Strain tuning of optical properties in Bi_2Se_3

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***Abstract*—Based on symmetry principles we determine the most general Hamiltonian for the low energy physics of Bi_2Se_3, including contributions due to a static electric field and strain. The full three-dimensional model is projected into the surface states at $k_{||} = 0$, giving an effective two-dimensional Hamiltonian for the surface states. Contributions from the strain tensor breaks the anisotropy of the surface state spectrum, giving an elleptical Dirac cone. Within this model we calculate the absorption spectrum for an ultra-thin film. We show that the fundamental absorption edge can be effectively tuned by application of uni-axial strain.**

I. Introduction

Topological insulators (TI) are a novel state of matter recently predicted and discovered in both two- and three-dimensional systems. While insulating in the bulk, the surface or edge states of topological insulators have linear dispersion. The dispersion of the surface states is linear, similar to graphene, but without the spin and valley degeneracies. The surface states show spin-momentum locking, and has attracted attention for possible applications spintronics and quantum information processing.

The crystal structure of Bi_2Se_3 consists of alternating atomic layers, with five atomic layers constituting a unit called a quintuple layer, with a width of approximately $1\,\mathrm{nm}$. The bonding is strong within the quintuple layer, whereas adjacent quintuple layers are bonded by Van der Waals forces, and thin films can usually only be fabricated with an integer number of quintuple layers.

Strain engineering is becoming an important tool in nanotechnology, since it offers a wide range of possibilities for modulating the physical properties of materials. For the topological insulator Bi_2Se_3 it has been shown by density functional theory calculations that the bulk band gap can be closed under tensile uni-axial strain, in [1], [2] and [3]. This is particularly interesting for topological materials, since a transition between a topologically trivial and a topological insulator phase involves the closing and reopening of a gap.

Both graphene and TI have been proposed as materials for photodetectors in the infrared region, and in [4] it was predicted that in particular thin films of topological insulators could improve the signal-to-noise ratio in comparison with conventional $Hg_{1-x}Cd_xTe$ photodetectors in the infrared spectrum. The linear dispersion of the 2D electrons results in a constant absorption rate. Here we will investigate the optical properties of thin films of topological insulators, in particular under the influence of strain.

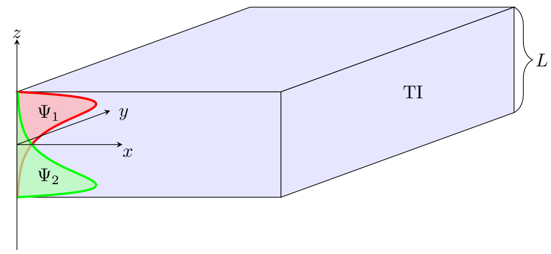

Fig. 1. Schematic of a TI slab of width L. The wave functions of the surface states on the upper/lower surface are shown in red/green. The overlap of the wave functions make them hybridize inducing a gap in the spectrum. This gap can be tuned by application of uni-axial strain.

II. Three-dimensional model Hamiltonian based on symmetry principles

In line with [5] we use the theory of invariants to derive the most general Hamiltonian for the lowest lying conduction band and highest lying valence band, which are both doubly degenerate. We include terms second order in the wave vector, first order in strain and first order in both strain and wave vector. The basisstates are denoted $|P1^+_-, \frac{1}{2}\rangle$, $-i|P2^-_+, \frac{1}{2}\rangle$, $|P1^+_-, -\frac{1}{2}\rangle$, $i|P2^-_+, -\frac{1}{2}\rangle$, derived from the p orbitals of the Bi and Se atoms. The upper sign denotes the inversion eigenvalue and the $\pm\frac{1}{2}$ the total angular momentum. We find a Hamiltonian of the form:

$$H^{3D} = \mathcal{E}_0 + \begin{pmatrix} \mathcal{M} & \beta_i^* k_i & 0 & \alpha_i^* k_i \\ \beta_i k_i & -\mathcal{M} & \alpha_i^* k_i & 0 \\ 0 & \alpha_i k_i & \mathcal{M} & -\beta_i k_i \\ \alpha_i k_i & 0 & -\beta_i^* k_i & -\mathcal{M} \end{pmatrix}, \tag{1}$$

where repeated indices are summed over and where:

$$\mathcal{E}_0 = C + C_1\epsilon_{zz} + C_2\epsilon_{||} + D_1 k_z^2 + D_2 k_{||}^2, \tag{2a}$$

$$\mathcal{M} = M + M_1\epsilon_{zz} + M_2\epsilon_{||} - B_1 k_z^2 - B_2 k_{||}^2. \tag{2b}$$

The parameters α_i and β_i can be modulated by shear strain, and $\epsilon_{xx} - \epsilon_{yy}$. The allowed Hamiltonian contribution due to an electric field perpendicular to the atomic layers can be written:

$$H_{E_z} \propto E_z(\sigma_y \otimes \tau_z), \tag{3}$$

where σ_y and τ_z are Pauli matrices.

For a semi-infinite topological insulator, we can derive the surface state dispersion by using hard-wall boundary conditions at the interface and demanding that the wave function goes to zero away from the interface. The surface state dispersion is shown in Fig. 2, together with the bulk dispersion which is obtained by diagonalizing (1).

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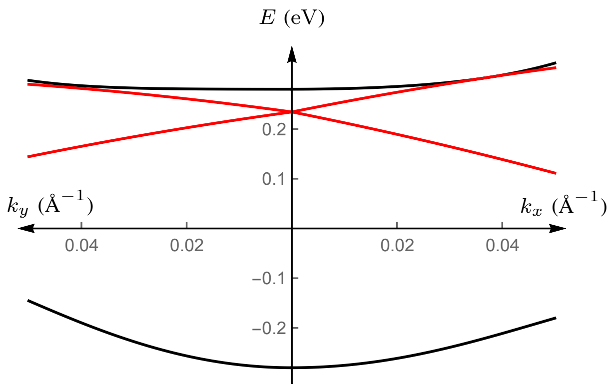

Fig. 2. Dispersion relation of the bulk bands for $k_z = 0$ (black) and the surface states of a semi-infinite TI (red). Here $\epsilon_{zy} = 5\%$, and we see that the in-plane rotational symmetry is broken, giving different group velocities in different directions.

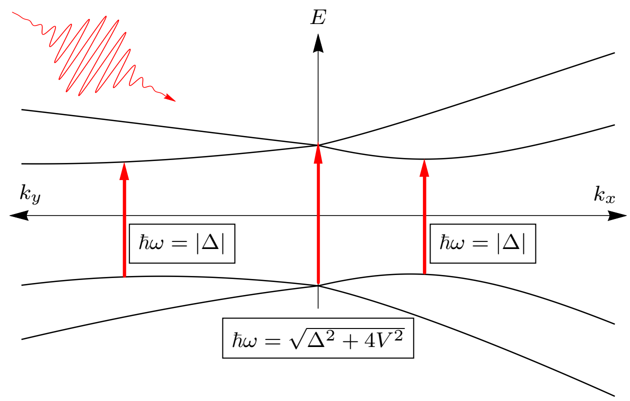

Fig. 3. Dispersion of the surface states of a strained thin film of topological insulator. The anisotropy seen is related to shear strain terms and the difference $\epsilon_{xx} - \epsilon_{yy}$. The absorption edge Δ is dependent on the film thickness, but also on the uni-axial strain ϵ_{zz} as well as the in-plane strain $\epsilon_{xx} + \epsilon_{yy}$.

III. Two-dimensional model for ultra-thin topological insulators

For a finite topological insulator the interactions of the surface states on opposite surfaces will induce a gap. Using hardwall boundary conditions the wave functions can be found analytically in the special case where $k_{||} = 0$ and no external fields. Projecting the full Hamiltonian into the surface states at $k_{||} = 0$ we derive an effective Hamiltonian for the surface states of a thin film.

$$H^{2D} = E_0 + Dk_{||}^2 + \begin{pmatrix} \frac{\Delta}{2} - Bk_{||}^2 & \tilde{\alpha}_i^* k_i & \tilde{\beta}_i k_i + iV & 0 \\ \tilde{\alpha}_i k_i & -\frac{\Delta}{2} + Bk_{||}^2 & 0 & \tilde{\beta}_i k_i - iV \\ \tilde{\beta}_i^* k_i + iV & 0 & -\frac{\Delta}{2} + Bk_{||}^2 & -\tilde{\alpha}_i^* k_i \\ 0 & \tilde{\beta}_i^* k_i - iV & -\tilde{\alpha}_i k_i & \frac{\Delta}{2} - Bk_{||}^2 \end{pmatrix}. \tag{4}$$

The parameter V is a potential breaking the mirror symmetry, which can be due to interaction with the substrate or an external electric field. Diagonalizing this Hamiltonian we get the dispersion of the surface states:

$$E = E_0 + Dk_{||}^2 \pm \Big((\Delta/2 - Bk_{||}^2)^2 + V^2 + |\tilde{\alpha}_i k_i|^2 + |\tilde{\beta}_i k_i|^2 \pm 2|V|\sqrt{|\tilde{\alpha}_i k_i|^2 + \mathrm{Im}(\tilde{\beta}_i k_i)^2} \Big)^{\frac{1}{2}}. \tag{5}$$

The dispersion of the gapped surface states is shown in Fig. 3. We see that the band gap at $k_x = k_y = 0$ is affected by V and therfore can be tuned by an electric field. The fundamendental absorption edge, however, is only dependent on the thickness of the slab and ϵ_{zz} and $\epsilon_{xx} + \epsilon_{yy}$.

The two-dimensional model can be in a topologically trivial or non-trivial state depending on the relative sign of B and Δ.

IV. Optical properties

Using minimal substitution, $\mathbf{k} \to \mathbf{k} - \frac{e}{c}\mathbf{A}$, in the two-dimensional model, we can derive the perturbation Hamiltonian due to the optical field. We calculate the absorption spectrum by using Fermi's golden rule:

$$W = \frac{2\pi}{\hbar} \sum_{k_x, k_y} \sum_{f \neq i} |\langle \psi_f | H' | \psi_i \rangle|^2 \delta(E_f - E_i - \hbar\omega), \tag{6}$$

and demonstrate strain tuning of the absorption edge and peaks in the optical absorption spectrum. We also examine the role of strain and topological effects for the absorbance of Bi_2Se_3 thin films.

V. Conclusion

We investigate the absorption spectrum of thin films of topological insulators under the influence of strain. The use of strain opens up new possibilities in the tuning of the electronic structures, and thereby the absorption spectrum of thin TI films. The fundamendental absorption edge can be tuned effectively by uniaxial strain perpendicular to the film, giving possibilities for applications in photodetectors. This can be done continuously with strain, in contrast to changing the thickness, which is only possible by single quintuple layers. The tuning of the band gap, also gives new possibilities for experimentally investigating and tuning the 2D topological nature of thin films of 3D TI.

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