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Density of Surface States in 3D Topological Insulators in the Presence of Magnetic Field with Hexagonal Warping Effect

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The behavior of the density of surface states (DOS) in 3D topological insulators of Rashba-type in the presence of static magnetic field is described in the paper. The influence of the hexagonal warping effect which is inherent to second generation of the topological insulator made on the basis of Bi_2Se_3 and Bi_2Te_3 is taken into account. In our work, a method is proposed for numerically determining the DOS, taking into account the influence of an external magnetic field. We have shown that the behavior of the DOS in these topological insulators has the qualitative differences from the behavior of 2D electron gas with spin-orbit interaction of Rashba-type without hexagonal warping effect. The results of our work have shown that in case of sufficiently weak fields, instead of the expected increase in the DOS with increasing applied magnetic field, there is observed its decrease. Estimated threshold values of the field are of the order of 1-10 G.

Keywords: Density of surface states, Topological insulator, Spin-orbit interaction, 2D electron gas, Rashba's interaction, Magnetic field, Hexagonal warping effect.

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1. INTRODUCTION

Recently, focused attention of researchers has been attracted to materials with gapless surface states, while the gap is present in the volume. They are called "topological insulators", since gapless surface states are topologically protected [1, 2]. The most important feature of topological insulators is a strong spin-orbit interaction in the volume of the material [3]. A two-dimensional electron gas with spin-orbit interaction was first considered as early as the first half of the 1980s [4], but almost immediately after the discovery of Bi_2Te_3-based topological insulators, both theoretical arguments and experimental evidence of warping of the Fermi surface form appeared [5].

The ARPES spectroscopy data convincingly show that the circular symmetry of isoenergetic curve peculiar to the Rashba Hamiltonian is replaced by a sixth-order rotation symmetry, due to the presence of a rhombohedral crystal lattice with the space group $R3\bar{m}$ in the material structure. On the sample surface, the symmetry of the crystal is reduced to the C_{3v} group, consisting of three-fold C_3 rotations around the spatial axis z and the mirror reflection operation M, thus it ultimately leads to the specified type of symmetry of surface states. As a result, the Fermi surface for 2D electrons instead of a circle acquires a shape resembling a snowflake [6]. This warping effect has a significant influence on both the energy spectrum and the density of electronic states (density of states, DOS) [7, 8].

Of considerable interest is the study of the dependence of the surface density of electronic states on an applied external magnetic field. Knowledge of this dependence is necessary to calculate a number of the most important observable characteristics of topological insulators, depending on the magnetic field, in particular, magnetic susceptibility. Nevertheless, despite the significant amount of both theoretical and experimental works in this field that have appeared in recent years [9-13], this aspect remains unexplored.

2. MODEL AND METHODS

2.1 Spectrum

In this article, topological insulators based on Bi_2Se_3 and Bi_2Te_3 are considered, for which a theory of tunneling density of surface states (TDOSS) has been developed taking into account hexagonal warping in the absence of a magnetic field [8]. The surface states are described by the Hamiltonian, with the spin-orbit interaction of Rashba and the hexagonal warping peculiar to these materials:

$$\mathcal{H} = \frac{\hbar^2(k_x^2+k_y^2)}{2m^*}\sigma_0 + \hbar v_F\left(k_x\sigma_y - k_y\sigma_x\right) + \frac{\lambda\hbar^3}{2}(k_+^3 + k_-^3)\sigma_z, \qquad (1)$$

where m^* is the effective mass, $k_\pm = k_x \pm ik_y$, $k_x = k\cos\theta$, $k_y = k\sin\theta$, σ_0 is the unit matrix, and σ_x, σ_y, σ_z are Pauli spin matrices. The field is introduced in the standard way: $\vec{p} \to \vec{p} - \frac{e}{c}\vec{A}$, the vector-potential is selected in the Landau calibration: (0, Bx, 0). Bismuth selenide is characterized by a positive, and telluride – by a negative effective mass m^* [14].

After substituting the vector-potential in (1), the Hamiltonian is written in the form:

$$\mathcal{H}(B) = \begin{pmatrix} \frac{\hbar^2}{2m^*}\left(k_x^2 + \left(k_y - \frac{eBx}{\hbar c}\right)^2\right) + \frac{\lambda\hbar^3}{2}\left[\left(k_x + i\left(k_y - \frac{eBx}{\hbar c}\right)\right)^3 + \left(k_x - i\left(k_y - \frac{eBx}{\hbar c}\right)\right)^3\right] & \hbar v_F\left(-ik_x - k_y + \frac{eBx}{\hbar c}\right) \\ \hbar v_F\left(ik_x - k_y + \frac{eBx}{\hbar c}\right) & \frac{\hbar^2}{2m^*}\left(k_x^2 + \left(k_y - \frac{eBx}{\hbar c}\right)^2\right) - \frac{\lambda\hbar^3}{2}\left[\left(k_x + i\left(k_y - \frac{eBx}{\hbar c}\right)\right)^3 + \left(k_x - i\left(k_y - \frac{eBx}{\hbar c}\right)\right)^3\right] \end{pmatrix} \qquad (2)$$

We confine ourselves to weak magnetic fields, when it is permissible to neglect the terms above the first order in the field. The diagonalization of the Hamiltonian (2) when taking into account the assumption made gives:

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$$E\left(k_x,k_y,B\right)=\frac{\hbar^2}{2m^*}\left(k^2-\frac{2e}{\hbar c}Bxk\sin\theta\right)\pm\sqrt{\hbar^2v_F^2\left(k^2-\frac{2e}{\hbar c}Bxk\sin\theta\right)+\lambda^2\hbar^6\left(k^6\cos^2 3\theta+6\frac{e}{\hbar c}Bxk^5\cos 3\theta\sin 2\theta\right)}. \quad (3)$$

The upper sign corresponds to the conduction band, the lower – to the valence band. In the following, we limit ourselves to a single-band approximation and we will make calculations only for the conduction band.

Following this research work [8], we will introduce energy parameters $\Delta=2|m^*|v_F^2$ and $E_0=\sqrt{v_F^3/\lambda}$, as well as a dimensionless parameter $\alpha=(\Delta/E_0)^4$. Then $=p/(2|m^*|v_F)=pv_F/\Delta$, $\lambda^2=\alpha v_F^6/\Delta^4$, $E=\varepsilon\Delta$, where ρ and ε are non-dimensional parameters corresponding to momentum and energy. In addition, we introduce another dimensionless parameter corresponding to the magnetic field: $\beta=eBx/(|m^*|cv_F)$. After substituting the specified parameters in the expression for $E\left(k_x,k_y,B\right)$ we obtain (for negative effective mass):

$$E(\eta,\theta,\beta)=\Delta\left(-\rho^2+\beta\rho\sin\theta+\sqrt{\rho^2+\alpha\rho^6\cos^2 3\theta-\beta(\rho\sin\theta-3\alpha\rho^5\sin 2\theta\cos 3\theta)}\right). \quad (4)$$

The graphs of isoenergetic curves (4) for $\alpha=0.4$ (bismuth selenide) and for $\alpha=22$ (bismuth telluride) for different values of the parameter β are shown in Fig. 1 and Fig. 2. It can be seen from the above figures that the influence of an external magnetic field breaks the 6th order rotational symmetry.

2.2 Density of States

The TDOSS is written as:

$$g(E,B)=\int_0^\infty\frac{kdk}{(2\pi)^2}\int_0^{2\pi}d\theta\delta\left(E-E_s(k,\theta)\right). \quad (5)$$

To calculate the DOS in order to be able to use the results of [8], we will use the parameterization:

$$\hbar^2k^2=\frac{\eta\Delta^2}{v_F^2}.$$

Then the dimensionless spectrum for negative effective mass will take the following form:

$$E(\eta,\theta,\beta)=\Delta\left(-\eta+\beta\eta^{\frac{1}{2}}\sin\theta+\sqrt{\eta+\alpha\eta^3\cos^2 3\theta-\beta\left(\eta^{\frac{1}{2}}\sin\theta-3\alpha\eta^{\frac{5}{2}}\sin 2\theta\cos 3\theta\right)}\right). \quad (4.1)$$

We take advantage of the smallness of the parameter β and decompose (4.1) in a row, limiting ourselves to the linear additive components:

$$-\eta+\beta\eta^{\frac{1}{2}}\sin\theta+\sqrt{\eta+\alpha\eta^3\cos^2 3\theta-\beta\left(\eta^{\frac{1}{2}}\sin\theta-6\alpha\eta^{\frac{5}{2}}\sin 2\theta\cos 3\theta\right)}\approx$$

$$\approx-\eta+\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}+\left(\frac{3\alpha\eta^{5/2}\sin 2\theta\cos 3\theta}{2\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}}-\frac{\eta^{\frac{1}{2}}\sin\theta}{2\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}}+\eta^{\frac{1}{2}}\sin\theta\right)\beta.$$

Substituting this expression into (5), we get:

$$g(\varepsilon,\alpha,\beta)=\frac{1}{(2\pi)^2}\frac{|m^*|\Delta}{\hbar^2}\int_0^\infty d\eta\int_0^{2\pi}d\theta\delta\left(\Delta\left(\varepsilon+\eta-\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}-\left(\frac{3\alpha\eta^{5/2}\sin 2\theta\cos 3\theta}{2\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}}-\frac{\eta^{\frac{1}{2}}\sin\theta}{2\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}}+\eta^{\frac{1}{2}}\sin\theta\right)\beta\right)\right).$$

Using the properties of the δ-function, the expression for the DOS can be given the form:

$$g(E,B)=\frac{|m^*|}{\pi\hbar^2}F(\varepsilon,\alpha,\beta), \quad (6)$$

where

$$F(\varepsilon,\alpha,\beta)=\frac{1}{4\pi}\int_0^\infty\frac{d\eta}{\left|\frac{\partial f(\varepsilon,\alpha,\beta,\eta,\theta)}{\partial\theta}\right|_{\theta_0}}$$

$$f(\varepsilon,\alpha,\beta,\eta,\theta)=$$
$$\varepsilon+\eta-\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}--\left(\frac{3\alpha\eta^{5/2}\sin 2\theta\cos 3\theta}{2\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}}-\right.$$
$$\left.\frac{\eta^{\frac{1}{2}}\sin\theta}{2\sqrt{\eta+\alpha\eta^3\cos^2 3\theta}}+\eta^{\frac{1}{2}}\sin\theta\right)\beta,$$

θ_0 are the roots of the equation $f(\varepsilon,\alpha,\beta,\eta,\theta)=0$.

The equation $f(\varepsilon,\alpha,\beta,\eta,\theta)=0$ was solved numerically by the iteration method with the given parameters ε, α and β. Having in mind the smallness of the field parameter β, and the fact that the dependence of the solution on it should be a continuous function, we can expect that the roots of this equation will be near the "unperturbed" solutions $\theta_0^{(0)}=\frac{1}{3}\arccos\sqrt{\frac{(\epsilon+\eta)^2-\eta}{\alpha\eta^3}}$ corresponding to the spectrum without a magnetic field [8]. Therefore, it is natural to take the point $\theta_0^{(0)}$ as a zero approximation when iterating. Solutions of the "perturbed" equation $\theta_0(\eta)$ are substituted into the expression for the derivative $\frac{\partial f(\varepsilon,\alpha,\beta,\eta,\theta)}{\partial\theta}$ and for given parameters ε,α,β the dependence $\varphi(\eta)=\frac{\partial f(\varepsilon,\alpha,\beta,\eta,\theta_0(\eta))}{\partial\theta}$ is approximated.

Then the latter is substituted into the integral and (numerically) integrated within the limits determined by the solutions of the system of inequalities:

$$\begin{cases}0\le\dfrac{(\epsilon+\eta)^2-\eta}{\alpha\eta^3}\le 1\\ \eta\ge 0,\end{cases}$$

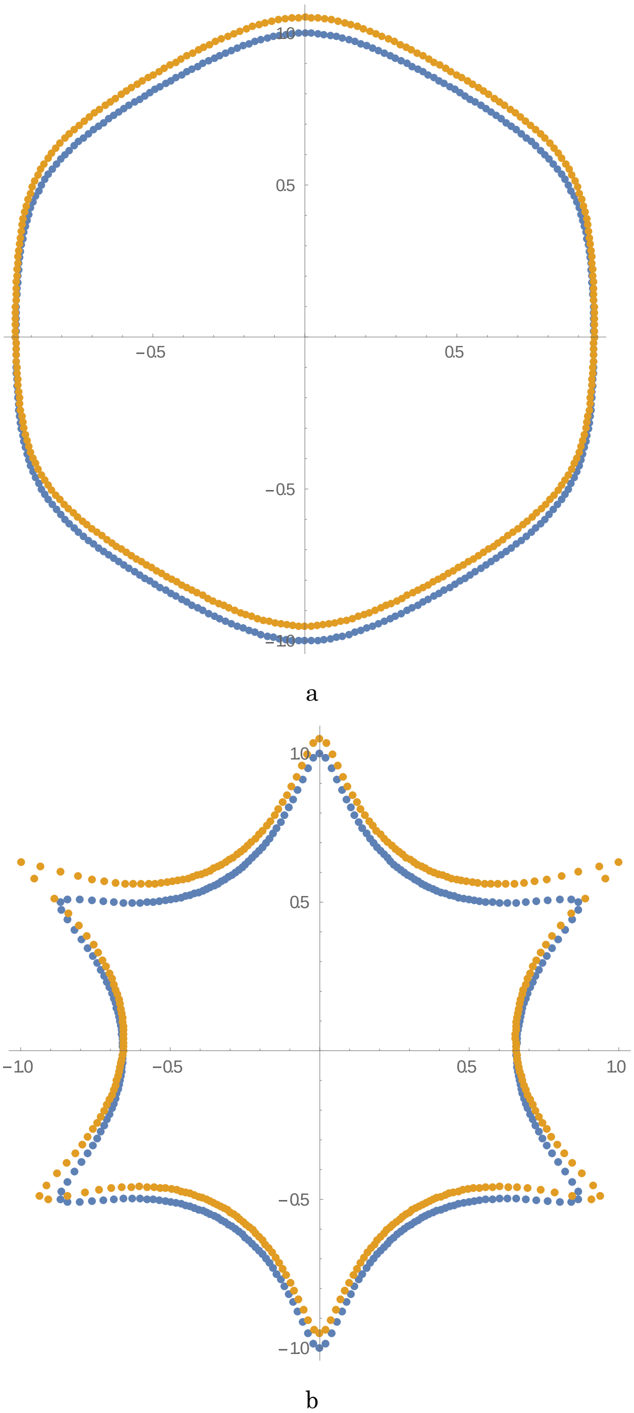

Fig. 1 – The isoenergetic curves with $\varepsilon = 2.0$ and $\alpha = 0.4$ for $\beta = 0$ (blue line) and $\beta = 0.1$ (orange line) (a), with $\varepsilon = 2.0$ and $\alpha = 25$ for $\beta = 0$ (blue line) and $\beta = 0.1$ (orange line) for a positive effective mass (b)

expressing the conditions for the existence of real solutions $\theta_0^{(0)}$.

The criterion of "weakness" of the field, which is necessary for numerical estimates, is obtained from the expanding $\left(k\sin\theta - \frac{e}{\hbar c}Bx\right)^2$:

$$\frac{2e}{\hbar c}Bxk\sin\theta \gg \left(\frac{e}{\hbar c}Bx\right)^2$$
$$Bx \ll \frac{2\hbar c}{e}k\sin\theta.$$

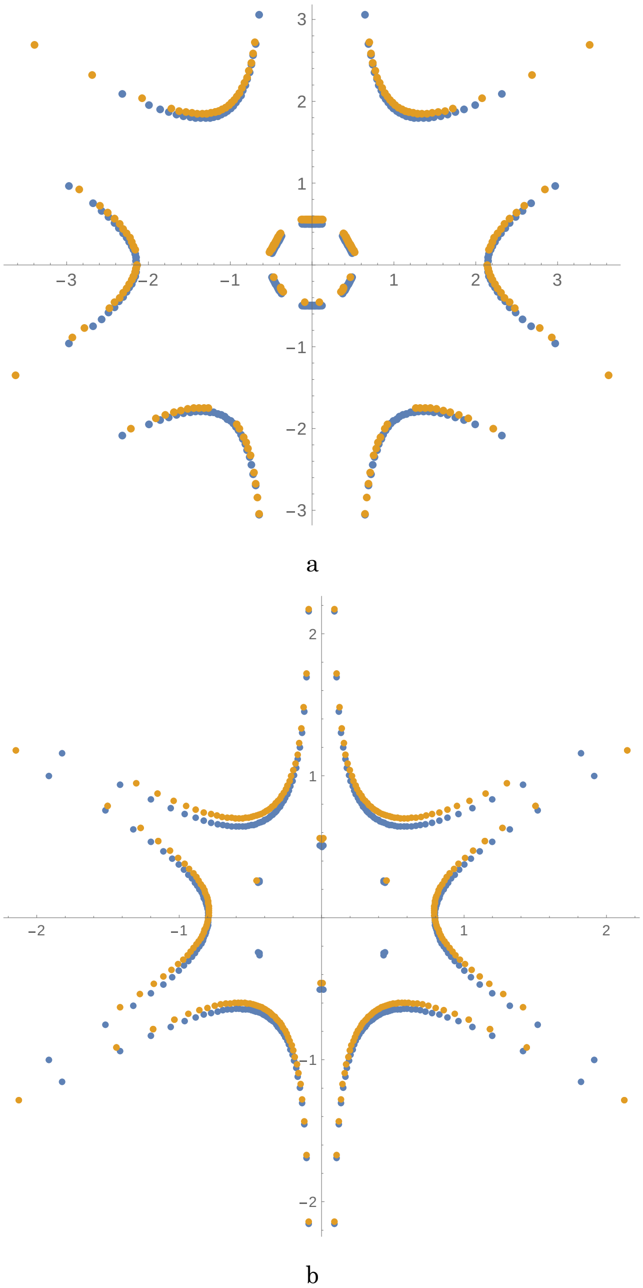

Fig. 2 – The isoenergetic curves with $\varepsilon = 2.0$ and $\alpha = 0.4$ for $\beta = 0$ (blue line) and $\beta = 0.1$ (orange line) (a), with $\varepsilon = 2.0$ and $\alpha = 25$ for $\beta = 0$ (blue line) and $\beta = 0.1$ (orange line) for a negative effective mass (b)

From here you can also get an estimate for β:

$$\beta = \frac{eBx}{|m^*|cv_F}$$
$$|m^*|v_F\beta \ll 2\hbar k\sin\theta$$
$$\beta \ll \frac{2\hbar k\sin\theta}{|m^*|v_F}.$$

Using the data given in [5] and [14] ($|m^*|/m = 0.3$; $v_F = 2.1$ eV·Å for Bi_2Se_3 and 3.8 eV·Å for Bi_2Te_3, $k \sim 0.1$) Å^{-1} and considering $\sin\theta \sim 1$, we have $\beta \ll 1$.

3. DISCUSSION

The graphs of the function of energy $F(\varepsilon, \alpha, \beta)$ for

$\alpha = 0.4$ (bismuth selenide) and for $\alpha = 22$ (bismuth telluride) for different values of the field are shown, respectively, in Fig. 3 and Fig. 4. The results in the absence of the field correspond to those obtained in [8]. In the case of Bi_2Se_3, there are two van Hove singularities at $\varepsilon \approx 0.175$ and 0.25. The magnitude of the magnetic field does not affect their location, and also has little effect on the behavior of the DOS up to the nearest neighborhood of the first singularity. For Bi_2Te_3, on the contrary, there is a single van Hove singularity with $\varepsilon \approx 0.25$. The effect of the field on the DOS is much more pronounced – it is significant over the entire energy range, and also significantly shifts the position of the van Hove singularity. In addition, in this case, the DOS in the investigated energy range is characterized by a very non-trivial behavior: to the left of the van Hove singularity, for $\varepsilon < 0.25$, the DOS decreases with increasing magnetic field, and to the right, for $\varepsilon > 0.25$, it increases (Fig. 4).

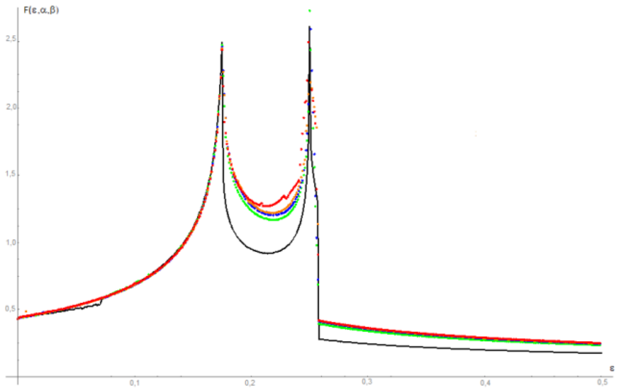

Fig. 3 – Density of states depending on the energy ε at $\alpha = 0.4$ for $\beta = 0$ (black line), $\beta = 0.001$ (green line), $\beta = 0.005$ (blue line), $\beta = 0.01$ (orange line) and $\beta = 0.02$ (red line)

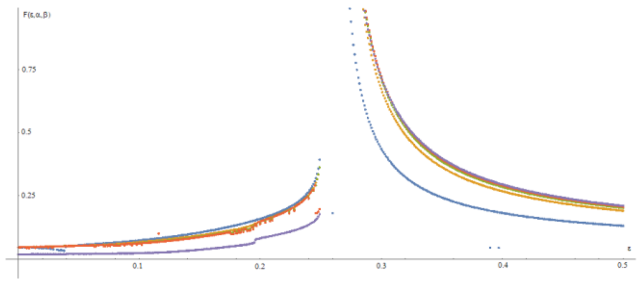

Fig. 4 – Density of states as a function of energy ε at $\alpha = 22$ for $\beta = 0$ (blue line), $\beta = 0.001$ (orange line), $\beta = 0.005$ (green line), $\beta = 0.01$ (red line) and $\beta = 0.02$ (purple line)

The dependence of the function *F(ε, α, β)* on the magnitude of the applied magnetic field is shown in Fig. 5-Fig. 8. Some general features of the behavior of the DOS for both materials can be noted. When the parameter $\varepsilon > 0.25$, a decrease in the DOS is observed with increasing parameter ε. Also common is the behavior of DOS as a function of the magnitude of the magnetic field β: a characteristic sharp increase at the beginning and a relatively slow decrease with a further increase in the “afield parameter”. Using the data from the previous section, it is easy to estimate the magnitude of the magnetic field and energy for which this effect can be expected. If we take $x = 10^{-2}$ cm, we get for $B \simeq 3$ G.

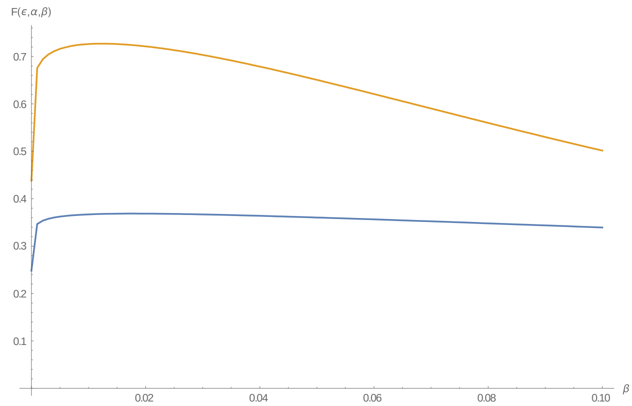

Fig. 5 – The dependence of the density of states on the magnitude of the magnetic field at $\varepsilon = 0.30$ for $\alpha = 0.4$ (blue line) and $\alpha = 22$ (orange line)

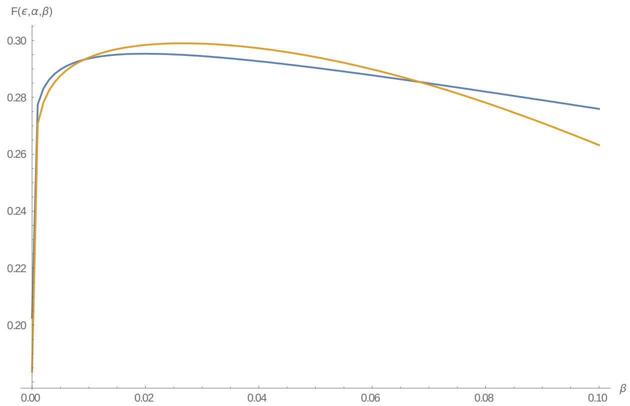

Fig. 6 – The dependence of the density of states on the magnitude of the magnetic field at $\varepsilon = 0.40$ for $\alpha = 0.4$ (blue line) and $\alpha = 22$ (orange line)

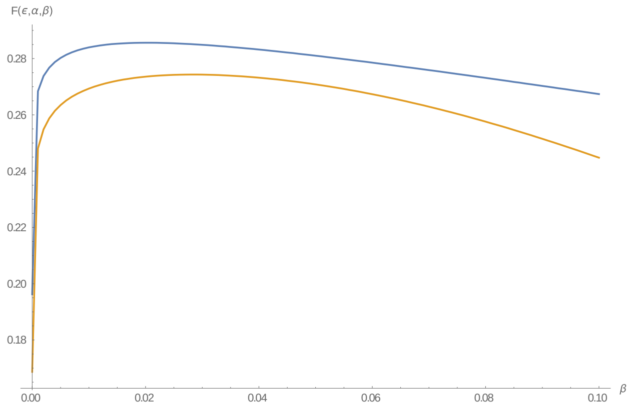

Fig. 7 – The dependence of the density of states on the magnitude of the magnetic field at $\varepsilon = 0.42$ for $\alpha = 0.4$ (blue line) and $\alpha =$ (orange line)

To explain this behavior of the DOS, it is convenient to first consider the case of the absence of hexagonal distortions. To do this, in the spectrum (4) it is enough to set $\alpha = 0$. As a result, we will have:

$$E(\rho,\theta) = \Delta\left(\rho^2 - \beta\rho\sin\theta \pm \sqrt{\rho^2 - \beta\rho\sin\theta}\right). \quad (7)$$

The isoenergetic curves corresponding to such a spectrum are circles with a center that is offset from the origin. The DOS in this case is:

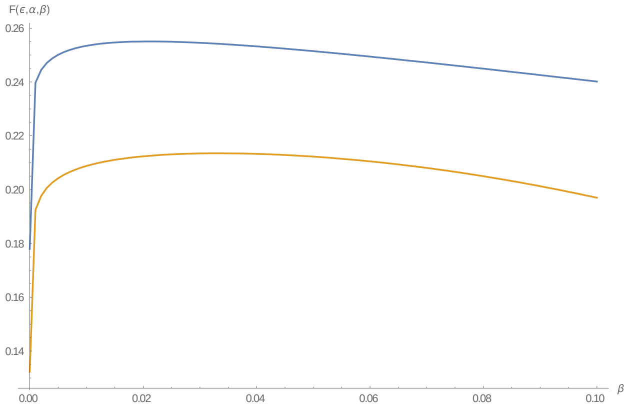

Fig. 8 – The dependence of the density of states on the magnitude of the magnetic field at $\varepsilon = 0.50$ for $\alpha = 0.4$ (blue line) and $\alpha = 22$ (orange line)

$$g(E) = \frac{2|m^*|\Delta}{(2\pi\hbar)^2}\int_0^\infty \rho d\rho \int_0^{2\pi} d\theta \delta\left(\Delta\left(\varepsilon - \rho^2 + \beta\rho\sin\theta \mp \sqrt{\rho^2 - \beta\rho\sin\theta}\right)\right).$$

After the transformations, which are generally similar to those carried out upon getting the expression (6), we obtain for the conduction band:

$$g(E,B) = \frac{|m^*|}{\pi\hbar^2}F_0(\varepsilon,\beta), \tag{8}$$

where

$$F_0(\varepsilon,\beta) = \frac{1}{2\pi}\int_{|\sin\theta|\le 1} \frac{\rho d\rho}{\left(1 + \frac{1}{2\sqrt{\frac{\rho^4 - \varepsilon^2}{2\rho^2 - 2\varepsilon - 1}}}\right)\sqrt{\frac{\beta^2\rho^2(2\rho^2 - 2\varepsilon - 1)^2 - (\rho^4 - (2\varepsilon + 1)\rho^2 + \varepsilon^2)^2}{(2\rho^2 - 2\varepsilon - 1)^2}}}$$

The region of the integration extends to all values of the momenta corresponding to the real θ determined by the roots of the equation $\varepsilon - \varepsilon(\rho,\theta) = 0$:

$$\left|\frac{\rho^4 - (2\varepsilon + 1)\rho^2 + \varepsilon^2}{\beta\rho(2\rho^2 - 2\varepsilon - 1)}\right| \le 1$$

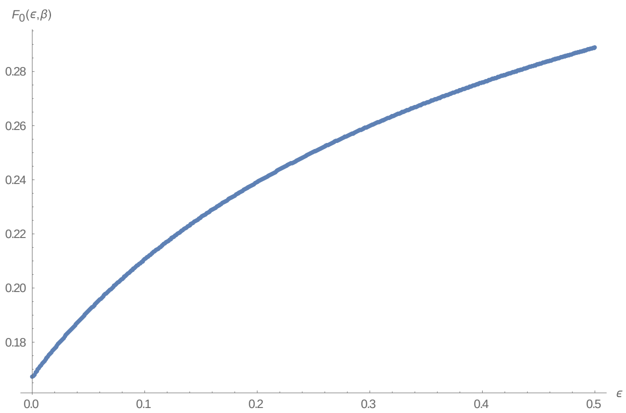

Fig. 9 – The dependence of the density of states on the energy in the case of the absence of hexagonal distortions with $\beta = 0.05$

Graphs of the function of energy $F_0(\varepsilon,\beta)$ and the magnitude of the magnetic field are shown in Fig. 9 and Fig. 10.

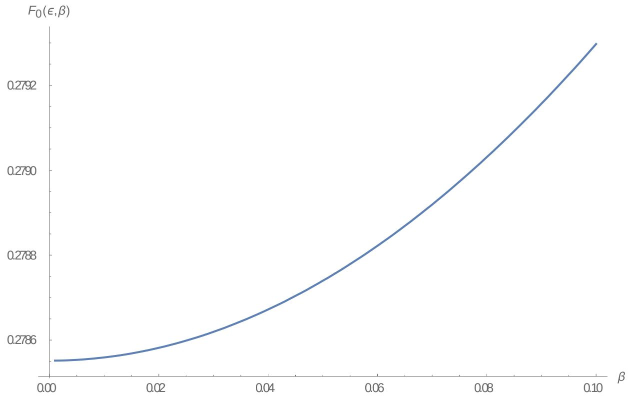

Fig. 10 – The dependence of the density of states on the magnetic field in the absence of hexagonal distortion with $\varepsilon = 0.42$

As L. Fu [5] points out, in the two-dimensional case for Fermi surfaces close in their shape to circles, there are only two stationary points at which the momenta are directed oppositely. Since in the topological insulators the spins and momenta of the electrons are interconnected, at the stationary points the spins will also be opposite. This circumstance makes scattering impossible and the electron states at stationary points turn out to be protected by symmetry with respect to time reversal. Therefore, in the absence of hexagonal distortions, an increase in the DOS due to the splitting of Landau levels is possible with increasing magnetic field (assuming that the field remains weak).

However, with a decrease in symmetry to the 6th order, several pairs of stationary points appear on the Fermi surface, in which, due to the complex shape of the Fermi surface, the momenta are no longer directed oppositely and therefore scattering is allowed between them, breaking symmetry with respect to time reversal. The applied external magnetic field also breaks symmetry with respect to time reversal and, in combination with the hexagonal distortion factor, the field growth leads first to a slowdown in the DOS, and later to its decrease (Fig. 5-Fig. 8). Thus, it can be assumed that the cause of a decrease in the DOS with an increase in the magnetic field is the breaking of the symmetry of the system caused by it with respect to time reversal, which results in a decrease in the symmetry of the spectrum of electronic states, which is clearly seen in Fig. 1 and Fig. 2. The results of a number of works [15-17] confirm this assumption. In particular, the authors of [15] note that with an increase in the external magnetic field, the form of the dependence of the nonlocal material resistance on the distance between the reading terminals from the power law to the exponential varies qualitatively. Experimental works [16, 17] describe a decrease in nonlocal resistance with the increase of external magnetic field, and also recorded the transition from the state of a topological insulator to the state of a trivial zone insulator when the field reaches a certain critical value, which corresponds to the disappearance of nonlocal resistance. The appearance of a gap in the energy spectrum of surface electrons due to the growth of the magnetic field applied to the topological insulator is a weighty argument in favor of our considerations.

4. CONCLUSIONS

Thus, we investigated the behavior of the DOS of Bi_2Se_3 and Bi_2Te_3 in an external constant magnetic field taking into account the hexagonal warping effect. The DOS in these materials is characterized by a very complex behavior under the influence of magnetic fields. We have obtained the dependences of the DOS on the energy for different values of the magnetic field strength. We also obtained the dependences of the DOS on the magnitude of the magnetic field. We have found that the behavior of DOS with an increase in the applied magnetic field in a structure with hexagonal warping effect is qualitatively different from its behavior in the usual 2D Rashba electron gas. The method we used to calculate the density of states is applicable only for weak fields. However, our study shows that even weak fields of the order of 1-10 G can break time reversal symmetry, thereby affecting the magnitude and behavior of the density of states.

We believe that the results of our work will be useful for calculating the macroscopic characteristics of topological insulators based on Bi_2Se_3 and Bi_2Te_3 (in particular, magnetic susceptibility).

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Щільність поверхневих станів в 3D топологічних ізоляторах у присутності магнітного поля з урахуванням гексагональних спотворень решітки

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Описано поведінку щільності поверхневих станів (DOS) в 3D топологічних ізоляторах Rashba-типу у присутності статичного магнітного поля. Враховується вплив гексагонального ефекту викривлення, властивого другому поколінню топологічного ізолятора, виконаного на основі Bi_2Se_3 і Bi_2Te_3. У роботі запропоновано метод чисельного знаходження DOS, що враховує вплив зовнішнього магнітного поля. Ми показали, що поведінка DOS в цьому топологічному ізоляторі має якісні відмінності від поведінки 2D електронного газу зі спін-орбітальною взаємодією Rashba-типу без гексагонального ефекту викривлення. Результати нашої роботи показали, що вже у випадку досить слабких полів замість очікуваного зростання DOS зі збільшенням прикладеного магнітного поля спостерігається її зменшення. Оцінки порогової величини поля дають порядок 1-10 Гс.

Ключові слова: Щільність поверхневих станів, Топологічний ізолятор, Спін-орбітальна взаємодія, 2D електронний газ, Взаємодія Rashba, Магнітне поле, Гексагональний ефект викривлення.