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CONDENSED MATTER

Splitting of the Spectrum of Fermionic Excitations in a Topological Insulator by Charge Fluctuations

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It is shown that the intersite Coulomb interaction of electrons in a topological insulator leads to the splitting of the initial energy structure and to the induction of two bands of fluctuation states. As a result, the total spectrum of Fermi excitations of the topological insulator has a four-band structure. The dielectric gap is determined by the energy interval between the bottom of the band of fluctuation states of conduction electrons and the top of the valence band of fluctuation states. Since the band of fluctuation states is narrow, quasiparticles with different effective masses appear.

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1. INTRODUCTION

The properties of topological insulators (TIs) and conditions for implementation of edge states were first considered for systems described by quadratic Hamiltonians [1–3], for structures with anomalously strong spin–orbit coupling [4], and within a model obtained using the formalism of wavefunction envelopes and boundary conditions [5]. The study of the properties of two-sublattice TIs has recently been begun [6].

A regime where the interaction between fermions cannot be considered as weak often occurs in real materials. This initiates works where the intersite Coulomb interaction (ISCI) is taken into account when calculating the spectrum of excitations in TIs and performing the topological classification [7–10].

In the presence of the ISCI, classical methods cannot be used to calculate the spectrum of fermionic excitations in TIs, and simple linearized schemes such as the generalized Hartree–Fock approximation are no longer correct when the Coulomb interaction parameters become comparable with the parameters determining the bare energy structure of TIs. Because of these factors, it is relevant to apply modern quantum statistical methods to develop the theory of mentioned materials.

The problem of correct description of the ISCI is complicated if bare bands overlap. As known [11–13], the Coulomb interaction in this case can significantly affect the system and form an excitonic insulator phase. The exchange part of the ISCI can induce edge states in the an excitonic insulator [14].

It was shown previously that the ISCI can lead to the splitting of the spectrum of fermionic excitations and to the formation of the band of fluctuation states in an ensemble of Hubbard fermions [15, 16]. This band is referred to as the band of fluctuation states (FSB) because the residues of the electron Green's function at the induced poles are proportional to the rms fluctuation of the electron density.

This result was obtained both with an extended set of basis operators [15] and within the diagrammatic technique in the atomic representation [16]. In the latter case, the exact summation of a subsequence of diagrams describing contributions from single-site charge fluctuations was significant to determine the mass operator for the fermionic Green's function.

Taking into account this result, one can expect that the inclusion of the ISCI under the conditions of the inverted band structure, which exists in TIs, can result in a more noticeable qualitative change in the energy structure. This occurs because the appearance of additional subbands both for conduction electrons and for electrons of the valence band, between which the spectrum of edge states lies, can significantly affect both the structure of the spectrum of the TIs and the behavior of the fermion density of states.

In this work, the spectrum of fermionic excitations is determined within the most popular model proposed by Bernevig, Hughes, and Zhang [1] (BHZ model), which describes the energy structure of the HgTe quantum well (see also [2, 3]) with an extended set of basis operators and the inclusion of the ISCI.

It is shown that charge fluctuations qualitatively change the energy structure of TIs: the spectrum of excitations includes not only the conduction and valence bands but also two FSBs, and edge states are

located between the upper and lower FSBs, for which the effective masses increase.

2. HAMILTONIAN OF THE BHZ + V MODEL

We recall the main features determining the characteristics of an ensemble of fermions with the spin–orbit coupling, which is described by the BHZ model.

Because of effects of the crystal field, relativistic corrections, and spin–orbit coupling, only two of six $5p$ spin orbitals play an important role in the formation of the band structure. These orbitals are $|l_z = 1, \sigma = +1/2\rangle$ and $|l_z = -1, \sigma = -1/2\rangle$, where l_z is the projection of the orbital angular momentum and σ is the spin projection [3]. These states form an actual basis for the description of the valence band.

The conduction band is formed from $6s$ states of Hg atoms, which hardly change for symmetry reasons.

In the quasimomentum representation, the Hamiltonian $\hat{H}_{\mathrm{BHZ}}$ can be written in the form

$$\hat{H}_{\mathrm{BHZ}} = \sum_{k\sigma}\left[\varepsilon_{ak}a^{+}_{k\sigma}a_{k\sigma} + \varepsilon_{bk}b^{+}_{k\sigma}b_{k\sigma}\right] + \sum_{k\sigma}(\Gamma_{k\sigma}a^{+}_{k\sigma}b_{k\sigma} + \Gamma^{*}_{k\sigma}b^{+}_{k\sigma}a_{k\sigma} + \mathrm{H.c.}), \quad (1)$$

where $a_{k\sigma}$ and $b_{k\sigma}$ are the secondary quantization operators used to describe the conduction and valence bands, respectively. The bare spectra of fermionic states are given by the expressions

$$\varepsilon_{ak} = \varepsilon_a + t_{ak}, \quad \varepsilon_{bk} = \varepsilon_b + t_{bk}, \quad (2)$$

where ε_a and ε_b include mean-field effects and specify the centers of the conduction and valence bands, respectively. The quasimomentum dependence of the spectrum corresponds to the inclusion of hoppings within the first coordination sphere,

$$t_{ak} = 2t_a(\cos(k_x) + \cos(k_y)), \quad t_{bk} = 2t_b(\cos(k_x) + \cos(k_y)), \quad (3)$$

where t_a and t_b are the hopping parameters for the conduction and valence bands, respectively.

The covalent mixing of states of Hg and Te ions is determined by the function

$$\Gamma_{k\sigma} = -2t_{sp}\left\{\eta_\sigma \sin\frac{k_1 + k_2}{2} - i\sin\frac{k_1 - k_2}{2}\right\}, \quad (4)$$

where t_{sp} is the parameter specifying the hybridization intensity and the phases of atomic spin orbitals are taken into account [3].

Effects of charge fluctuations are described by the additional operator

$$\hat{V} = \sum_{f\in F,\delta} V\Delta\hat{n}_f\Delta\hat{n}_{f+\delta}. \quad (5)$$

Here, V is the parameter determining the interaction energy of electrons on the nearest Hg and Te ions connected by the vector δ, the subscript f specifies the sites of the F sublattice where Hg ions are located, the subscript g specifies the sites of the G sublattice where Te ions are located, and the operators of fluctuations of the electron density at the site are determined by the expressions

$$\Delta\hat{n}_f = \hat{n}_f - \langle\hat{n}_f\rangle, \quad \hat{n}_f = \sum_\sigma a^{+}_{f\sigma}a_{f\sigma}, \quad \Delta\hat{n}_g = \hat{n}_g - \langle\hat{n}_g\rangle, \quad \hat{n}_g = \sum_\sigma b^{+}_{g\sigma}b_{g\sigma}. \quad (6)$$

Here, the Wanier representation is used in the form

$$a_{f\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{ikf}a_{k\sigma}, \quad b_{g\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{ikg}b_{k\sigma}, \quad (7)$$

where N is the number of unit cells and $\langle\hat{n}_{f(g)}\rangle$ is the equilibrium number of electrons at the site in the $F(G)$ sublattice.

The Hamiltonian of the BHZ + V model under consideration is the sum of the Hamiltonian $\hat{H}_{\mathrm{BHZ}}$ and the operator $\hat{V}$ given by Eq. (5):

$$\hat{H}_{\mathrm{BHZ}+V} = \hat{H}_{\mathrm{BHZ}} + \hat{V}. \quad (8)$$

3. FLUCTUATION RENORMALIZATION OF LOCALIZED LEVELS AND SPLITTING OF BANDS

The first exact equations of motion including correlation effects have the form

$$\left(i\frac{d}{dt} - \varepsilon_a - t_{ak}\right)a_{k\sigma} = \Gamma_{k\sigma}b_{k\sigma} + VA_{k\sigma}, \quad \left(i\frac{d}{dt} - \varepsilon_b - t_{bk}\right)b_{k\sigma} = \Gamma^{*}_{k\sigma}a_{k\sigma} + VB_{k\sigma}, \quad (9)$$

where

$$A_{k\sigma} = \frac{1}{N}\sum_{f\in F,q\delta} e^{if(q-k)}a_{q\sigma}\Delta\hat{n}_{f+\delta}, \quad (10)$$

$$B_{k\sigma} = \frac{1}{N}\sum_{g\in G,q\delta} e^{ig(q-k)}b_{q\sigma}\Delta\hat{n}_{g+\delta} \quad (11)$$

are operators reflecting the coupling of fermions to charge fluctuations.

According to Eq. (9), V serves as a coupling constant between fermions and fluctuations of electron densities. If this parameter is not small, this coupling should be correctly described.

This description can be performed with the following expansion of the set of basis operators:

$$\{a_{k\sigma}, b_{k\sigma}\} \to \{a_{k\sigma}, b_{k\sigma}, A_{k\sigma}, B_{k\sigma}\}. \quad (12)$$

Writing equations for $A_{k\sigma}$ and $B_{k\sigma}$ and using the Zwanzig–Mori method [17, 18], we obtain

$$\begin{aligned}\left(i\frac{d}{dt}-\tilde{\varepsilon}_a-t_{ak}/2\right)A_{k\sigma}&=M^*_{k\sigma}a_{k\sigma}+L_{k\sigma}b_{k\sigma},\\ \left(i\frac{d}{dt}-\tilde{\varepsilon}_b-t_{bk}/2\right)B_{k\sigma}&=P_{k\sigma}a_{k\sigma}+M_{k\sigma}b_{k\sigma}.\end{aligned} \quad (13)$$

Here, only principal contributions are retained on the right-hand sides and the coefficients being functions of quasimomentum are given by the expressions

$$M_{k\sigma}=2h(2-h)V-\Gamma_{k\sigma}\frac{1}{N}\sum_q\Phi_{kq}\langle b^+_{q\sigma}a_{q\sigma}\rangle,$$

$$L_{k\sigma}=\frac{1}{N}\sum_q\Phi_{kq}[(t_{bq}-t_{aq}-t_{bk})\langle b^+_{q\sigma}a_{q\sigma}\rangle+\Gamma^{ab}_{q\sigma}], \quad (14)$$

$$P_{k\sigma}=\frac{1}{N}\sum_q\Phi_{kq}[(t_{aq}-t_{bq}-t_{ak})\langle a^+_{q\sigma}b_{q\sigma}\rangle+(\Gamma^{ba}_{q\sigma})^*],$$

where

$$\Phi_{kq}=4\cos((k_x-q_x)/2)\cos((k_y-q_y)/2),$$

$$\Gamma^{ab}_{q\sigma}=\Gamma_{q\sigma}(n^a_{q\sigma}-n^b_{q\sigma}).$$

Furthermore, it is taken into account that the site concentration of electrons in the valence band is slightly different from 2 and is described in terms of the concentration of holes h as

$$n_G=\frac{1}{N}\sum_g\langle\hat{n}_g\rangle=\frac{1}{N}\sum_{g\sigma}\langle b^+_{g\sigma}b_{g\sigma}\rangle=2-h. \quad (15)$$

The equation for calculating the chemical potential follows from the condition of the equality of concentrations of conduction electrons and holes

$$n_F=\frac{1}{N}\sum_f\langle\hat{n}_f\rangle=\frac{1}{N}\sum_{f\sigma}\langle a^+_{f\sigma}a_{f\sigma}\rangle=h. \quad (16)$$

According to (13), charge fluctuations shift the centers of bands associated with the composition operators $A_{k\sigma}$ and $B_{k\sigma}$ because the equations contain renormalized quantities $\tilde{\varepsilon}_a$ and $\tilde{\varepsilon}_b$ rather than bare ones ε_a and ε_b. It is substantial that fluctuation renormalization occurs through different scenarios:

$$\varepsilon_a\to\tilde{\varepsilon}_a=\varepsilon_a-(1-h)V, \quad (17)$$

$$\varepsilon_b\to\tilde{\varepsilon}_b=\varepsilon_b+(1-h)V. \quad (18)$$

As a result, the FSB induced by the composition operator $A_{k\sigma}$ is shifted by $(1-h)V$ toward the valence band. It should be emphasized that this FSB, as seen in Eq. (10), is due to the coherent superposition of states, each combined from fermions of the conduction band and fluctuations of the electron density in the valence band that are coupled to these fermions. It is substantial that the FSB is below the bare conduction band in energy. Consequently, the FSB serves as the renormalized conduction band in the rearranged energy structure of the TI.

The valence FSB generated by the operator $B_{k\sigma}$ is shifted toward the conduction band by the same value $(1-h)V$. In this case, the FSB is formed through the coupling of fermions of the valence band to fluctuations of the electron density from the conduction band. It is important that this FSB is shifted toward higher energies and, thereby, can serve as the valence band in the renormalized spectrum of the TI. The difference in the behavior of these two FSBs is due to the different values of the square of fluctuations of the electron density for the valence and conduction bands. In the former case, fluctuations occur against the background of the almost complete filling of electronic levels; then,

$$(\Delta\hat{n}_g)^2=h(2-h)/2-(1-h)\Delta\hat{n}_g. \quad (19)$$

Fluctuations of the electron density in the conduction band occur at insignificant filling of levels. Therefore, the square of the fluctuation operator of the electron density is given by the expression

$$(\Delta\hat{n}_f)^2=h(2-h)/2+(1-h)\Delta\hat{n}_f. \quad (20)$$

Opposite signs of the second terms in Eqs. (19) and (20) lead to different shifts of fluctuation bands because the ISCI couples a conduction electron to fluctuations of the electron density in the valence band, whereas the ISCI couples an electron of the valence band to fluctuations of the electron density in the conduction band.

4. SPECTRUM OF EXCITATIONS AND THE ELECTRON DENSITY OF STATES IN THE BHZ + V MODEL

It follows from Eqs. (9) and (13) that the spectrum of excitations of the TI is determined by solutions of the dispersion equation

$$\begin{aligned}&[(\omega-\varepsilon_{ak})(\omega-\varepsilon_{bk})-|\Gamma_{k\sigma}|^2](\omega-\tilde{\varepsilon}_{ak})(\omega-\tilde{\varepsilon}_{bk})\\ &-V[M_{k\sigma}(\omega-\varepsilon_{ak})+\Gamma_{k\sigma}P_{k\sigma}](\omega-\tilde{\varepsilon}_{ak})\\ &-V[M^*_{k\sigma}(\omega-\varepsilon_{bk})+\Gamma^*_{k\sigma}L_{k\sigma}](\omega-\tilde{\varepsilon}_{bk})\\ &+V^2(|M_{k\sigma}|^2-P_{k\sigma}L_{k\sigma})=0,\end{aligned} \quad (21)$$

where

$$\tilde{\varepsilon}_{ak}=\tilde{\varepsilon}_a+t_{ak}/2,\quad \tilde{\varepsilon}_{bk}=\tilde{\varepsilon}_b+t_{bk}/2. \quad (22)$$

The coefficients of the equation are functions of the quasimomentum and self-consistently depend on the thermodynamic averages $\langle a^+_{q\sigma}b_{q\sigma}\rangle$, $\langle a^+_{q\sigma}a_{q\sigma}\rangle$, and $\langle b^+_{q\sigma}b_{q\sigma}\rangle$. They can be calculated using the method of two-time Green's functions, matrix description, and field operator

$$\hat{\Psi}_{k\sigma}=(a_{k\sigma},b_{k\sigma},A_{k\sigma},B_{k\sigma})^T.$$

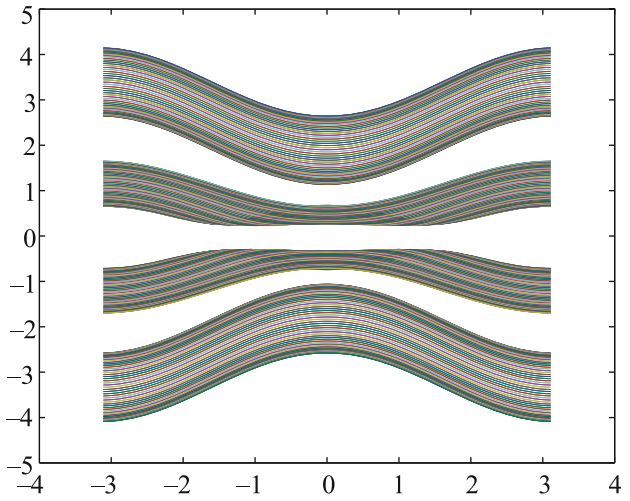

Fig. 1. (Color online) Energy spectrum of fermion states of the topological insulator including Coulomb correlations obtained with the parameters $V = 1$, $t_a = -0.45$, $t_b = 0.45$, $t_{sp} = 0.2$, and $h = 0.25$.

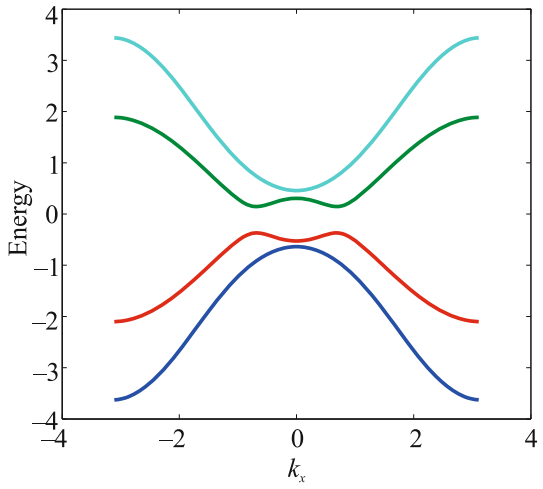

Fig. 2. (Color online) Fermion spectrum of the topological insulator for $k_x = k_y$ obtained with the parameters $V = 0.5$, $h = 0.2$, and the other parameters the same as in Fig. 1.

The 16-component matrix Green's function $\hat{G}_{k\sigma}(t-t')$ can be defined in terms of this field operator as

$$\hat{G}_{k\sigma}(t-t') = -i\theta(t-t')\langle\{\hat{\Psi}_{k\sigma}(t), \hat{\Psi}^{+}_{k\sigma}(t')\}_{+}\rangle, \qquad (23)$$

where $\theta(t-t')$ is the Heaviside step function and $\{...\}_{+}$ means the anticommutator.

The equation for the Green's function has the form

$$[\omega\hat{I} - \hat{M}_{k\sigma}]\hat{G}_{k\sigma}(\omega) = \hat{S}_{k\sigma}, \qquad (24)$$

where ω is the frequency, $\hat{I}$ is the identity matrix, the elements of the matrix $\hat{M}$ are determined by comparing Eqs. (9) and (13) with Eq. (24), and

$$\hat{S}_{k\sigma} = \langle\{\hat{\Psi}_{k\sigma}, \hat{\Psi}^{+}_{k\sigma}\}_{+}\rangle. \qquad (25)$$

The self-consistent equations for thermodynamic averages can be easily obtained from the solution of Eq. (24). They were analyzed using the symmetry classification of allowed phases [14, 19–21].

Omitting intermediate calculations, we present the results on the effect of charge fluctuations.

Figure 1 shows the spectrum of fermionic excitations. It is seen that, at a fixed value of one of the projections of the quasimomentum (in this case, k_x), four energy bands appear; the energy of the fermion state depends on the second projection of the quasimomentum (k_y). In this case, relatively narrow FSBs are adjacent to the dielectric gap.

The presented results show that charge fluctuations initiate the appearance of heavy fermions. Correspondingly, the authors of [22] used the possibility of existence of light and heavy holes in the HgTe quantum well to interpret experimental data on the magnetic properties of two-dimensional fermions.

Taking into account this result, we demonstrate that charge fluctuations can initiate the appearance of heavy holes. Figure 2 shows the energy spectrum for the $k_x = k_y$ direction. It is seen that states with heavy holes will be filled at low carrier densities in the quantum well. As the carrier density increases, the filling of states with light holes will begin because the spectral intensity for heavy holes corresponding to the valence FSB is low since it is proportional to the rms fluctuation of the charge density in the conduction band. This circumstance promotes a fast transition to the filling of valleys with light holes [22].

It is noteworthy that the FSB for Hubbard fermions, located much below the chemical potential, leads only to the redistribution of filling of fermion states. The situation is significantly different in the case under consideration because the FSB plays a decisive role in the thermodynamic properties of TIs.

Since the energy intervals of bands at different k_x values are different, split parts of the conduction and valence bands are overlapped. As a result, the total density of states holds only one gap in the spectrum of states. This case is demonstrated in Fig. 3, where the fermion density of states of the TI is shown. The density of states decreases strongly with the distance from the upper edge of the gap, but it does not vanish because of the overlapping of bands.

The overlapping of energy bands for TIs with narrower bare bands is smaller and a decrease in the density of states is stronger. In a narrow-gap TI where hopping parameters in absolute value are much smaller than the intersite Coulomb interaction parameter, the complete separation of the FSB occurs and is accompanied by the appearance of dielectric gaps and by vanishing of the density of states. This case is demonstrated in Fig. 4.

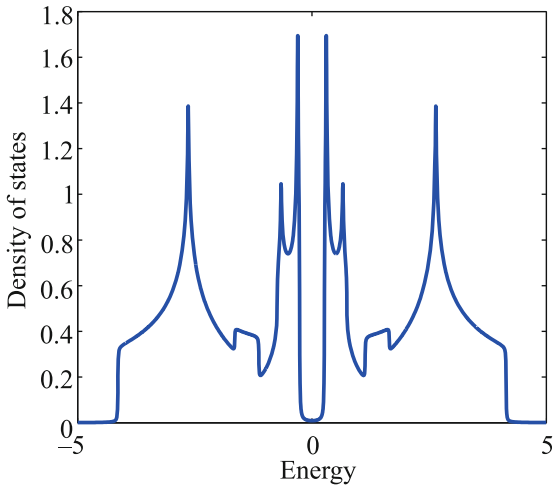

Fig. 3. (Color online) Fermion density of states of the topological insulator within the BHZ + V model. The parameters are the same as in Fig. 1.

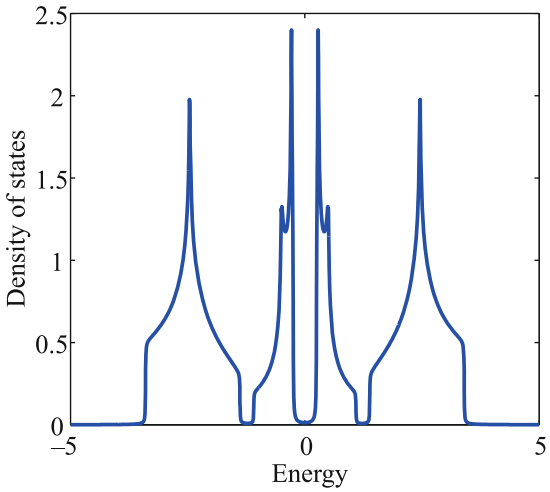

Fig. 4. (Color online) Fermion density of states of the narrow-gap topological insulator within the BHZ + V model obtained with the parameters $t_a = -0.3$, $t_b = 0.3$, and the other parameters the same as in Fig. 1.

5. SPECTRUM OF EDGE STATES IN THE BHZ + V MODEL

It is a relevant problem to determine the position of the spectrum of edge states in TIs with the split band structure. To solve this problem, the above system of self-consistent equations was solved for cylinder geometry. The calculated energy structure is shown in Fig. 5. For the sake of clarity, the spectrum is shown for the part of the Brillouin zone corresponding to relatively low quasimomenta in the direction for which periodic boundary conditions are used. It is seen that the energies of edge states are between the valence FSB and FSB of conduction electrons.

This result means that the features of the energy structure caused by charge fluctuations are of significant importance for the interpretation of the properties of Tis. Since changes are expected in materials where the intersite Coulomb interaction parameter is not small, some remarks are in order concerning the parameter V in the CdTe/CdHg/CdTe quantum well described within the BHZ model.

In this model, spin–orbit coupling enters into the zeroth Hamiltonian used to construct the actual basis of electronic states of the Te ion [3]. Only the two lowest spin orbitals are taken into account, whereas the upper spin orbitals are ignored.

This approach is justified if the hopping parameter between spin orbitals belonging to neighboring Te ions is smaller than the spin–orbit coupling constant. This condition restricts the allowed hopping parameter values of the valence band: $|t_b| \lesssim |\lambda|$, where λ is the spin–orbit coupling constant. Taking into account real λ values, one can expect that the Coulomb interaction between electrons located on neighboring Te and Hg ions corresponds to the case where V is not smaller than other energy parameters of the BHZ model and the energy structure of the quantum well with the width corresponding to the TI regime should be described by the BHZ + V model. As seen in Fig. 5, edge states in this case are adjacent to two FSBs, where effective masses are significantly renormalized. Correspondingly, the electronic specific heat, magnetic susceptibility, and other characteristics change significantly.

6. CONCLUSIONS

To conclude, we emphasize that the ISCI between electrons in the TI phase, where the top of the valence band and the bottom of the conduction band are inverted, qualitatively changes the energy spectrum

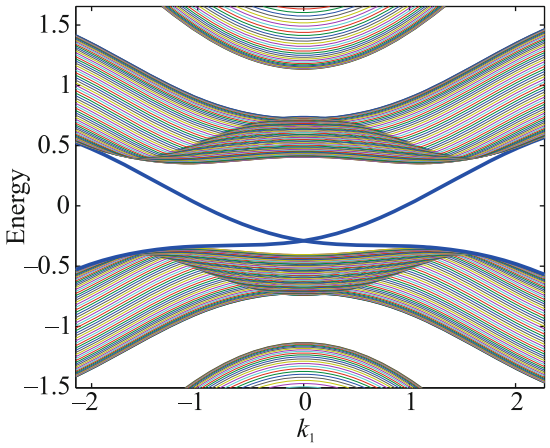

Fig. 5. (Color online) Spectrum of bulk and edge states of the topological insulator within the BHZ + V model. The parameters are the same as in Fig. 1.

and the fermion density of states when the ISCI parameter is not small compared to hopping integrals.

The main modification is due to the generation of two FSBs; as a result, the total spectrum of fermionic excitations in the TI has the four-band energy structure.

It is substantial that FSBs play the main role in the spectral and thermodynamic properties because these bands are in the immediate vicinity of the gap in the spectrum of bulk states and the spectrum of edge states in the TI is between them. Quasiparticles from FSBs with renormalized effective masses (in our case, $m^* \gtrsim 2m$) correspond to the top of the valence band and the bottom of the conduction band. Such an increase in the mass of quasiparticles is due to the correlated motion of fermions with surrounding charge fluctuations. An increase in the energy near the bottom of the conduction band is accompanied by a decrease in the density of states corresponding to a pseudogap behavior.

In the *p*-type narrow-gap topological insulator, where the intersite Coulomb interaction parameter exceeds the hopping parameters, the density of states vanishes and an additional energy gap appears.

The picture for the electron density of states near the top of the valence band is similar.

It is noteworthy that the predicted features of the energy structure caused by charge fluctuations will be characteristic not only of the model under consideration but also of other multiband models of semimetals.

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CONFLICT OF INTEREST

The author declare that he has no conflicts of interest.

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