme, and W. H. Zurek, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 454, 365 (1998).
[8] D. Gottesman, Stabilizer Codes and Quantum Error Correction, Ph.D. thesis, California Institute of Technology (1997).
[9] P. Zanardi and M. Rasetti, Physics Letters A 264, 94 (1999).
[10] E. Hahn, Physical Review 80, 580 (1950).
[11] H. Carr and E. Purcell, Physical Review 94, 630 (1954).
[12] S. Meiboom and D. Gill, Review of Scientific Instruments 29, 688 (1958).
[13] K. Khodjasteh and D. A. Lidar, Physical Review Letters 95, 180501 (2005).
[14] G. S. Uhrig, Physical Review Letters 98, 100504 (2007).
[15] L. Viola and E. Knill, Physical Review Letters 90, 037901 (2003).
[16] K. Khodjasteh and L. Viola, Physical Review Letters 102, 080501 (2009).
[17] K. Khodjasteh and L. Viola, Physical Review A 80, 032314 (2009).
[18] K. Khodjasteh, D. A. Lidar, and L. Viola, Physical Review Letters 104, 090501 (2010).
[19] T. Green, H. Uys, and M. J. Berczik, Physical Review Letters 109, 020501 (2012).
[20] G. A. Paz-Silva and L. Viola, “A general transfer-function approach to noise filtering in open-loop quantum control,” arXiv:1408.3836.
[21] B. Kane, Nature 393, 133 (1998).
[22] A. J. Skinner, M. E. Davenport, and B. E. Kane, Physical Review Letters 90, 087901 (2003).
[23] J. J. L. Morton, “A silicon-based cluster state quantum computer,” arXiv:0905.4008.
[24] M. J. Calderón, B. Koiller, and S. Das Sarma, Physical Review B 75, 125311 (2007).
[25] J. M. Elzerman, R. Hanson, L. H. Willems van Beveren, B. Witkamp, L. M. K. Vandersypen, and L. P. Kouwenhoven, Nature 430, 431 (2004).
[26] A. Morello, J. J. Pla, F. A. Zwanenburg, K. W. Chan, K. Y. Tan, H. Huebl, M. Mtnen, C. D. Nugroho, C. Yang, J. A. van Donkelaar, A. D. C. Alves, D. N. Jamieson, C. C. Escott, L. C. L. Hollenberg, R. G. Clark, and A. S. Dzurak, Nature 467, 687 (2010).
[27] C. B. Simmons, J. R. Prance, B. J. Van Bael, T. S. Koh, Z. Shi, D. E. Savage, M. G. Lagally, R. Joynt, M. Friesen, S. N. Coppersmith, and M. A. Eriksson, Physical Review Letters 106, 156804 (2011).
[28] R. Rahman, C. J. Wellard, F. R. Bradbury, M. Prada, J. H. Cole, G. Klimeck, and L. C. L. Hollenberg, Physical Review Letters 99, 036403 (2007).
[29] G. Feher, Physical Review 114, 1219 (1959).
[30] D. A. Lidar, A. T. Rezakhani, and A. Hamma, Journal of Mathematical Physics 50, 102106 (2009).