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Abstract
Motivated by applications to quantum computer architectures we study the
change in the exchange interaction between neighbouring phosphorus donor
electrons in silicon due to the application of voltage biases to surface control
electrodes. These voltage biases create electro-static fields within the crystal
substrate, perturbing the states of the donor electrons and thus altering the
strength of the exchange interaction between them. We find that control gates
of this kind can be used to either enhance or reduce the strength of the interaction,
by an amount that depends both on the magnitude and orientation of the donor
separation.

1. Introduction

Phosphorus donors in silicon have been the subject of increased research interest in recent
years due to their status as either nuclear [1] or electron [2] spin qubits in various proposals
for a scalable quantum computer. In both cases the exchange energy between neighbouring
donor electrons is of fundamental importance as the mediator of the qubit coupling.
Although proposals exist for implementing quantum information processing with this exchange
interaction fixed [3], it is none the less desirable to have some control over this parameter,
particularly for the readout process. Recent studies have shown that the magnitude of the
exchange interaction for donor electrons in silicon is strongly dependent on not only the
magnitude of the donor separation, but also on the relative orientation of the donors within the
silicon crystal lattice [4–6].

In a previous article [6] the effect of J-gate biases on the exchange coupling was computed
for donor separations along the [100] axis only. Here we extend the calculations to include
separations in other orientations relative to the host silicon lattice, in particular separations
along the [110] and [111] crystallographic axes. A two-qubit Kane device, figure 1, consists
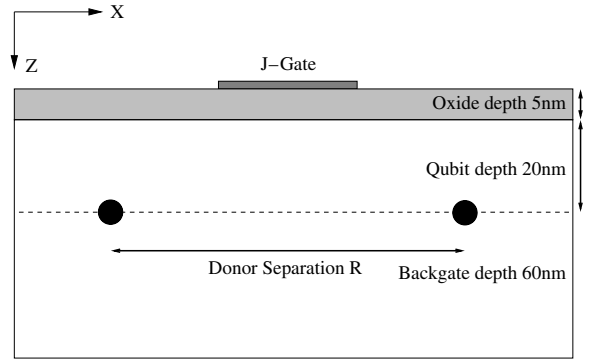
Figure 1. The Kane architecture based on buried phosphorus dopants in a silicon substrate.

of two phosphorus donors at substitutional sites in a silicon substrate at a depth 20 nm below a 5 nm layer of silicon oxide. On top of this oxide, and between the donors, is a metallic J-gate electrode, which, for the purposes of these calculations, is assumed to be 7 nm wide and infinitely long in the y-direction (out of page). A grounded back plane lies at a depth of 60 nm below the silicon-oxide interface. The distance R, between the donors is varied, as is their orientation relative to the silicon crystallographic lattice. The electro-static potential created inside the device by the application of a voltage bias to the J-gate electrode, while the remaining electrodes are held at ground, is calculated by means of a commercial package that solves the Poisson equation for such semiconductor systems[4], details of these calculations for Kane type devices can be found in [7].

2. Donor electron wavefunctions

In the absence of a perturbing potential the electron wavefunction for a phosphorus donor centred at a position $\mathbf{R}/2$ in a silicon substrate can be expressed in the Kohn–Luttinger [8, 9] form:

$$\psi(\mathbf{r} - \mathbf{R}/2) = \sum_{\mu} F_{\mu}^{1,0,0}(\mathbf{r} - \mathbf{R}/2)e^{i\mathbf{k}_{\mu}\cdot(\mathbf{r}-\mathbf{R}/2)}u_{\mu}(\mathbf{r}). \tag{1}$$

The functions $u_{\mu}(\mathbf{r})$ are the periodic part of the Bloch functions for the pure silicon crystal, with wavevectors $\mathbf{k}_{\mu}$ located at each of the degenerate conduction band minima. The envelope functions,

$$F_{\pm z}^{1,0,0}(\mathbf{r}) = \varphi_{1,0,0}(x, y, \gamma z), \tag{2}$$

are correctly normalized non-isotropic hydrogen like wavefunctions, with effective Bohr radius $a_{\perp}$. The above example is for functions localized around the conduction band minima $\mathbf{k}_{\pm z} = 2\pi/a(0, 0, \pm 0.85)$, with $a = 5.43$ Å the lattice spacing for silicon. The parameter $\gamma = a_{\perp}/a_{\parallel}$, where the values $a_{\perp} = 25.09$ Å, $a_{\parallel} = 14.43$ Å are the transverse, and longitudinal effective Bohr radii, respectively, and are determined variationally [8, 4]. The subscripts refer to the electronic, orbital and magnetic (n, l, m) quantum numbers, respectively.

To control the strength of the exchange coupling it is proposed that a voltage bias be applied to a surface 'J-gate' electrode, see figure 1. This voltage bias produces an electric potential within the substrate, perturbing the donor electron wavefunctions, and thus altering
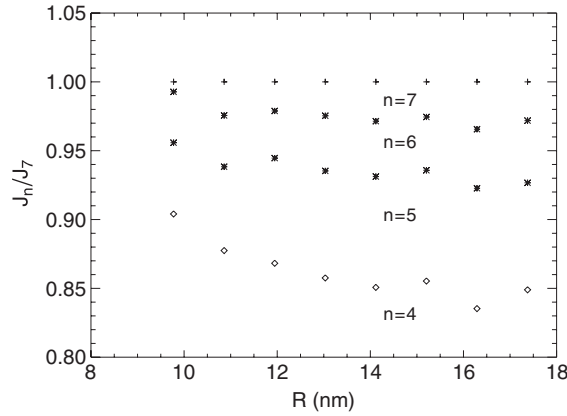
Figure 2. Comparison of the exchange coupling as calculated using various basis sizes. The calculations were performed for donors separated along a crystallographic [100] axis, in the presence of the electro-static potential produced by a 1 V gate bias. This is the largest voltage bias considered in this paper, and so requires the largest basis.

the exchange coupling. To model this process we have calculated the electro-static potential produced inside the device by the application of a J-gate potential. The potential matrix is then calculated in the basis of generalized Kohn–Luttinger states given in equation (1), using hydrogenic envelope functions up to and including $n = 7$, a basis of 140 states in total. The decision to truncate the basis at $n = 7$ was based on the fact that reasonable convergence was achieved for a basis of this size, and to increase the basis beyond this involves a significant increase in computational cost, for little improvement in the accuracy of the result. The convergence of a typical calculation is illustrated in figure 2 where we compare values for the exchange coupling with a 1 V bias applied to the J-gate. This is the largest voltage bias considered in this paper, and as such, a calculation which requires the largest basis.

The Hamiltonian is diagonalized in this basis to find the ground-state donor electron wavefunction:

$$\psi(\mathbf{r} - \mathbf{R}/2; V) = \sum_{n,l,m} c_{n,l,m}(V) \sum_{\mu} F_{\mu}^{n,l,m}(\mathbf{r} - \mathbf{R}/2) e^{i\mathbf{k}_{\mu} \cdot (\mathbf{r} - \mathbf{R}/2)} u_{\mu}(\mathbf{r}). \quad (3)$$

In the Heitler–London approximation the two donor system is treated as a correctly symmetrized product of single donor wavefunctions. The fermion anti-symmetry of the overall wavefunction ensures that the spin singlet (s) and triplet (t) states are, respectively, represented as even and odd superpositions of single electron wavefunctions. This approximation is valid when the donor separation is large compared to the effective Bohr radii of the single electron wavefunctions. For donors centred at positions $\pm\mathbf{R}/2$, the spatial part of the triplet/singlet wavefunctions are thus:

$$\Psi_{t/s}(\mathbf{r}_1, \mathbf{r}_2; V) = \frac{1}{\sqrt{2(1 \pm S^2)}} \{\psi_R(\mathbf{r}_1 - \mathbf{R}/2; V)\psi_L(\mathbf{r}_2 + \mathbf{R}/2; V)$$
$$\pm \psi_L(\mathbf{r}_1 + \mathbf{R}/2; V)\psi_R(\mathbf{r}_2 - \mathbf{R}/2; V)\}, \quad (4)$$

where $S = \int \psi_L^*(\mathbf{r} + \mathbf{R}/2; V)\psi_R(\mathbf{r} - \mathbf{R}/2; V)\,d\mathbf{r}$ is the overlap integral and the subscripts (L, R), refer to the wavefunctions of donors located on the (left, right) of the J-gate.

3. Exchange coupling

In the Kane proposal for a phosphorus nuclear spin quantum computer in silicon [1], the effective Hamiltonian between neighbouring donors is given by

$$
\begin{aligned}
H_{\text{eff}} = {}& g_n \mu_n B (\sigma_{n1}^z + \sigma_{n2}^z) + g \mu_B B (\sigma_{e1}^z + \sigma_{e2}^z) \\
& + A_1(V) \vec{\sigma}_{n1} \cdot \vec{\sigma}_{e1} + A_2(V) \vec{\sigma}_{n2} \cdot \vec{\sigma}_{e2} + J(V) \vec{\sigma}_{e1} \cdot \vec{\sigma}_{e2}.
\end{aligned}
\tag{5}
$$

Here the σ represent the usual Pauli operators, and the subscripts n, e represent operation on nuclei and electrons, respectively. The controllable parameters, through which quantum information processing is implemented, are the contact hyperfine coupling A between the donor nucleus and its associated electron and the exchange coupling J between neighbouring donor electrons. Both these quantities are to be controlled through manipulation of the electron wavefunction via the application of bias voltages to control gates. The contact hyperfine coupling is dependent on $|\psi(0)|^2$, that is, the probability density of the electron wavefunction located at the position of the nucleus. This can be changed by drawing the electron wavefunction away from the nucleus via the application of a positive bias to an A-gate or J-gate [10, 11].

The exchange coupling, as can be seen from equation (5), is equal to a quarter of the energy difference between the two electron spin single and spin triplet states. In the Heitler–London approach, this is evaluated by calculating the energy difference between the even and odd superpositions of single donor wavefunctions, equation (4). The origin of this difference in energy between the spin singlet and triplet states is due to the fact that the even superposition state has a higher probability density in the region located between the two donors, a region that has a relatively low potential. The odd superposition state has a lower probability density in this region, which is compensated by a higher probability density in the higher potential regions located outside the two donors. This energy difference can be manipulated by application of a voltage bias to a J-gate located above and between the two donors. Application of a positive bias will decrease the potential in the region between the two donors, thus increasing the exchange coupling, while a negative bias will have the opposite effect.

4. Results

It has been well documented that in the absence of a bias potential, the exchange coupling between neighbouring phosphorus donor electrons in a silicon substrate is strongly dependent on both the magnitude and the orientation of the donor separation with respect to the host silicon lattice [4, 6].

With this in mind it is not unexpected that this orientation dependence remains in the presence of a bias potential. Indeed we find that the presence of this potential enhances the oscillations observed in the zero bias case. This is illustrated in figure 3 for separations of increasing magnitude along three high symmetry crystallographic axes.

It is evident from these plots, that application of a voltage bias to a J-gate can exert significant control over the strength of the exchange coupling, both increasing and decreasing the strength depending on the polarity of the bias. The range over which the exchange coupling can be changed is, however, extremely sensitive to the donor separation. This is well illustrated in figure 4 where we have plotted the value of the exchange coupling as a function of applied voltage bias for donor separations of different magnitudes along the same crystallographic axes.

For all separations studied it was found to be possible, via the application of a suitable negative voltage bias, to reduce the exchange coupling to zero, and thus to turn the inter-
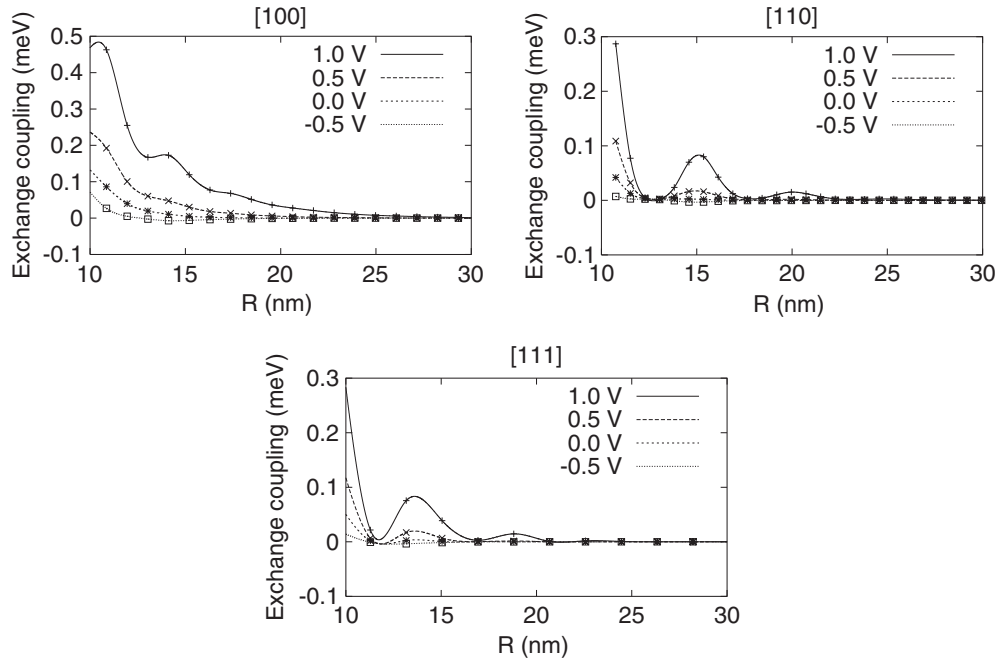
Figure 3. Exchange coupling as a function of donor separation along high symmetry crystal directions for different J-gate biases. The points represent the position of fcc substitutional sites.
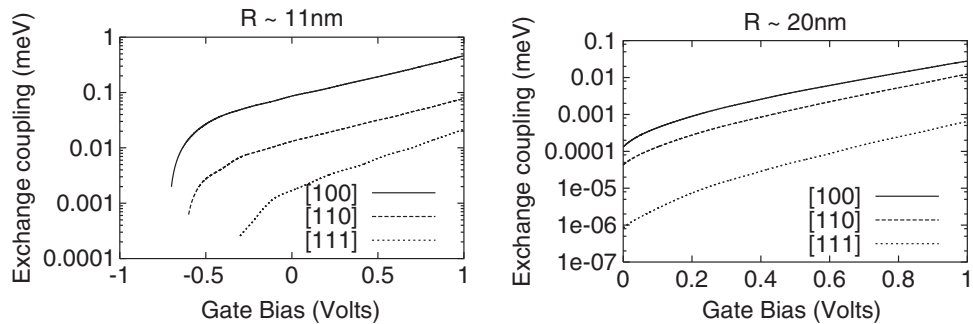
Figure 4. Semi-log plot of the exchange coupling as a function of applied gate bias along high symmetry crystal axes for different separation magnitudes. Because of the discrete positioning of possible substitutional sites, the exact magnitude of the separation is different for each direction with $R = 10.86$ nm in the [100] direction, $R = 11.51$ nm for the [110] separation and $R = 11.28$ for the donor separations along the [111] axis.

qubit interaction off. Indeed calculations at large negative bias, particularly for large donor separations, give negative values of the exchange coupling, a result that is unphysical for two electron systems. We attribute this result to a breakdown of the Heitler–London approximation in this regime due to the strongly delocalized nature of the single donor wavefunctions. In fact we find that even at large, (1 V), positive gate biases, for donors separated by large distances, $R \approx 30$ nm, the single donor wavefunctions are highly delocalized. In such a situation it is no longer valid to treat the two particle wavefunction as a simple superposition of two
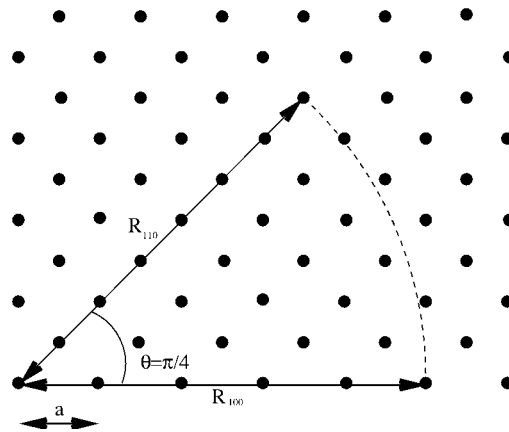
Figure 5. Schematic of the crystallographic structure of a [001] plane in silicon, showing donors separated by vectors along a [100] axis ($\mathbf{R}_{100}$) and a [110] axis ($\mathbf{R}_{110}$). For two donors in the same [001] plane, we can define the separation R_θ relative to the [100] axis.

localized single electron wavefunctions, as is done in the Heitler–London approximation, and more sophisticated methods are required to obtain a reliable estimate of the exchange coupling between the two electrons.

The speed of two-qubit gates, for both electron and nuclear spin architectures, increases with the strength of the exchange coupling and so it would be desirable to achieve the largest exchange coupling possible. To this end it is clear that a donor separation along the [100] axis would be preferable, with the magnitude of the separation being as small as possible. Of course there are limits on the precision to which these donors can be placed, and on the separations that can be achieved. Technical issues will probably set a lower bound on reliable donor separation of approximately 20 nm. Due to the process by which the silicon is doped in the so called 'bottom up' approach [12], it is possible to place donors with near-atomic precision in the same [001] plane (that is a plane perpendicular to a crystallographic [001] axis), reliably, using atomic force microscopy techniques and thermal incorporation. The surface is then over-grown with silicon, resulting in a device in which the dopants are located to within no more than several lattice sites of their intended position. The fact that the deposition is onto a silicon surface means that the uncertainty of the donor position in that plane is significantly greater than the out-of-plane uncertainty. With this in mind we have calculated the expected exchange coupling for donors located at various substitutional sites within the same [001] plane, with a separation magnitude of approximately 20 nm for different donor orientations, the results are presented in figure 6. The first plot shows the exchange coupling for donors separated by a vector $\vec{R}_\theta = R(\cos\theta, \sin\theta, 0)$, that is the donors are in the same [001] plane, and when $\theta = 0$ are separated by a vector in the [100] direction. The second and third plot show the strength of the exchange coupling when the two donors are not in the same [001] plane. In the second plot one of the donors has been displaced to its nearest neighbour substitutional site and the donor separation is now $\vec{R} = \vec{R}_\theta + a/4(1, 1, 1)$. In the third plot the donor is displaced by one lattice constant perpendicular to the [001] plane, $\vec{R} = \vec{R}_\theta + a(0, 0, 1)$. The plots show that even small displacements from the ideal [100] separation significantly decrease the strength of the exchange coupling, indeed a displacement of just one lattice site can halve the coupling strength.
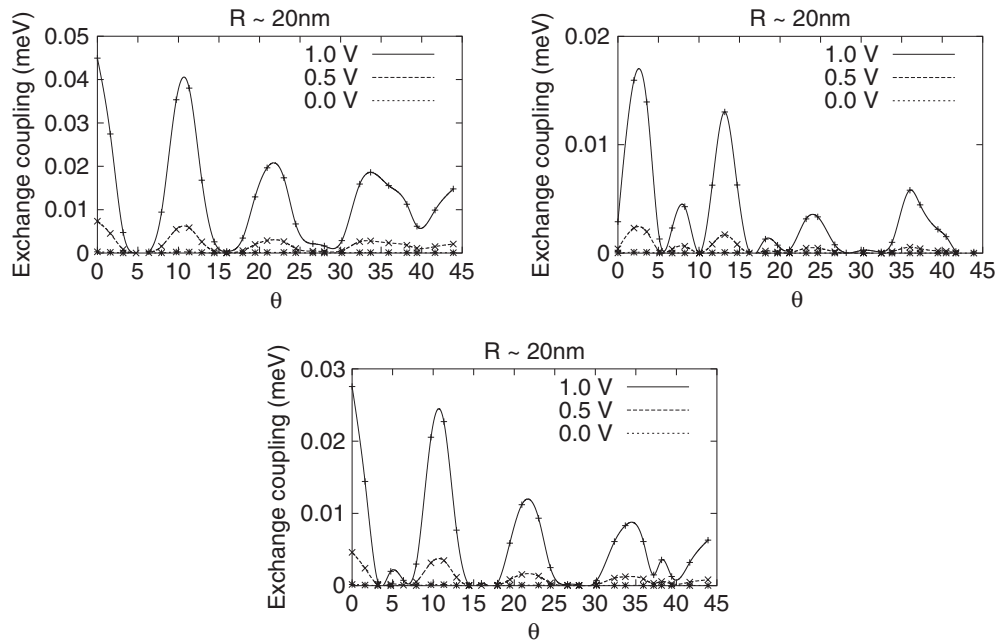
Figure 6. Exchange coupling as a function of donor separation angle from the [100] direction for donors separated by approximately 200 Å in various planes. In the first figure both donors are in the same [100] plane, and the angle θ refers to the donor orientation with respect to separation along the [100] axis, as shown in figure 5. In the second figure one donor has been moved to a nearest-neighbour site, a displacement of $\delta = a/4(1, 1, 1)$ relative to the positions of the first plot. The final plot contains data for which the second donor has been displaced by one lattice constant in a direction out of the plane, $\delta = a(0, 0, 1)$. Here the points represent the position of substitutional fcc sites. The exact magnitude of the donor separation at these points varies slightly due to the discrete distribution of such sites.

5. Conclusions

We find that the strength of the exchange coupling between neighbouring phosphorus donor electrons in a silicon substrate can be significantly increased or decreased by the application of a bias voltage to a surface 'J-gate' electrode placed above and between the donor qubits. The bare (zero-bias) coupling is strongly dependent on the magnitude and orientation of the donor separation, and this dependence is amplified by the application of the voltage bias which has the affect of altering the coupling strength by a voltage dependent factor. Regardless of the donor orientation the exchange coupling strength can be reduced to zero, via the application of a negative J-gate bias, and so ideal donor placement is determined by the maximum value to which the coupling can be increased. To maximize the achievable coupling strength the donors would ideally be separated along a crystallographic [100] axis, however even small deviations from this ideal placement, of the order of one lattice spacing, can decrease the coupling strength by more than a factor of two.

Acknowledgments

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