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On the photon-drag effect of photocurrent of surface states of topological insulators

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ABSTRACT

The photocurrent of surface states of topological insulator due to photon-drag effect is computed, being based on pure Dirac model of surface states. The scattering by disorder is taken into account to provide a relaxation mechanism for the photocurrent. The Keldysh–Schwinger formalism has been employed for the systematic calculation of photocurrent. The helicity dependent photocurrent of sizable magnitude transverse to the in-plane photon momentum is found, which is consistent with experimental data. Other helicity independent photocurrents with various polarization states are also calculated.

1. Introduction

The topological insulators (TIs) have been intensively studied recently [1,2]. TIs have bulk energy gap but they have conducting (namely gapless) states at *boundary* [3]. There exist 3-dimensional TIs, and they have conducting *surface* states (SS) which are protected against backscattering by Z_2 topological invariants of time reversal symmetry in the bulk [4–6]. The energy band of SS takes the form of (perturbed) Dirac cone where the spin and the momentum are locked into each other, producing helical spin structure [1,3].

The SS are expected to have diverse exotic physical properties such as Majorana fermion [7]. Among these properties we focus on the *photocurrent* response. The photocurrent response is a very unique probe of the SS since it should originate only from the surface where the bulk inversion symmetry is naturally broken [8]. Also the spin–momentum locking structure is naturally sensitive to the circular polarization (or the helicity) of incident light, so that the *helicity dependent* DC photocurrent is expected. The helicity dependent photocurrent of Bi_2Se_3 has been observed experimentally in Ref. [9]. For a laser intensity of $60\,\mathrm{W\,cm^{-2}}$, the observed current density is the order of $10\,\mu\mathrm{A/mm}$ (see Fig. 1 of Ref. [9]). This experiment bears an importance also from the viewpoint of opto-spintronics.

Evidently the interband transition between lower and upper Dirac cones of SS is expected to play a dominant role (see Fig. 1). For most of the interband transitions in optical regime, the momentum of photon is neglected. Surprisingly, in the limit of negligible photon momentum, the pure Dirac model of SS with usual orbital coupling of photons gives *vanishing* photocurrent [8,10]. It turns out that to obtain non-zero photocurrent, the trigonal distortion perturbation of Dirac cone, the correction to Fermi velocity, and the *Zeeman* coupling of photon have to be included. (For normal incidence, the Zeeman coupling to external magnetic field is also required [8]). The above perturbations are rather minor effects, and accordingly they yield non-zero but small photocurrents compared to experimental data.

From the above inversion symmetry argument, it is clear that SS should contribute a major component to photocurrent (if not all), so we must seek another mechanism which can give a substantial photocurrent *without* relying on small perturbations to Dirac structure of SS. In this paper, we claim that *the photon-drag effect can provide such mechanism* and we show this by explicit microscopic Feynman diagram calculation. The electric current by the photon-drag effect is the current *due to the momentum imparted by the absorbed photons*, (so we should keep photon momentum finite in our calculation) and it often plays an important role in interband absorption [11]. In general the photon-drag current is in the direction of light propagation [11], but in the case of SS where spin and momentum is locked, the photocurrent for circular polarization from the photon-drag effect can be transverse to the direction of light propagation as argued in Ref. [8] from symmetry consideration and dimensional analysis.

In this paper we study the photon-drag effect of the photocurrents of SS based on a pure Dirac model of SS. Also, to obtain physically relevant results we introduce a mechanism for momentum relaxation. In our study we will consider the scattering by disorder [12] as a possible source of momentum relaxation.

In actual computation Keldysh–Schwinger (KS) formalism is

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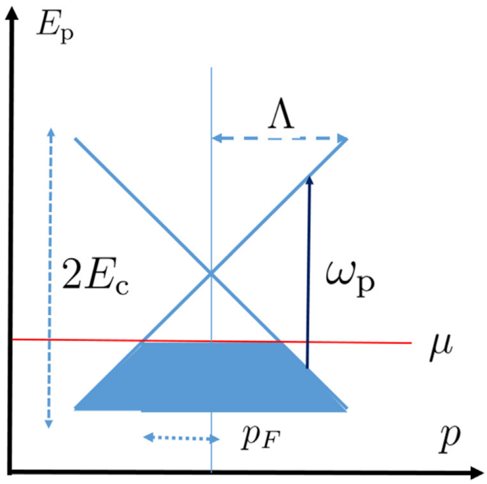

Fig. 1. The energy band of pure Dirac model of SS. $\omega_{\rm p}$ is the energy of incident photon. $p_F = |\mu|/v$ is a Fermi momentum, and $\Lambda \approx 0.05$ Å^{-1}, $E_c \approx 0.13$ eV is the cutoff momentum and the cutoff energy of our pure Dirac model, respectively.

employed [13,14]. There are a few reasons for this choice: the first is that the photocurrent belongs to a class of real time Green's function (the so-called *less* Green's function) [18], for which KS formalism provides the most natural framework for perturbation theory. The second reason is that the average of Green's function over disorder can be done very easily thanks to the property of unit partition function $Z=1$ in KS formalism [15–17]. Third, the photocurrent is nonlinear in photon vector potentials, so that the standard imaginary time Green's function theory of linear response theory cannot be used.

We have obtained the *helicity dependent photocurrent transverse to the photon direction originating from photon-drag effect* (see Eq. (55)) which is *not* suppressed by small perturbations of pure Dirac model, thus it is of sizable magnitude *being consistent with experimental data*. Other helicity independent photocurrents for various photon polarization states also have been obtained. We also observe that a new component of relaxation time by disorder scattering appears due to the Dirac cone spin–momentum locking structure (see Section 4). The main results of this paper are Eqs. (30), (55), (57) and (58).

This paper is organized as follows: we set up the Hamiltonians for our problem in Section 2. Then the Hamiltonians and the current operator are mapped to KS functional integral formulation in Section 3. In Section 4, the self-energy of KS Green's function which incorporates the scattering by disorder is computed. The photocurrent is computed in Section 5, and we conclude this paper with discussions and summary in Section 6.

2. Setup

We will consider a pure two-dimensional Dirac fermion model of SS, neglecting trigonal distortion [19] and correction to Fermi velocity [20]. The second quantized Hamiltonian in momentum space for the SS is given by (α, β are spin indices, and $\hbar = 1$ convention will be used in this paper)

$$\mathrm{H_{SS}} = \sum_{\alpha,\beta=\uparrow,\downarrow} \sum_{\mathbf{p}} \hat{c}^{\dagger}_{\mathbf{p}\alpha} \mathrm{h}_{\alpha\beta} \hat{c}_{\mathbf{p}\beta},$$
$$\hat{\mathrm{h}} = (\mathrm{h}_{\alpha\beta}), \quad \hat{\mathrm{h}} = v(p_x\sigma_y - p_y\sigma_x), \tag{1}$$

where $\mathbf{p}$ is a two-dimensional momentum in x–y plane of SS. $\sigma_{x,y}$ are Pauli matrices acting on spin space, and $\hat{c}_{\mathbf{p}\alpha}$ is the destruction operator for SS electron with wavenumber $\mathbf{p}$ and spin α. Since we are neglecting the correction to Fermi velocity, v can be regarded as the Fermi velocity. The numerical value of v is $v \sim 5 \times 10^5$ m/s [19]. The energy band is given by

$$E_{\pm}(\mathbf{p}) = \pm vp, \quad p = \sqrt{p_x^2 + p_y^2}. \tag{2}$$

The eigen-spinor is a function of momentum which reflects the locked spin–momentum structure [19]. We will choose the chemical potential μ to lie in the lower Dirac cone (see Fig. 1). The precise experimental determination of chemical potential is well-known to be very difficult. We will assume that the chemical potential is away from the apex of Dirac cone to ensure a substantial density of states at Fermi energy, and the typical value is taken to be around $\mu \sim -0.04$ eV. Also, the photon energy is chosen to be in the range of 0.1–0.13 eV.

The pure Dirac fermion model is valid only in the restricted range of momentum. Fig. 4 of Ref. [19] suggests the wavenumber cutoff (for the validity of Dirac cone structure) be $\Lambda \approx 0.05$ Å^{-1}, which implies that the energy cuttoff $E_c = v\Lambda$ for our problem is around 0.13 eV (see Fig. 1).

Next we consider the interaction of SS with photon. In our study, the usual orbital coupling of photon will produce non-zero photocurrent owing to photon-drag effect. In the notation of Eq. (1) the second quantized Hamiltonian (in momentum space) for the interaction between light (incoming photon) and SS can be expressed as

$$\mathrm{H}' = -\frac{1}{c}\sum_{\mathbf{q}} \vec{J}(\mathbf{q})\cdot\vec{A}(-\mathbf{q}), \tag{3}$$

where $\vec{A}(-\mathbf{q})$ is the vector potential of photon, and $\vec{J}(\mathbf{q})$ is the current density operator:

$$\vec{J}(\mathbf{q}) = (-e)\sum_{\mathbf{p},\alpha,\beta} \hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q}\alpha} \frac{\partial h_{\alpha\beta}(\mathbf{p}+\frac{\mathbf{q}}{2})}{\partial \mathbf{p}} \hat{c}_{\mathbf{p}\beta}. \tag{4}$$

From Eq. (1) we can obtain the explicit form of current density operator ($i, j = x, y = 1, 2$ and ϵ^{ij} is a totally antisymmetric tensor in two indices):

$$J^i(\mathbf{q}) = (-e)v\sum_j \epsilon^{ij} \sum_{\mathbf{p},\alpha,\beta} \hat{c}^{\dagger}_{\mathbf{p}+\mathbf{q}\alpha}(\sigma_j)_{\alpha\beta}\,\hat{c}_{\mathbf{p}\beta}. \tag{5}$$

Owing to the rotation symmetry of pure Dirac model in x–y plane, the incoming photon momentum $\mathbf{k}_{\rm p}$ can be taken to be in y–z plane:

$$\mathbf{k}_{\rm p} = |\mathbf{k}_{\rm p}|(-\cos\theta\hat{\mathbf{z}} + \sin\theta\hat{\mathbf{y}}) = |\mathbf{k}_{\rm p}|\,\hat{\mathbf{k}}_{\rm p}. \tag{6}$$

For the basis of photon polarization, we will take $\hat{\mathbf{e}}_2 = \hat{\mathbf{x}}$ to be S-polarization (perpendicular to y–z plane) and $\hat{\mathbf{e}}_1 = \hat{\mathbf{e}}_2 \times \hat{\mathbf{k}}_{\rm p} = \cos\theta\hat{\mathbf{y}} + \sin\theta\hat{\mathbf{z}}$ to be P-polarization (in y–z plane). Then a general *linear* polarization state can be represented as

$$\hat{\mathbf{e}}_{\mathbf{k}_{\rm p}} = \cos\varphi\hat{\mathbf{e}}_1 + \sin\varphi\hat{\mathbf{e}}_2, \tag{7}$$

and the corresponding vector potential (a certain profile function characterizing laser beam size is implicitly assumed) is given by

$$\vec{A}_{\rm linear}(\mathbf{r}, t) = A_0\,\hat{\mathbf{e}}_{\mathbf{k}_{\rm p}}\cos(\mathbf{k}_{\rm p}\cdot\mathbf{r} - \omega_{\rm p}t), \tag{8}$$

where $\omega_{\rm p} = |\mathbf{k}_{\rm p}|c > 0$ (a factor like e^{0^+t} is implicitly assumed in Eq. (8) to insure slow turning of interaction. 0^+ is an infinitesimally small positive quantity).

The *circularly* polarized state is represented by

$$\hat{\mathbf{e}}_{\pm} = \frac{\hat{\mathbf{e}}_1 \pm i\,\hat{\mathbf{e}}_2}{\sqrt{2}}, \tag{9}$$