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On the Spin States of Electrons in a Double Quantum Dot in a Two-Dimensional Topological Insulator with Spin-Orbit Interaction

A. A. Sukhanov[a],* **and V. A. Sablikov**[a]

[a] *Kotel'nikov Institute of Radio Engineering and Electronics (Fryazino Branch), Russian Academy of Sciences, Moscow oblast, Fryazino, 141190 Russia*

**e-mail: AASukhanov@yandex.ru*

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Abstract—The spectra and spin structure of the states of two interacting electrons localized in a double quantum dot in a two-dimensional topological insulator with spin-orbit interaction are investigated. It is found that, in such a system, a singlet-triplet transition in the ground state without a magnetic field can be implemented. Spin-orbit interaction leads to the splitting of polarized triplet levels and to anticrossing, when one of them crosses the singlet.

Keywords: topological insulators, spin-orbit interaction, singlet-triplet transition, quantum dot

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1. INTRODUCTION

The spin of the ground state of interacting electrons is a fundamental problem of the quantum physics of a small number of particles, which is of great importance for creating spin-polarized states and implementing spin qubits on quantum dots [1, 2]. The spin state of localized electrons is determined by the balance of the spin-dependent components of the system energy, which include, first of all, exchange coupling, but not only this, since direct interaction, interaction with a potential forming bound states, and the kinetic energy are also spin-dependent. Of greatest interest is a model system of two electrons. In this case, there is a clear result that is associated with Wigner's name. According to Wigner's theorem, the ground state is a singlet for any spin-independent pairwise interaction [3]. Therefore, the singlet-triplet transition can only occur in an applied magnetic field. Another, equally well-known classical result is related to a system consisting of a rather large number of electrons. This is the semi-empirical Hund's rule [4, 5], according to which the state with the highest spin has the lowest energy. It cannot be definitively answered what the number of spins at which this rule is valid is; it is known, however, that, for two electrons, it does not work. Nevertheless, the triplet state can still be made the ground state if a two-electron system is coupled with a close additional quantum dot containing a large number of electrons. Electrons in a large quantum dot serve as mediators, which enhance the exchange interaction between the investigated electrons [6, 7].

These conclusions were made for systems with a conventional spectrum. However, as applied to modern topologically nontrivial electronic systems, the problem of the ground-state spin and singlet-triplet transitions is understudied. We examined this for two electrons in systems with a two-band spectrum in the topological and trivial phases in two-dimensional (2D) systems [8]. It was established that, in the topological phase, Wigner's theorem is violated under certain conditions and the ground state of two electrons can become a polarized triplet.

In this study, we investigate the effects caused by spin-orbit interaction (SOI) and related to spatial asymmetry in a double quantum well in a 2D topological insulator (TI). It is shown that SOI leads to significant rearrangement of the triplet states, but, at weak SOI, pronounced transitions between the changed singlet and triplet states remain. Interestingly, the polarized triplets split into two states and, consequently, there are two such transitions and anticrossing occurs only when one of the triplet levels crosses the singlet. The spin structure of the states in an isolated quantum well and a double-well structure is investigated and the nature of the singlet-triplet transition is discussed.

2. DOUBLE QUANTUM DOT MODEL

Electrons in a double quantum well in a 2D TI are described by the Hamiltonian

$$H = H_{\mathrm{TI}} + V_A(|\mathbf{r} - \mathbf{R}_A|) + V_B(|\mathbf{r} - \mathbf{R}_B|), \quad (1)$$

where H_{TI} is the Hamiltonian of an electron in the TI, which is presented as a sum of the standard Hamiltonian H_{BHZ} in the Bernevig–Hughes–Zhang (BHZ) model [9] and the SOI Hamiltonian H_{SOI}

$$H_{\mathrm{TI}} = H_{\mathrm{BHZ}} + H_{\mathrm{SOI}}. \quad (2)$$

The Hamiltonian of the BHZ model in the dimensionless form is

$$H_{\mathrm{BHZ}} = \begin{pmatrix} h(\hat{k}) & 0 \\ 0 & h^*(-\hat{k}) \end{pmatrix}, \quad (3)$$

where $h(\hat{k}) = (\mu - \hat{k}^2)\hat{\tau}_z + a(\hat{k}_x\hat{\tau}_x + \hat{k}_y\hat{\tau}_y)$; $\hat{\tau}_i$ is the Pauli matrices for a pseudo-spin; the energy is normalized to the mass term in the Hamiltonian $|M|$ and the pulse, to $\sqrt{|M|B|}$; $\mu = M/|M|$, and $a = A/\sqrt{|MB|}$. Here, A, M, and B are the BHZ-model parameters [9]. The parameter μ determines the topological ($\mu = -1$) and trivial ($\mu = 1$) phases.

In this study, we took into account SOI caused by spatial asymmetry with regard to asymmetry both in the bulk [10] and at the interface [11]. The two SOI types yield qualitatively similar results in the spectra, but the emerging spin textures have different spin directions. In the first case, the SOI Hamiltonian is written in the form

$$H_{\mathrm{SOI}} = \Delta\hat{\tau}_y \otimes \hat{\sigma}_y, \quad (4)$$

where Δ is the SOI constant.

For the sake of simplicity, the quantum-well potentials V_A and V_B are assumed to be the same ($V_A = V_B = V$) and vectors $\mathbf{R}_A$ and $\mathbf{R}_B$ indicate the positions of the wells.

The states of two interacting electrons are described by the Hamiltonian

$$H(1,2) = H(1) \oplus H(2) + U(1,2)I_{16}, \quad (5)$$

where $H(1)$ and $H(2)$ are the above-presented single-particle Hamiltonians of electrons denoted by 1 and 2, $U(1, 2)$ is the pair interaction potential, and I_{16} is the unity matrix. The two-particle wave function is described by a 16-rank spinor.

To find the spectrum and wave functions, we assume the distance d between the quantum wells to be rather large so that the configuration splitting of the quantum-well levels due to electron tunneling between potential wells and the electron-electron interaction can be taken into account using perturbation theory. In this case, as basic functions, we take the two-particle ones representing antisymmetrized products of the single-particle wave functions of the Hamiltonian of isolated quantum wells (A and B).

These single-particle wave functions are determined by the Hamiltonian

$$H_0 = H_{\mathrm{TI}} + V(|\mathbf{r} - \mathbf{R}_{A,B}|), \quad (6)$$

where H_{TI} is the Hamiltonian of the BHZ model with SOI included (see Eq. (2)) and V is the potential of the isolated quantum wells.

The Schrödinger equation with Hamiltonian (6) is solved by the method presented in [12, 13]. This technique is based on the assumption that the quantum-dot potential is highly localized, so that the wave function in the potential localization region changes insignificantly. As a result, one can analytically find the wave functions of an electron localized in a well. The energy levels and wave functions are determined by the dimensionless parameters ν, Λ, and $\delta/|M|$.

The parameter $\nu = |B|^{-1}\int V(r)d^2\mathbf{r}$ determines the quantum-well potential amplitude and $\Lambda = \sqrt{|M/B|}/l$ is the ratio between the characteristic length in the BHZ model to the width l of the potential localization region. In addition, the energy of states depends on the parameter of hybridization of the electron and hole bands (a).

As in the absence of SOI, at each sign of the quantum-well potential in the 2D TI, two states, electron and hole type, with different energies can occur. Each of these states is doubly degenerate, since, in virtue of the time reversal symmetry, each state is a Kramers pair. Thus, single-particle wave functions are represented by four-component spinors indicated by the subscript e or h, which correspond to the electron or hole type of the state, and the subscript α or β, which show the state of the Kramers pair.

Simple analysis and comparison with the data of numerical calculations showed that perturbation theory for calculating the tunnel splitting of quantum-well levels is valid for a rather large distance between the wells ($d > 6\sqrt{|B/M|}$) in a wide range of the SOI parameter Δ.

The zero-approximation two-particle basis functions of perturbation theory for electron-electron interaction are formed by single-particle wave functions $\Psi_{n\gamma}(\mathbf{r})$ determined using perturbation theory for two tunnel-coupled wells

$$\Psi^{(0)}_{n\gamma,m\gamma'}(1,2) = \frac{1}{\sqrt{2}} \times [\Psi_{n\gamma}(1) \otimes \Psi_{m\gamma'}(2) - \Psi_{m\gamma'}(1) \otimes \Psi_{n\gamma}(2)]. \quad (7)$$

Here, the index $n(m)$ denotes the symmetric (s) or antisymmetric (a) double-well wave functions for the electron or hole states and γ, $\gamma' = (\alpha, \beta)$ are the indices of the Kramers-pair states.

The problem can be further simplified if we limit the consideration to only one pair of single-particle levels formed under tunnel splitting of one level in an isolated quantum well. This simplification is justified

when the quantum well is rather narrow and the distance between the wells is rather large. The conditions for these simplifications were discussed in [8] and correspond to the above inequality $d > 6\sqrt{|B/M|}$.

In this case, the single-particle states in the coupled wells are classified only as symmetric (bonding) and antisymmetric (antibonding), which are denoted by us by the subscripts s and a, respectively. Thus, we have six basic single-particle wave functions

$$(\Psi^{(0)}_{s\alpha,s\beta}, \Psi^{(0)}_{s\alpha,a\beta}, \Psi^{(0)}_{a\alpha,s\beta}, \Psi^{(0)}_{s\alpha,a\alpha}, \Psi^{(0)}_{s\beta,a\beta}, \Psi^{(0)}_{a\alpha,a\beta})^T. \quad (8)$$

Below, they are numerated, for simplicity, by the same subscript $j = (1, 6)$.

The wave function of Hamiltonian (5) is presented in the form

$$\Psi(1,2) = \sum_{j=1}^{6} C_j \Psi^{(0)}_j(1,2). \quad (9)$$

Using Eqs. (5) and (9), we can easily obtain a homogeneous system of equations for the coefficients C_j, the determinant of which determines the spectrum. The determinant matrix and matrix coefficients are not presented because they are too complex.

3. SPECTRUM AND SINGLET-TRIPLET TRANSITION

In the topological phase of a 2D TI, the short-range potential $V(r)$ creates two levels at any potential sign, in contrast to the trivial phase, when there is only one level for a potential of any sign within the BHZ model [12, 13].

The localized states corresponding to these levels are classified as electron- and hole-like. They significantly differ in distribution of the electron density and density of the spinor wave function components. In a double quantum well, these levels are split into two due to configuration interaction between the wells. We consider each pair of formed levels separately, assuming them to be sufficiently distant in energy and the splitting of each pair to be small. The properties of the two-particle spectra generated by each of these levels are significantly different. In particular, at a positive potential, the singlet-triplet transition can occur only for hole-like states [8]. Therefore, below we considered only these states.

The energy spectrum has six ε_j levels. We examined their dependence on the amplitude of the electron-electron interaction potential u, which is normalized, as the well potential, to $|M|$, and found which effects are caused by SOI and what the combined action of SOI and electron-electron interaction leads to. Figure 1 shows the calculated spectrum of SOI caused by bulk asymmetry [10] with the parameter $\Delta = 0.2$ determined as in [10] and normalized to $|M|$.

The problem contains three characteristic energies, $2\varepsilon_s$, $\varepsilon_a + \varepsilon_s$, and $2\varepsilon_a$, which determine the spectrum in the absence of SOI and electron-electron interaction. Here, ε_s and ε_a are the energies of the symmetric and antisymmetric single-particle states. In this limiting case, the levels are classified conventionally: line *1* is the singlet $|s\uparrow s\downarrow\rangle$, lines *2* and *3* are polarized triplets $|s\uparrow a\uparrow|$ and $|s\downarrow a\downarrow\rangle$, line *4* is the nonpolarized triplet consisting of the states $|s\uparrow a\downarrow\rangle$ and $|s\downarrow a\uparrow\rangle$, line *5* is a singlet consisting of the states $|s\uparrow a\downarrow\rangle$ and $|s\downarrow a\uparrow\rangle$, and line *6* is the singlet $|a\uparrow a\uparrow\rangle$. In view of this conventional terminology, it should be noted that, in the investigated case, the latter is not quite accurate. The fact is that the full spin is not conserved in the BHZ model, since the operator S^2 does not commutate with the Hamiltonian. Only S_z has a definite value. Therefore, at a nonzero interaction between electrons, there is no triply spin-degenerate state. There is only a doubly degenerate one, which is often also called a triplet.

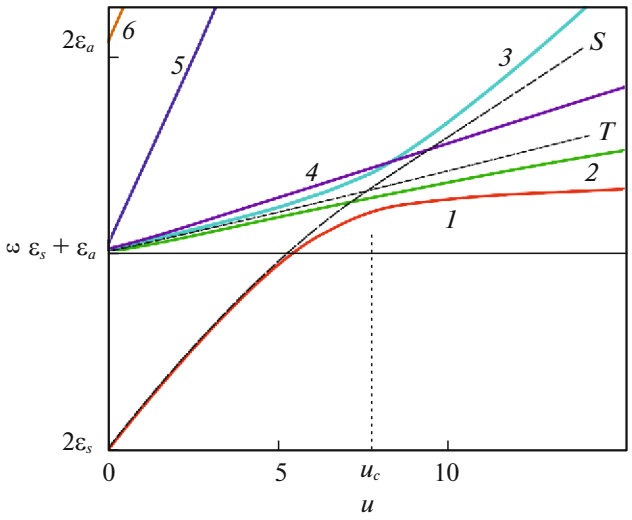

Fig. 1. Two-particle electron spectrum in a double symmetric quantum well in the presence of SOI. The calculation was performed at $\nu = 20$, $\Lambda = 3$, $a = 2$, $\Delta = 0.2$, and $d = 8$.

As the interaction amplitude u increases in the absence of SOI, the singlet states $|s\uparrow s\downarrow\rangle$ and $|a\uparrow a\downarrow\rangle$ mix, the states $|s\uparrow a\uparrow\rangle$ and $|s\downarrow a\downarrow\rangle|$ remain degenerate, and the compositions in the mixture of the states $|s\uparrow a\downarrow\rangle$ and $|s\downarrow a\uparrow\rangle$ forming a nonpolarized triplet and singlet change. In this case, the singlet $|s\uparrow s\downarrow\rangle$ indicated by line *1* intersects the triplets (*2* and *3*), as was shown earlier in [8]. The behavior of these terms is shown by the dotted lines *S* and *T* in Fig. 1. A nontrivial feature is the intersection of the singlet and triplet terms at a critical value of $u = u_c$. At $u > u_c$, the triplet state becomes the ground state, i.e., Wigner's theorem is violated. It is worth noting that this behavior of the terms is only possible when the band spectrum is inverted, i.e., only in the topological phase and at a small hybridization parameter a ($a < 10$), when the system is rather far from the topological transition point.

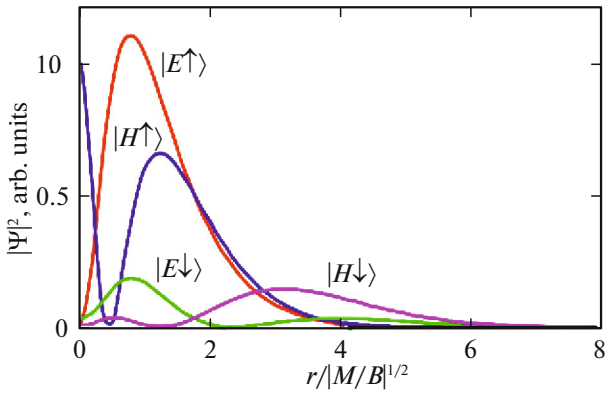

Fig. 2. Radial distribution of the spinor components of the hole-like electron state localized in an isolated quantum well. The components with spin (↓) are enlarged fourfold. The calculation was performed for the parameters $a = 2$, $\Lambda = 4$, $\Delta = 0.2$, and $\nu = 40$. The bound state energy is $\varepsilon = 0.3289$.

The u_c value critical for the singlet-triplet transition depends on the potential ν of the quantum wells, so the intersection of the terms and the singlet-triplet transition can be implemented by changing this potential.

The effect of SOI consists, first of all, in the fact that the doubly degenerate triplet level (dotted line *T*) splits into two levels (curves *2* and *3*). Near the singlet-triplet transition point, repulsion (anticrossing) of the singlet level and the upper split triplet level occurs.

Interestingly, all the projections of the spin density S_i in the states formed during splitting of the doubly degenerate triplet level (lines *2* and *3* in Fig. 1) are zero: $\Psi^+_{j=2,3}(\mathbf{r})S_i\Psi_{j=2,3}(\mathbf{r}) = 0$; i.e., the formed two-electron states are nonpolarized.

4. ON RECONSTRUCTION OF THE GROUND STATE

The answer to the question of which state of two electrons—with parallel or opposite spins—is energetically more favorable is determined by the ratio between the spin-dependent energy components, which, in the investigated system, are, first of all, the exchange and direct Coulomb interaction energies. In addition, of great importance are the energy of interaction of an electron with charges forming a quantum well and the kinetic energy, but, for quantum wells with a highly localized potential, which are rather distant from each other, these latter components are insignificant.

The spin dependence of the electron interaction energy is related to the presence of several components of the spinor describing this state, which have different spatial distributions at different spin configurations. In the usual situation, when Wigner's theorem is established, electrons are considered in a system with a single-band spectrum and states are described by a spinor of the second rank. In this case, the spectrum evolves with increasing amplitude of the electron-electron interaction potential in the following manner. The energy of the lower singlet increases due to an increase in the Coulomb repulsion energy. The energy of polarized triplets grows much slower due to the fact that the repulsion energy is compensated, to a great extent, by exchange coupling. However, with an increase in the electron–electron interaction, the exchange energy decreases and, at the limit $u \to \infty$, becomes insignificant, so the singlet and triplet terms asymptotically approach each other, yet do not intersect [14].

In the system under study, the single-particle wave functions have four components corresponding to two spin directions and two basic orbitals. In the BHZ model, the basis is formed by electron and hole bands with different angular moments: $\{|E, 1/2\rangle, |H, 3/2\rangle, |E, -1/2\rangle, |H, -3/2\rangle\}$. The energies of the direct (W_C) and exchange (W_{ex}) interactions of electrons described by the wave functions $\Psi(\mathbf{r}_1) = (\psi_1, \psi_2, \psi_3, \psi_4)^T$ and $\Phi(\mathbf{r}_2) = (\phi_1, \phi_2, \phi_3, \phi_4)^T$ have the form

$$W_C = \int\int d^2\mathbf{r}_1 d^2\mathbf{r}_2 \Psi^+(\mathbf{r}_1)\Psi(\mathbf{r}_1)U(|\mathbf{r}_1 - \mathbf{r}_2|)\Phi^+(\mathbf{r}_2)\Phi(\mathbf{r}_2)$$

and

$$W_{ex} = \int\int d^2\mathbf{r}_1 d^2\mathbf{r}_2 \Psi^+(\mathbf{r}_1)\Phi(\mathbf{r}_1)U(|\mathbf{r}_1 - \mathbf{r}_2|)\Phi^+(\mathbf{r}_2)\Psi(\mathbf{r}_2).$$

Obviously, the presence of pseudospin components significantly changes the values of both direct and exchange interactions and their spin dependence, especially taking into account that the exchange integral values are determined not only by the spin components, but also by the pseudospin ones.

The contribution of the wave spinor components to the charge and spin densities, which are usually attributed to direct and exchange interactions, can be easily demonstrated by the example of a bound state for a single isolated quantum well. Figure 2 shows the radial distribution of the components $|\psi_{i=(1,4)}(\mathbf{r})|^2$ for the hole-type bound state. The spin density distribution is presented in Fig. 3. The spin density component S_z (Fig. 3a) normal to the system plane changes nonmonotonically with distance and even changes its sign upon removal from the center. The tangential component is much smaller, but still exists and changes with distance in a completely unusual manner, as shown in Fig. 3b for the S_x component.

Obviously, extraordinary, as compared with the trivial system, charge and spin density distributions can significantly change both the direct and exchange interactions of electrons in two wells, which causes the violation of Wigner's theorem.

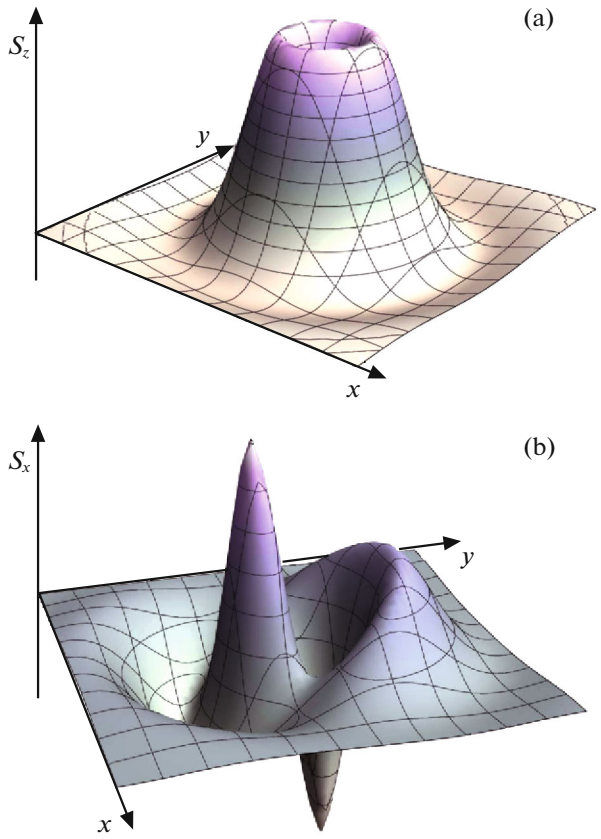

Fig. 3. Distribution of (a) the S_z and (b) S_x components of the spin density of an electron localized in an isolated quantum well in the hole-like state. The component S_x is enlarged twentyfold. The parameters used are as in Fig. 2.

5. CONCLUSIONS

Our calculations showed that with an increase in the electron-electron interaction amplitude the singlet and triplet terms intersect under certain conditions if SOI is absent. At weak SOI, triplet splitting occurs. In this case, one of the split levels intersects with the singlet, whereas for the other anticrossing is observed. Formally, in the calculations within perturbation theory, due to the presence of spinor pseudospin components, the exchange interaction is described by three matrix elements in the absence of SOI and six elements in the presence of it and the direct interaction in both cases is described by only three matrix elements. All together, they determine the energies of different spin configurations.

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CONFLICT OF INTEREST

The authors declare they have no conflict of interest.

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