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CONDENSED MATTER

Edge States of an Excitonic Insulator with the Spin–Orbit Interaction

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The effect of the spin–orbit and Coulomb interactions on the symmetry and topological properties of the *s*, *p*, *d*, and *s* + *d* phases of an excitonic insulator has been considered by example of the inverted two-band structure of the HgTe quantum well. It has been found that only the *p* phase has a nontrivial topology, but it is metastable. It has been shown that the exchange interaction between fermions induces the ground state with the *s* + *d* symmetry of the excitonic order parameter. This phase of the excitonic insulator has zero Chern number; nevertheless, edge states occur in the case of open boundaries.

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1. INTRODUCTION

The first studies of an excitonic insulator showed that the Coulomb interaction between fermions in a semiconductor can induce spontaneous appearance of the excitonic order parameter with the generation of the dielectric gap at a nonzero quasimomentum [1–3]. The most important condition of the formation of the excitonic insulator is the existence of an inverted band structure with the overlapping of the valence and conduction bands. It is substantial that the effective hybridization of states in these bands occurs in the excitonic insulator phase.

At the same time, the inverted band structure and spin–orbit interaction are necessary conditions for the formation of a topologically nontrivial phase in the Bernevig–Hughes–Zhang (BHZ) model [4], which describes the band structure of the HgTe quantum well (see also [5, 6]). A nontrivial topology of the ground state is in particular responsible for the formation of edge states in such system with open boundaries.

In view of these circumstances, it is of current interest to analyze whether topologically nontrivial phases and edge states could appear in an excitonic insulator with the spin–orbit interaction, where the appearance of the excitonic order parameter results in the hybridization of states formally the same as that caused by the bare parameter of interband hybridization in the BHZ model.

In this work, it is shown for the first time that the exchange interaction depending on the spin degrees of freedom is of particular importance for solving this problem. It is found that this interaction, violating the classification of excitonic phases induced by an interaction of density–density type, results in the ground state of the system with edge states.

The role of the Coulomb interaction was already considered in the problem of the formation of topological phases and edge states in solid-state systems. It was involved in the classification of topological materials [7], the problem of appearance of Majorana bound states [8, 9], and the development of renormalization group methods for the density matrix [10] in application to the strong correlation regime.

2. EXCITONIC INSULATOR WITH THE SPIN–ORBIT INTERACTION

Excitonic insulator phases induced by the Coulomb interaction between fermions in a system with the spin–orbit interaction are considered within the BHZ model [4].

As shown in [6], because of crystal field effects, relativistic corrections, and spin–orbit interaction, only the following two of six Te 5*p* orbitals play an important role in the formation of the band structure: $|l_z = 1, \sigma = +1/2\rangle$ and $|l_z = -1, \sigma = -1/2\rangle$, where $|l_z$ and σ are the projections of the orbital angular momentum and spin, respectively. These states constitute an actual basis for describing the valence band and its rearrangement under the effect of other fields.

The conduction band is formed from Hg 6*s* states, which do not change for symmetry reasons.

In the second quantization representation, the bare Hamiltonian has the form

$$H_0 = \sum_{g\sigma}(\varepsilon^b - \mu)b^+_{g\sigma}b_{g\sigma} + \sum_{gg'\sigma}t^b_{gg'}b^+_{g\sigma}b_{g'\sigma} + \sum_{f\sigma}(\varepsilon^a - \mu)a^+_{f\sigma}a_{f\sigma} + \sum_{ff'\sigma}t^a_{ff'}a^+_{f\sigma}a_{f'\sigma}. \quad (1)$$

Here, the operator $a_{f\sigma}$ ($b_{g\sigma}$) annihilates an electron with the spin projection σ at the site f (g), which belongs to the sublattice F (G) and is occupied by an Hg (Te) atom; $\varepsilon^a(\varepsilon^b)$ is energy of a single-site state in the conduction (valence) band; $t^a_{ff'}$ ($t^b_{gg'}$) are the electron hopping parameters between sites f' and f (g' and g); and μ is the chemical potential of the system.

The covalent mixing of s and p electronic states of Hg and Te atoms is described by the operator

$$\hat{T}_{sp} = \sum_{g\delta\sigma}t^\sigma_{sp}(\delta)a^+_{g+\delta,\sigma}b_{g\sigma} + \text{H.c.} \quad (2)$$

The matrix element $t^\sigma_{sp}(\delta)$ depending on σ and the vector δ connecting the Hg atom with one of the four nearest Te atoms can be represented in the form

$$t^\sigma_{sp}(\delta_l) = -t_{sp}(i\eta_\sigma)^l, \quad \eta_\sigma = 2\sigma, \quad l = 1, 2, 3, 4. \quad (3)$$

Here, the phases of atomic orbitals and the spin–orbit interaction are taken into account [6]. It is substantial that the matrix elements $t^\sigma_{sp}(\delta)$ are transformed according to a two-dimensional irreducible representation of the point group D_4.

The operator of the intersite Coulomb interaction between electrons in neighboring Te and Hg atoms has the form

$$\hat{V} = \sum_{g\delta\sigma\sigma'}Va^+_{g+\delta,\sigma}b^+_{g\sigma'}b_{g\sigma'}a_{g+\delta,\sigma} + \sum_{g\delta\sigma\sigma'}J_{\sigma\sigma'}(\delta)a^+_{g+\delta,\sigma}b^+_{g\sigma'}a_{g+\delta,\sigma'}b_{g\sigma}, \quad (4)$$

here, the first term corresponds to the density–density interaction with the parameter

$$V = \int d\mathbf{r}_1 d\mathbf{r}_2|\psi_s(r_{1x})|^2 v_{12}u^\perp_1|R_p(r_2)|^2, \quad (5)$$

where $r_{1x} = \sqrt{(x_1 - 1/2)^2 + y_1^2 + z_1^2}$,

$$v_{12} = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad u^\perp_1 = \frac{x_1^2 + y_1^2}{r_1^2}, \quad r_i = |\mathbf{r}_i|,$$

ψ_s is the Hg 6s orbital, and R_p is the radial part of the Te 5p orbital. The second term in Eq. (4) is due to the exchange contribution. For further analysis, the specific dependence of the exchange parameter on the direction of the vector δ and spin variables σ and σ' is important:

$$J_{\sigma\sigma'}(\delta) = \begin{cases}\eta_\sigma\eta_{\sigma'}J_1 + J_2, & \delta = \delta_1, \delta_3,\\ \eta_\sigma\eta_{\sigma'}J_2 + J_1, & \delta = \delta_2, \delta_4.\end{cases} \quad (6)$$

Here,

$$J_1 = \int d\mathbf{r}_1 d\mathbf{r}_2 u_s(1_x, 2_x)v_{12}\frac{x_1x_2}{r_1r_2}u_p(1, 2),$$
$$J_2 = \int d\mathbf{r}_1 d\mathbf{r}_2 u_s(1_x, 2_x)v_{12}\frac{y_1y_2}{r_1r_2}u_p(1, 2), \quad (7)$$

where

$$u_s(1_x, 2_x) = \psi_s(r_{1_x})\psi_s(r_{2_x}), \quad u_p(1, 2) = R_p(r_1)R_p(r_2).$$

3. SELF-CONSISTENCY EQUATION FOR THE EXCITONIC ORDER PARAMETER

To consider the properties of the excitonic insulator with the spin–orbit interaction, we set $t_{sp} = 0$ and use the theory presented in [1, 2] (see also [11]).

Omitting details, we write the integral self-consistency equation for the excitonic order parameter in the form

$$\Delta_\sigma(k) = \frac{2\tilde{V}}{N}\sum_q\Phi(k, q)\frac{\Delta_\sigma(q)}{\nu_q}L_q(T) - \frac{2J}{N}\sum_q\Psi(k, q)\frac{\Delta_{\bar\sigma}(q)}{\nu_q}L_q(T), \quad (8)$$

where the kernels and parameters are given by the expressions

$$\Phi(k, q) = \cos\frac{k_1 - q_1}{2}\cos\frac{k_2 - q_2}{2}, \quad \tilde{V} = V - J_1 - J_2,$$
$$\Psi(k, q) = \sin\frac{k_1 - q_1}{2}\sin\frac{k_2 - q_2}{2}, \quad J = J_1 - J_2, \quad (9)$$

and $L_q(T)$ is expressed in terms of the Fermi–Dirac functions and the energy spectrum as

$$L_q(T) = f(E^-_q/T) - f(E^+_q/T),$$
$$f(x) = (\exp(x) + 1)^{-1},$$
$$E^\pm_q = \frac{\varepsilon^a_q + \varepsilon^b_q}{2} \pm \nu_q, \quad \nu_q = \sqrt{(\varepsilon^a_q - \varepsilon^b_q)^2/4 + |\Delta_\sigma(q)|^2},$$
$$\varepsilon^{a,b}_q = \varepsilon^{a,b} + 2t_{a,b}(\cos q_1 + \cos q_2).$$

When deriving Eq. (8), we take into account that

$$\Delta_\sigma(k) = \sum_\delta\Delta_\sigma(\delta)\exp(-ik\delta),$$
$$\Delta_\sigma(\delta) = \tilde{V}\langle b^+_{g\sigma}a_{g+\delta,\sigma}\rangle - J_{\sigma\bar\sigma}\langle b^+_{g\bar\sigma}a_{g+\delta,\bar\sigma}\rangle. \quad (10)$$

It follows from Eq. (8) that the exchange contribution is responsible for a relation between the parameters $\Delta_\uparrow(k)$ and $\Delta_\downarrow(k)$. The dependences of these parameters on the spin projection σ are such that $|\Delta_\sigma(k)|$ is independent of σ. As shown below, the exchange interaction is important because it induces a specific state of the excitonic insulator where edge states are formed under the open boundary conditions.

Further, it is convenient to classify excitonic phases in terms of their symmetry properties for the case $J_1 = J_2 (J = 0)$.

4. SYMMETRY OF PHASES OF THE EXCITONIC INSULATOR AT $J = 0$

To determine the quasimomentum dependence $\Delta_\sigma(k)$, we use the symmetry properties of the square lattice, as in [12, 13], when determining the chiral order parameter for the triangular lattice.

Using the characters of the irreducible representations of the group D_4 [14], it is easy to find that, when only the Coulomb interaction between electrons located at the nearest sites is taken into account, there are three types of basis functions:

$$\varphi_s(k) = \cos(k_1/2)\cos(k_2/2),$$

$$\varphi_d(k) = \sin(k_1/2)\sin(k_2/2), \tag{11}$$

$$\varphi_{p\sigma}(k) = \eta_\sigma \sin\frac{k_1 + k_2}{2} - i\sin\frac{k_1 - k_2}{2}, \quad \sigma = \pm 1/2.$$

The first function corresponds to the identity representation and characterizes the s-type symmetry. In this case,

$$\Delta_s(k) = \Delta_s\varphi_s(k), \tag{12}$$

and the amplitude Δ_s is determined from the solution of the equation

$$1 = \frac{V - 2J_1}{2N}\sum_k \frac{1 + 2\cos k_1 + \cos k_1 \cos k_2}{\nu_{sk}} L_{sk}(T). \tag{13}$$

Here and below, the additional subscripts s, d, and p of the functions ν_k and $L_k(T)$ indicate that the excitonic order parameter appearing in these functions is taken in the form corresponding to the s, d, and p symmetries, respectively.

For the second one-dimensional representation corresponding to the d symmetry, the excitonic order parameter

$$\Delta_d(k) = \Delta_d\varphi_d(k) \tag{14}$$

is a solution of Eq. (8) if the amplitude Δ_d satisfies the equation

$$1 = \frac{V - 2J_1}{2N}\sum_k \frac{1 - 2\cos k_1 + \cos k_1 \cos k_2}{\nu_{dk}} L_{dk}(T). \tag{15}$$

The solution of Eq. (8) corresponding to the two-dimensional representation of the group D_4 with the p symmetry has a complex form with the phase depending on the spin projection

$$\Delta_{p\sigma}(k) = \Delta_p\varphi_{p\sigma}(k). \tag{16}$$

Here, the amplitude Δ_p is determined from the solution of the self-consistency equation

$$1 = \frac{V - 2J_1}{2N}\sum_k \frac{1 - \cos k_1 \cos k_2}{\nu_{pk}} L_{pk}(T). \tag{17}$$

5. TOPOLOGICAL CLASSIFICATION OF EXCITONIC PHASES AND EDGE STATES AT $J = 0$

We use an additional classification of the states of the excitonic insulator in terms of such topological invariant as the Chern number [15]:

$$Q^{(\lambda)} = -\frac{1}{2\pi}\int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 B^{(\lambda)}(k_1, k_2). \tag{18}$$

Here, $B^{(\lambda)}(k_1, k_2)$ is the Berry curvature for a quantum state described by the Bloch wavefunction $\psi_{\lambda k}$ and is given by the well-known formula

$$B^{(\lambda)}(k_1, k_2) = \frac{\partial A_2^{(\lambda)}(k_1, k_2)}{\partial k_1} - \frac{\partial A_1^{(\lambda)}(k_1, k_2)}{\partial k_2}, \tag{19}$$

where

$$A_j^{(\lambda)}(k_1, k_2) = -i\left\langle \psi_{\lambda k}\left|\frac{\partial}{\partial k_j}\right|\psi_{\lambda k}\right\rangle, \quad j = 1, 2, \tag{20}$$

are averages over this quantum state. The calculations for the phases of the excitonic insulator with the s and d symmetries of the excitonic order parameter show that $Q^{(s)} = 0$ and $Q^{(d)} = 0$ at all parameters of the system. In this case, edge states do not appear under the open boundary conditions.

A different situation occurs for the excitonic insulator with the p symmetry of the order parameter. The calculation of the topological invariant $Q^{(p)}$ in this case can be reduced to the calculation of the following integral over the two-dimensional Brillouin zone:

$$Q^{(p)} = -\frac{1}{2\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dk_1 dk_2 \left(\frac{\eta_\sigma\Delta_p^2}{4\nu_{pk}^3}\right)\Phi_Q^{(p)}(k). \tag{21}$$

Here,

$$\Phi_Q^{(p)}(k) = \left\{(t_a - t_b)(\sin^2 k_1 + \sin^2 k_2) + \frac{\varepsilon_k^a - \varepsilon_k^b}{1 - \cos k_1 \cos k_2}\,\frac{\cos k_1 \sin^2 k_2 + \cos k_2 \sin^2 k_1}{4}\right\} \tag{22}$$

is the function obtained with the quasimomentum dependence of the excitonic order parameter for the p symmetry given by Eq. (16).

In the inverted regime, where a nontrivial solution exists for the excitonic order parameter, we find that $Q^{(p)} = 1$ if $\sigma = +1/2$ and $Q^{(p)} = -1$ if $\sigma = -1/2$.

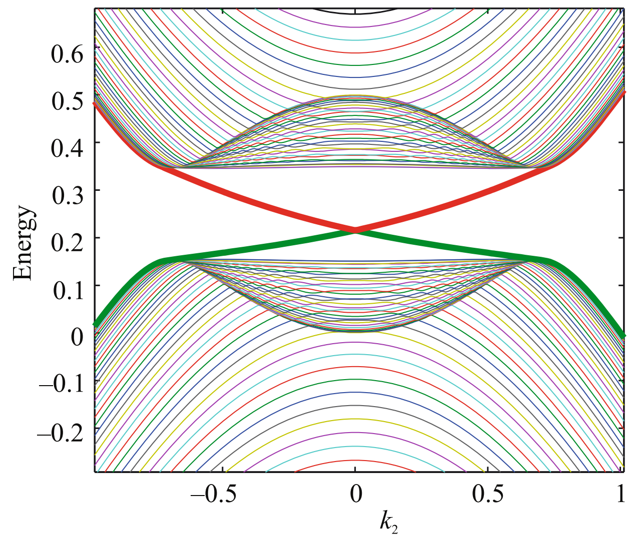

Fig. 1. (Color online) Energy spectrum of Fermi states of the excitonic insulator with the $p + ip$ symmetry of the excitonic order parameter at open boundaries (geometry of the cylinder) obtained with the parameters $\tilde{V} = 2.5$, $t_a = -0.5$, $t_b = 0.5$, $\varepsilon_a = -4t_a$, and $\varepsilon_b = 0.5 - 4t_b$.

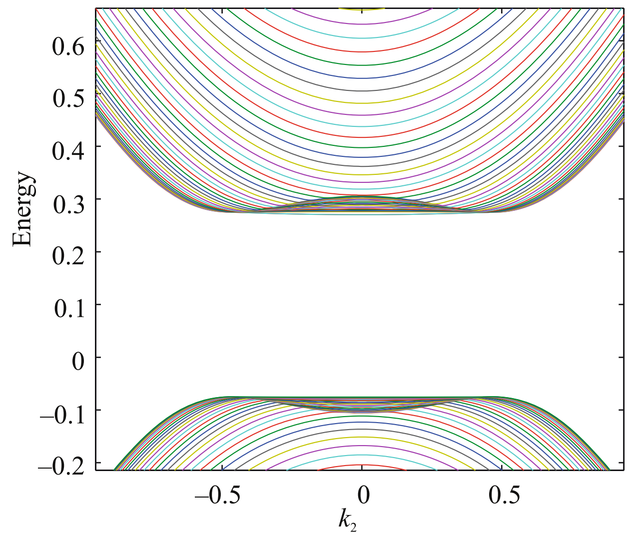

Fig. 2. (Color online) Energy spectrum of Fermi states of the excitonic insulator with the s symmetry of the excitonic order parameter at open boundaries (geometry of the cylinder) obtained with $V = 1$ and the other parameters the same as in Fig. 1.

This means that the p phase of the excitonic insulator is topologically nontrivial. It is noteworthy that the quasimomentum dependence $\Delta_{p\sigma}(k)$ for this phase coincides with the dependence of the covalent mixing intensity for the BHZ model taken with opposite sign:

$$t_{sp}(k) = -2t_{sp}\varphi_{p\sigma}(k). \quad (23)$$

Since the Chern number corresponds to the nontrivial topology of the p phase, edge states should be expected in this phase under open boundary conditions. To test this statement, we calculated the energy spectrum of Fermi states at $T = 0$ in the geometry of the cylinder. The results of the calculation are shown in Fig. 1. The parameters were chosen such that the bare structure of energy bands corresponds to the inverted case. The self-consistent amplitude is $\Delta_p = 0.19$.

According to the structure of the spectrum in Fig. 1, because of edge effects, the considered system has not only ordinary bulk states but also states with energies inside the band gap. The latter states include states with quasimomenta k_2 near the point of intersection of intragap branches; these states are edge states: most of the wavefunction weight for them is within three layers adjacent to the boundary. According to the Chern number value, the phase of the excitonic insulator with the p symmetry of the excitonic order parameter is simultaneously a topological phase.

It is noteworthy that edge states are formed in the excitonic insulator only when the excitonic order parameter corresponds to the two-dimensional representation of the group D_4. The calculations of the energy spectrum of the excitonic insulator with the s and d symmetries of the excitonic order parameter demonstrate no edge states. The structure of the energy spectrum for the s symmetry is shown in Fig. 2. The picture for the d symmetry of the excitonic order parameter is qualitatively the same. This completely correlates with the Chern numbers obtained for these phases.

Is the excitonic insulator simultaneously a topological insulator? To answer this question, it is necessary to determine which phase is stable and which two others are metastable. To this end, we calculate the dependences of the amplitudes of the order parameters on the effective Coulomb interaction parameter. The results are shown in Fig. 3.

It is seen that the s phase has the largest amplitude of the excitonic order parameter among the three possible phases. Since the condensation energy of the excitonic phase increases with this amplitude (this rule is confirmed by direct calculations), the s phase is stable and the two others are metastable. Consequently, the transition of the system to the excitonic phase at $J = 0$ does not lead to the formation of edge states under open boundary conditions.

6. EDGE STATES OF THE EXCITONIC INSULATOR FOR $J_1 \neq J_2$

At $J_1 \neq J_2$, the exchange term in the self-consistency equation for the excitonic order parameter qualitatively changes the character of the ground state of the considered two-band semiconductor with the

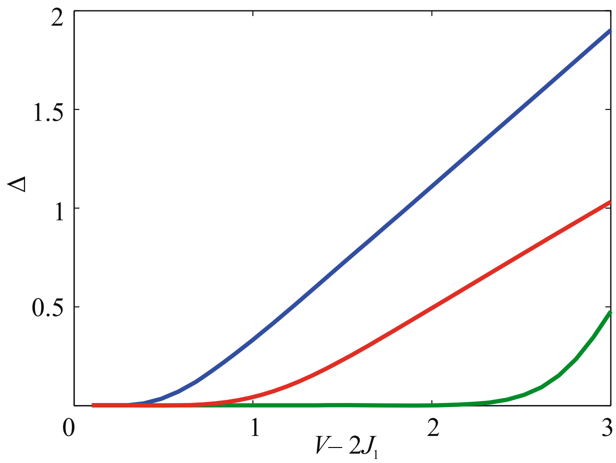

Fig. 3. (Color online) Amplitudes (upper line) Δ_s, (middle line) Δ_p, and (lower line) Δ_d of the respective the excitonic order parameters versus $\tilde{V} = V - 2J_1$ (at $J_1 = J_2$).

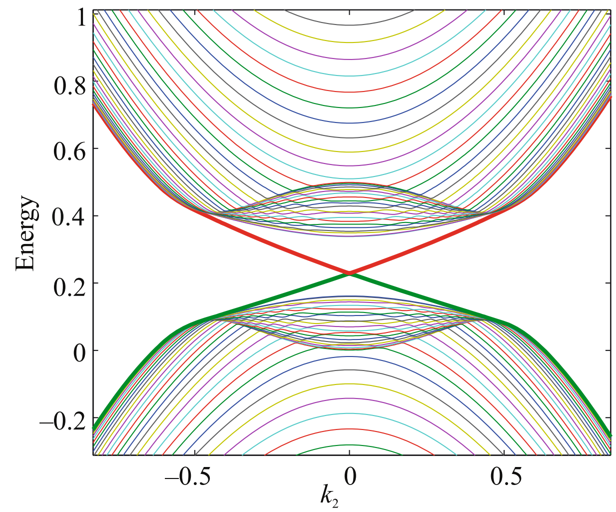

Fig. 4. (Color online) Energy spectrum of Fermi states of the excitonic insulator with the $s + d$ symmetry of the excitonic order parameter at open boundaries (geometry of the cylinder) obtained with $J = 1$, $t_a = -0.5$, $t_b = 0.5$, and the other parameters the same as in Fig. 1.

spin–orbit interaction. We now discuss this important problem.

First, the p phase of the excitonic insulator is still a solution of Eq. (8). The excitonic order parameter $\Delta_{p\sigma}(k)$ is also given by Eq. (16) and its amplitude Δ_p is determined from Eq. (17).

The situation with the s and d phases of the excitonic insulator is different. At $J_1 \neq J_2$, each of these phases is no longer a solution.

In the considered case, a qualitatively new type of solutions of Eq. (8) has the form of the superposition

$$\Delta_{sd,\sigma}(k) = \Delta_s(i + \eta_\sigma)\varphi_s(k) + \Delta_d(i - \eta_\sigma)\varphi_d(k). \quad (24)$$

Here, the amplitudes Δ_s and Δ_d satisfy the system of equations

$$\begin{aligned} (1 - \tilde{V}C_s)\Delta_s + JC_d\Delta_d &= 0, \\ JC_s\Delta_s + (1 - \tilde{V}C_d)\Delta_d &= 0, \end{aligned} \quad (25)$$

where

$$\begin{aligned} C_s &= \frac{1}{2N}\sum_k \frac{1 + 2\cos k_1 + \cos k_1 \cos k_2}{\nu_{sd}(k)} L_{sd}(k), \\ C_d &= \frac{1}{2N}\sum_k \frac{1 - 2\cos k_1 + \cos k_1 \cos k_2}{\nu_{sd}(k)} L_{sd}(k). \end{aligned} \quad (26)$$

The solution of these equations makes it possible to determine the characteristics of the excitonic insulator with the combined $s + d$ symmetry of the excitonic order parameter. The important properties of this excitonic insulator are as follows.

The Chern number for the $s + d$ phase of the excitonic insulator is $Q^{(s+d)} = 0$. This seems not surprising because the excitonic order parameter in the considered phase is represented in the form of the superposition of basis functions, each corresponding to an excitonic phase with zero Chern number.

The situation with the $s + d$ phase of the excitonic insulator is nontrivial: the calculated energy spectrum of the system with open boundaries includes states with energies inside the band gap of the bulk spectrum (see Fig. 4). In this case, states with energies sufficiently deep in the band gap are edge states (according to the criterion used above).

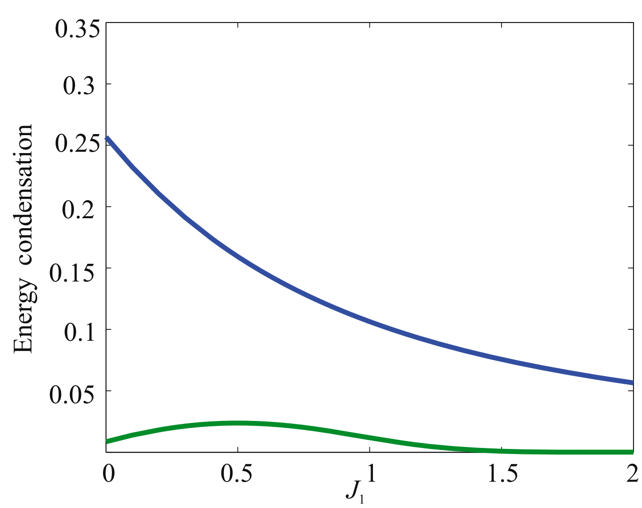

Fig. 5. (Color online) Energies of condensation of the (upper line) $s + d$ and (lower line) p phases of the excitonic insulator versus the parameter J_1 calculated with the model parameters $t_a = -0.5$, $t_b = 0.5$, $\varepsilon_a = -4$, $\varepsilon_b = 1 - 4t_b$, $V = 3.5$, and $J_2 = 0.5$.

It is remarkable that the $s + d$ phase of the excitonic insulator is the ground state of the considered semiconductor. This follows from the comparison of the condensation energy of the $s + d$ phase with the corresponding energy for the p phase (see Fig. 5). It is seen that the condensation energy of the $s + d$ phase at all J_1 values is much higher than the condensation energy of the p phase.

According to the results reported above, the exchange interaction between fermions in the two-band semiconductor with the spin–orbit interaction and an inverted band structure can induce a specific state of the excitonic insulator, where edge states are formed in the presence of open boundaries, whereas the Chern number for such phase is zero.

7. CONCLUSIONS

To summarize, the symmetry and topological properties of an excitonic insulator with the spin–orbit interaction have been studied for the first time. Such an excitonic insulator has been theoretically considered by the example of the band structure of the HgTe quantum well described by the BHZ model.

It has been shown that the Coulomb and exchange interactions between fermions with allowance for the spin–orbit coupling, differently affect the characteristics of the induced excitonic insulator state under the conditions of the inverted band structure.

The symmetry classification of the excitonic insulator phases has been performed in terms of the irreducible representations of the group D_4. The topological classification of these phases has been performed in terms of the Chern number.

It has been shown that three phases correspond to the solutions of the integral self-consistency equation without the exchange interaction. The excitonic order parameter for them is characterized by the s, d, and p symmetries. The excitonic order parameter in the p phase is transformed according to the two-dimensional representation of the group D_4, and the topological invariant corresponds to a nontrivial topology. Edge states exist in such a phase of the system with open boundaries. However, this phase is metastable, and the ground state is the s phase with a trivial topology.

It has been shown that the exchange interaction qualitatively changes the properties of the excitonic insulator. As a result, the ground state is the mixed $s + d$ phase, where the excitonic order parameter is the superposition of the s and d basis functions with the coefficients depending on the spin projection. An important feature of the mixed $s + d$ phase is that the topological invariant for it is zero, whereas edge states occur in the system with open boundaries.

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