Twisted Singlet in Semiconductor Artificial Molecules

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The spin-configuration of semiconductor artificial molecules consisting of quantum dots and spin field effect transistors is studied theoretically. We find that the antiferromagnetic spin configuration can be changed to the ferromagnetic one by applying a gate voltage to the spin field effect transistors. We show that the square-norm of the total spin of an artificial molecule oscillates with the twist angle \( \theta \) and has maxima at \( \theta = \text{an odd integer times } \pi \). We also show that the square-norm of the total spin of the ring-shaped artificial molecule changes drastically at certain values of \( \theta \) where the lowest two energy levels cross each other.

Nanospintronics is an emerging research field of physics and engineering focused on spin degrees of freedom of electrons confined in nano-structures \[1\]. One attractive nanospintronics device is the spin field effect transistor (spin-FET) proposed by Datta and Das \[2\], where the precession of the spin of a conduction electron is dominated by the Rashba spin-orbit (RSO) interaction \[3\]. The strength of the RSO interaction and therefore the precession of spin can be controlled by applying a gate voltage. The RSO interaction in semiconductor nano-structures has been extensively studied both theoretically \[4, 5\] and experimentally \[6, 7\].

Semiconductor quantum dot is a basic element of current nanotechnology and is often considered as an artificial atom \[8\]. We are able to construct an artificial molecule (AM) of quantum dots by connecting the dots either laterally \[9, 10\] or vertically \[11, 12\]. It is important to study the spin configuration of electrons in such semiconductor AMs. The AMs can be described by the Hubbard Hamiltonian \[13, 14\], which has been extensively studied in the context of strongly correlated electron systems \[15, 16, 17, 18\]. Lieb proved that the ground state of the Hubbard model with a bipartite lattice and a half filled band has the antiferromagnetic spin configuration \[19\]. Lieb’s theorem cannot be applied to the lattice with odd number of sites. However, as we shall show later by using the exact diagonalization method, the linear-shaped and the ring-shaped one-dimensional lattices with \( N = 3 \) and 5 sites also have the antiferromagnetic ground states. Thus we can say that the ground state of the semiconductor AM with a small number of quantum dots prefers the antiferromagnetic spin configuration as long as the system is described by the usual half-filled Hubbard model.

However, if the dots are coupled via spin-FETs as shown in Fig. 1(a) we can control the spin configuration of the AM by applying a gate voltage to the spin-FETs. The key concept is “twisted singlet”. The spin-FET can twist the singlet spin-wavefunction, which is the essence of the antiferromagnetism, in the spin space. If we set the twist angle to an odd integer times \( \pi \), we have the triplet spin-wavefunction instead of the singlet one.

In this letter, we theoretically study the spin configuration of AMs consisting of quantum dots and spin-FETs and show that the spin configuration of such an AM can be controlled by the RSO interaction. Both linear-shaped and ring-shaped one-dimensional AMs are considered. It is shown that the square-norm of the total spin of the AM oscillates with the twist angle \( \theta \) and has maxima at \( \theta = \text{an odd integer times } \pi \). It is also shown that the square-norm of the total spin of the ring-shaped AM changes drastically at certain values of \( \theta \) where the lowest two energy levels cross each other. These results provide a powerful guiding principle of making a gate-controllable nano-magnet.

The RSO interaction in the spin-FET (See Fig. 1(a)) is described by the Hamiltonian

\[
H_{SO} = \alpha \left[ \sigma_y \nabla_z + \sigma_z \nabla_y \right],
\]

where \( \sigma_y \) and \( \sigma_z \) are respectively the \( y \) and \( z \)-component of the Pauli spin matrix and \( \alpha \) represents the strength of the RSO interaction. Experimentally, one typically observes values for \( \alpha \) on the order of \( 10^{-11} \) eV m \[10, 11, 12\]. We assume that in the spin-FET the wavefunction in the \( y \)-direction has the form \( \sin(m\pi y/W) \), where \( W \) is...
the width of the wire and $m$ is an integer, the expectation value of $\nabla_y^2$ is zero. Hence we can neglect the last term in Eq. (1) and we have

$$ H_{SO} = \alpha \sigma_y \nabla_z. \quad (2) $$

The RSO interaction rotates the spin around the $y$-axis. The rotation of the spin by angle $\theta$ in the spin-FET can be represented by the matrix

$$ R(\theta) = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}. \quad (3) $$

We consider the one-dimensional AM of quantum dots coupled via spin-FETs described by the Hamiltonian

$$ H = -t \sum_{\sigma} \sum_{\langle i,j \rangle} \left\{ c_{i\sigma}^\dagger R_{\sigma\sigma'}(\theta_{ij}) c_{j\sigma'} + U \sum_n n_{i\uparrow} n_{i\downarrow} \right\}, \quad (4) $$

where $t$ is the hopping matrix elements, $U$ is the on-site Coulomb energy, $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$ and operators $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are, respectively, the creation and annihilation operators for an electron of spin $\sigma$ at $i$th quantum dot. The sum $\langle i,j \rangle$ is restricted to nearest-neighbor sites and $\theta_{ij}$ is the rotation angle of spin when the electron is transferred from the $i$th dot to the $j$th one. We assume that system is half-filled, i.e., the number of electrons is the same as that of dots. Since we are interested in the spin configuration of AMs, the physical quantity of central importance is the square-norm of the total spin defined as

$$ S^2 = (S^z)^2 + \frac{1}{2} (S^+ S^- + S^- S^+) \quad (5) $$

where

$$ S^z = \frac{1}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow}) $$

$$ S^+ = \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}, \quad S^- = \sum_i c_{i\downarrow}^\dagger c_{i\uparrow}. \quad (6) $$

Without RSO interaction, Eq. (4) reduces to the usual Hubbard Hamiltonian

$$ H_t = -t \sum_{\sigma} \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (7) $$

The basic properties of the Hubbard Hamiltonian with a finite number of sites and a half filled band have been investigated intensively by several authors $[20, 21, 22, 23]$. The Hamiltonian is commutable with the operator $S^2$ and the total spin $S$, $S^2 = S(S+1)$, is the conserved quantity. According to Lieb’s theorem $[21]$, the total spin of the ground state of the bipartite AM of even number of quantum dots is $S = 0$ without RSO interaction. For the AMs with $N = 3$ and 5 quantum dots, we numerically diagonalize the Hamiltonian given by Eq. (7) and confirm that the ground states of the linear-shaped and the ring-shaped AMs with $N = 3$ and 5 have the antiferromagnetic spin configuration with $S = 1/2$. Without RSO interaction, all AMs we consider here have antiferromagnetic ground state with $S = 0$ or $1/2$.

Let us first consider the simplest AM, two quantum dots connected via a spin-FET, shown in Fig. 1(a). The Hamiltonian can be easily diagonalized and the energy spectrum is independent of the angle $\theta_{12}$. The ground state energy is given by

$$ E = \frac{1}{2} \left( U - \sqrt{16t^2 + U^2} \right). \quad (8) $$

The corresponding spin-wavefunction of the ground state is

$$ \psi = C \left[ \cos \left( \frac{\theta}{2} \right) (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \sin \left( \frac{\theta}{2} \right) (|\uparrow, \uparrow\rangle + |\downarrow, \downarrow\rangle) \right] $$

where $C$ is the normalization constant, $\theta \equiv \theta_{12}$, $|\sigma, \sigma'\rangle$ represents the basis where the left dot has an electron with spin $\sigma$ and the right dot has an electron with spin $\sigma'$, and $|\uparrow, \downarrow\rangle$ represents the basis where the left(right) dot has two electrons with spin $\uparrow$ and $\downarrow$.

From Eqs. (8) and (9), the square-norm of the total spin of the ground state is obtained as

$$ S^2 = \frac{2 \sin^2 \left( \frac{\theta}{2} \right)}{2 \sin^2 \left( \frac{\theta}{2} \right)} \frac{(U + \sqrt{16t^2 + U^2})^2}{16t^2 + (U + \sqrt{16t^2 + U^2})^2}. \quad (10) $$

As shown in Fig. 1(b), the square-norm $S^2$ oscillates with a period of $2\pi$ and has maxima at $\theta = \pi$ and $3\pi$. The maximum value of the square-norm $S^2$ is slightly smaller than two since the ground state consists not only of the nearest-neighbor singlet but of the on-site singlet. As the on-site Coulomb energy $U/t$ increases, the occupation probability of the on-site singlet decreases and the maximum value of $S^2$ increases as shown in Fig. 1(c).

These results for two-dot AM can be easily understood by introducing the following local gauge transformation in the spin space:

$$ c_{2\sigma}^\dagger \rightarrow c_{2\sigma}^\dagger(\theta) \equiv \sum_{\sigma'} R_{\sigma\sigma'}(\theta) c_{2\sigma'}, $$

$$ c_{2\sigma} \rightarrow c_{2\sigma}(\theta) \equiv \sum_{\sigma'} R_{\sigma\sigma'}(\theta) c_{2\sigma'} \quad (11) $$

The creation and annihilation operators $c_{2\sigma}^\dagger(\theta)$ and $c_{2\sigma}(\theta)$ satisfy the usual fermion anti-commutation relations. The Hamiltonian given by Eq. (7) is expressed as

$$ H = -t \sum_{\sigma} \left\{ c_{1\sigma}^\dagger c_{2\sigma}(\theta) + c_{2\sigma}(\theta) c_{1\sigma} \right\} $$

$$ + U \left\{ n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow}(\theta) n_{2\downarrow}(\theta) \right\}, \quad (12) $$
where \( n_{2\theta}(\theta) \equiv c_{1,2}^\dagger(\theta)c_{2,1}(\theta) \). Therefore, the energy spectrum is invariant under the gauge transformation defined by Eq. (11) and is independent of the angle \( \theta \). The above gauge transformation corresponds to the twist of the spin quantization axis of the 2nd dot by angle \( \theta \). In such a \( \theta \)-twisted spin space, the Hamiltonian is identical to Eq. (11). The spin operators in the \( \theta \)-twisted spin space are given by

\[
S^z(\theta) = (S^z(\theta))^2 + \frac{1}{2} (S^+(\theta)S^-(\theta) + S^-(\theta)S^+(\theta))
\]

\[
S^\pm = c^\dagger_{1,1}c_{1,1} + c^\dagger_{2,1}c_{2,1}(\theta)
\]

\[
S^- = c^\dagger_{1,1}c_{1,1} + c^\dagger_{2,1}c_{2,1}(\theta).
\]

The total spin in the \( \theta \)-twisted spin space \( S(\theta), S^2(\theta) = S(\theta)^2 + S(\theta) \), is the conserved quantity and the ground state has \( S(\theta) = 0 \).

The \( \pi \)-rotation operator \( R(\pi) \) maps \( |\uparrow\rangle \) to \( |\downarrow\rangle \) while \( |\downarrow\rangle \) to \( |\uparrow\rangle \). Therefore, the singlet in the \( \pi \)-twisted spin space \( |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle \), which is the dominant component of the ground state of \( S(\theta) = 0 \), is in fact the triplet \( |\uparrow,\uparrow\rangle + |\downarrow,\downarrow\rangle \) in the real spin space. The dominant component of the spin-wavefunction in the real spin space, changes from singlet \( \rightarrow \) triplet \( \rightarrow \) singlet \( \rightarrow \) triplet as shown on the top of Fig. 1(b).

In Figs. 2 (a)-(d), we show the square-norm of the ground state \( S^2 \) for the linear-shaped AM consisting of \( N = 3, 4, 5, \) and 6 quantum dots. The energy levels and corresponding spin-wavefunctions are obtained by using the exact diagonalization method. We assume that the on-site Coulomb energy is \( U/t = 10 \) and the twist angle takes the same value \( \theta \) for all spin-FETs. Without RSO interaction, \( \theta = 0 \), the ground state has the antiferromagnetic spin configuration with \( S = 0 \) or 1/2. The square-norm \( S^2 \) is again an oscillating function of \( \theta \) with a period of 2\( \pi \). However the shoulders appear at \( \theta = \pi/2, 3\pi/2, 5\pi/2 \) and 7\( \pi/2 \) for \( N = 4, 5 \) and 6. The shoulders correspond to the formation of the next-nearest-neighbor twisted singlet. For \( N = 6 \) we have other shoulder structures at \( \theta = \pi/3, 5\pi/3, 7\pi/3, \) and 11\( \pi/3 \) corresponding to the next-next-nearest-neighbor twisted singlet.

The operators in the twisted spin space are obtained by using the following local gauge transformation in the spin space:

\[
c_{i,\sigma} \rightarrow c_{i,\sigma}^\dagger(\theta_i) = \sum_{\sigma'} R_{\sigma\sigma'}(\theta_i)c_{i,\sigma'}^\dagger,
\]

\[
c_{i,\sigma} \rightarrow c_{i,\sigma}(\theta_i) = \sum_{\sigma'} R_{\sigma\sigma'}(\theta_i)c_{i,\sigma'}.
\]

The Hamiltonian and spin operators in the twisted spin space are obtained by replacing operators \( c_{i,\sigma}^\dagger \) and \( c_{i,\sigma} \) in Eqs. (3) and (4) by \( c_{i,\sigma}^\dagger(\theta_i) \) and \( c_{i,\sigma}(\theta_i) \) as

\[
H_i = -t \sum_{\sigma,j} c_{i,\sigma}(\theta_j)c_{j,\sigma}(j) + U \sum_{i} n_{i,\uparrow}(\theta_i)n_{i,\downarrow}(\theta_i),
\]

where \( n_{i,\sigma}(\theta_i) = c_{i,\sigma}^\dagger(\theta_i)c_{i,\sigma}(\theta_i) \). The energy spectrum is independent of the twist angle. The spin operators in the twisted spin-space are given by

\[
S^2(\theta) = (S^z(\theta))^2 + \frac{1}{2} (S^+(\theta)S^-(\theta) + S^-(\theta)S^+(\theta)),
\]

![FIG. 2: The square-norm of the total spin \( S^2 \) of the ground states of linear-shaped AMs with \( N = 3, 4, 5 \) and 6 are plotted against the twist angle \( \theta \) in panels (a), (b), (c) and (d), respectively. The on-site Coulomb energy is \( U/t = 10 \) and the twist angle takes the same value \( \theta \) for all spin-FETs.](image)

![FIG. 3: The square-norm of the total spin \( S^2 \) of the ground states and energy levels of ring-shaped AMs with \( N = 3, 4, 5 \) and 6 are plotted against the twist angle \( \theta \) in panels (a), (b), (c) and (d), respectively. The energy is normalized by the hopping matrix element \( t \). The on-site Coulomb energy is \( U/t = 10 \) and the twist angle takes the same value \( \theta \) for all spin-FETs.](image)
where
\[ S^2(\theta) = \frac{1}{2} \sum_i (n_{i\uparrow}(\theta_i) - n_{i\downarrow}(\theta_i)) \]
\[ S^+ = \sum_i c_{i\uparrow}^\dagger(\theta_i) c_{i\downarrow}(\theta_i), \quad S^- = \sum_i c_{i\downarrow}^\dagger(\theta_i) c_{i\uparrow}(\theta_i). \] (17)

The ground state has the antiferromagnetic spin configuration in the twisted spin space with \( S(\theta) = 0 \) or 1/2.

On the contrary to the linear-shaped AM, the square-norm \( S^2 \) of the ring-shaped AM is not a smooth function of the twist angle. In Figs. 3 (a)-(d), we show the square-norm \( S^2 \) and the energy levels for the ring-shaped AMs with \( N = 3, 4, 5 \) and 6 dots obtained by using the exact diagonalization method. We assume that the on-site Coulomb energy is \( U/t = 10 \) and the twist angle takes the same value \( \theta \) for all spin-FETs. Without RSO interaction, \( \theta = 0 \), the ground state has the antiferromagnetic spin configuration with \( S = 0 \) or 1/2. Due to the boundary condition of the ring-shaped AMs, it is difficult to twist the spin configuration by an arbitrary angle. Therefore, the square-norm \( S^2 \) jumps at a certain value of angle \( \theta \) where the lowest two energy levels cross each other as shown in Figs. 3 (a)-(b).

In conclusion, we theoretically study the spin-configuration of artificial molecules which consists of quantum dots and spin field effect transistors. We show that we can change the antiferromagnetic spin configuration to the ferromagnetic one by applying a gate voltage to the spin field effect transistors. We note that the approach of twisting the singlet by using the spin field effect transistor is a very powerful tool for making the ferromagnetic spin configuration in non-magnetic semiconductor nano-structures. The periodic oscillation of the square-norm of the total spin in artificial molecules against the twist angle can be applied to the future nano-spintronics devices, for example, a gate-controllable nano-magnet.

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