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Non-ideal experimental Berry phase in the topological insulator Bi_2Se_3 single crystal

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Abstract. Magnetoresistivity and Hall resistivity of a bulk Bi_2Se_3 single crystal are investigated. It is found that in high magnetic fields (above 7 T), the Shubnikov – de Haas effect is observed. The Berry phase determined using the standard Lifshitz – Onsager formalism is $\Phi_B \approx 0.8\pi$, which indicates the presence of Dirac fermions in the system. At the same time, Φ_B deviates from the ideal π value. It is shown that it is important to take into account the Zeeman interaction and the non-ideality of the Dirac dispersion relation for surface states for correct description of topological effects.

Keywords: Berry phase, magnetoresistivity, Shubnikov – de Haas oscillations, Landau level fan diagram, Hall effect, topological insulator, Bi_2Se_3

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Материалы конференции
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Неидеальная экспериментально наблюдаемая фаза Берри в монокристалле топологического изолятора Bi_2Se_3

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Аннотация. Проведено исследование магнитосопротивления и сопротивления Холла объемного монокристалла Bi_2Se_3. Обнаружено, что в сильных магнитных полях выше 7 Т наблюдается эффект Шубникова – де Гааза. Определенная с помощью стандартного формализма Лифшица – Онсагера фаза Берри $\Phi_B \approx 0.8\pi$, что говорит о наличии дираковских фермионов в исследуемой системе. В то же время значение Φ_B отлично от идеального, равного π. Показано, что для корректного описания этого эффекта важен учет зеемановского расщепления и неидеальности дираковского закона дисперсии для поверхностных состояний.

Ключевые слова: фаза Берри, магнитосопротивление, осцилляции Шубникова – де Гааза, веерная диаграмма уровней Ландау, эффект Холла, топологический изолятор, Bi_2Se_3

Финансирование: Исследование магнитосопротивления, эффекта Холла и осцилляций Шубникова – де Гааза (раздел 3.1) выполнено за счет гранта Российского научного фонда (проект №24-72-00168, https://rscf.ru/project/24-72-00168/, Институт физики металлов имени М.Н. Михеева Уральского отделения Российской академии наук, Свердловская обл.). Анализ фазы Берри (раздел 3.2) выполнен в рамках государственного задания Министерства науки и высшего образования Российской Федерации (тема «Спин» № 122021000039-4).

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Introduction

One of the interesting concepts in condensed matter physics is the concept of the Berry phase. In general, the Berry phase is defined as the phase acquired by the wave function when the system changes adiabatically along a closed loop in the parameter space [1, 2]. Attention to it has increased significantly with the discovery of topological insulators (TIs), since it allows to evaluate the topology of the system and the presence of Dirac fermions. The Berry phase, or the so-called topological invariant, occurs when an electron moves along a two-dimensional Fermi surface around a Dirac point in the 2D Brillouin zone. It is equal to π for Dirac fermions with a linear dispersion relation and vanishes for ordinary electrons with a quadratic dispersion relation [3]. The discovery of this concept has made it possible to explain many effects in condensed matter physics, such as a topological electric polarization, weak antilocalization, anomalous Hall effect, etc.

Magnetotransport studies remain one of the most powerful tools for determining the Berry phase to this day [4–6]. An electron inevitably moves along closed trajectories in a magnetic field and, as a result, acquires the Berry phase reflected in the phase of Shubnikov – de Haas (SdH) oscillations

$$\Delta\rho_{xx} \propto \cos\left[2\pi\left(\frac{F}{B}+\frac{1}{2}-\beta\right)\right], \tag{1}$$

where F is the oscillation frequency and β is the phase factor related to Berry phase $\Phi_B = 2\pi\beta$.

The experimental Berry phase was found to be different from the ideal π value in most TIs, which still remains one of the subjects of discussion [6–8]. In the present work, the magnetotransport properties of a TI Bi_2Se_3 single crystal were investigated. We found that the Berry phase, determined from SdH oscillations, deviates from π. We show that it is possible to explain the shift in the observed Berry phase using a simple model that takes into account the Zeeman interaction and the curvature of the Dirac dispersion relation.

Materials and Methods

The single crystal of the TI Bi_2Se_3 was synthesized by the Bridgman – Stockbarger method and this is described in detail in our previous work [9]. The magnetoresistivity and Hall resistivity were measured by the four-contact method in magnetic fields up to 9 T at a temperature of 8 K using the Physical Property Measurement System (PPMS–9, Quantum Design) at the Collaborative Access Center of IMP UB RAS.

Results and Discussion

3.1. Magnetoresistivity, Hall effect and SdH oscillations.

Fig. 1, *a* shows the field dependence of the magnetoresistivity $MR = (\rho_{xx} - \rho_0)/\rho_0 \cdot 100\%$ of the investigated Bi_2Se_3 single crystal. Here ρ_0 is the resistivity measured in zero field, and ρ_{xx} is the resistivity measured in non-zero field. It can be seen that the magnetoresistivity increases monotonously, reaching small values of ~ 1.45%, which is strongly related to low value of carrier mobility, $\mu \approx 600$ cm^2/Vs, determined from the Hall resistivity measurement (Fig. 1, *b*). The dependence ρ_{xy}(B) is negative and linear, and the slope of this gives the bulk electron concentration $n_h \approx 4.5 \cdot 10^{19}$ cm^{-3}. Such a high value of carrier concentration and a low value of mobility indicates the presence of a large number of defects in our sample [10].

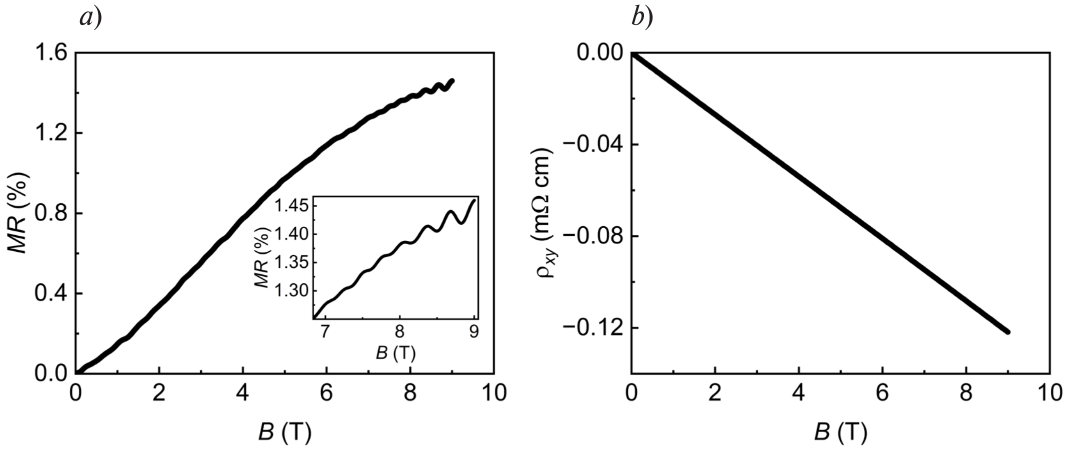

Fig. 1. Field dependence of magnetoresistivity of the Bi_2Se_3 single crystal at T = 8 K (*a*), the inset shows the SdH oscillations; field dependence of Hall resistivity for Bi_2Se_3 single crystal at T = 8 K (*b*)

SdH oscillations caused by the formation of Landau levels in a high magnetic field (see inset in Fig 1, *a*) can be detected in fields above ~7 T. Quantum oscillations are clearly observed in the second derivative $-d^2MR/dB^2$, plotted as a function of the inverse magnetic field (Fig. 2, *a*). Fig. 2, *b* shows the fast Fourier transform, which determines that the observed oscillations correspond to a single frequency F = 217 T. Using the Onsager relation

$$F = \left(\frac{\hbar}{2\pi e}\right)\pi k_F^2, \tag{2}$$

we can determine the Fermi wave vector k_F = 0.081 Å^{-1}, as well as the 2D $n_{SdH}^{2D} = k_F^2/4\pi = 5.22 \cdot 10^{12}$ cm^{-2} and 3D $n_{SdH}^{3D} = k_F^3/3\pi^2 = 1.8 \cdot 10^{19}$ cm^{-3} carrier concentrations. It should be noted that the k_F is in good agreement with that determined from ARPES for surface states in [11].

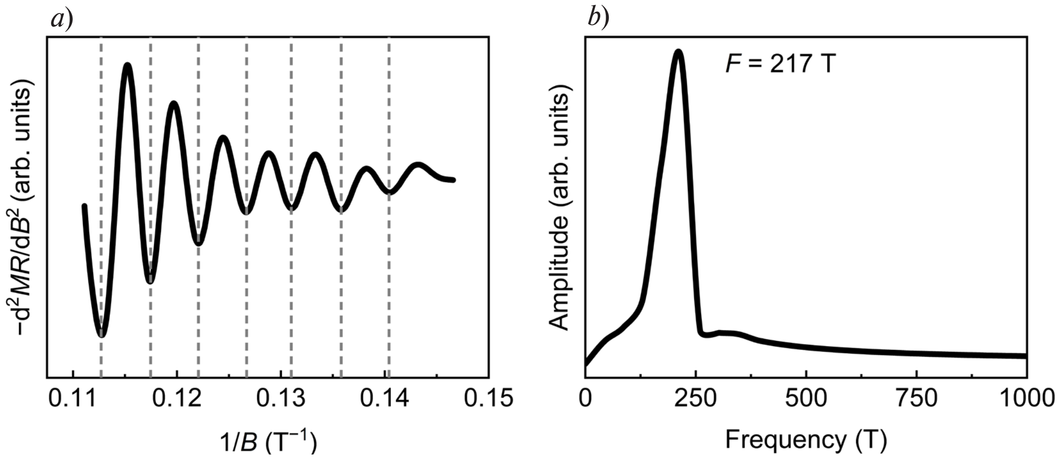

Fig. 2. Dependence of $-d^2MR/dB^2$ on inverse magnetic field (*a*).
Fast Fourier transform with single oscillation frequency equal to 217 T (*b*)

3.2. Berry phase analysis.

A standard way to determine the Berry phase from the SdH oscillations is to construct a Landau level (LL) fan diagram using the Lifshitz – Onsager quantization rule [3]

$$n = \frac{F}{B} + \beta. \quad (3)$$

The LL indexes n are a linear function of the inverse magnetic field, the slope of which determines the oscillation frequency, and the intercept determines β, which is equal to 0.5 for Dirac fermions and 0 for ordinary electrons [6]. We used the standard method and assigned integer LL indexes to the minima and half-integer ones to the maxima of $-d^2MR/dB^2$. Fig. 3, *a* shows the LL fan diagram, which gives F = 218 T and $\beta \approx 0.4$ (see Fig. 3, *b*). It is clearly seen that the Berry phase is different from 0, which indicates the presence of Dirac fermions in our system. At the same time, Φ_B, determined in such a way is also different from the ideal π value.

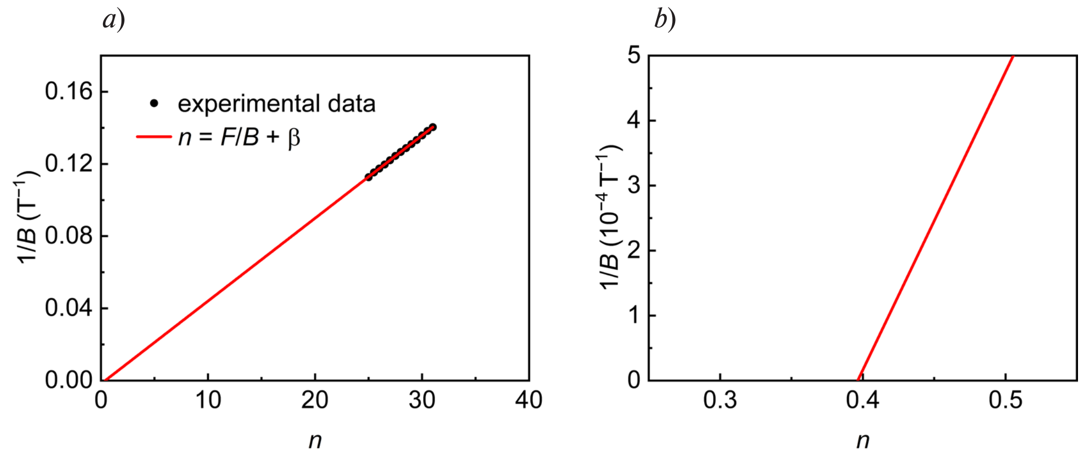

Fig. 3. LL fan diagram constructed using the Lifshitz – Onsager quantization rule
Black dots show the experimental values of the integer and half-integer LL indexes (*a*); LL fan diagram near zero Landau level (*b*), indicating that the intercept is close to 0.4

It is well-known that the surface dispersion relation in topological insulators has a non-ideal linear dependence on the wave vector. On the other hand, it is also known that strong spin-orbit coupling can give rise to strong Zeeman interaction. Both of these factors will lead to an additional shift of the Landau levels and, accordingly, the observed Berry phase. The minimal model that takes these factors into account is given by the Hamiltonian [6]

$$\widehat{H} = v_F\left(\Pi_x\sigma_y - \Pi_y\sigma_x\right) + \frac{\Pi^2}{2m^*} - \frac{1}{2}g_s\mu_B B\sigma_z, \quad (4)$$

where $\Pi = \hbar\mathbf{k} + e\mathbf{A}$ with $\mathbf{A} = (0, B_x, 0)$, σ_i are the Pauli matrices, m^* is the effective mass, v_F is the Fermi velocity, μ_B is the Bohr magneton, and g_s is the surface g-factor. The eigenvalues of the LL energies are determined as [6]

$$E_N = \hbar\omega_c N + \sqrt{2\hbar v_F^2 eBN + \left(\frac{1}{2}\hbar\omega_c - \frac{1}{2}g_s\mu_B B\right)^2}, \quad (5)$$

where $\omega_c = eB/m^*$ is the cyclotron frequency. Taking into account that $E_N(B_N) = E_F$ with $E_F = \hbar v_F k_F + \hbar^2 k_F^2/2m^*$, where k_F is given by Eq. (2), we can use Eq. (5) to fit our experimental data. We took $m^* = 0.25m_0$ and $v_F = 3\cdot10^5$ m/s from the ARPES experiments [12] and used F and g_s as two free parameters. Fig. 4, *a* shows the LL fan diagram, where the green and blue dashed lines correspond to fermions with linear and quadratic dispersion relation, respectively, and the solid red line corresponds to the best fitting parameters (g_s = 55 or − 39 and F = 217.6 T) given by Eq. (5). For comparison, we also calculated the curve for zero g-factor, shown as a violet solid line. The inset in Fig. 4, *a* shows the experimental and calculated data after subtracting the contribution corresponding to ideal Dirac fermions. From this, it is clearly seen that taking into account only the finite effective mass leads to only a very small deviation from the ideal situation with the π Berry phase. Taking into account also the g-factor best describes the experimental data and leads to a stronger deviation from the ideal line, which explains the non-ideal value of the observed Berry phase.

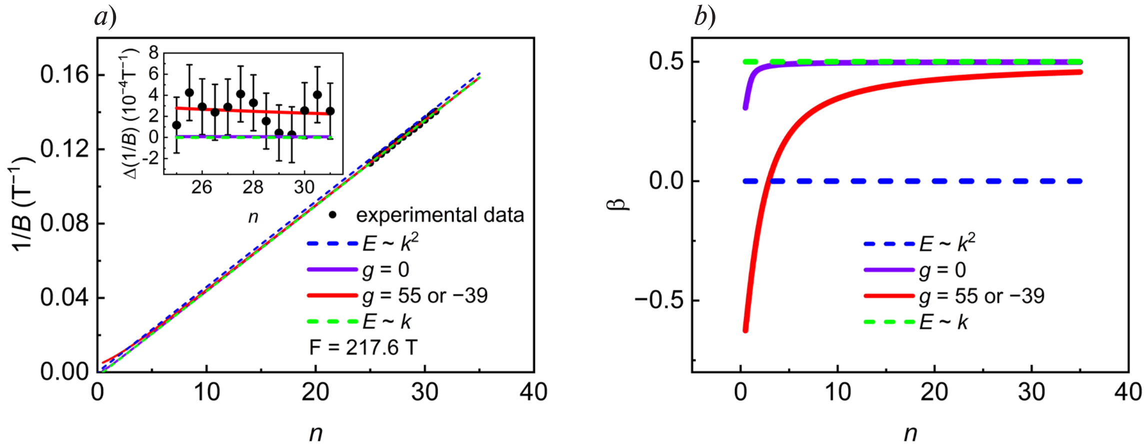

Fig. 4. Analysis of LL fan diagram using Eq. (5) (*a*). Green and blue dashed lines correspond to fermions with dispersion relation $E \sim k$ and $E \sim k^2$, respectively, the red line shows the fit with Eq. (5) taking into account the finite effective mass and *g*-factor. The violet line corresponds to zero *g*-factor. Inset shows the experimental and calculated curves after subtracting the Dirac contribution $\Delta(1/B) = (1/B) - (1/B)_{\text{Dirac}}$
Dependence of the Berry phase factor on the Landau level (*b*)

Using the fitted lines, the Berry phase factor can be calculated as [6]

$$\beta = \frac{1}{2} - \frac{mv_F^2}{\hbar\omega_c}\left(1 + \frac{E_N}{\hbar\omega_c} - \sqrt{1 + \frac{2E_N}{\hbar\omega_c}}\right) + N. \quad (6)$$

As shown in Fig. 4, *b* the observed Berry phase strongly depends on the magnetic field, which is especially pronounced for low Landau levels. Such a strong dependence of $\Phi_B(n)$ indicates that it is not fully correct to use the simple Lifshitz – Onsager quantization rule to determine the Berry phase. Note also that the values of the *g*-factor obtained in our work are in a good agreement with the values in other works for Bi_2Se_3 and other Bi-based topological insulators [6, 7, 13].

Conclusions

To conclude, we have performed a study of the magnetoresistivity and Hall effect of a single crystal of the topological insulator Bi_2Se_3. The SdH oscillations observed in the $-d^2MR/dB^2$ dependence demonstrate occurrence of topological surface states with a non-zero Berry phase and $k_F = 0.081$ Å^{-1}. The Berry phase determined in the simplest way using the Lifshitz – Onsager quantization rule, $\Phi_B \approx 0.8\pi$, is different from the ideal π value. We have shown that taking into account the Zeeman effect plays one of the crucial roles in determining the correct Berry phase value in topological insulators with strong spin-orbit coupling. The rather simple model used can describe the non-ideal value of the observed Berry phase. To construct a full theoretical approach, more complex models are required that take into account disorder in the system, the dependence of the chemical potential on the magnetic field, etc. (see, e.g., [5]).

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