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Collective excitonic and plasmonic excitations on a surface of 3D topological insulator

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Abstract. Properties of collective excitonic and plasmonic excitations on the surface of three-dimensional topological insulator are reviewed. Due to spin-momentum locking for electrons populating the surface states plasmonic excitation manifests itself as coupled spin- and density-wave and can be called "spin-plasmon". Its excitation induces spin polarization of topological insulator surface that is perpendicular to the spin-plasmon momentum. Excitons appear on the surface when the gap in the surface spectrum is magnetically induced. Excitons correspond to the set of subgap levels with unusual dependence of the energy on orbital angular momentum quantum number and can be called "chiral". Contrary to conventional excitons chiral ones resonantly contribute to Hall component of optical conductivity tensor and play significant role in magneto-optical Faraday and Kerr effects. They resonantly enhance Faraday effect and reduce Kerr effect.

1. Introduction

Topological insulator (TI) is new class of solids that has nontrivial topology of the band structure (see [1] and references therein). TIs as conventional insulators have forbidden band in the bulk but also contain exotic topologically protected conducting states on their surface (3D) or border (2D). Recently a “new generation” of three-dimensional topological insulators (the binary compounds Bi₂Se₃, Bi₂Te₃ and others), retaining topologically protected behavior at room temperatures, were investigated experimentally [2]. Surface states of these materials are described by the Dirac-like Hamiltonian for two-dimensional massless particles that is given by

$$H_0 = v_F (p_x \sigma_y - p_y \sigma_x),$$

(1)

where $v_F$ is the Fermi velocity of electron; the Pauli matrices $\sigma_x$ and $\sigma_y$ act in the spaces of its spin projections. Spectrum is formed by conduction ($\gamma = 1$) and valence ($\gamma = -1$) bands that have linear dispersion low $\epsilon_{p\gamma} = \gamma v_F p$ and touch each other. This Hamiltonian is similar to one that describes electrons in graphene but electron spin is substituted by pseudospin which is connected with lattice degree of freedom [3].

The direction of spin projection of electrons populating the surface states of TI is determined by their momentum. Such spin-momentum locking manifests itself in different transport phenomena that include coupled diffusion of charge and spin [4], inverse galvanomagnetic effect [5] and contact effects [6]. Collective plasmonic excitation in degenerate electron gas populating...
TI surface states manifests itself as coupled charge- and spin- density waves and can be called spin-plasmon [7, 8]. Latter it was proposed to apply spin-plasmons in spin accumulator [9]. Comprehensive analysis of the physical properties of spin-plasmons was made in the paper [8].

The surface spectrum is protected from external perturbations that do not break the time reversal symmetry, for example, from nonmagnetic disorder [10]. External exchange field that can be created by ordered magnetic impurities introduced to a TI bulk or surface [11] acts only on magnetic moment of the surface states and leads to the gap formation in the spectrum. The Hamiltonian describing electrons on the surface of TI in the presence of external exchange field is given by

$$H_0 = v_F(p_x\sigma_y - p_y\sigma_x) + m\sigma_z,$$

where value $m$ parameterizes coupling strength of the $z$-component of exchange field with electron’s spin. Other components of exchange field can be excluded by the gauge transformation that shifts Dirac point in momentum space. Exchange field leads to the formation of the gap in the spectrum $\epsilon_{p,\gamma} = \gamma\sqrt{v_F^2 + m^2}$. Excitonic states that correspond to bound states of electron from conduction band and hole from valence were considered in [12]. It interesting that the excitonic state with minimal energy has finite value of orbital momentum quantum number and can be called chiral.

Breaking of the time reversal symmetry leads to half-integer quantum Hall effect on the TI surface that causes topological magnetoelectric effect in the TI bulk [13]. The topological magnetoelectric effect leads to quantized magneto-optical Kerr and Faraday effect [14] without external magnetic field. In thin film of topological insulator which width is less then length of magnetoelectric effect leads to quantized magneto-optical Kerr and Faraday effect [14] without TI surface that causes topological magnetoelectric effect in the TI bulk [13]. The topological is given by

$$F_{p,\gamma} = \frac{\pi e^2}{4\hbar c}$$

where $F_{p,\gamma}$ is the two-dimensional Fourier transform of Coulomb interaction potential and $\varepsilon$ is effective dielectric permittivity of half-space formed by topological insulator surface.

$$\sum_{p\gamma} \xi_{p,\gamma}^a p_{p\gamma}^a \sigma_{p\gamma} + \frac{1}{2} \sum_{qpp'} \sum_{\gamma_1\gamma_2\gamma_1'\gamma_2'} V_c(q) \langle f_{p+q\gamma_1'} | f_{p\gamma_1} \rangle \langle f_{p'-q\gamma_2'} | f_{p'\gamma_2} \rangle a_{p+q\gamma_1'}^a a_{p'\gamma_2}^a a_{p'\gamma_2}^a a_{p\gamma_1},$$

2. Equation of motion approach

Excitations are called collective ones if they can not be described within single-particle picture. Starting point of their investigation is the Hamiltonian that includes interaction between particles. For electrons populating surface states of TI the Hamiltonian is given by

$$H = \sum_{p\gamma} \xi_{p,\gamma}^a p_{p\gamma}^a \sigma_{p\gamma} + \frac{1}{2} \sum_{qpp'} \sum_{\gamma_1\gamma_2\gamma_1'\gamma_2'} V_c(q) \langle f_{p+q\gamma_1'} | f_{p\gamma_1} \rangle \langle f_{p'-q\gamma_2'} | f_{p'\gamma_2} \rangle a_{p+q\gamma_1'}^a a_{p'\gamma_2}^a a_{p'\gamma_2}^a a_{p\gamma_1},$$

where $a_{p,\gamma}$ is the destruction operator for the electron with momentum $p$ from the band $\gamma$: $|f_{p,\gamma}\rangle$ denotes the corresponding wave function in spinor space that is eigenvectors of Hamiltonians (1) or (2), respectively; $\xi_{p,\gamma} = \epsilon_{p,\gamma} - E_F$ is the dispersion law of electrons that includes chemical potential $E_F$; $V_c(q) = 2\pi e^2/\varepsilon q$ is the two-dimensional Fourier transform of Coulomb interaction potential and $\varepsilon$ is effective dielectric permittivity of half-space formed by topological insulator surface.
Creation operators for plasmons and excitons have the same form and are given by

$$Q_{q}^{+} = \sum_{p\gamma\gamma'} C_{pq}^{\gamma\gamma'} a_{p+q\gamma'}^{+} a_{p\gamma},$$  \(4\)

where \(C_{pq}^{\gamma\gamma'}\) are weights of intraband \((\gamma = \gamma')\) and interband \((\gamma \neq \gamma')\) single-particle transitions. Plasmonic excitation contains both interband and intraband contributions while exciton contains only interband ones. Both of them can be represented as composite bosons and their creation operators satisfy corresponding commutation relations \([Q_{q}, Q_{q'}^{+}] = \delta_{qq'}\). Creation operator of collective excitation obeys equation of motion \([H, Q_{q}^{+}] = E_{q} Q_{q}^{+}\), where \(E_{q}\) is its energy and \(H\) is Hamiltonian of interacting electrons (3).

There is only single dimensionless parameter that determines physical properties of the collective excitations on the surface of TI that is given by \(\alpha_{c} = e^{2}/\hbar v_{F}\). In case of spin-plasmons it corresponds to ratio between Coulomb interaction energy of degenerate electron gas to its kinetic energy and is usually denoted as parameter \(r_{s}\). In case of excitons it corresponds to the ratio between electron-hole interaction energy to their kinetic energies. Weak-coupling regime \(\alpha_{c} \ll 1\) corresponds to experimental relevant conditions [2]. In this case Random phase approximation (RPA) [18] can be employed for solution of equation of motion for creation operator of spin-plasmon and equation of motion of excitons has the simple approximate analytical solution [17]. Also we considered the case of zero temperature.

3. Spin-plasmons

3.1. Internal structure of plasmons

We find that in RPA wave function of spin-plasmon is given by

$$C_{pq}^{\gamma\gamma'} = \frac{\langle f_{p+q\gamma'}|f_{p\gamma}\rangle N_{q}}{E_{q} + \xi_{p\gamma'} - \xi_{p+q\gamma'} + i\delta},$$  \(5\)

Figure 1. Plasmon dispersion at different values of parameter \(\alpha_{c}\). Dotted lines denote borders of intraband \((w < v_{F}q)\) and interband \((w > 2E_{F} - v_{F}q)\) single particle continua.

Figure 2. Dependence of total weight of intraband transitions that contribute to wave function of plasmon at different values of dimensionless parameter \(\alpha_{c}\).
where $N_q$ is normalization factor and $E_q$ is the dispersion law of plasmons that can be obtained from the following equation

$$1 - V_c(q) \sum_{p,\gamma,\gamma'} |\langle f_{p+q,\gamma'} | f_{p,\gamma} \rangle|^2 \frac{(n_{p,\gamma} - n_{p+q,\gamma'})}{E_q + \xi_{p,\gamma} - \xi_{p+q,\gamma'} + i\delta} = 0. \quad (6)$$

Here $n_{p,\gamma}$ is occupation number of electronic states $|p,\gamma\rangle$. The same equation was obtained within diagrammatic approach based on RPA to plasmonic excitations in Dirac electronic gas on a surface of topological insulator [7] and graphene [19].

For numerical calculations we used the following set of parameters $v_F = 0.62 \cdot 10^6$ m/s and $\epsilon_{TI} = 80$ that corresponds to $\alpha_c = 0.09$. Dispersion law of spin-plasmons on the surface of TI is presented in Fig.1. The dispersion laws for plasmons in Dirac electronic gas in suspended graphene ($\alpha_c = 8.8$) and graphene on SiO$_2$ substrate ($\alpha_c = 2.2$) are presented for comparison. (For graphene parameter $\alpha_c$ is given by $ge^2/hv_F$ where $g = 4$ is degeneracy factor of Dirac cones). For $\alpha_c = 0.09$ dispersion law of plasmon tends to the border of continuum of intraband single-particle transitions ($w < v_Fq$). At $q \simeq k_F$ it intersects continuum of iterband single-particle transitions ($w > 2E_F - v_Fq$) and spin-plasmon become damped since conservation laws of energy and momentum allow transfer energy between spin-plasmon and electron-hole pairs.

Plasmonic excitation consists of intraband and interband single-particle transitions. Their total contribution can be characterized by their weight $D_{\gamma,\gamma'}$ that is given by

$$D_{\gamma,\gamma'} = \sum_p |C_{pq}^{\gamma,\gamma'}|^2 (n_{p,\gamma} - n_{p+q,\gamma'}). \quad (7)$$

Dependence of weight of the intraband contribution $D_{11}$ on momentum of the spin-plasmon for different values of dimensionless coupling $\alpha_c$ is presented in Fig.2. The undamped plasmon for all values of parameter $\alpha_c$ consists mainly of intraband transitions. In single-particle continuum contributions of the interband and the interband transitions approximately coincide.

### 3.2. Spin- and density- waves

In the spin-plasmon state distribution of the electrons is shifted along its momentum $q$ in the momentum space and spin-polarization of the TI surface appears due to the locking between spin and momentum of single electron. By the same reason spin polarization of the surface of TI appears in the current-carrying state [5]. Value of the spin polarization of the TI surface in the spin-plasmon state versus its momentum is presented in Fig.3.

Due to spin-momentum locking plasmonic excitations manifests themselves as coupled spin- and density- waves. Direction of spin polarization is perpendicular to plasmon momentum. Dependence of amplitudes of spin- and density- waves ($A_s$ and $A_d$) on momentum of spin-plasmon in dimensionless units $\sqrt{n - n_q}$ ($\rho$ is the concentration of electrons and $n_q$ is the concentration of plasmons with momentum $q$) is presented in Fig.3. The values of their amplitudes have the same order. Similar effect appears in electron gas in the presence of spin-orbital interaction in which plasmonic excitation is also accompanied by the spin-density wave. But for the experimental relevant parameters its amplitude is considerable less then amplitude of the charge wave.

### 3.3. Scattering of spin-plasmons

We considered scattering of spin-plasmons on the external potential and magnetic field. Fermi’s Golden rule was used for the calculation of the probability of the spin-plasmon scattering. The angle probability distribution of plasmon scattering can be presented in the form:

$$w_V(q, \phi) = |V(2q \sin \frac{\phi}{2})|^2 |\Phi_V(q, \phi)|^2, \quad (8)$$
Here momentum is given by
\[
\text{of single-particle spectrum can be omitted [17] the equation of motion for exciton with zero total}
\]

Only excitons with zero momentum contribute to the optical conductivity tensor, hence we will

4. Chiral excitons

4.1. Structure of the set of excitonic states

Only excitons with zero momentum contribute to the optical conductivity tensor, hence we will

suppose below that their momentum is zero and omit momentum index. If the renormalization

of single-particle spectrum can be omitted [17] the equation of motion for exciton with zero total

momentum is given by
\[
2\epsilon_k C_k + \sum_{k'} V_{\text{eff}}(k, k') C_{k'} = EC_k. \tag{10}
\]

Here \( V_{\text{eff}}(k, k') \) is the efficient electron-hole interaction that is given by
\[
V_{\text{eff}}(k, k') = V_c(k - k') \left\{ \frac{v_F^2 k^2}{k' k} + (1 + \frac{m^2}{\epsilon_k \epsilon_{k'}}) \cos(\phi_k - \phi_{k'}) + i \left( \frac{m}{\epsilon_k} + \frac{m}{\epsilon_{k'}} \right) \sin(\phi_k - \phi_{k'}) \right\}. \tag{11}
\]

Equation (10) have been numerically solved in [12]. Excitonic state with minimal energy

has with finite value of orbital angular momentum and there is no symmetry between the

states with opposite values of orbital angular momentum. Hence excitons can be called

"chiral". We find that in weak coupling regime \( \alpha_c \ll 1 \) the energy spectrum and effective

interaction can be approximated in following way: \( \epsilon_k \approx |m| + \frac{1}{2} v_F^2 k^2 / 2 |m| \) and \( V_{\text{eff}}(k, k') \approx V_c(k - k') \left[ \cos(\phi_k - \phi_{k'}) + i \sin(\phi_k - \phi_{k'}) \right] \). In this case the equation (10) coincides with Schrodinger equation for 2D hydrogen atom in which: 1) multipole momenta of Coulomb potential Fourier transform are shifted by \( \delta l = 1 \); 2) effective reduced mass of electron in 2D hydrogen atom problem is \( \mu^* = |m| / 2 v_F^2 \). The chiral excitons can be characterized by radial \( n = 0, 1, \ldots \) and

Figure 3. Amplitudes of spin- and charge-density waves and value of spin polarization

versus momentum of spin-plasmon.

Figure 4. Dependence of squared electric and magnetic form-factors on scattering angle of spin-plasmon \( \phi \).
orbital angular \( l = 0, \pm 1, \ldots \) quantum numbers with \( |l - 1| \leq n \). Their energy spectrum \( \Omega_{nl} \) and wave functions in momentum space \( C_{k}^{nl} \) can be obtained by shift of well-known ones for a 2D hydrogen atom. State \( |0, 1\rangle \) with minimal energy has orbital quantum number \( l = 1 \). Sign of the orbital quantum number that corresponds to the lowest-energy state depends on sign of \( m \) and therefore on the direction of exchange field.

### 4.2. Excitonic contribution to conductivity tensor

We used the linear response theory and the equation of motion approach for calculation of the excitonic contribution of optical conductivity tensor. Its components are given by

\[
\sigma_{xx}^{ex}(\omega) = i\frac{e^2}{\hbar} 2\pi \sum_{nl} |M_{nl}^{xx}|^2 \frac{\omega}{E_{nl} (\omega + i\gamma)^2 - E_{nl}^2},
\]

\[
\sigma_{yx}^{ex}(\omega) = -\frac{e^2}{\hbar} 2\pi \sum_{nl} |M_{nl}^{yx}|^2 \frac{2m^2}{(\omega + i\gamma)^2 - E_{nl}^2},
\]

where the summation is performed over all exciton quantum numbers; \( \gamma \) is phenomenologically introduced exciton decay rate; \( M_{nl}^{xx} \) is dimensionless matrix element that depends only on dimensional coupling strength \( \alpha_c \) and is given by

\[
M_{nl}^{xx} = \frac{\hbar}{m} \sum_{k} C_{k}^{nl}(k,v)|J_{k,c}|,
\]

where vector \( J = v_F(\sigma_y, -\sigma_x) \) is the single-particle current operator. Value \( M_{nl}^{xx} \) characterizes coupling strength between exciton and external electromagnetic field. It has nonzero value only for levels with \( l = \pm 1 \) and all other states are optically inactive. Dependence of squared absolute value of matrix element \( |M_{nl}^{xx}|^2 \) on dimensional coupling strength for states for four optical active states that has the lowest energy is presented in Fig. 5. Matrix elements are decreasing with increasing of quantum number \( n \) due to destructive interference of interband transitions in (14) since wave functions \( C_{k}^{nl} \) for high energy levels oscillate in momentum space. Also optical activity of levels with angular momentum \( l = -1 \) is considerable less then \( l = 1 \).
For all numerical calculations we used the following parameters: $m = 12.5$ meV, $\gamma = 0.25$ meV and $v_F = 0.62 \times 10^6$ m/s. Also we used three values of dimensionless parameter $\alpha_c$. Value $\alpha_c = 0$ corresponds to the case of noninteracting electrons on TI surface. Values $\alpha_c = 0.18$ and $\alpha_c = 0.35$ correspond to values of effective permittivity $\epsilon = 20.5$ and $\epsilon = 10.5$, respectively (If the TI surface is subjected to the air with $\epsilon' = 1$ the corresponding values dielectric permittivity of TI are $\epsilon_{TI} = 40$ and $\epsilon_{TI} = 20$, respectively).

Contribution of the excitonic level $|n, l\rangle$ to Hall conductivity has the same sign as it orbital quantum number $l$. States with opposite orbital quantum numbers $l$ and $-l$ are connected by the time reversal transformation. Due to the time reversal symmetry breaking by external exchange field chiral excitons on the surface of TI do resonantly contribute to optical Hall conductivity. Frequency dependence of real part of Hall conductivity is presented in Fig.6.

4.3. Magneto-optical effects in thin film of TI

We theoretically investigated magneto-optical effects at normal incidence in thin film of topological insulator which width is considerably less then wave length of electromagnetic field. The results can be easily generalized for more complicated geometry and oblique incidence.

Dependencies of Faraday angle $\theta_F$ and Kerr angle $\theta_K$ on frequency of incident electromagnetic wave are presented in Fig.7 and Fig.8 respectively. Values of Faraday and Kerr angles in low frequency limit where excitonic contribution is negligible tend to their universal values: $\tan \theta_F = \alpha$ and $\tan \theta_K = 1/\alpha$, where $\alpha \approx 1/137$ is fine structure constant. Resonance contribution of chiral excitons to Hall conductivity of the TI surface lead to resonant enhancement of Kerr effect. At resonant condition longitudinal part of the conductivity has sharp maximum that leads to resonant absorption of energy of electromagnetic field and resonant reduction of Kerr effect.

Conventional excitons in two- and three- dimensional systems in presence of time reversal symmetry do not contribute to Hall conductivity and, hence, do not manifests in magneto-optical effect in absence of magnetic field.

5. Summary

We reviewed properties of spin-plasmons in degenerate electronic gas populating the surface states and chiral excitons in presence of the magnetically induced gap in the surface spectrum. They both can be represented as composite bosons that are superposition of single-particle electron-hole transitions and can be effectively described within equation of motion based

\[\begin{align*}
\alpha_c = 0 & \quad ... \\
\alpha_c = 0.18 & \quad ... \\
\alpha_c = 0.35 & \quad ...
\end{align*}\]
approach. But their physical properties are different. Spin-plasmons manifest themselves as coupled spin- and density- waves and their excitation also induces spin polarization of topological insulator that is perpendicular to their momentum. Chiral exciton that manifest itself as bound state of electron and hole and has unusual dependence of energy on its angular quantum number. Contrary to conventional ones chiral excitons resonantly contribute to Hall component of conductivity tensor. Chiral excitons resonantly enhance Faraday effect and resonantly reduce Kerr effect.

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