

Chirality in Quantum Computation with Spin Cluster Qubits

V.W. Scarola, K. Park, and S. Das Sarma

Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA
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We study corrections to the Heisenberg interaction between several lateral, single-electron quantum dots. We show, using exact diagonalization, that three-body chiral terms couple triangular configurations to external sources of flux rather strongly. The chiral corrections impact single-qubit encodings utilizing loops of three or more Heisenberg coupled quantum dots.

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Qubits based on electron spin in semiconductor structures play a central role in solid state quantum information processing [1–4]. In particular, the extremely long [5] spin coherence times ($T_2 \gg \mu\text{s}$) coupled with the enormous lithographic and fabrication scalability advantages of existing semiconductor technology have led to a large number of proposed quantum computer architectures using electron spin qubits in semiconductor nanostructures. Most of these proposals [1–4] utilize the Heisenberg exchange coupling (“the exchange gate” [1]) between two electrons localized in individual quantum dots [1] or in shallow donor states (e.g., P atoms in Silicon [2]) in order to carry out the required two-qubit operations. The original proposals involve control, tuning, and manipulation of one-qubit and two-qubit gates through externally applied, local magnetic and electric field pulses, respectively, but it was soon realized that controlling *single* localized electron spins through local magnetic field (and/or microwave) pulses is problematic [6–8], perhaps even prohibitively so, and therefore a number of interesting theoretical proposals have recently been made [7–10] for using a cluster of spins (“spin cluster”) rather than a single spin, as the suitable qubit unit in solid state spin-based quantum computing architectures. In particular, some elegant, recent theoretical literature [7–13] has convincingly demonstrated as a matter of principle the nonessential and therefore disposable character of single-spin qubit operations altogether, showing that the Heisenberg exchange coupling between electron spins by itself can actually carry out quantum computation in spin-based architectures, provided each *logical* qubit is encoded in a number of *physical* spins (i.e., spin cluster encoded qubits).

One important perceived advantage of such collective spin-based logical qubits (avoiding single-electron spin qubits altogether) is that the system can be placed in a decoherence free subsystem or subspace [14,15] (where the encoding scheme strongly suppresses decoherence of single logical qubits) making such encoded spin cluster qubits highly desirable from the perspective of scalable and coherent fault-tolerant quantum computation. Not surprisingly, therefore, the idea of using spin clusters

rather than single spins as the basic building block of exchange gate-based solid state quantum computation has attracted a great deal of recent theoretical attention.

In this Letter we point out and theoretically formulate an important conceptual, topological aspect of spin cluster qubits in solid state architectures. In particular, we show that the proposed solid state two (or three)-dimensional spin cluster qubits will necessarily generate topological chiral terms in the qubit Hamiltonian in the presence of external sources of flux, which will necessarily modify the Heisenberg exchange interaction bringing into question, in the process, the applicability of the exchange gate idea which has been the centerpiece of spin-based solid state quantum computation architectures. Thus the proposed spin cluster qubits involving looped arrays of localized, tunnel coupled electron spins will not behave as originally envisaged in the exchange gate scenarios discussed in many recent publications. Even the proposed encoded spin qubits, which specifically exclude all single-qubit operations (and hence do not employ any applied external magnetic field), will have severe single-qubit decoherence problems (thus undermining the decoherence free properties of the logical qubit) since any temporally fluctuating external sources of enclosed flux will cause dephasing through the chiral term discussed here. Contributions to the mean field component of an external magnetic field may arise, for example, from the nuclear dipolar field of the host lattice [5]. Alternatively, we find that the chiral term plays no role in clusters which do *not* contain three simultaneously tunnel coupled sites. The chiral term may also be considered negligible when the area enclosed by three tunneling channels is small. Atomic clusters, with small lattice spacings $\sim 1 \text{ \AA}$, require large external magnetic fields, $\sim 10^4 \text{ T}$, to see a sizable chiral contribution. We show that the large lattice spacing in looped quantum dot arrays enhances the role of three-body chiral terms in the spin Hamiltonian.

We study the low energy Hilbert space of N lateral quantum dots containing N electrons lying in the $x - y$ plane by exact diagonalization of the following Hamiltonian:

$$H = \sum_{i=1}^N \left[\frac{\mathbf{P}_i^2}{2m^*} + V(\mathbf{r}_i) \right] + \sum_{i < j}^N \frac{e^2}{\varepsilon |\mathbf{r}_i - \mathbf{r}_j|} + H_Z, \quad (1)$$

where we define the canonical momentum, $\mathbf{P} = \mathbf{p} + \frac{e}{c} \mathbf{A}$, and the Zeeman term $H_Z = g^* \mu_B \mathbf{S} \cdot \mathbf{B}$. In GaAs, we have an effective mass $m^* = 0.067m_e$, dielectric constant $\varepsilon = 12.4$, and g -factor $g^* = -0.44$. We work in the symmetric gauge with magnetic field $\mathbf{B} = B\hat{z}$. The field couples directly to the total spin, \mathbf{S} , through the Zeeman term. The single particle potential confines the electrons to lie at the vertices of an equilateral triangle and square for $N = 3$ and 4, respectively, as shown in Fig. 1. In diagonalizing the $N = 3$ system we choose $V(\mathbf{r}_i) = (m^* \omega_0^2/2) \min_j \{ |\mathbf{r}_i - \mathbf{R}_j|^2 \}$, where a parabolic confinement parameter, $\hbar\omega_0 = 6$ meV, effectively localizes the electrons at the sites \mathbf{R}_j separated by 40 nm.

Prior to exact diagonalization of Eq. (1), we seek a perturbative expansion in terms of on-site spin operators. We consider the single band, tight binding limit, a good approximation in the limit that the excited states of the quantum dot lie higher in energy than the lowest spin split states. We also take the on-site Coulomb interaction to be much larger than the tunneling energy. (We verify numerically that, for the $N = 3$ system, the following approximations are self consistent *only* at low B , $\omega_c \lesssim \omega_0/3$, where $\omega_c = eB/m^*c$ is the cyclotron frequency.) As a result, we obtain the Hubbard Hamiltonian:

$$H_H = - \sum_{i,j,\alpha} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_i (U n_{i\uparrow} n_{i\downarrow} + g^* \mu_B \mathbf{B} \cdot \mathbf{S}_i), \quad (2)$$

where $c_{i\alpha}^\dagger$ creates a fermion at the site i with spin $\alpha \in \{\uparrow, \downarrow\}$ and $n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha}$. We have defined the spin operators $\mathbf{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\alpha'} c_{i\alpha'}$ where $\boldsymbol{\sigma}$ are the Pauli matrices. As a consequence of the magnetic field, the tunneling coefficients are complex: $t_{ij} = |t_{ij}| \exp(2\pi i \Phi_{ij}/\Phi_0)$, where $\Phi_0 \equiv hc/e$. The magnetic vector potential generates the Peierls phase: $\Phi_{ij} = \int_i^j \mathbf{A} \cdot d\mathbf{r}$. The integral is taken along a path connecting the sites i and j . Working in the small $|t_{ij}|/U$ limit we confine our attention to single occupancy states. Here we expand H_H [16] by applying a unitary transformation $\exp(iK)H_H \exp(-iK)$, where K

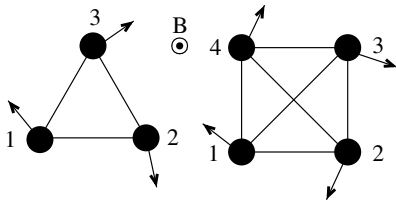


FIG. 1. Two possible looped configurations of lateral quantum dots in a magnetic field. The triangular configuration contains three tunneling channels with one loop formed by the vertices 123. The square configuration contains, in general, six tunneling channels with four three-site loops formed by the vertices 123, 234, 341, and 412.

is an operator changing the number of doubly occupied states. Up to third order in this expansion we find [17,18]:

$$H_{\text{eff}} = g^* \mu_B \mathbf{B} \cdot \sum_i \mathbf{S}_i + \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{ijk \in \Delta} \mu_{ijk} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) + \vartheta \left(\frac{t^4}{U^3} \right), \quad (3)$$

where $t \sim |t_{ij}|$. The second term is the usual Heisenberg interaction, where $J_{ij} = 2|t_{ij}|^2/U$, while the third term is a three-site sum over chiral [19] terms $\chi_{ijk} \equiv \mu_{ijk} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$ around loops, Δ . In H_{eff} we have excluded fourth order terms of the form $(\mathbf{S}_i \times \mathbf{S}_j) \cdot (\mathbf{S}_k \times \mathbf{S}_l)$ and $(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l)$. It was shown that the latter plays a role at $B = 0$ in a four spin, tetrahedral configuration [20]. The coefficients in the chiral term $\mu_{ijk} = (24/U^2) \times |t_{ij}| |t_{jk}| |t_{ki}| \sin(2\pi \Phi_{ijk}/\Phi_0)$ depend on the flux enclosed by the three-site loop, Φ_{ijk} . As a result, the chiral term generates an energy splitting between third order, virtual tunneling processes which run along and counter to the applied vector potential. The phase, $2\pi \Phi_{ijk}/\Phi_0$, is the Aharonov-Bohm phase generated by the virtual current moving around the flux enclosed by the three-site loop. The chiral term is Hermitian but breaks time reversal symmetry and vanishes on bipartite lattices as a result of particle hole symmetry [18].

We may now ask whether or not three coupled quantum dots containing three electrons may support a noiseless subsystem in the presence of a fluctuating, perpendicular magnetic field [15]. The set of states comprising a noiseless subsystem remain invariant under the application of a suitable noise operator. We may, for example, choose the first term in Eq. (3) as a noise source. We then find the simplest example of a quantum dot, noiseless subsystem in the $S = 1/2$ sector of the $N = 3$ system. This encoding makes use of a fourfold, $B = 0$ degeneracy found in this sector to protect quantum information stored in the qubit defined by $|\lambda\rangle_3$, where $\lambda = 0$ or 1. The subscript denotes the number of quantum dots and electrons used to define the qubit. The four states may be written:

$$|\lambda\rangle_3 \otimes \left| -\frac{1}{2} \right\rangle = \frac{-1}{\sqrt{3}} (|\uparrow\uparrow\downarrow\rangle + \omega^{\lambda+1} |\uparrow\downarrow\uparrow\rangle + \omega^{2-\lambda} |\downarrow\uparrow\uparrow\rangle) \\ |\lambda\rangle_3 \otimes \left| \frac{1}{2} \right\rangle = \frac{1}{\sqrt{3}} (|\uparrow\uparrow\uparrow\rangle + \omega^{\lambda+1} |\uparrow\uparrow\downarrow\rangle + \omega^{2-\lambda} |\uparrow\downarrow\uparrow\rangle), \quad (4)$$

where $\omega \equiv \exp(2\pi i/3)$. In the presence of a fluctuating Zeeman energy, the first term in the tensor product preserves the quantum information stored in the quantum number λ while the z -component of spin, the second term in the tensor product, may fluctuate. Application of H_{eff} up to second order shows that the magnetic field only weakly affects $|\lambda\rangle_3$ through the Heisenberg term. In fact, several proposals [7,9–11,21] suggest use of the Heisenberg term, with anisotropic couplings J_{ij} , to implement Pauli gates on encoded qubits. In Heisenberg gating

schemes, the expectation value of the individual Heisenberg terms, and hence gates formed from them, remain insensitive to fluctuations in the Zeeman term because $[\mathbf{S}_i \cdot \mathbf{S}_j, \sum_i \mathbf{S}_i] = 0$ for all i and j .

Up to second order, H_{eff} also allows an encoding against Zeeman-like or collective noise. Here collective noise implies symmetry among all spins when coupling to a bath. However, the third order chiral term acts as a *noncollective* system-bath interaction between the encoded qubit and a potentially noisy source of enclosed flux. The chiral and Zeeman terms remove all degeneracies required to establish a qubit encoding immune to fluctuations in the perpendicular magnetic field. Explicitly: $\chi_{123} |\lambda\rangle_3 \otimes |\pm \frac{1}{2}\rangle = \mu_{123} (2\lambda - 1)(\sqrt{3}/4) |\lambda\rangle_3 \otimes |\pm \frac{1}{2}\rangle$, where $\mu_{123} = (12tJ/U)\sin(2\pi\Phi_{123}/\Phi_0)$ in the case $J_{ij} = J$ and $|t_{ij}| = t$ for all i and j . Therefore, χ_{123} yields an *effective* Zeeman splitting between the encoded basis states of the three spin qubit. The size of the splitting depends on $6J(J/t)$ which, under reasonable conditions, cannot be neglected as long as the second order term, $J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j$, remains large. Gates constructed from the exchange interaction must operate on time scales shorter than typical spin relaxation times supplying, in turn, a necessary minimum to the exchange interaction.

To test the accuracy of H_{eff} , we diagonalize Eq. (1) with $N = 3$. We construct the matrix representing H in the Fock-Darwin [22] basis centered in the triangle formed by the three parabola centers defined by $V(\mathbf{r})$. We find it necessary to include up to $\sim 10^5$ origin centered, Fock-Darwin basis states with z -component of angular momentum less than 12 to obtain convergence. We use a modified Lanczos routine to obtain the ground and excited states. We focus on the three lowest energy states in the absence of the Zeeman term. Figure 2 shows the energy of the lowest states obtained from exact diagonalization of H in the $S^z = 1/2$ sector as a function of magnetic field. The ground state energy is set to zero. The two lowest energy states have total spin $S = 1/2$. They are degenerate at $B = 0$ as expected from the reflection symmetry of the triangular confining potential. The next highest state has $S = 3/2$, which corresponds to $6t^2/U \approx 0.125$ meV. Above this state we find (not shown) the higher excited states to lie near 3.8 meV.

As we increase magnetic field, the magnetic vector potential breaks the reflection symmetry of the confining potential leading to a splitting between the two lowest states. The splitting is linear in B for small B , which suggests that the splitting is due to χ_{123} . The chiral term annihilates $S = 3/2$ states. We therefore expect that the energy of the $S = 3/2$ state, $E_{S=3/2}$, does not change with magnetic field at low fields (while $E_{S=3/2} - E_{|0\rangle_3}$ should increase linearly). Here the relevant length scale is a modified magnetic length, $a = \sqrt{\hbar c/eB}(1 + 4\omega_0^2/\omega_c^2)^{-1/4}$. As a result, the magnetic field increases the Coulomb energy ($\sim e^2/\epsilon a$) only above $B \sim 0.7$ T. At

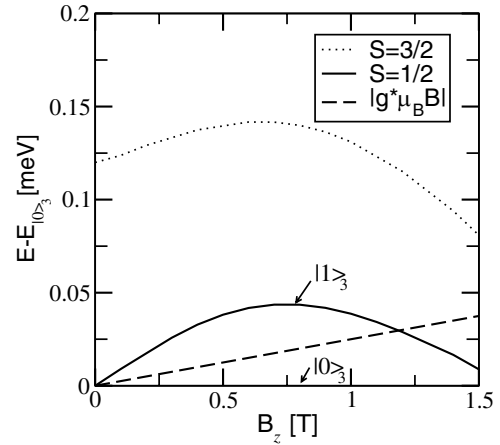


FIG. 2. The energy of the lowest states of three electrons confined in three adjacent, parabolic quantum dots obtained from exact diagonalization of Eq. (1). The dot centers form an equilateral triangle in the $x - y$ plane with 40 nm side lengths. The energies are plotted as a function of perpendicular magnetic field. The total z -component of spin is taken to be $1/2$. The energy of the state $|0\rangle_3$ in Eq. (4) is set to zero. The solid and dotted lines show the energy of the states with total spin $S = 1/2$ and $S = 3/2$, respectively. The dashed line plots the Zeeman splitting in GaAs, $\approx 0.025B[T]$ meV, for comparison. The energy splitting between the three-electron encoded qubit states $|0\rangle_3$ and $|1\rangle_3$ is larger than the Zeeman splitting between the spin up and down states of a single electron.

fields above $B \sim 0.7$ T, the energies slope down, indicating an eventual sign change in J , as for double quantum dots [23]. Here the chiral contribution starts to become suppressed, along with the exchange interaction. At larger fields, the long range part of the Coulomb interaction becomes relevant. We must then keep extended terms in H_{H} of the form $V \sum_{i,(\alpha,\alpha') \in \{1,2,3\}} n_{i,\alpha} n_{i+1,\alpha'}$. We note that inclusion of these terms into H_{H} merely renormalizes the on-site contact term U for $U \gg V$ [24]. For large V , the extended Hubbard term favors double occupancy of the dots and eventually leads to a sign change in J [23]. This suggests that H_{eff} is qualitatively accurate below $B \sim 0.7$ T.

The slope of the energy splitting between the two lowest states in Fig. 2 allows us to estimate t/U for this system. Using the area of the equilateral triangle defined by the dot centers, we obtain $t/U \approx 0.09$ which shows that our expansion in t/U is consistent at low fields [25]. For $N = 3$, only odd powers of t_{ij} allow linear magnetic field dependence in the splitting, showing that the magnetic field dependence captured by the chiral term is accurate up to $\mathcal{O}(t^3/U^3)$.

The dashed line in Fig. 2 shows, for comparison, the Zeeman splitting between the spin states of a single electron. The Zeeman splitting is smaller than the energy difference $E_{|1\rangle_3} - E_{|0\rangle_3}$, suggesting that, in the chosen parameter regime, quantum information encoded in the “noiseless” spin states of a three-electron, triangular set

of quantum dots is *more* sensitive to a perpendicular magnetic field than a single electron.

We now study magnetic field effects on a decoherence free subspace (DFS) [14] formed from quantum dot loops. The lowest number of physical spins supporting a DFS is four. For simplicity, we begin with four quantum dots containing four electrons lying at the vertices of a square with equal tunneling $|t_{ij}| = t$, including diagonal terms shown schematically in Fig. 1. In this case we find a DFS among two $S = 0$ states corresponding to $\lambda = 0$ and 1:

$$|\lambda\rangle_4 = |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + \omega^{\lambda+1}|\uparrow\downarrow\uparrow\downarrow\rangle + \omega^{\lambda+1}|\downarrow\uparrow\downarrow\uparrow\rangle \\ + \omega^{2-\lambda}|\uparrow\uparrow\downarrow\downarrow\rangle + \omega^{2-\lambda}|\downarrow\downarrow\uparrow\uparrow\rangle. \quad (5)$$

These states have equal Zeeman energies and, up to second order in Eq. (3), show no direct magnetic field dependence in their energy spectra. As for the third order term, the spin Hamiltonian must respect the exchange symmetry inherent in the lattice. Therefore, the sum over asymmetric chiral terms must vanish with equal tunneling among all sites. In the $|\lambda\rangle_4$ basis we find:

$$\sum_{ijk \in \Delta} \chi_{ijk} \otimes I_l |\lambda\rangle_4 = \frac{\sqrt{3}}{4} (2\lambda - 1) \sum_{ijk \in \Delta} \mu_{ijk} \epsilon_{ijkl} |\lambda\rangle_4, \quad (6)$$

where ϵ_{ijkl} is the four component Levi-Civita symbol and I_l is the identity operator. The sums run over three-site loops excluding $l = i, j$ or k . The sum vanishes with tunneling $|t_{ij}| = t$ for all i and j . However, if we impose some asymmetry in tunneling, as is done when applying a Pauli gate to the encoded qubit, this sum is not zero. Consider a simple case: $|t_{31}| = |t_{23}| = |t_{34}| = t(1 + \delta)$, where δ is a number and all other $|t_{ij}| = t$. The sum over chiral terms then induces an energy splitting $\approx 24\pi\sqrt{3}tJ\delta AB_z/(U\Phi_0)$ between the states with $\lambda = 0$ and 1 for $\Phi_{ijk}/\Phi_0 \ll 1$. Here, A is the area of the triangle defined by the vertices 123. As in the $N = 3$ system, the energy splitting acts as an effective Zeeman splitting on the $N = 4$ encoded qubit with the exception that here the parameters A and δ may be included in an effective g -factor of the encoded two-level system.

As mentioned earlier, Pauli gating sequences may be applied to encoded, multispin qubits by tuning the Heisenberg couplings, and therefore t_{ij} , in an asymmetric fashion. When applied to a DFS, a Pauli gate composed of Heisenberg terms must, by construction, involve a spin specific asymmetry with, for example, large δ . As shown above, the $N = 4$ encoded qubit will, during a gate pulse, be sensitive to sources of enclosed flux because the scalars forming the Heisenberg interaction do not commute with the individual chiral terms where, for example: $[\mathbf{S}_i \cdot \mathbf{S}_3, \chi_{123}] \neq 0$, with $i = 1$ or 2.

We have shown that, in multiple quantum dot architectures containing tunnel coupled loops, fluctuations in enclosed flux provide a potential source of phase flip error in noiseless subsystems and subspaces through chiral currents generated by virtual hopping processes around

three-site loops. In systems for which fluctuations in the phase of t_{ij} can be ignored, we have shown that a well controlled source of flux may also be a good candidate for implementing a logical Pauli Z gate on a three or four spin encoded qubit. Quantum algorithms using only exchange based quantum gates require several accurate applications of the exchange Hamiltonian [7]. The chiral term may then supplement the exchange interaction and therefore potentially reduce the overhead in exchange based algorithms. However, the phase in t_{ij} is in general a Berry's phase [26] arising from symmetry breaking terms in the original Hamiltonian. Spin orbit coupling can contribute to Berry's phase effects in triangular lattices [27] and may therefore play a role in effective spin Hamiltonians modeling tunnel coupled quantum dots.

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