

Electron exchange coupling for single-donor solid-state spin qubits

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Intervalley interference between degenerate conduction band minima has been shown to lead to oscillations in the exchange energy between neighboring phosphorus donor electron states in silicon [B. Koiller, X. Hu, and S. Das Sarma, Phys. Rev. Lett. **88**, 027903 (2002); Phys. Rev. B **66**, 115201 (2002)]. These same effects lead to an extreme sensitivity of the exchange energy on the relative orientation of the donor atoms, an issue of crucial importance in the construction of silicon-based spin quantum computers. In this article we calculate the donor electron exchange coupling as a function of donor position incorporating the full Bloch structure of the Kohn-Luttinger electron wave functions. It is found that due to the rapidly oscillating nature of the terms they produce, the periodic part of the Bloch functions can be safely ignored in the Heitler-London integrals as was done by Koiller, Hu, and Das Sarma, significantly reducing the complexity of calculations. We address issues of fabrication and calculate the expected exchange coupling between neighboring donors that have been implanted into the silicon substrate using an 15 keV ion beam in the so-called “top down” fabrication scheme for a Kane solid-state quantum computer. In addition, we calculate the exchange coupling as a function of the voltage bias on control gates used to manipulate the electron wave functions and implement quantum logic operations in the Kane proposal, and find that these gate biases can be used to both increase and decrease the magnitude of the exchange coupling between neighboring donor electrons. The zero-bias results reconfirm those previously obtained by Koiller, Hu, and Das Sarma.

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I. INTRODUCTION

Solid state systems have emerged as a promising candidate for the construction of a large scale quantum computer (QC). In particular, spin based architectures take advantage of the relatively long spin dephasing times of donor electrons or nuclei in silicon. Single qubit operations are performed by tuning the spin Zeeman energy to be resonant with an oscillating field which drives the transition while neighboring qubits are coupled via the electron exchange interaction, whether it be directly in the case of electron-spin proposals,¹ or indirectly in the case of nuclear spin quantum computers.

In this work we concentrate on the Kane² concept of single phosphorus donor nuclear spin qubits embedded in a silicon substrate, which is a leading candidate in the search for a scalable QC architecture. The Kane architecture (shown in Fig. 1) calls for the placement of phosphorus donors at substitutional [face-centered cubic (fcc)] sites in the host silicon matrix, with interdonor spacings of order 200 Å. Quantum logic operations on the nuclear-spin qubits are implemented through coherent control of the donor electron wave functions which are coupled to the donor nuclei through the contact hyperfine interaction. This control of the electron wave functions is achieved through application of voltage biases to control gates placed on the substrate surface above (*A* gate), and between (*J* gate) the phosphorus donors, which create electrostatic potentials within the device thus altering the form of the electron wave functions.

In a recent paper, Koiller, Hu, and Das Sarma (KHD)³ presented theoretical evidence for oscillations in the electron-mediated exchange coupling as a function of inter-

donor separation, and a strong dependence of this coupling on the relative orientation of the two donors with respect the structure of the silicon substrate. They calculate the exchange coupling using an approximate version of the Heitler-London formalism and by essentially ignoring the periodic part of the Bloch wave functions in the expression for the donor electron wave functions. In this article we eliminate both these approximations, by calculating the exchange coupling in the full Heitler-London formalism and by including the full Bloch structure of the donor electron wave function. We show that while the first approximation breaks down for small donor separations, as discussed by KHD themselves,⁴ the second approximation, that of ignoring the periodic part of the Bloch functions, is in excellent agreement with the full calculations regardless of the donor orientation.

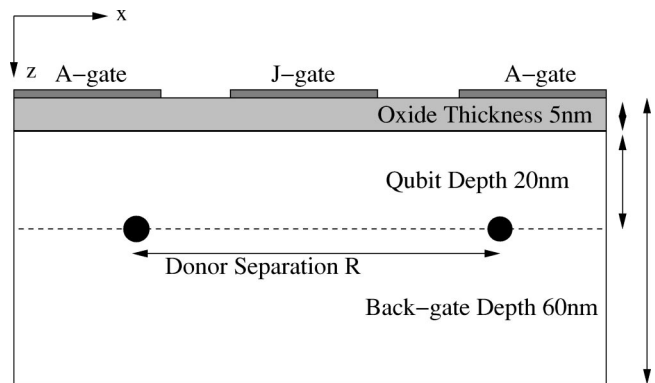


FIG. 1. The Kane architecture based on buried phosphorus dopants in a silicon substrate.

This paper is organized as follows. In Sec. II we review the calculation of the valence electron wave functions for phosphorus donors in silicon, in the Kohn-Luttinger effective mass formalism. In Sec. III we discuss the Heitler-London formalism used to calculate the exchange coupling between neighboring donor electrons, and we show that the terms that arise due to the periodic part of the Bloch functions oscillate sufficiently rapidly so as to average to zero over the range of the integrals. Section IV contains a discussion of some of the fabrication issues that arise from the strong position dependence of the exchange energy on the production of a phosphorus donor based solid state quantum computer.

Section V is devoted to a calculation of the dependence of the exchange coupling between neighboring donor electrons on voltage biases applied to the control J gate, used to tune the interqubit coupling. By extending the conventional effective mass formalism we construct a basis of nonisotropic hydrogenlike envelope functions in which we expand the donor-electron wave function in the presence of the electric potentials. The potential created inside the device due to the J -gate bias is calculated using a commercial software package specifically designed for the modeling of semiconductor devices. Donor wave functions are obtained by direct diagonalization, and the Heitler-London formalism is used to determine the exchange coupling for various gate biases and donor separations oriented in the silicon [100] direction.

II. THE DONOR ELECTRON WAVE FUNCTION

Although the qubits of the Kane quantum computer are encoded by the nuclear spins, it is the donor electron which

mediates both single and coupled gate operations. Therefore, the crucial element in the quantum description of the device is the donor electron wave function. Initial attempts to describe the operation of the device, particularly in response to external time dependent gate potentials which complicate the situation considerably, have focused on effective hydrogenic-type approximations for the donor electron wave function,^{5,6} or the use of simplified potentials.⁷ These calculations provide some useful estimates, however, more detailed calculations are required, using realistic models of both the donor electron wave function and the potentials induced inside the device by the application of control gate biases.

In going beyond the effective hydrogenic treatment of the ground-state electron wave function for phosphorus donors in silicon it is recognized that the underlying crystal structure of the silicon must have an effect. The wave function is thus expanded in the basis of the Bloch functions for silicon,^{8,9}

$$\Psi(\mathbf{r}) = \int F(\mathbf{k}) \phi_{\mathbf{k}}(\mathbf{r}) d\mathbf{k}. \quad (1)$$

The coefficients $F(\mathbf{k})$ are obtained by substituting the above form into the Schrödinger equation, with the Hamiltonian $H = H_0 - U(r)$, where H_0 is the Hamiltonian for the pure silicon crystal and $U(r)$ is the donor-potential for phosphorus. The Bloch functions can be written in the form $\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$, where $u_{\mathbf{k}}(\mathbf{r})$ is a function that shares the periodicity of the lattice, and can be expanded in a basis of plane waves with wave vectors equal to the reciprocal lattice vectors for silicon \mathbf{G} , $u_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} A_{\mathbf{k},\mathbf{G}}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}$. The result is that the Schrödinger equation can be written as

$$\begin{aligned} EF(\mathbf{k}) &= E_{\mathbf{k}}^0 F(\mathbf{k}) + \sum_{\mathbf{G},\mathbf{G}'} \int A_{\mathbf{k}',\mathbf{G}'}^* A_{\mathbf{k},\mathbf{G}} U(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}} F(\mathbf{k}') d\mathbf{r} d\mathbf{k}' \\ &= E_{\mathbf{k}}^0 F(\mathbf{k}) + \sum_{\mathbf{G},\mathbf{G}'} \int A_{\mathbf{k}',\mathbf{G}'}^* A_{\mathbf{k},\mathbf{G}} \tilde{U}(\mathbf{k} + \mathbf{G} - \mathbf{k}' - \mathbf{G}') F(\mathbf{k}') d\mathbf{k}', \end{aligned} \quad (2)$$

where $\tilde{U}(\mathbf{k}) = \int U(\mathbf{r}) e^{-i\mathbf{r}\cdot\mathbf{k}} d\mathbf{r}$ is the Fourier transform of the impurity potential. The $E_{\mathbf{k}}^0$ are the eigenenergies of the Bloch functions $\phi_{\mathbf{k}}(\mathbf{r})$, for the pure silicon lattice. We make the approximation that due to the increased energies of the higher bands, only conduction band states contribute to the impurity wave function. Further, in silicon there are six degenerate conduction band minima, located along the $\langle 100 \rangle$ directions in \mathbf{k} space, 85% of the way between the center (Γ point) and the zone boundary (X point). Because of the reduced energies in these regions the envelope functions can be expressed as a sum of functions localized around each of the conduction band minima $F(\mathbf{k}) = \sum_{\mu} F_{\mu}(\mathbf{k})$.

In the effective-mass treatment⁸⁻¹⁰ the Bloch energies are expanded to second order around the conduction band minima $E_{\mathbf{k}}^0 \approx (\hbar^2/2)(\mathbf{k}_{\perp}^2/m_{\perp} + k_{\parallel}^2/m_{\parallel})$, where \mathbf{k}_{\perp} is the component of $\mathbf{k} - \mathbf{k}_{\mu}$ perpendicular to \mathbf{k}_{μ} and k_{\parallel} is the parallel

component. The m_{\perp}, m_{\parallel} are effective masses and the inequality of these two values reflects the anisotropy of the conduction band minima. An additional approximation is made whereby only the terms with $\mathbf{G} = \mathbf{G}'$ in the potential term of the Schrödinger equation are included. The assumption is that $U(\mathbf{k} - \mathbf{k}' + \mathbf{G} - \mathbf{G}') \ll U(\mathbf{k} - \mathbf{k}')$ for $\mathbf{G} \neq \mathbf{G}'$. This approximation is well satisfied for a Coulombic potential $U(\mathbf{k}) = 1/(\kappa\pi^2|\mathbf{k}|^2)$, with $\kappa = 11.9$ the dielectric constant for silicon, and with the reciprocal lattice vectors of magnitude $|\mathbf{G}| = n2\pi/d$, where n is an integer and $d = 5.43 \text{ \AA}$ is the lattice spacing for silicon. Another way of viewing the approximation is that the terms $e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}}$ in the first line of Eq. (2) oscillate on a scale sufficiently short compared to variations in $U(\mathbf{r})$, that they average the integrand to zero. We will show in the next section that the same approximation allows us to ignore the periodic part of the Bloch functions in

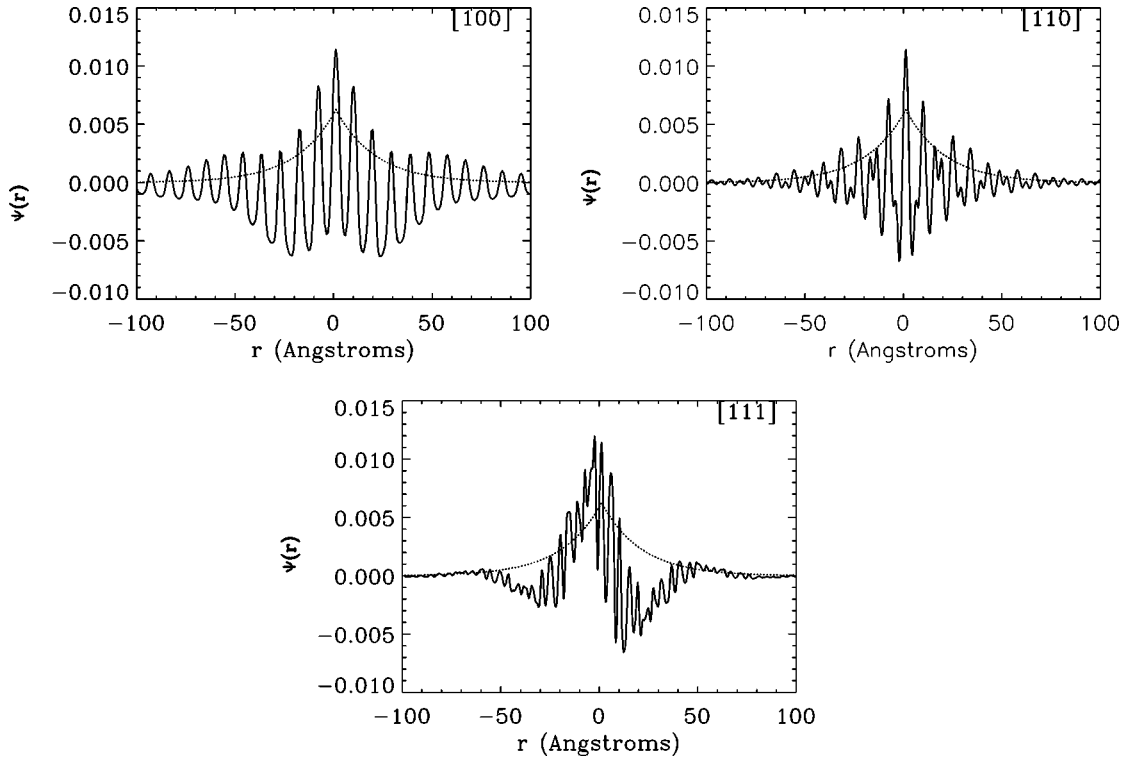


FIG. 2. The solid line shows Kohn-Luttinger wave function for a phosphorus donor electron in silicon, plotted along directions of high symmetry within the crystal. The dotted line shows an isotropic $1s$ hydrogenic wave function, with an Bohr radius of 20.13 \AA .

the donor electron wave functions when performing Heitler-London integrations.

One further approximation is necessary, $A_{\mathbf{k}',\mathbf{G}} \approx A_{\mathbf{k},\mathbf{G}}$, which coupled with the relation $\sum_{\mathbf{G}} |A_{\mathbf{k},\mathbf{G}}|^2 = 1$ gives the effective mass Schrödinger equation

$$\begin{aligned} \frac{\hbar^2}{2} \left(\frac{k_{\perp}^2}{m_{\perp}} + \frac{k_{\parallel}^2}{m_{\parallel}} \right) \sum_{\mu} F_{\mu}(\mathbf{k}) + \int \tilde{U}(\mathbf{k}-\mathbf{k}') \sum_{\mu} F_{\mu}(\mathbf{k}') d\mathbf{k}' \\ = E \sum_{\mu} F_{\mu}(\mathbf{k}). \end{aligned} \quad (3)$$

In the standard effective mass treatment the so-called valley-orbit terms, which couple the envelope functions at different conduction band minima are ignored, and we are left with six independent equations, one for each minimum. With a Coulombic impurity potential the solutions are nonisotropic hydrogenic wave functions of the form

$$F_{\pm z}(\mathbf{r}) = \frac{\exp[-\sqrt{(x^2+y^2)/a_{\perp}^2 + z^2/a_{\parallel}^2}]}{\sqrt{6\pi a_{\perp}^2 a_{\parallel}}}, \quad (4)$$

where $F_{\mu}(\mathbf{r}) = \int F_{\mu}(\mathbf{k}-\mathbf{k}_{\mu}) e^{i\mathbf{k}\cdot\mathbf{r}} d\mathbf{k}$, and we have used the example of the envelope function localized around the z minima of the conduction band. The Kohn-Luttinger^{8,9} form for the electron wave function of a donor situated at any position \mathbf{R} is then given by

$$\Psi(\mathbf{r}-\mathbf{R}) = \sum_{\mu} F_{\mu}(\mathbf{r}-\mathbf{R}) e^{i\mathbf{k}_{\mu}\cdot(\mathbf{r}-\mathbf{R})} u_{\mu}(\mathbf{r}), \quad (5)$$

where the periodic part of the Bloch function is independent of the position of the substitutional impurity. The values $a_{\perp} = 25.09 \text{ \AA}$, $a_{\parallel} = 14.43 \text{ \AA}$ are the effective Bohr radii, and are determined variationally.^{3,8}

It is well known that the valley orbit coupling does contribute to the energy of the state,¹¹ particularly if the donor potential is not Coulombic as is the case in the immediate vicinity of the donor nucleus. The consequence of this is that the donor electron binding energy given by this wave function is $E = 28.95 \text{ meV}$, significantly lower than the experimental value of $E = 45.5 \text{ meV}$.^{12,13} This discrepancy is thought to arise from the deviation of the donor potential from a purely Coulombic potential as well as the effect of a nonstatic dielectric constant in silicon.¹⁴ It is expected, however, that at distances of more than approximately an effective Bohr radius from the donor nucleus, the donor potential should be approximately Coulombic and so Eq. (5) will provide a good description of the true donor electron in this region.⁸ Thus the Kohn-Luttinger form of the donor-electron wave function should be adequate for the purposes of calculating exchange energies for donor separations in the range considered in this article.

A plot of the donor electron wave function along three directions of high symmetry, calculated using effective Bohr radii as determined by Koiller *et al.*,³ is shown in Fig. 2 for a donor placed at a substitutional lattice site. The coefficients $A_{\mathbf{k}_{\mu},\mathbf{G}}$, were calculated using the simple local empirical pseudopotential method as outlined in Ref. 15, and a basis of 125 states. This method accurately reproduces the electronic

band structure for silicon, particularly in the region of interest for this calculation, the lowest conduction bands, as obtained using more complicated nonlocal pseudopotential techniques. The donor electron wave functions obtained in this manner clearly display oscillations produced by the interference between the Bloch functions located at the different conduction band minima. The wave functions are real, and in the [111] direction slightly asymmetric, the asymmetry being a consequence of the presence of the second sublattice. In the [111] orientation the silicon atoms are not evenly spaced, and so the neighboring silicon atom on one side of the phosphorus donor is much closer than that on the other side. Superimposed over the donor wave function is an isotropic $1s$ hydrogenic envelope with a Bohr radius of 20.13 \AA , reflecting the effect of the superposition of the nonisotropic envelope functions F_μ .

III. THE HEITLER LONDON FORMALISM

The two electron Hamiltonian for a system of two donors separated by a vector \mathbf{R} , in effective Rydberg units, is

$$H = -\frac{\hbar^2}{2m^2}\nabla_1^2 - \frac{\hbar^2}{2m^2}\nabla_2^2 - \frac{e^2}{4\pi\epsilon\mathbf{r}_1} - \frac{e^2}{4\pi\epsilon|\mathbf{R}-\mathbf{r}_1|} - \frac{e^2}{4\pi\epsilon\mathbf{r}_2} - \frac{e^2}{4\pi\epsilon|\mathbf{R}-\mathbf{r}_2|} + \frac{e^2}{4\pi\epsilon|\mathbf{r}_1-\mathbf{r}_2|} + \frac{e^2}{4\pi\epsilon\mathbf{R}} + V_{Si}(\mathbf{r}_1, \mathbf{r}_2). \quad (6)$$

In the standard Heitler-London approximation¹⁶ one assumes that the lowest energy two electron wave function of the two-donor system is simply a correctly symmetrized superposition of single electron wave functions centered around each of the two donors

$$\Psi_\pm(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2(1 \pm S^2)}} [\Psi(\mathbf{r}_1 - \mathbf{R}/2)\Psi(\mathbf{r}_2 + \mathbf{R}/2) \pm \Psi(\mathbf{r}_1 + \mathbf{R}/2)\Psi(\mathbf{r}_2 - \mathbf{R}/2)], \quad (7)$$

where the two donors are located at positions $\pm \mathbf{R}/2$. This approximation is asymptotically exact and should hold for separations greater than the effective Bohr radii $|\mathbf{R}| \gg a_\perp, a_\parallel$. The antisymmetry of the fermion wave function then tells us that the exchange splitting, the difference in energies between the spin singlet and triplet spin states, is simply equal to the difference in energy between the states Ψ_\pm , that is $E_{\text{triplet}} - E_{\text{singlet}} = E_- - E_+$.

In this article we present our results in terms of the exchange, or J coupling, in the exchange term of the effective spin Hamiltonian $J\vec{\sigma}_1^e \cdot \vec{\sigma}_2^e$, which is common to the quantum computing literature. We make this decision despite the observation that it is the exchange splitting, the energy difference between the single and triplet states, that is most commonly presented in the solid-state literature. These quantities are related by the expression $J = (E_{\text{triplet}} - E_{\text{singlet}})/4$.

In the Heitler-London formalism the exchange coupling can be expressed in terms of matrix elements of the Hamiltonian one can rewrite this as

$$J(\mathbf{R}) = \frac{1}{2} [S(\mathbf{R})^2 I_1(\mathbf{R}) - I_2(\mathbf{R})] / [1 - S(\mathbf{R})^4], \quad (8)$$

where the overlap integrals are given explicitly by

$$I_1(\mathbf{R}) = \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \Psi^*(\mathbf{r}_1 + \mathbf{R}/2)\Psi^*(\mathbf{r}_2 - \mathbf{R}/2) \times H\Psi(\mathbf{r}_1 + \mathbf{R}/2)\Psi(\mathbf{r}_2 - \mathbf{R}/2),$$

$$I_2(\mathbf{R}) = \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \Psi^*(\mathbf{r}_1 + \mathbf{R}/2)\Psi^*(\mathbf{r}_2 - \mathbf{R}/2) \times H\Psi(\mathbf{r}_2 + \mathbf{R}/2)\Psi(\mathbf{r}_1 - \mathbf{R}/2),$$

$$S(\mathbf{R}) = \int d^3\mathbf{r} \Psi(\mathbf{r} + \mathbf{R}/2)^* \Psi(\mathbf{r} - \mathbf{R}/2). \quad (9)$$

Computation of these expressions using the Kohn-Luttinger wave function without approximation is rather tedious, given the large number reciprocal lattice vectors it is necessary to sum over to evaluate the periodic part of the Bloch functions for each of the six Bloch states in the donor electron wave function. We have used an adaptive Monte Carlo quadrature program to evaluate all overlap integrals, taking due care to obtain reasonable precision.

In Fig. 3 we plot the exchange energy as a function of donor separation in each of the major lattice directions. For comparison the result using an isotropic hydrogenic wave function is also given. We compare our results with those obtained using the method of KHD in their original paper,³ who used two major approximations in order to make the calculation more tractable, some of which are discussed in detail in references.^{4,17} First, the Heitler-London expression for the exchange energy is approximated by the Coulomb exchange integral alone, an approximation that is asymptotically quite good, however it is this approximation that is responsible for the difference between our result and that obtained by KHD in Ref. 3. In Ref. 4, the authors have used the complete form for the Heitler-London expression, and obtained results that match those presented here.

The other approximation made is to effectively ignore the contribution of the periodic part of the Bloch functions $u_\mu(\mathbf{r}) = 1$; this is an excellent approximation as can be seen from the figures in which it is almost impossible to distinguish between the results obtained in this approximation and those for which the detailed Bloch structure was included. The ability to ignore the periodic part of the Bloch structure in the computation of the Heitler-London integrals significantly reduces the complexity of the calculation by eliminating the sums over reciprocal lattice vectors. It is worth examining this approximation in more detail as we find it is effectively the same approximation as is made in effective mass formalism to obtain the Kohn-Luttinger form for the donor electron wave function.

The Heitler-London integrals are all of the form

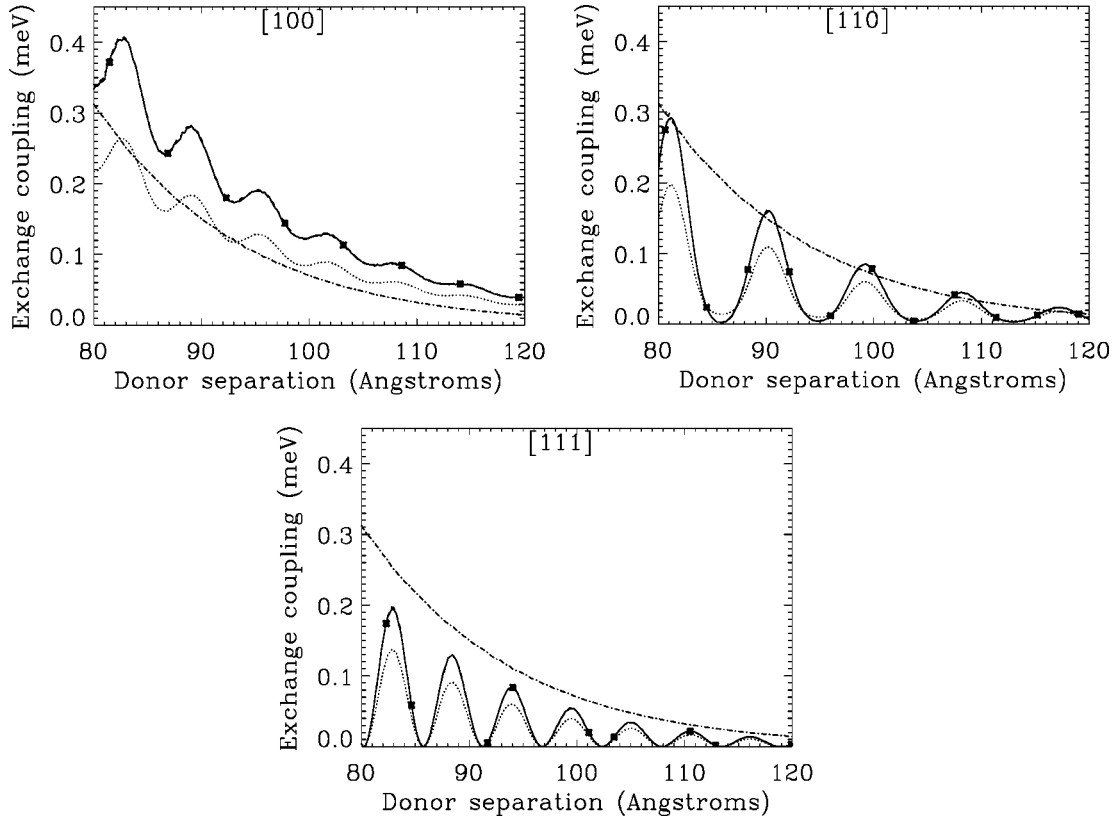


FIG. 3. Calculated exchange couplings as a function of donor separations along three high symmetry directions. In each case we plot with a solid line the results obtained when the periodic part of the Bloch function $u(r)$ is included, a dashed line indicates the results obtained with $u(r)=1$. In each plot these lines cannot be separately resolved. The dotted line gives the results obtained when using the approximations of KHD and the dotted-dashed line gives the exchange coupling calculated using a 1s hydrogenic orbital with an effective Bohr radius of 20.13 Å. The asterisks denote the positions of lattice sites.

$$\begin{aligned}
I &= \int \Psi^*(\mathbf{r}_1 - \mathbf{R}/2) \Psi^*(\mathbf{r}_2 + \mathbf{R}/2) V(\mathbf{r}_1, \mathbf{r}_2) \Psi(\mathbf{r}_2 - \mathbf{R}/2) \\
&\quad \times \Psi(\mathbf{r}_1 + \mathbf{R}/2) d\mathbf{r}_1 d\mathbf{r}_2 \\
&= \int \sum_{\alpha, \beta, \gamma, \delta} \sum_{i, j, l, m} F_i(\mathbf{r}_1 - \mathbf{R}/2) F_j(\mathbf{r}_2 + \mathbf{R}/2) \\
&\quad \times F_l(\mathbf{r}_2 - \mathbf{R}/2) F_m(\mathbf{r}_1 + \mathbf{R}/2) V(\mathbf{r}_1, \mathbf{r}_2) \\
&\quad \times e^{i(\mathbf{k}_i + \mathbf{k}_m - \mathbf{k}_j - \mathbf{k}_l) \cdot \mathbf{R}/2} e^{i(\mathbf{k}_m - \mathbf{k}_i) \cdot \mathbf{r}_1} e^{i(\mathbf{k}_l - \mathbf{k}_j) \cdot \mathbf{r}_2} \\
&\quad \times A_{\mathbf{k}_i, \mathbf{G}_\alpha}^* A_{\mathbf{k}_j, \mathbf{G}_\beta}^* A_{\mathbf{k}_l, \mathbf{G}_\gamma} A_{\mathbf{k}_m, \mathbf{G}_\delta} e^{i(\mathbf{G}_\alpha - \mathbf{G}_\delta) \cdot \mathbf{r}_1} \\
&\quad \times e^{i(\mathbf{G}_\beta - \mathbf{G}_\gamma) \cdot \mathbf{r}_2} d\mathbf{r}_1 d\mathbf{r}_2. \tag{10}
\end{aligned}$$

The various potentials represented in the above expression as $V(\mathbf{r}_1, \mathbf{r}_2)$ are all impurity potentials of a similar nature to those encountered in the effective mass formalism, and so we expect that they are sufficiently slowly varying that we can safely ignore the rapidly oscillating terms in the above integrand, in exactly the same manner. This immediately gives

$$\begin{aligned}
I &= \int \sum_{i, j} F_i(\mathbf{r}_1 - \mathbf{R}/2) F_j(\mathbf{r}_2 + \mathbf{R}/2) F_i(\mathbf{r}_2 - \mathbf{R}/2) \\
&\quad \times F_j(\mathbf{r}_1 + \mathbf{R}/2) V(\mathbf{r}_1, \mathbf{r}_2) e^{i(\mathbf{k}_i + \mathbf{k}_m - \mathbf{k}_j - \mathbf{k}_i) \cdot \mathbf{R}/2} d\mathbf{r}_1 d\mathbf{r}_2, \tag{11}
\end{aligned}$$

which is equivalent to setting $u_\mu(\mathbf{r})=1$ in Eq. (10). The “rapidly oscillating” terms include the exponentials containing the values of \mathbf{k} at the conduction band minima, which are separated by a minimum magnitude of $\delta\mathbf{k}=2\sqrt{2} \times 0.85\pi/d$. This separation is sufficiently large to allow us to ignore terms except those for which $i=m, l=j$. Since $\sum_{\mathbf{G}} A_{\mathbf{k}, \mathbf{G}}^* A_{\mathbf{k}, \mathbf{G}} = 1$, this allows us to ignore the periodic part of the Bloch functions in the Heitler-London integrals.

IV. FABRICATION

The observed extreme sensitivity of the exchange coupling on the relative orientation of the two phosphorus donors sets stringent requirements on the placement of donors for any quantum computer architecture that is reliant on the exchange interaction to couple qubits. In this section we discuss these implications for the construction of a Kane nuclear spin quantum computer.

Fabrication of the Kane solid-state quantum computer is being pursued along two parallel paths.¹⁸ In the so-called “bottom up” approach, individual phosphorus donors are effectively placed with atomic precision on a phosphorus surface by application of phosphine gas to a hydrogen terminated silicon surface in which individual hydrogen atoms have been removed at the proposed donor site using a scanning-tunneling microscope tip. The hydrogen monolayer

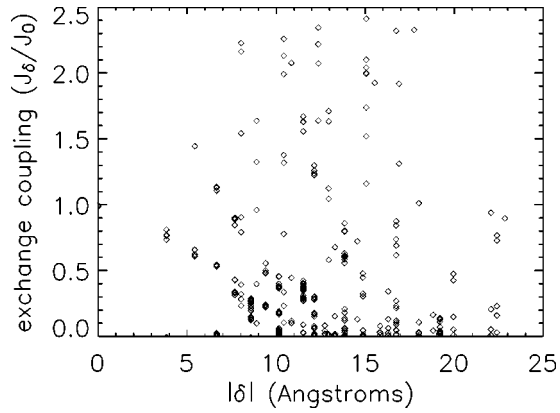


FIG. 4. Calculated exchange couplings for donors at fcc lattice sites that are displaced by a vector δ from their ideal separation of 200.91 \AA in the $[100]$ direction. The couplings are plotted as a fraction of the expected exchange coupling $J(200.91 \text{ \AA}) = 0.18 \mu\text{eV}$.

is then removed and the surface overgrown with phosphorus.¹⁹ Although this approach has not been fully developed, it is likely that it will be able to produce an array of donors located at precise fcc substitutional sites, to within a few lattice spaces. Small displacements are inevitable, however, and can have dramatic effects on the exchange coupling between the donors. This is illustrated in Fig. 4 where we show a plot of the exchange coupling as a function of the magnitude of the displacement $|\delta|$ of the second phosphorus dopant from its desired position at a fcc substitutional site a distance of 200.91 \AA , in the $[100]$ direction, from the first dopant. These dopants have been displaced by no more than four fundamental lattice spacings on either of the two fcc lattices that make up the silicon matrix, however, the exchange coupling varies by more than an order of magnitude emphasizing the need for precise placement.

The second approach, known as the top down approach calls for the implantation if the phosphorus donors into the silicon using an ion beam of phosphorus ions incident on the substrate.²⁰ The precision of such a technique in the placement of dopants is fundamentally limited by the phenomenon known as “stragglng,” whereby the implanted ions scatter from the nuclei of the host silicon atoms. Simulations of this process for a beam of 15 keV phosphorus ions implanted into silicon, an energy appropriate for an implantation depth of approximately 200 \AA into the silicon substrate, give a roughly Gaussian distribution for the final position of the dopant with a variance of about 90 \AA in the transverse direction, and 100 \AA in the longitudinal direction. Using these data, for two dopants implanted 200 \AA apart in the $[100]$ direction, we have calculated the distribution of exchange couplings between the donor electrons, assuming that after thermal annealing the phosphorus donors take up a position on a fcc substitutional site. Figure 5 shows a plot the integrated probability, $\int_J^\infty P(J') dJ'$, that is the probability that the exchange coupling is greater than a value J , for two dopants implanted in the manner just described.

In the case of electron spin quantum computers where it is the exchange energy that directly couples neighboring qubits,

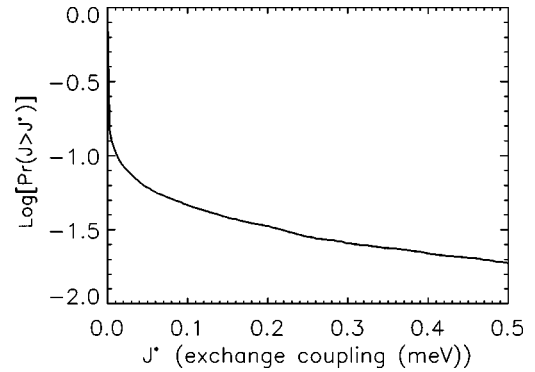


FIG. 5. A plot of the logarithm of the integrated probability for the exchange coupling between donor electrons for donors implanted 200 \AA apart in the $[100]$ direction, using a 15 keV phosphorus ion beam. The donors are assumed to take a substitutional fcc lattice site.

a coupling of $50 \mu\text{eV}$ corresponds to a gate time of the order of 10 GHz . The top down approach can in this case produce qubits coupled by extremely fast gates with a very high probability. In nuclear spin quantum computers however, the exchange interaction only mediates the interqubit coupling and the resulting gates are slower. The original Kane proposal calls for an adiabatic implementation of a controlled-NOT gate that requires a exchange coupling of approximately $50 \mu\text{eV}$.^{2,21} Additional proposals exist for nonadiabatic implementations^{22,23} for which controlled-NOT gates can be accurately implemented with a lower exchange coupling. Figure 5 shows the probability that the bare exchange coupling for implanted donors being greater than $50 \mu\text{eV}$, is about 6%. What is more important than the bare coupling however is the values of the exchange coupling that can be achieved with the application of J -gate biases.

We note that KHD have performed calculations that suggest a method for overcoming the strong dependence of the exchange coupling on the donor orientation.⁴ They calculate the exchange coupling, in the same approximations as discussed earlier, for phosphorus donor electrons in uniaxially strained silicon. The strain is a product of the silicon host being fabricated on a layer of $\text{Si}_{1-\delta}\text{Ge}_\delta$, and is found to suppress the oscillations in the coupling for donors that lie within a plane perpendicular to the direction of the uniaxial strain. The coupling remains highly sensitive to displacements away from this plane.

V. EXTERNAL CONTROL OF THE EXCHANGE COUPLING

Inherent in the Kane proposal for a solid state quantum computer is the ability to control the exchange coupling of neighboring donor electrons through the application of voltage biases to a control J -gate placed on the substrate surface between the position of the phosphorus donors, as illustrated in Fig. 1. In this section we calculate the effect on the exchange coupling on the J -gate bias. Some results have been reported on similar calculations. Fang *et al.*⁷ used an unrestricted Hartree-Fock method, which avoids some of the ap-

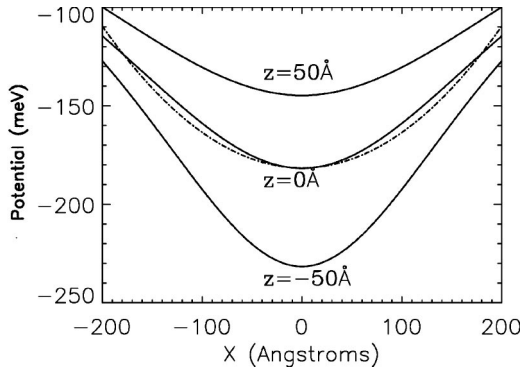


FIG. 6. Potential produced inside the device by a voltage bias of 1 V applied to a metallic J gate. Here x is the interdonor axis, the donors are located at $x = \pm 100$ Å and at $z = 0$. The potential is independent of the y coordinate, mimicking a very long electrode. The dashed line is the one-dimensional potential used by Fang *et al.* with $\mu = 0.15$ and shifted to match our potential at $x, z = 0$.

proximations inherent in the Heitler-London approach, to calculate the exchange coupling between phosphorus donor electrons as a function of a simplified electric potential. They use a trial wave function of the form $\Psi(\mathbf{r}) = F(r)\phi_{\mathbf{k}_\mu}(\mathbf{r})$, including only one of the six degenerate conduction band minima, with a spherical envelope function, that is one of the same form as Eq. (4), but with $a_\perp = a_\parallel = 20$ Å. As a result of their single minimum approximation they cannot possibly reproduce the oscillatory nature of the coupling which results from interference between the terms localized at the six minima. They model the potential produced inside the device by the control gate as one-dimensional potential of the form $V_J(x) = \mu[(x - R/2)(x + R/2)/(R/2)^2] \times 30$ meV, where x is the distance is along the direction between the two donors which are situated at $x = \pm R/2$, as defined in Fig. 1.

In our calculation we compute the potential produced inside the device due to the application of a voltage bias to a metallic J gate by numerical solution of the Poisson equation using a commercial package TCAD,²⁴ designed for the semiconductor industry. In Fig. 6 we plot the potential parallel to the interdonor axis, for several values of the z coordinate, which denotes the distance below the oxide barrier, located at $z = -200$ Å. For more information on the details of the potential calculation see Ref. 25. We compare the potential obtained for a J -gate voltage of 1 V, with the one-dimensional potential of Fang *et al.* and see that the two potentials agree well for $z = 0$, the plane of the donors, provided we set $\mu = 0.15$. However, we see that for this value of μ the two potentials are quite different in the planes 50 Å above and below the donors. We must therefore conclude that the one-dimensional approximation is not a good one.

To calculate the effect of the applied potential on the electron we expand the wave function as follows:

$$\Psi(\mathbf{r} - \mathbf{R}/2, V_J) = \sum_{n,l,m} c_{n,l,m}(V_J) \sum_{\mu} F_{\mu}^{n,l,m}(\mathbf{r} - \mathbf{R}/2) e^{i\mathbf{k}_\mu \cdot (\mathbf{r} - \mathbf{R}/2)}, \quad (12)$$

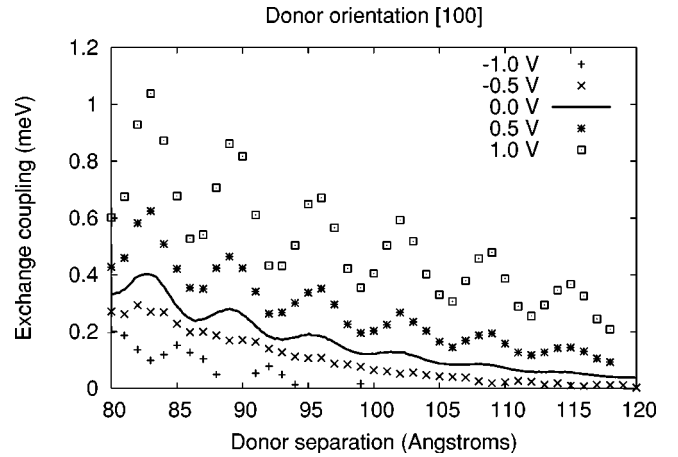


FIG. 7. Exchange coupling as a function of donor separation for donors oriented along the [100] direction and various J -gate biases.

where the $F_{\mu}^{n,l,m}(\mathbf{r} - \mathbf{R}/2)$ are nonisotropic hydrogenic envelope functions defined by Faulkner.¹² The μ is a label for the six degenerate conduction band minima and determines the direction of the anisotropy of the envelope function, for example, $F_{\pm z}^{n,l,m}(\mathbf{r}) = F^{n,l,m}(x, y, \gamma z)$, is the hydrogenic function with a Bohr radius $a = a_\perp$ and $\gamma = a_\parallel/a_\perp$. The orthonormality of this basis is enforced by the $e^{i(\mathbf{k}_\mu - \mathbf{k}_\nu) \cdot (\mathbf{r} - \mathbf{R}/2)}$ terms which appear in the matrix elements and due to their rapidly oscillating nature average to zero unless $\mathbf{k}_\mu = \mathbf{k}_\nu$. The coefficients $c_{n,l,m}$ are determined by direct numerical diagonalisation of the Hamiltonian in the presence of the electrostatic potential. We use a basis of 140 states, which includes all states with principle quantum number up to and including $n = 7$, and we rescale the energies such that the unperturbed ground-state energy gives the experimentally observed value of 45.5 meV for phosphorus donors in silicon.

The donor electron wave functions obtained in this way are then used in the Heitler-London formalism to calculate the electron exchange energy, as a function of both the donor separation, and applied J -gate bias. The results are plotted in Fig. 7, for donor separations from 80–120 Å in the [100] direction. We see that application of a positive bias will tend to increase the exchange coupling, while a negative bias decreases the strength of the coupling. It is also worth noting that the relative increase in the exchange coupling produced by a given bias increases with the donor separation. Also the change in coupling is strongest at the peaks, the application of a positive bias enhances the oscillations in the exchange coupling whereas a negative bias of magnitude 1 V inverts the oscillations such that points that were originally at peaks become troughs.

The range of separations shown in these plots is far less than the approximately 200 Å donor separation called for in the original Kane proposal—we have plotted values over range for ease of comparison with our previous results, and more particularly those of KHD. In Fig. 8 we plot the exchange coupling as a function of the J -gate bias for donors separated by 200.91 Å in the [100] direction. At this separation a 1 V J -gate bias can increase the exchange coupling by over two orders of magnitude up to a value of approximately

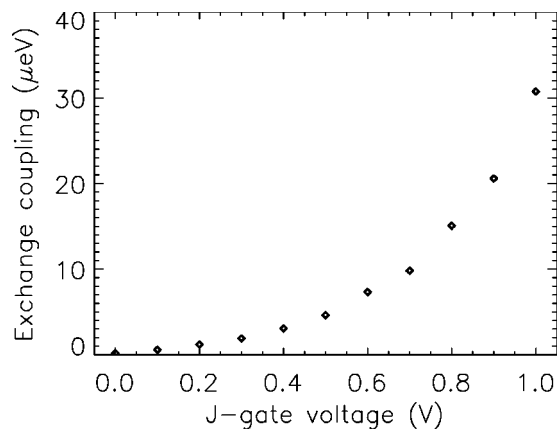


FIG. 8. Exchange coupling as a function of J -gate bias for donors at fcc lattice sites separated by 200.91 \AA in the $[100]$ direction.

$30 \mu\text{eV}$. The exchange coupling can also be reduced via application of a negative bias.

Although it is difficult to compare our results with those of Fang *et al.* due to the different potentials, the shift of an order of magnitude obtained for separation of 200 \AA and a bias of 1 V is greater than the shift they predict. For a value of $\mu = 0.15$, Fang *et al.* predict a shift of less than an order of magnitude. This discrepancy can in part be attributed to the 1D approximation for the gate potential which does not account for the fact that the magnitude of the potential increases as the J gate is approached from below (in the z direction). We note that it may not be possible to apply voltages much greater than one volt to these nanoscale devices without exceeding the breakdown fields of the various materials involved.²⁵

VI. DISCUSSION AND CONCLUSIONS

In agreement with the approximations implicit in the calculations of donor electron exchange energy of Koiller, Hu, and Das Sarma,³ we show explicitly that the periodic part of the Bloch functions in the donor electron wave functions can be ignored in the Heitler-London integrals, greatly reducing the complexity of the calculation. This has allowed the calculation of the intrinsic exchange coupling for a large number of donor pairs distributed according to the probability distribution for donors implanted 200 \AA apart by 15 keV ion beams. In this manner we have determined the probability distribution of the exchange coupling for the top-down approach for the fabrication of a Kane solid-state quantum computer.

In addition we have investigated the application of control gate biases to increase the exchange coupling between donor pairs using both realistic potentials and realistic donor electron wave functions. We find that as expected the exchange coupling can be increased by the application of a positive bias, and decreased with a negative bias. Over the range of donor separations investigated it was found that the relative increase of the exchange coupling produced by a given bias increases with the separation, and for donors separated by 200 \AA in the $[100]$ direction a 1 V bias can increase the coupling by over two orders of magnitude.

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