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FAST TRACK COMMUNICATION

Electron dynamics in quantum gate operation

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Abstract

We model the evolving time-dependent electronic structure of a solid-state quantum gate as it performs basic quantum operations. Our time-dependent configuration-interaction method follows the evolution of two donor electron spin qubits interacting with a third, optically excited, control spin in an applied magnetic field, a possible realization of the basic component of a proposed quantum information processor. We identify unitary operations which approximately disentangle the control spin, and use them to construct high-accuracy two-electron operations that are locally equivalent to CNOT, SWAP and $\sqrt{\text{SWAP}}$ operations. From our evaluation of the accuracy of a set of candidate gates we estimate the residual entanglement of the control electron and overall gate operation times. These results attest to the feasibility of the silicon-based quantum gates proposed by Stoneham, Fisher and Greenland.

Quantum phenomena offer a route to radical developments in information technology. On the one hand, devices using such technology could provide opportunities to tackle problems not feasible with classical computing methods, e.g. [1–3]. On the other hand, such devices might bypass fast-approaching technological problems, such as the massive heat production anticipated in ultra-small processors.

Just as classical computers manipulate logical bits with universal gates, so quantum computers manipulate qubits with universal quantum gates. Many physical systems have been proposed, e.g. [4–6], some satisfying the DiVincenzo criteria [7]. Most discussions assessing the efficacy of such realizations are based on formal treatments of model components. Our aim here is to demonstrate realistic modelling of a representative solid-state gate operation: we follow the evolving electronic structure of qubits as they respond to the fields driving the gate.

Our concern here is with the dynamics of a basic component of a quantum computer, the quantum gate. Specifically, we shall discuss the so-called SFG gate suggested by Stoneham, Fisher and Greenland [8], in which electron spins are manipulated optically. This optical control of the entanglement of two electron spin qubits is achieved by optical excitation of

a third 'control' electron. We simulate the evolving time-dependent electronic structure of this solid-state quantum gate and show how several of the 'standard' gate operations might be performed. The SFG gate has several potentially important practical advantages. It could be fabricated with relatively standard silicon technology, exploiting the randomness of dopants as available from a typical fabrication plant. No precise placement of dopants is needed: gate operations are chosen to use those structures available. With suitable dopants, operation at convenient temperatures should be possible, possibly at room temperature.

In the SFG proposal, the electron spin qubits are randomly distributed deep donors. Their spacings are sufficient that they interact negligibly in their ground states, in which they store quantum information. Entanglement is mediated by the optical excitation of distinct control electrons that, in their excited states, interact with the two qubits to be entangled. Singling out a particular gate is achieved by a combination of spatial and spectral resolution, exploiting the system's spatial randomness. When entangling two-qubit gate operations are effected via the direct exchange coupling of each qubit spin to the control electron, quantum information must not be lost to the control electron at the end of the operation. The control spin must be disentangled, leading to a criterion that can be expressed explicitly for given magnitudes of exchange and magnetic field coupling strengths [9]. A key quantity is the real number

$$f = (B - B_{\mathrm{C}})/J_{\mathrm{C}}, \tag{1}$$

where J_{C} gives the qubit-control exchange coupling when the control electron is in an optically excited state, and B_{C} (where $B_{\mathrm{K}} = |\mathbf{B}|\mu_{\mathrm{K}}$) measures the difference between the couplings of the qubit and the control to the applied magnetic field. In turn f can be redefined in terms of two integers N and M [9]. Identification of N and M gives a gate operation time t, and hence identifies the specific two-qubit operation defined by N and M that perfectly disentangles the control electron. This operation may be a recognizable one (e.g. a CNOT operation), but will typically be some entangling operation with no classical analogue.

We shall consider a system consisting of two deep (binding energy 71 meV) donors, similar to Bi donors in Si, and a deeper control donor. The fact that the donor is deep is treated explicitly by established methods. The donor electron spins provide the qubit states. In our example, the qubit centres are 13.25 nm (=500 au) apart, sufficient to ensure negligible direct qubit–qubit coupling J_{Q}, that is $J_{\mathrm{Q}} \ll J_{\mathrm{C}}$. We place the control donor (binding energy 150 meV) equidistant from the qubits. Our approach allows us to choose any geometry; this specific geometry is a useful reference case. Optical excitation of the control electron from its ground state to a p-like state 'switches on' the exchange coupling between qubits and control. Subsequent optical de-excitation of the control returns the system to its ground state, with the interpulse duration giving the gate operation time.

We now describe our electronic structure calculations which allow us crucially to bridge the gap between the analysis of [9] and the evolution of the system in a realistic physical environment. In particular, we can use our calculated one-electron states to evaluate J_{C} and $B - B_{\mathrm{C}}$, and hence identify the dimensionless quantity f. This ability to identify f should be emphasized, since to a large extent f characterizes the nature of the gate itself. We envisage that a future operator of our proposed device would know f, so these simulations could form the basis of successful device operation and future algorithm optimization.

In following the evolution of the electronic system during gate operation, we exploit both Hartree–Fock (HF) theory and configuration-interaction methods in conjunction with an extension of effective mass theory (EMT) [10]. This extension has previously been employed to good effect in, for example, the study of exciton [11] and donor–acceptor [12] systems, and in the modelling of the susceptibility of Si:P [13]. In EMT, there are scalings involving the effective mass and dielectric screening of Coulomb interactions in the potential $V(r)$. EMT

has a good record for shallow donor states with Bohr radii on the nanometre scale. We shall take m^* as the isotropic effective mass (generalizations allow an anisotropic effective mass). We note further that silicon also has a six-fold degenerate conduction band minimum. This degeneracy can be built into effective mass theory and into our approach but there is good reason to believe [13–15] that this would lead to only a small quantitative alteration of our results. Here we assume simple spherical bands.

In the simplest EMT, with a purely Coulombic potential $V(r) = -1/\varepsilon_r r$, ground state energies are in poor agreement with experiment because short-range terms are omitted. We modify $V(r)$ with a 'central-cell correction' (see e.g. section 4.3 of [14]), and so the potential energy term becomes

$$V(r) = \frac{1}{\varepsilon_r r}(1 + (\varepsilon_r - 1)\exp(-\sigma r^2)), \tag{2}$$

which has previously been shown [16] to give the ground state energies of P, As, Sb and Bi donors in silicon to within 10%, while maintaining the EMT excited state spectra. The second term in (2) provides the form of the core part of the effective mass Hamiltonian in our scaled Hartree–Fock calculations. The two-electron component of the Fock Hamiltonian is simply scaled to $1/\varepsilon_r r$, in keeping with earlier studies [11, 12]. We add a spatially varying magnetic field of the form

$$\mathbf{B} = \mathbf{B}_0 \sum_i \lambda_i \exp(-\rho(\mathbf{r} - \mathbf{r}_i)^2), \tag{3}$$

which, in principle, allows us to model any spatial field profile we require, including contributions from nearby magnetic moments. In practice a summation in (3) over as few as three Gaussians suffices to simulate the differences in electron g-factors between the control and qubit states, so ensuring that $B - B_C$ is non-zero (as required by [8]), whilst still allowing the self-consistent-field (SCF) method to be applied. No standard electronic basis set was suitable for our needs, and so we formed a customized Gaussian basis with (suitably scaled) contracted 'atomic-like' states and uncontracted diffuse functions. Details of this basis and non-SCF calculations using it can be found in [16].

A feature of molecular-orbital calculations on molecule-like systems, analogues of H_2, is their unphysical delocalization of one-electron states over both centres at large separation, making it hard to predict exchange splittings accurately. Several methods of resolving this difficulty have been presented, see [17, 18] for example. In particular, one successful method [18] involves the construction of localized 'broken-symmetry' spin states. We take a similar approach by finding a unitary transformation U_L that can be applied to the scaled HF eigenstates in order to localize the qubit states on single centres. Typically, the explicit form of U_L is found numerically, and this allows us to construct a configuration-interaction basis analogous to the three-electron computational basis used throughout the quantum computational literature, i.e. $\{|\uparrow\uparrow\uparrow\rangle = |000\rangle = |0\rangle, |\uparrow\uparrow\downarrow\rangle = |001\rangle = |1\rangle, \ldots, |\downarrow\downarrow\downarrow\rangle = |111\rangle = |7\rangle\}$. Our notation here means that, for example, $|\uparrow\uparrow\downarrow\rangle = |\uparrow_A\uparrow_B\downarrow_C\rangle$, where A and B label the qubit centres and C the control centre. For our present purposes we shall take the control electron to be in its excited state, so our configuration-interaction basis consists of eight configurations. We shall order this basis as $\{|0\rangle, |2\rangle, |4\rangle, |6\rangle, |1\rangle, |3\rangle, |5\rangle, |7\rangle\}$ for ease of later analysis.

We construct our 8×8 configuration-interaction Hamiltonian $\mathbf{H}^{CI}$ in the standard way, noting that off-diagonal matrix elements of $\mathbf{H}^{CI}$ can be immediately identified with exchange couplings between localized states, whereas on-diagonal elements H^{CI}_{nn} give the total energy of the nth configuration. This allows us to evaluate B and B_C, and therefore f. Table 1

Table 1. Summary of system parameters used throughout this communication.

r_{DD} (nm)	J_C (meV)	J_Q (meV)	$B - B_C$ (meV)	f
26.5	0.253	0.253×10^{-3}	0.136	0.535

summarizes the relevant results for the system considered here. Perfect disentanglement of the control electron is achieved when the two integers N and M satisfy the condition [19]

$$\frac{M}{N} = \sqrt{\frac{f^2 - 2f + 9}{f^2 + 2f + 9}}. \tag{4}$$

The disentangling gate operation time t is then given by

$$t = \frac{M\pi}{J_C\sqrt{f^2 - 2f + 9}} = \frac{N\pi}{J_C\sqrt{f^2 + 2f + 9}}. \tag{5}$$

Equation (5) holds even in the presence of direct qubit–qubit coupling.

Whilst we can appreciate the advantages of time-dependent multi-configurational self-consistent-field (TDMC-SCF) methods for optically controlled spintronics, we believe that a time-dependent configuration-interaction (TDCI) approach is sufficient for the purposes of demonstrating quantum gate operation. Such TDCI methods also show more clearly the parallels with the analytical approaches employed in quantum information processing (QIP). Thus the time evolution of our system is described by

$$\mathbf{U}(t) = \exp(-\mathrm{i}\mathbf{H}^{\mathrm{CI}}t) = \begin{pmatrix} \mathbf{U}_+(t) & \boldsymbol{\chi}_+(t) \\ \boldsymbol{\chi}_-(t) & \mathbf{U}_-(t) \end{pmatrix}. \tag{6}$$

If the control electron is perfectly disentangled, then the 4×4 submatrices $\boldsymbol{\chi}_\pm(t)$ are zero matrices, and the $\mathbf{U}_\pm(t)$ are two-electron unitary operators acting on the qubit degrees of freedom that return the control electron to its initial state at the end of the operation. For an imperfectly disentangling operation, $\boldsymbol{\chi}_\pm(t)$ give a measure of the residual entanglement of the control electron: the greater the value of the Euclidean norm of $\boldsymbol{\chi}_\pm(t)$,

$$\|\chi\| = \sqrt{\sum_{i,j} |\chi_{ij}|^2}, \tag{7}$$

the greater the degree of non-unitarity of $\mathbf{U}_\pm(t)$. Note, however, $\|\chi\|$ is not an entanglement monotone. An analytical expression for $\|\chi\|$ can be derived [19], and its time dependence studied. For the system considered here, we find a maximum value $\|\chi\|_{\mathrm{Max}} = 1.32$, and in the remainder of this communication all calculated values $\|\chi\|$ are scaled relative to this maximum.

There prove to be some benefits of permitting some finite but small residual entanglement with the control electron in our simulations. We emphasize that a future operator of our device would not need to know the details, but would instead use information gained from a one-off configuration process based on simulations like ours. However, an approach that allows residual control entanglement leads to an efficient method for identifying useful gate operations. If one permits such finite entanglement with the control after a gate operation, approximate solutions to (4) become valid, and can be found using the method of continued fractions [19]. In turn, this leads to a set of elementary approximate SFG gates, defined by pairs of integers $\{N_i, M_i\}$, that we shall combine to construct gate operations locally equivalent to CNOT, SWAP and $\sqrt{\mathrm{SWAP}}$.

The operation times of the members of this set of gates, t_{N_i} and t_{M_i}, will differ; a difference that introduces an error in the gate operation, analogous to that introduced by timing jitter (see e.g. [16]). We therefore only accept as members of our set of approximate gates those

pairs $\{N_i, M_i\}$ for which the associated gate operation times differ by less than 1%. The gate operation time for this pair of integers is then taken to be the optimal value [19] of $t_i = (t_{N_i} + t_{M_i})/2$, ensuring that gate operation times should be accurate. Since these times must also be short relative to decoherence timescales, we define an upper limit of 1 ns on all elementary gates accepted into our gate set (see section 5 of [9]), and reject those of longer duration. Finally, we note that, in general, multiplying $\{N_i, M_i\}$ by an integer k results in a different, yet still valid, approximately disentangling gate, with operation time given by kt_i. If kt_i is less than 1 ns, then this gate, denoted by the integers $\{kN_i, kM_i\}$, is added to the set. For the system discussed here, we find a set of 55 approximate SFG gates. To this we add the identity operation (in this case an operation with $t = 0$) to allow greater flexibility in the algorithm we use to identify combined gate operations locally equivalent to CNOT, SWAP and $\sqrt{\text{SWAP}}$. These gates are defined below, along with their associated local invariants G_1 and G_2, as defined by Makhlin [20]. Two gates with identical local invariants are said to be locally equivalent, and one gate can be made identical to the other using only local (i.e. one-electron or non-entangling) transformations.

$$\text{CNOT:} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad G_1 = 0, \qquad G_2 = 1$$

$$\text{SWAP:} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad G_1 = -1, \qquad G_2 = -3$$

$$\sqrt{\text{SWAP}}\text{:} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1-\mathrm{i}}{2} & \frac{-1-\mathrm{i}}{2} & 0 \\ 0 & \frac{-1-\mathrm{i}}{2} & \frac{1-\mathrm{i}}{2} & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \qquad G_1 = -\frac{\mathrm{i}}{4}, \qquad G_2 = 0.$$

Our combined gates are constructed from our approximate set in a straightforward manner, and it is knowledge of these combined gates which would be available to a future operator. If we label the nth gate in our approximate set as $\mathbf{U}_n$, then, for example, a three-operation combined gate is defined as $\mathbf{U}_{nml} = \mathbf{U}_l \cdot \mathbf{U}_m \cdot \mathbf{U}_n$. We note that since $\mathbf{H}^{\text{CI}}$ is not itself time dependent, every member of the elementary gate set commutes with every other, and so the combined gate operation time will be $t_{nml} = t_n + t_m + t_l$. For our present purposes, we restrict the number of approximate elementary gates used in a combined operation to five or less. We employ a simulated-annealing algorithm [21, 22] to identify near-optimal combinations of elementary gate operations. The cost function ϵ to be minimized by this algorithm measures the difference in local invariants between the computed and target gate operation, as well as the Euclidean norm of the off-diagonal submatrix $\boldsymbol{\chi}_{\pm}(t)$,

$$\epsilon = \sqrt{\Delta^2 + \|\chi\|^2}, \tag{8}$$

where $\Delta = \sqrt{\Delta_1^2 + \Delta_2^2}$ with $\Delta_1 = G_1^{\text{T}} - G_1^{\text{C}}$, $\Delta_2 = G_2^{\text{T}} - G_2^{\text{C}}$, and the superscripts T and C identify target and computed quantities.

Table 2 gives the results of applying the simulated annealing algorithm to the approximate elementary gate set considered here. n_{e} represents the number of elementary gates used in the combined operation, and $\bar{p}$ gives the probability of measuring the control spin to have flipped during the operation, averaged over the eight states defining the computational basis. Table 2 shows that combined gate operations of high accuracy can be constructed from our elementary gate set. Moreover, the entangling properties of these elementary gates show that the simulated

Table 2. Combined gates obtained using the time-dependent configuration-interaction method and the simulated annealing algorithm.

Gate operation	n_e	Δ	$\|\chi\|$	t (ns)	$\bar{p}$ (%)
CNOT	2	0.0579	0.0151	0.789	0.0100
SWAP	2	0.0127	0.0613	0.672	0.162
SWAP	3	0.115	0.0257	2.00	0.0287
$\sqrt{\text{SWAP}}$	1	0.0891	8.48×10^{-3}	0.162	3.19×10^{-3}
$\sqrt{\text{SWAP}}$	2	0.0248	0.0524	0.510	0.120

annealing algorithm allows us to construct error-cancelling combinations. Some cases we find yield combined operations which reduce Δ at the expense of $\|\chi\|$, and vice versa. This is to be expected, since the relative weights of these two quantities in the cost function ϵ are equal. Other cost functions could easily be defined to emphasize the importance of minimizing a particular quantity. This may be of value when combined with the well-studied [23, 24] error-correction methods which could be applied to the effective two-qubit gates calculated here. It is not obvious that such methods could be applied to the problem of residual control entanglement, and so a cost function that minimizes $\|\chi\|$ may be of benefit. For several purposes, the general cost function which we have implemented seems to be the most useful to illustrate our method.

In summary, we have shown for the first time that self-consistent time-dependent electronic structure methods can be used to study gate operation in QIP devices. This has been achieved in a way that allows for the inclusion of a more physically realistic environment than that possible with most analytical methods. We have used these methods to study the detailed behaviour of a set of two-qubit gate operations which might form the basis of a potential realization of a QIP device. Our analysis shows that accurate two-qubit operations are possible within this realization. Thus the original SFG proposal [8] remains feasible under our improved analysis. Moreover, our new approach offers a potential opportunity to optimize SFG gates, whether by judicious choice of specific qubit–qubit couplings from a random distribution or by biasing of the initial spatial distribution during fabrication itself by taking advantage of specific features of the variety of available deposition techniques. Our approach might also be used to analyse other important aspects of solid-state QIP devices, such as the potentially one-off critical configuration process for the SFG system that identifies optical excitation energies with specific control-qubit groups, whilst the explicit time dependence of the method makes it a natural choice for studying initialization/readout proposals. Further work will consider the effects of a larger configuration-interaction basis (so that, for example, double occupation of qubit centres will be allowed), asymmetric qubit-control coupling, i.e. $J_{AC} \neq J_{BC}$, and the presence of 'spectator' spins on two-qubit gate operations. Our approach may have broader implications, since it allows for more detailed study of the quantum dynamics of a variety of solid-state proposals for QIP devices. In itself, it may form the basis for more sophisticated theoretical treatments of such systems. This will allow for direct quantitative comparison of alternative proposals for solid-state quantum computing.

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