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Effect of high-frequency pumping on thin-film topological insulators

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Abstract. Thin-film topological insulators (TIs) with the thickness below 10 nm are characterized by the presence of a gap in the spectrum of topologically protected surface states. This unusual behavior, also known as anomalous finite size effects, is associated with the hybridization between the states propagating along the opposite boundaries of thin-slab TI. In this work we consider a bismuth-based TI and show how an intense high-frequency linearly polarized light can be used for the tuning of the value of a gap. We also theoretically predict the effect of band inversion in the spectrum of the surface states under external electromagnetic pumping.

1. Introduction

The interest towards the studying of topological matter represents the mainstream in modern condensed matter physics [1, 2, 3]. Among such systems are the recently predicted [4, 5, 6] and experimentally realized [7, 8] three-dimensional topological insulator (TI), a structure which behaves as an insulator in the bulk but has gapless conducting electronic modes at the two-dimensional boundaries. Despite enormous progress TIs still remain an extremely active area of research due to their unique properties and potential applications [9, 10]. As an example of a strong three-dimensional TI one can consider Bi₂Se₃ that has the gapful spectrum of surface states, if the thickness of a structure is below 10 nm due to the interference between top and bottom states and gapless for larger thicknesses [11, 12, 13].

The idea of utilizing off-resonant pumping to drive low-dimensional electronic systems to non-trivial topological phases has recently been pushed forward [14, 15, 16]. Nevertheless, almost no attention was paid to the idea of using high-frequency electromagnetic radiation to the finite-size systems despite their potential impact on the realization of all-optical control in topological systems. In this paper we show that high-frequency pumping leads to renormalization of the bare Hamiltonian of a three-dimensional TI by studying as an example a thin slab of Bi₂Se₃ within the paradigm of Brillonin-Wigner perturbation theory [15], and demonstrate that the anomalous finite size effects in the spectrum of surface states are sensitive to the intensity of the driving.
2. Effective Hamiltonian

We introduce the coordinate system so that the $z$ axis to be normal to the surface plain of the TI. The $k \cdot p$ Hamiltonian of Bi$_2$Se$_3$ in the vicinity of the $\Gamma$-point with no external pumping can be written as

$$H = \mathcal{E}_k + \begin{pmatrix} \mathcal{M}_k & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -\mathcal{M}_k & A_2 k_- & 0 \\ 0 & A_2 k_+ & \mathcal{M}_k & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -\mathcal{M}_k \end{pmatrix},$$

(1)

where the three-dimensional wave vector $k = (k_x, k_y, k_z)$ specifies the electron states, $\mathcal{E}_k = C + D_1 k_x^2 + D_2 k_y^2$, $\mathcal{M}_k = B_0 - B_1 k_x^2 - B_2 k_y^2$, with $k_{\pm} = k_x \pm ik_y$ and $k_{\perp}^2 = k_x^2 + k_y^2$, while the parameters $A_1$, $A_2$, $B_0$, $B_1$, $B_2$, $D_1$, and $C$ have to be fit to the results of ab-initio simulations [8].

Assume that the TI is pumped with a time-periodic electromagnetic field $E = E_0 \sin \omega t$ with the amplitude $E_0$ and the frequency $\omega$ propagating along the $z$ axis. Restricting to linearly polarized electromagnetic field (along $y$ direction) we take account of the external field by virtue of Peierls substitution $k_y \rightarrow k_y - eE_0 \cos(\omega t)/(\hbar \omega)$. To find the renormalized parameters of the Hamiltonian (1) we use the high-frequency expansion in the form of Brillouin-Wigner perturbation theory. Performing the expansion up to terms proportional to $1/\omega^2$ we arrive at the effective Hamiltonian

$$H_{\text{eff}} = \mathcal{E}_k + \left( \begin{array}{cccc} \tilde{\mathcal{M}}_k \tilde{\tau}_z + \tilde{A}_1 k_z \tilde{\tau}_x & (\tilde{A}_2 x k_x - i \tilde{A}_2 y k_y) \tilde{\tau}_x \\ (\tilde{A}_2 x k_x + i \tilde{A}_2 y k_y) \tilde{\tau}_x & \tilde{\mathcal{M}}_k \tilde{\tau}_z - \tilde{A}_1 k_z \tilde{\tau}_x \end{array} \right),$$

(2)

with $\tilde{A}_1 = A_1 (1-a-b)$, $\tilde{A}_2 = A_2 (1-a-b)$, $\tilde{A}_2 y = A_2 (1-2aB_0B_2/A_2^2 + 7b)$, and $\tilde{\mathcal{M}}_k = \tilde{\mathcal{M}} - \tilde{B} - \tilde{B}_1 k_z^2 - \tilde{B}_2 k_{\perp}^2 - 2aB_2 k_y^2$, where we have set $a = [A_2 \gamma/(\hbar \omega)]^2$, $b = [B_2 \gamma^2/(4\hbar \omega)]^2$, $\gamma = eE_0/(\hbar \omega)$, $\tilde{B}_1 = (1-a)\tilde{B}_1$, and $\tilde{\mathcal{M}} = \tilde{B}_0 - (2-a)\tilde{B}_2 \gamma^2/4$. In the expression (2) we have also defined a set of Pauli matrices $\tilde{\tau}_x$ and $\tilde{\tau}_z$. As one can clearly see the effect of renormalization in (2) brings is a certain anisotropy to the bare Hamiltonian (1).

3. Band structure of surface states

Consider a three-dimensional TI of the thickness $L$ in the $z$ direction, yet being infinite along $x$ and $y$. To calculate the spectrum of surface states of the TI subjected to high-frequency pumping one has to solve the Schrödinger equation with the renormalized Hamiltonian (2), on condition that boundary conditions $\psi(x, y; z = 0, L) = 0$ are imposed, meaning that the wave function should be zero at the surface of the TI. Solving the eigenvalue problem with the Hamiltonian (2) we arrive at the dispersion relation in the form

$$\sum_{\pm} \left[ \frac{\tanh(\lambda \pm L/2)}{\tanh(\lambda \pm L/2)} \frac{\lambda \pm}{\lambda \pm} \left( 1 \pm \frac{D^2_1 - B^2_1 \sqrt{R}}{D^2_2 - B^2_2 A^2_1} \right) \right] = 0 \text{ with } \lambda \pm = \frac{F \pm \sqrt{R}}{2(D^2_1 - B^2_1)},$$

(3)

where $F = (l_+ + l_-)D_1 + (l_+ - l_-)\tilde{B}_1 - \tilde{A}_1^2$, $R = F^2 - 4(D^2_1 - \tilde{B}^2_1)(l_+ l_- - (\tilde{A}_2 x k_x)^2 - (\tilde{A}_2 y k_y)^2)$, and $l_\pm = C \pm \tilde{\mathcal{M}}_k + \tilde{B}_2 k_{\perp}^2 - \varepsilon$.

The expression (3) implicitly determines the spectrum of the surface states $\varepsilon_k(L)$ as a function of the layer thickness $L$. Solving this equation numerically we find that an external field allows to reduce the value of the energy gap. To model the properties of Bi$_2$Se$_3$ we utilize the following parameters [8]: $C = 6.8 \times 10^{-3}$ eV, $B_0 = 0.28$ eV, $A_1 = 2.2$ eV Å, $A_2 = 4.1$ eV Å, $B_1 = 10$ eV Å$^2$, $B_2 = 56.6$ eV Å$^2$, $D_1 = 1.3$ eV Å$^2$, and $D_2 = 19.6$ eV Å$^2$. The phase diagram that shows an
interplay between the thickness of a thin-film TI and the intensity of the driving field in terms of the gap value is plotted in Fig. 1.

As one can see the external electromagnetic field not only leads to the suppression of anomalous finite size effects, but also may be used to induce band inversion in the spectrum of surface states. In particular, for a given layer thickness, slightly below 7 nm, the system undergoes topological phase transition along the black line in Fig. 1 where the gap collapses from topologically non-trivial phase (yellow area) to topologically trivial state (blue area).

4. Conclusions
We have investigated anomalous finite size effects in a thin-film TI subjected to an intense off-resonant linearly polarized electromagnetic radiation. The high-frequency expansion reveals that the gap in the spectrum of surface states is quite sensitive to the parameters of the field, and can be suppressed upon increasing the intensity of the field within experimentally accessible range. Moreover, a further increase of the intensity can also lead to the light-induced band inversion.

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