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ABSTRACTS

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Interplay of ferromagnetism and nontrivial topology in triple layers Te-Mn-Te of $MnBi_2Te_4$

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Considering the structure of triple layers Te-Mn-Te, as a part of septuple layers Te-Bi-Te-Mn-Te-Bi-Te of the van der Waals single crystal $MnBi_2Te_4$ [1, 2], the effects of the crystal field, spin-orbit interaction, and covalent mixing between $3d$ orbitals of Mn^{2+} ions and $5p$ orbitals of Te^{2-} ions are studied. We propose the effective tight-binding model with strong electron correlations between d electrons and analyze the topology of the Fermi excitation spectrum in the ferromagnetic state.

In the framework of the formalism of the Zubarev Green's functions and Zwanzig-Mori projection technique the system of equations is obtained in the form

$$\left(\omega - \hat{M}_{k\sigma}\right)\hat{D}_{k\sigma}(\omega) = \hat{P}_{\sigma}\,,$$

where $\hat{D}_{k\sigma}$ is the Fourier transform of the matrix Green's function formed by the three-component field operator of p- and d-electrons, $\hat{P}_{k\sigma}$ is the diagonal matrix with elements (1, $N_{0\sigma}$, 1), and

$$\hat{M}_{k\sigma} = \begin{pmatrix} \varepsilon_{pk\sigma} & -t^{*}_{1k\sigma} & -t_{12k} \\ -N_{0\sigma}t_{1k\sigma} & \varepsilon_{dk\sigma} & -N_{0\sigma}t_{2k\sigma} \\ -t^{*}_{12k} & -t^{*}_{2k\sigma} & \varepsilon_{pk\sigma} \end{pmatrix}.$$

Here $N_{0\sigma} = 1 - n_d/2 + 2\sigma M$ with concentration n_d and magnetization M of d-electrons, $\varepsilon_{pk\sigma}$ and $\varepsilon_{dk\sigma}$ are the bare energies of p- and d-electrons, respectively, renormalized by

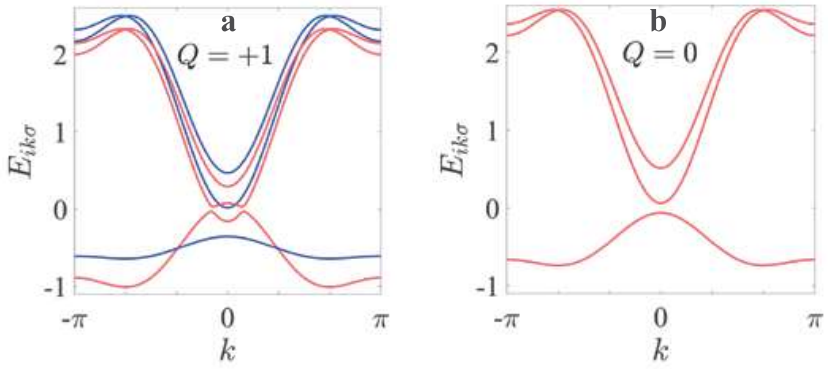

Fig. 1. Fermi excitation spectrum for two phases: **a** unsaturated ferromagnetic phase (red and blue lines correspond to the spin-splitted energy branches); **b** paramagnetic phase with the energy branches which are degenerated with respect to spin projection. In both cases chemical potential is in a gap at zero energy. The Chern number Q is nontrivial (Q = 1) in the presence of ferromagnetism and trivial (Q = 0) for paramagnetic state.

the p-d exchange interaction and kinematic interaction of Hubbard fermions [3]. The p-d hybridization is described by the functions $t_{1k\sigma}$ and $t_{2k\sigma}$, and t_{12k} is the hopping integral of p-electrons between different Te-layers.

It is crucial that $t_{1k\sigma}$ and $t_{2k\sigma}$ are complex functions depending on spin index. Therefore, nontrivial topology of the energy structure can exist when d- and p-bands are overlapped and long-range magnetic ordering is realized. It is shown that the Chern number Q of the lower filled band has the value +1 in the ferromagnetic phase which is caused by the kinematic interaction. This corresponds to the nontrivial topology of the energy structure of triple layers Te-Mn-Te in $MnBi_2Te_4$. On the contrary, the Chern number is zero and the topology is trivial in the paramagnetic phase.

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1. Otrokov M.M., Klimovskikh I.I., Bentmann H. et al.: Nature **576**, 416–422 (2019)
2. Shikin A.M., Estyunin D.A., Glazkova D.A. et al.: JETP Lett. **115**, 213–225 (2022)
3. Zaitsev R.O.: JETP **96**, 286–300 (2003)
4. Val'kov V.V., Zlotnikov A.O., Gamov A.: JETP Lett. **118**, No. 5 (2023)