Quantum Information Protectorates in Coupled Quantum Dot Exchange Gates

V.W. Scarola and S. Das Sarma
Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742-4111

Using exact diagonalization we study the low energy Hilbert space of the two-electron, two-quantum dot artificial molecule under a perpendicular magnetic field. We show that electrons bind to vortices to induce several spin transitions among ground states. Furthermore, the lowest excited states of either even or odd vorticity mix, opening an anticrossing which protects the quantum information stored in the spin states of the strongly correlated quantum dot molecule.

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Exchange gate, the key idea underlying spin quantum computation in semiconductor quantum dots, involves the tunable exchange coupling between two electrons localized in neighboring quantum dots. This system can be thought of as a two-electron quantum molecule (i.e. an artificial H₂ molecule) in an external magnetic field with external gates controlling the “molecular” coupling between the two quantum dots. In this Letter we show that the effective exchange coupling in such an artificial quantum dot molecule manifests highly non-trivial and unexpected magnetic field dependence which can be used to “protect” quantum information.

The Heisenberg model captures the essential, low energy spin physics of neighboring, single electron quantum dots [1]. For well separated and therefore weakly coupled electrons in the perturbative regime, recent studies [2, 3] indicate that such an artificial two-dot molecule may indeed be thought of as a two-level spin system with an effective exchange interaction. However, there is no direct experimental probe of the average inter-electron distance or confinement. Bearing this in mind we study the nature of the ground and excited states of the strongly coupled, two electron system using both exact diagonalization and variational techniques in a regime inaccessible to perturbation theory.

We first solve the problem of two electrons in one parabolic dot in a large, perpendicular magnetic field analytically. We find ground and excited state transitions as a function of magnetic field. At special magnetic fields correlations force the excited states to become degenerate potentially destroying the two-level approximation invoked in applying the Heisenberg model to two laterally separated dots. To explore this possibility in detail we examine the two-electron-two dot problem using exact diagonalization. We find, as in a previous study [3], striking evidence for several spin transitions as a function of magnetic field. The two lowest states still map onto a Heisenberg model but with an exchange interaction which oscillates with magnetic field, clearly a non-trivial, Coulombic effect. As for the higher excited states, we find that rotational symmetry breaking creates an anticrossing which, with the correct parameters, can be used to protect the quantum information stored in the two electron entangled state. We explore the nature of the states making up the anticrossing. We show conclusively that trial states based on the composite fermion theory of the fractional quantum Hall effect accurately capture the ground and excited states. We classify these states according to the number of vortices attached to each electron, or vorticity. Our principal conclusion is twofold: Ground state spin transitions occur as a result of a unit increase in vorticity, and the lowest excited states of either even or odd vorticity mix, opening an energy gap which acts as a protectorate for quantum information.

We begin with a general Hamiltonian describing two, lateral, single electron quantum dots:

\[ H(\omega_0, R) = \sum_{i=1}^{2} \left[ \frac{1}{2m^*} \left( p_i + eA_i \right)^2 + V(\omega_0, R; r_i) \right] + \frac{e^2}{4\pi\varepsilon|\mathbf{r}_1 - \mathbf{r}_2|} + g^\ast \mu_B \mathbf{S} \cdot \mathbf{B}. \]  

(1)

For GaAs we take the effective mass to be \( m^* = 0.067m_e \) and the dielectric constant \( \varepsilon = 12.4\varepsilon_0 \). The two dimensional coordinates \( \mathbf{r} = (x, y) \) lie in the plane perpendicular to the magnetic field, \( \mathbf{B} \), which points along the z-axis. In the symmetric gauge we have: \( \mathbf{A} = \frac{B}{2}(-y, x, 0) \). The confinement potential consists of two parabolas separated by a distance \( R \) along the x-axis:

\[ V(\omega_0, R; \mathbf{r}) = \frac{m^*\omega_0^2}{2} \min \left\{ \left( \frac{x - \frac{R}{2}}{2} \right)^2 + y^2, \left( \frac{x + \frac{R}{2}}{2} \right)^2 + y^2 \right\}, \]  

(2)

where we choose the confinement parameter to be \( \hbar\omega_0 = 3 \text{ meV} \). The last term in \( H \) is the Zeeman contribution where \( \mathbf{S} \) is the total electron spin and \( g^\ast \) is the \( g \)-factor in GaAs. In GaAs the Zeeman splitting, \( \sim -0.025S_zB[T] \text{ meV} \), is an additive constant which may be taken into account after solving for the orbital degrees of freedom. We may therefore restrict our attention to the \( S_z = 0 \) subspace with no loss of generality. We seek solutions of the above Hamiltonian of the form \( A[\psi\chi] \) where \( \psi \) and \( \chi \)
are the orbital and spin parts of the wave function and \( A \) is the antisymmetrization operator.

The above model is analytically soluble in two extreme regimes: Two well-separated one-electron “artificial atoms” and a two-electron artificial atom in a high magnetic field. The first case is trivial and consists of two well separated quantum dots (akin to two well-separated one electron atoms not in a molecular state) with one electron in each dot, \( R \gg a \). Here \( a = \sqrt{\hbar/eB(1+4\omega_0^2/\omega_c^2)} \) is a modified magnetic length and \( \omega_0 = eB/m^* \) is the cyclotron frequency. In this case we may ignore the Coulomb interaction. The non-interacting ground state consists of degenerate singlet and triplet states.

In the second soluble limit (a two-electron artificial atom) two electrons lie in one parabolic dot in a strong magnetic field. In this case we take \( \omega_0 \ll \omega_c \) and \( R = 0 \). Correspondingly, the relative and \( z \)-component of angular momentum commute with the Hamiltonian. At large magnetic fields we may project onto the lowest Landau level (LLL), giving:

\[
H(\omega_0, R) \left| \omega_0 \ll \omega_c, R = 0 \right. = \gamma \hat{L}_z + \sum_{m=0}^{\infty} V_m \hat{P}_m, \tag{3}
\]

where \( \gamma \equiv \frac{\hbar}{4}(\sqrt{\omega_c^2 + 4\omega_0^2} - \omega_c) \) and \( \hat{L}_z \) is the total angular momentum in the \( z \) direction. The second term represents the LLL Coulomb interaction, projected onto eigenstates of relative angular momentum, \( m \), via the projection operator \( \hat{P}_m \). The coefficients, \( V_m \), are the Haldane pseudopotentials which, for the Coulomb interaction, decrease with increasing \( m \), at large \( m \). The unnormalized eigenstates of relative angular momentum are:

\[
|m\rangle = (z_1 - z_2)^m \exp \left( \frac{-|z_1|^2 - |z_2|^2}{4a^2} \right), \tag{4}
\]

where \( z = x + iy \). It can be shown by direct calculation that, because there is no center of mass motion, the above wave functions are also eigenstates of \( \hat{L}_z \), with eigenvalue \( m \). Thus the set of states \( |m\rangle \) form an orthogonal set of eigenstates of Eq. (3), with eigenvalues \( E_m = \gamma m + V_m \). The relative angular momentum of the lowest energy state depends on the parameters in \( \gamma \) and the form of the interaction. For the LLL Coulomb interaction, in the artificial zero field limit, the lowest energy state has \( m = 1 \). Increasing \( B \) lowers the confinement energy cost, \( \gamma m \sim m/B \), and raises the Coulomb cost, \( V_m \sim \sqrt{B}/(m+1) \), thereby raising \( m \) by one. The transition from one eigenstate to the next occurs when \( E_m = E_{m+1} \) which, for \( \omega_0 \ll \omega_c \), occurs at magnetic fields:

\[
B_m \approx \left( \frac{C}{V_m - V_{m+1}} \right)^{\frac{1}{2}}, \tag{5}
\]

where \( V_m \equiv V_m/(e^2/4\pi\varepsilon a) \) and \( C \equiv 4\pi\varepsilon h^{3/2}\omega_0^2m^*e^{-7/2} \).

FIG. 1: Energy of the four lowest states of a two electron quantum dot under a perpendicular magnetic field in the lowest Landau level plotted as a function of perpendicular magnetic field. The ground state energy is set to zero. The ground state alternates between spin singlet \((S = 0)\) and triplet \((S = 1)\) as a function of magnetic field. The spin singlet and triplet states correspond to even and odd angular momentum quantum numbers, \( m \).

For the parameters used here we find \( C \sim 1.2 \ T^{3/2} \). The states \(|m\rangle\) are symmetric (antisymmetric) with respect to particle exchange if \( m \) is even (odd). The total wave function, \( A|\psi\rangle \), must be antisymmetric. Therefore \( \chi \) is spin singlet (triplet) for \( m \) even (odd). Here, the index \( m \) may be interpreted as the number of zeros or vortices attached to each electron, allowing us to assign a vorticity to each spin state. We show that vorticity plays an important role in the protection of quantum information in the GaAs coupled quantum dot exchange gate architecture.

Fig. 1 plots \( E_m - E_{\text{ground}} \) versus \( B \) for the four lowest energy states, \( m = 1, 2, 3, \) and 4. Cusps appear at \( E_m - E_{\text{ground}} = 0 \) where the ground state changes at \( B_m \) signaling a change in the number of vortices per electron. (Note that the relation for \( B_m \) is valid for \( \omega_0 \ll \omega_c \).) The ground state clearly shows a number of spin transitions with increasing magnetic field. Furthermore, the second highest excited state becomes degenerate with the third at level crossings which occur at magnetic fields between ground state transitions. This suggests that quantum information stored in the two lowest energy spin states in neighboring quantum dots becomes susceptible to leakage when the dots are brought very close together. Below, we address this issue quantitatively using both exact diagonalization and a new set of variational states.

We now diagonalize the full Hamiltonian, Eq. (4), in regimes not amenable to perturbation theory, for \( R \sim a \) and \( \omega_0 \ll \omega_c \). We construct the matrix representing \( \hat{H} \) in the Fock-Darwin basis centered between the two dots. Previous studies have involved diagonalization of similar Hamiltonians using several dot centered basis states. This technique requires lengthy, numerical routines to generate an orthogonal set of basis states. The
limited number of basis states allows for high accuracy only in a regime where the Coulomb interaction may be treated perturbatively. However, to access the strongly correlated regime, 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 twelve. We use a modified Lanczos routine to obtain the ground and excited states. This technique yields the entire spectrum. However, here we focus on the four lowest energy states. The energies converge to within \( 1 \mu eV \) upon inclusion of more basis states and may therefore be considered exact. Details, including the matrix elements, will be published elsewhere.

The top panel in Fig. 2 shows the four lowest energies obtained from exact diagonalization of Eq. (1) versus magnetic field. The energy zero is taken to be the ground state. We have chosen an inter-dot separation of \( R = 10 \) nm. The energy of the first excited state gives the effective exchange splitting which changes sign through successive spin transitions at each cusp. The results are qualitatively similar to the results shown in Fig. 1 but are entirely unexpected. Vortex attachment non-perturbatively lowers the Coulomb energy of uniform states but does not necessarily apply to highly disordered systems. Yet, the intriguing oscillations in the effective exchange interaction seen in Fig. 2 suggest just this and therefore require further study.

In comparing Figs. 1 and 2 we find further differences. At low fields, the top panel of Fig. 2 correctly shows a spin singlet ground state at \( B = 0 \) rather than a triplet state as shown in the LLL limit of Fig. 1. Most importantly the degeneracies in excited states at \( B = 0, 2.4, 5.2 \) and \( 8 \) T begin to lift. As opposed to the level crossing in the single dot, \( R = 0 \) case discussed earlier, the breaking of rotational symmetry forces an anticrossing among the first and second excited states. Where, at small to intermediate inter-dot separations, \( R \lesssim a \), the higher excited states are perturbed, single dot states with a nearly uniform charge density. A large anticrossing among the two lowest excited states protects the quantum information stored in the entangled state of two strongly coupled quantum dots. Experimental uncertainties in \( R \) and \( \omega_0 \) may eventually lead to the strongly coupled regime. Careful study of the states making up the anticrossing is therefore crucial.

We now construct variational states which reproduce the exact results discussed above. The composite fermion theory \( \Phi \) of the fractional quantum Hall effect offers an accurate variational ansatz describing two dimensional electron systems at high magnetic field. A composite fermion is the bound state of an electron and an even number of quantum mechanical vortices of the many-body wave function. The corresponding orbital wave function is \( \psi = J \phi \), where \( \phi \) is a weakly interacting fermion state, \( J \) a Jastrow factor, and \( \psi \) the highly correlated state of electrons. In isotropic, spinless systems \( J \) attaches an even number of vortices to the fermions in the antisymmetric state \( \phi \) yielding an antisymmetric electron wave function. In anisotropic systems with additional quantum numbers one may bind an even or odd number of vortices to each particle while preserving the antisymmetry of the overall wave function \( \Phi \). Applying the composite fermion ansatz to the Hamiltonian studied here we take \( \phi \) to be the non-interacting ground state. We also take \( J = (z_1 - z_2)^p \), where \( p = 0, 1, 2, ..., \) giving:

\[
\psi_p = (z_1 - z_2)^p \phi. \tag{6}
\]

This is our initial, high field solution of \( H \). \( \psi_p \) clearly reduces to \( |m\> \) at \( R = 0 \). For \( R \gg a \) the fermions in the state \( \phi \) become localized on each dot leaving \( J \) constant \( \sim R^p \). In which case \( \psi_p \) reduces to the limit of two independent electrons.

The bottom panel of Fig. 2 plots the overlap of the exact ground state and the variational state \( \psi_p \) at \( R = 10 \) nm. Triplet (singlet) spin states correspond to odd (even) values of \( p \), as in the \( R = 0 \) case. The overlaps drop to zero when the particle exchange symmetry of the orbital wave function changes. We have checked by direct calculation of the density that, by \( B \sim 9 \) T, the modified magnetic length has become small enough to localize the electrons on each dot. The surprisingly high overlaps prove that vortex attachment is a valid ansatz even in the highly localized regime. At large dot separations, \( R \geq 40 \) nm, the Coulomb interaction lowers to a point where
the four variational states remain. The bottom panel in Fig. 3 shows the energy of electrons localized on each dot suppresses the exchange splitting obtained with the variational states compared well with the exact value. Furthermore, in the range $B = 1$ to $4$ T, the second excited state captures the essential features of the corresponding exact results. Rotational symmetry breaking forces the higher excited states to open an anticrossing observed near $B = 0, 2, 4$, and $4.3$ T. The states at the anticrossings in Fig. 3 are similar to the states making up the level crossings in Fig. 4. For example the electrons in the first excited state at $2.4$ T in Fig. 3 form a two and zero vortex mixed state in a $56\%$ to $44\%$ ratio, as opposed to the ground state which holds one vortex per electron, to within $98\%$. To evaluate the anticrossing explicitly we note that for $R \ll a$ the asymmetry in confinement acts as a perturbation. We may rewrite the confinement potential up to an overall constant:

$$V(\omega_0, R; r) = \frac{m^* \omega_0^2}{2} \left( |r|^2 - |x| R \right). \quad (8)$$

The second term breaks rotational symmetry and forces an anticrossing among the lowest two excited states. It is crucial that the two lowest excited states involve states of even vorticity. Symmetry allows these two states to mix yielding an anticrossing as one may find by diagonalizing the rotational symmetry breaking term in the even-vorticity subspace. The matrix elements are: $m^* \omega_0^2 R/2 \langle \psi_p | x_1^2 + x_2^2 | \psi_p \rangle$, where, near $B = 2.4$ T for example, $p$ and $p'$ may be 0 or 2. These matrix elements give an anticrossing $\sim m^* \omega_0^2 Ra$. This is in contrast to ground state transitions between states with even and odd vorticity. Here the states $\psi_p$ and $\psi_{p+1}$ cannot mix, allowing the exchange splitting to change sign.

We stress that the top panel in Fig. 3 is obtained by diagonalization of the full Hamiltonian with $\sim 10^5$ basis states while the lower panel is obtained by the same method but with four, physically relevant basis states. The agreement breaks down at larger fields, $B \sim 5.6$ T, where the excited states should include the $p = 4$ variational state. Inclusion of variational states with large $p$ is necessary at larger fields. The excellent agreement obtained thus far demonstrates that the plethora of spin transitions in strongly coupled quantum dots originates from a swapping of the particle exchange symmetry associated with vortex attachment.

To conclude, we have discussed the surprisingly rich and unexpected vortex structure found in the exchange coupling of a two-electron artificial molecule in coupled semiconductor quantum dots which should be important both for constructing quantum gates and for studying strongly correlated quantum dot electronic states.

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