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Superexchange Driven Singlet-Triplet Transition in

Quantum Dots Array Embedded in Kagome Lattice System

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Abstract

The envisaged revolutionary impact of the quantum computer has continued to elucidate diverse means to design and build physical quantum computers. In condensed matter physics, one of the means is to design materials to host two-electron quantum dots (QDs) which can be manipulated into singlet-triplet (S-T) transition. This transition which is read as the quantum bits (qubits) that is considered as a possible logic gate for the quantum computers is enhanced by external magnetic field which is a potential source of decohenrence. In the study here therefore, the possibility of using a superexchange induced internal magnetic field to drive the S-T transition in QDs embedded in a kagome lattice system (KLS) is examined. The design is by embedding the two-electron QDs into the frustrated sites of the KLS and then filling the other sites with single electrons. The parameter space of this KLS to achieve the S-T in the QDs array are obtained from the superexchange interaction in correlated variational study of the system.

Keywords: frustrated system, kagome lattice, quantum dot, singlet-triplet transition, quantum computer

1. Introduction

Since the Peter Shor's demonstration in the mid 1990s of an efficient algorithm for factorizing prime numbers, the race to design and build quantum computers has continued to advance. Researchers have proposed several ways to implement quantum computers, ranging from systems that store information in trapped atoms (Pellizzari et. al., 1995), ions (Cirac and Zoller, 1995; Monz et. al., 2009) or molecules (Hosaka et. al., 2010) to those based on condensed matter systems such superconductivity (Devoret and Martinis, 2004; Catelani et. al., 2011) and quantum dots (Akpojotor and Akpojotor, 2009). Such computers would rely on the phenomena of quantum coherence and quantum entanglement among a set of quantum bits (qubits). In general, quantum computers store information in qubits which are quantum combinations of ones and zeros. In practice, to perform quantum computation, it is sufficient to implement certain elementary one- and two-qubit operations, forming universal sets. These operations are analogous to the fundamental building block OR, AND, NOT operations of conventional microelectronics. Such a set of operations on qubits can be used to simulate any quantum computation with arbitrary precision (Sjöqvist, 2008). A first goal for holonomic quantum computation is to find physical implementations of universal sets of gates that are all-geometric, that is, based entirely upon quantum holonomies. Traditionally, qubits have been recorded in some intrinsic property of an isolated system, like the spin of a trapped electron. The trouble is that any slight interaction with the environment will force the qubit to collapse into a specific state and lose information (Bonderson and Lutchyn, 2011). This is known as decoherence which has made large-scale quantum computers hard to construct because quantum systems easily lose their coherence through interaction with the environment (Sjöqvist, 2008). In their study in 1995, Pellizzari and co-workers use the theory of continuous measurement to analyze the effects of decoherence on a realistic model of a quantum computer based on cavity QED. They demonstrated how decoherence affects the computation and methods to prevent it. One possible solution to this problem is to use topological quantum computers, which store information in intertwined particle states, called anyons. If one imagines these

anyons as checkers on a board, a computation would consist of swapping the pieces in a precise sequence. The quantum information is not localized on individual checkers, but is instead encoded in the way the anyon trajectories weave around each other in spacetime. Topological qubits have yet to be fully realized, but they show promise as robust quantum storage units. (Bonderson and Lutchyn, 2011). Another highly sought after method which is being investigated to achieve quantum computers is to use man made quantum dots (QDs) fabricated in solid state materials. The basic idea is to develop a means to read the state of the quantum particles inside the dot which then become a viable quantum bit and a combination of them culminate in quantum procession of information (QPI). The electronic spins of a two-electron QD has a qubit of singlet or triplet state and the transition between these two states can be considered as a possible logic gate for the quantum computers. Consequently, the singlet-triplet (S-T) transition in the two-electron QDs has received a deluge of studies and there seems to be a general consensus that this transition is enhanced by the presence of external magnetic field (Ellenberger et al., 2006). In a challenging report in 2008, however, Amasha and co-workers observed a puzzling behavior in the spin-dependent tunneling of electrons into a quantum dot in the presence of an external magnetic field. When a magnetic field is applied parallel to the dot, it splits the energy levels (Zeeman splitting) on it. Ignoring the spin-orbit interaction, one would expect the tunneling rates for electrons with spin-up and spin-down to be the same, since the energy levels in the leads are similarly shifted by the field. Instead, Amasha and co-workers find that with increasing magnetic field, the tunneling rate for the spin-down state is less than that of the spin-up state, and is completely suppressed by ~7.5 T. But, by adjusting the metallic gates to make the quantum confinement potential more symmetric, they can make the tunneling rates for the spin-up and spin-down states identical. The implication is that the external magnetic influence is a possible additional source of decoherence which as already stated, is widely regarded as the major obstacle to designing quantum computer made of quantum dots in solid state systems. Therefore, to eliminate this additional source, it will be interesting to investigate the possibility of designing a host that can provide the desired magnetic field to induce the S-T transition in the embedded QDs. A preliminary report to theoretically demonstrate that this may be achieved in Kagome lattices systems (KLS) has earlier been presented (Akpojotor and Akpojotor, 2009). In that study, we demonstrated that it is possible to utilize decoherence as a positive influence on QDs. This is by embedding the two-electron ODs at appropriate sites in the the KLS to make them magnetically ordered. It is then possible to tune the lattice parameters to make KLS provide the magnetic field to achieve the singlet-triplet transitions in the QDs. We then characterize the role of these parameters in that study and thereby giving a useful description of the underlying physics. That study was recently boosted by the study of Edlund et. al., (2011a; 2011b) which demonstrated a new method of the particle-particle potential that gives a targeted geometry as a unique ground state. As a proof of principle, they find the potential needed to produce a kagome lattice, where the particles form a lattice of interconnected triangles. Therefore in the current study, the possibility of designing a two-electron QDs array embedded in a kagome lattice system is further investigated. This will be done using the following plan. In section 2, there will be a theoretical description of the possible experimental set-up of the QDs array embedded in a KLS. The theoretical calculation of the parameter space to manipulate the KLS hence the QDs array into the S-T transition will be presented in section 3 while the presentation of results and discussion will be in section 4. This will be followed by a summary and a conclusion in section 5.

2. Theoretical description of the possible experimental set-up of the QDs array

In general, the Kagome lattice systems which are two-dimensional (2D) systems and are composed of corned-shared triangles are believed to be magnetically frustrated materials. Frustration here means all the constraints imposed by the Hamiltonian cannot be simultaneously fulfilled. The main interest of most studies of the prospect of QDs using KLS has been to fabricate artificial kagome lattices using QDs as the building block and then investigating the possibility of obtaining ferromagnetism in these systems (Kimura et. al., 2002). The approach here is in tandem with our earlier study (Akpojotor and Akpojotor, 2009) based on using the magnetic ordering of the kagome lattice system to induce the S-T transition in the QDs. Therefore, as done in that study, the first step is to eliminate the frustration in the spin ordering of the third site of a frustrated equilateral triangular lattice (see Figure 1a). This can be achieved by embedding a two-electron QDs at this third site (see Figure 1b). These triangular lattices with embedded quantum dots are then used to build an n x 3 cluster of KLS and thereby mapping the KLS into a bipartile-like lattice of an array of chains of the initial kagome atoms separated by an array of the QDs (See Figure Ic).

Now if we start with the chains of the initial kagome atoms having Neel type antiferromagnetic ordering, then they

will orientate each of the electrons in the QDs in the opposite directions as depicted in Figure Ic. Then by manipulating all the chains of the initial kagome atoms to orientate in the same direction, the two electrons in the QDs will orientate in this direction (See Figure 4). Thus we see from this simplified scenario that if the Kagome atoms are manipulated into singlet-triplet transition, they may provide an internally generated magnetic field to induce the S-T transitions in the QDs.

3. Theoretical calculation

The most probable mechanism to manipulating the singlet-triplet transition is by superexchaneg interaction which emanates from the quantum mechanical process of virtual hopping of a spin from its site to a neighbouring site while a spin in this neighbouring site or the same spin will hop back to the initial site (Trotzky et. al., 2008, Bloch, 2008). This kind of hopping preserves the sites configurations but not the spin ordering of the atoms. It is therefore a virtual localization process that enables spin flips and can lead to singlet-triplet transition depending on the lattice parameters (Duan et. al, 2003; Akpojotor and Li, 2009). In a recent study (Akpojotor, 2012), I demonstrated superexchange interaction in the double well and resonating valence bond (RVB) states in kagome lattice which is important for understanding the CuO_2 plane of the superconducting cuprates and other magnetic frustrated materials. In earlier study (Akpojotor and Li, 2009), we have developed a phenomenological approach to a model of superexchange interactions in optical wells which theoretically demonstrated the seminal work of Trotzky et. al. (2008) wherein superexchange interaction was first demonstrated with cold atoms in optical lattices. The mathematical formulation in all these studies has been the highly simplified correlated variational approach which we have shown to be a powerful theoretical tool for investigating superexchange interactions (see the details of the method in Akpojotor, 2008;Akpojotor and Li, 2009; Akpojotor, 2012).

The superexchange Hamiltonian is the the t-U-V-J model

$$H = -t\left[\sum_{<i,j>,\sigma} C^{+}_{i\sigma}C_{j\sigma} + H.C.\right] + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{<i,j>} n_i\, n_j + J\sum_{<i,j>\sigma,\bar{\sigma}} C^{+}_{i\sigma}C^{+}_{j\bar{\sigma}}C_{i\bar{\sigma}}C_{j\sigma} \tag{3.1}$$

where t is the hopping term, U is the on-site Coulombic interaction term, V is the nearest neighbour (NN) interaction term and J is the NN exchange interaction term.

The wavefunction for the n x 3 cluster is given by

$$/\psi>=\sum_{i=1}^{N} X\,/i\sigma, i\bar{\sigma}> + \sum_{i=1,j=1;i\neq j}^{N} X[/i\sigma, j\bar{\sigma}> - /i\sigma, j\bar{\sigma}>]$$
$$+ \sum_{i=1,j=1;i\neq j}^{N} Y[/\sigma\uparrow, \sigma\uparrow> + \sum_{i=1,j=1;i\neq j}^{N} Z[/i\downarrow, j\downarrow> \tag{3.2}$$

where the electronic state $/i\sigma, j\bar{\sigma}>$ means that one electron is on lattice site i with spin σ and the other electron is on lattice site j with spin $\bar{\sigma}$, while the R (= X, Y, Z) are the expansion coefficients with X for the singlet states, Y for the spin-up triplet states and Z for the spin-down triplet states.

To obtain the matrix representation for the n x 3 cluster will be computational cumbersome. Therefore in the study here, only a small array (n = 3) yielding a 3 x 3 cluster will be considered and it is expected that this will give a useful insight into the trend. The superexchange matrix representation for this cluster is (Akpojotor, 2008;Akpojotor and Li, 2009; Akpojotor, 2012)

$$\begin{bmatrix} E-4(U/4t) & 8 & 0 & 0 & 0 & 0 & 0 \\ 2 & E+2+4(V/4t)-4(J/4t) & 4 & 0 & 0 & 0 & 0 \\ 0 & 4 & E+4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E+2+4(V/4t)-4(J/4t) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & E+4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & E+2+4(V/4t)-4(J/4t) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & E+4 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ Y_1 \\ Y_2 \\ Z_1 \\ Z_2 \end{bmatrix} \quad (3.3)$$

where U/4J is the on-site interaction strength which determines the response of the kinetic energy of the electrons to the varying on-site Coulombic interaction U, V/4J is the NN inter-site interaction strength which determines the response to the varying NN Coulombic interaction V and J/4J is the NN superexchange interaction strength which determines the response to the varying superexchange interaction J. All these quantities are physically dimensionless as they are ratios of the same unit.

4. Presentation and discussion of results

The energy spectrum of the superexchange interaction in the 3 x 3 cluster KLS hosting the array of QDs is obtained by diagonalizing Eq. (3.3). This energy spectrum provides both the ground state energies for the singlet states, E_s and and the triplet states, E_t. The smallest of them becomes the ground state of the system, that is, if $E_s < E_t$ the spins in the KLS hence those of the QDs array will anti-align so that the QDs will read singlet states as shown in Figure 1c. However, when $E_s > E_t$ the spins in the KLS hence those of the QDs array will align in the same direction, either all spin-up or all spin-down, so that the QDs will read triplet states. We have observed in previous studies that the domineering term which is the exchange term J must be finite for the S-T transition to be initiated (Akpojotor, 2008, Akpojotor and Li, 2009 and Akpojotor, 2012). This is easily shown by making J = 0 as shown in Table 1. The large energy differences between E_s and E_t implies that the spins will anti-align for all finite values of the negative U and negative V as well as even the physically unrealistic positive U and positive V. The inclusion of this unrealistic regime of U and V is to have a complete investigation for all finite values of U and V.

Since the J is the domineering parameter to drive the system into the S-T transition, the value of J at which the system transits into the triplet state will be called the transition point here, T_p. The value of J/4t at which there is the S-T transition as the other parameters, U and V, are varied, are shown in Table 2 with the lowest energies for both the singlet and triplet states. Observe in Table 2 that the T_p is not always sharp as there are parameters combinations that will result to mixed spin ordering. In Table 2, when U/4t = V/4t = 5, $E_s = E_t$ = -5.0939 at the T_p of J/4t = 0.1170 while when U/4t = 5 and V/4t = 0, $E_s = E_t$ = -7.285 at the T_p of J/4t = 0.1037. Observe also in Table 2 that when U = V = 0, there is still a S-T transition at J/4t = 0.1261 as expected which clearly depicts the domineering role of J. For the role of the other lattice parameters, U and V, the former enhances the S-T transition while the latter suppresses it. For example, from Table 2, observe that at U/4t = V/4t = 5, the S-T transition is at J/4t = 0.1170 and this increases to J/4t = 0.3866 at U/4t = 0 and V/4t = 5 while it reduces to J/4t = 0.1037 at U/4t = 5 and V/4t = 0. It is pertinent to point out that the limitation of the range of U and V to U/4t = V/4t = 5 to U/4t = V/4t = -5 is simply because the trend from our numerical calculation is the same for all finite values of U and V.

5. Summary and Conclusion

The proposed quantum computer will be a device which is used for computation that makes the direct use of quantum mechanical phenomenon such as entanglement and superposition to perform operations on different kinds of data. Therefore the quantum computer, following the laws of quantum physics, would gain enormous processing power through the ability to be in multiple states, and to perform tasks using all possible permutations simultaneously. The reason being that quantum computers exploit the fact that a quantum system can be in a superposition of two states, say 1 and 0, at the same time. n such qubits could be combined or entangled to represent 2^n values simultaneously, which could lead to the parallel processing of information on a massive scale. However, qubits are very fragile and can be adversely affected by decohenrece due to the environment which can degrade the quantum nature of the qubits. Thus the use of external magnetic field to enhance the performance of QDs will create decoherence. Though there are a number of suggestions in the literature to eliminate or reduce decoherence such as

encoding quantum information in the so-called decoherence-free subspacewill (Monz et. al., 2009) and designing equispaced energy levels QDs (Ejere and Akpojotor, 2013), the decoherence due to the external magnetic field cannot be eliminated by these methods. Therefore designing QDs hosted in materials that can be manipulated to provide the magnetic field to drive the singlet-triplet transition in the QDs becomes a viable option (Akpojotor and Akpojotor, 2009). In the study here, it has been demonstrated that by embedding the two-electron QDs in the frustrated sites of KLS to form a bipartile-like lattice of an array of chains of the initial kagome atoms separated by an array of the QDs, a superexchange interaction at the appropriate parameter space will provide the magnetic field to drive the QDs array into the S-T transition. Interestingly, in addition to the singlet and triplet states, the QDs array can also be manipulated to be in mixed states (Akpojotor, 2013). This is the superposition state which is expected to increase the computing power of the quantum computer.

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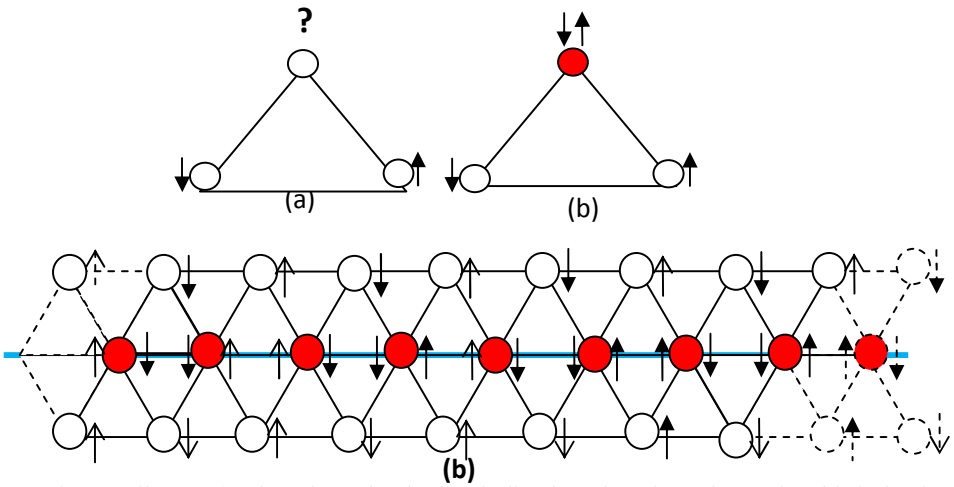

Figure 1 (Colour online): (a) The triangular lattice indicating that the spin at the third site is frustrated thereby making it a geometrically frustrated spin system (b) The triangular lattice indicating the embedment of a quantum dot hosting two electrons with opposite spins at the third site thereby cancelling the geometrical frustration (c) The combination of the triangular lattice with embedded quantum dots to possibly form an n x 3 cluster of Kagome lattice with the embedded quantum dots forming an qubit array for a quantum computer channel.

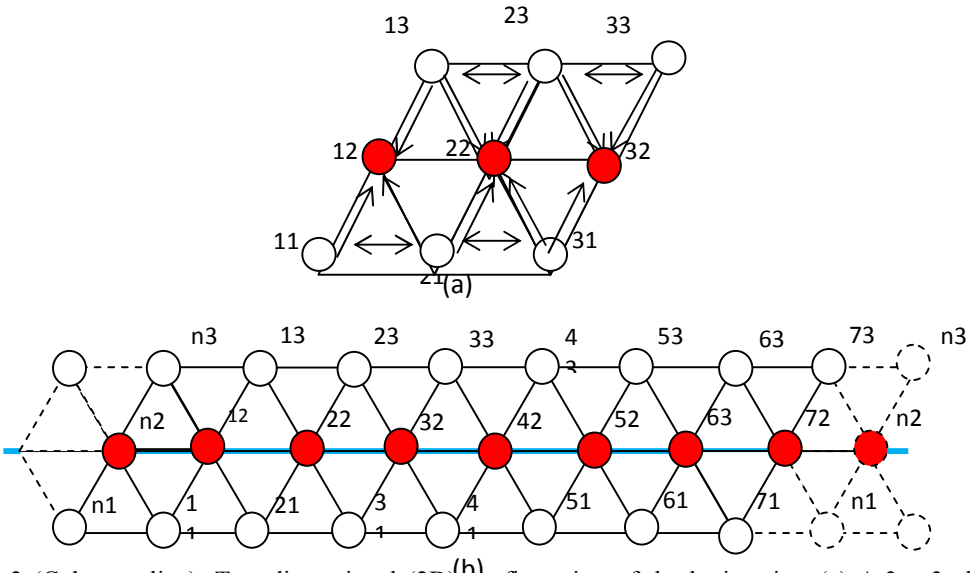

Figure 2 (Colour online): Two dimensional (2D) configuration of the lattice sites (a) A 3 x 3 cluster of Kagome lattice with the embedded quantum dots (b) An n x 3 cluster of Kagome lattice with the embedded quantum dots.

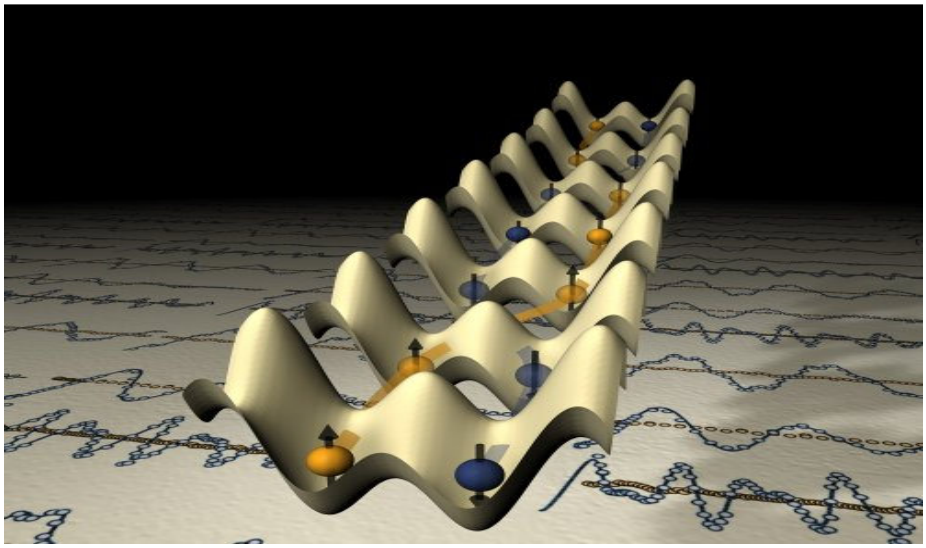

Figure 3 (Colour online): Artistic impression of the 1D lattice of double wells used by Trotzky et. al., (2008) to observe superexchange interactions. In this representation, each double well contains a spin up (amber spheres) atom and a spin down (blue spheres) atom. Courtesy: Immanuel Bloch

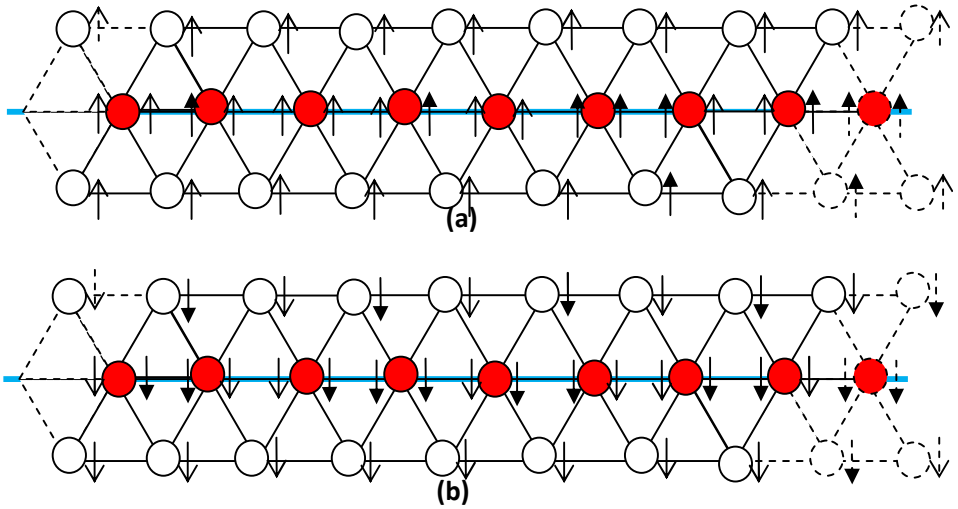

Figure 4 (Colour online): The triplet spin ordering of the two electrons of the quantum dots induced by the spin ordering of the one-electron spin lattice sites chain (a) Spin-up triplet states and (b) Spin-down triplet states.

Table 1 The lowest energy for singlet state E_s, lowest energy for triplet state E_t and their energy difference when the J = 0 as the on-site interaction strength and NN interaction strength are varied.

On-site interaction strength U/4t	NN interaction strength V/4t	Lowest energy for singlet state E_s	Lowest energy for triplet state E_t	Energy difference
5	5	-5.1273	-5.0623	-0.0650
	0	-7.4543	-7.1231	-0.3319
	-5	-15.9159	-15.4031	-0.5128
0	5	-5.3024	-5.0623	-0.2400
	0	-8.0000	-7.1231	0.8769
	-5	-16.2849	-15.4031	0.8818
-5	5	-12.7641	-5.0623	7.7071
	0	-13.6090	-7.1231	6.4859
	-5	-17.8760	-15.4031	2.4729

Table 2 The parameter space to achieve the singlet-triplet transition in the arrays of quantum dots as the on-site interaction strength and NN interaction strength are varied.

On-site interaction strength U/4t	NN interaction strength V/4t	NN exchange interaction strength J/4t	Lowest energy for singlet state E_s	Lowest energy for triplet state E_t
5	5	0.1170	-5.0939	-5.0939
	0	0.1037	-7.2852	-7.2852
	-5	0.0723	-15.6613	-15.6613
0	5	0.3866	-5.1740	-5.1741
	0	0.2647	-7.5568	-7.5570
	-5	0.1262	-15.8541	-15.8545
-5	5	5.1210	-12.3906	-12.3908
	0	2.2699	-12.8811	-12.8812
	-5	0.4098	-16.8810	-16.8813