Study of Dirac plasmons on the surface of a topological insulator based on spin quantum hydrodynamics

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Abstract

Starting from the Dirac equation, the nonlinear relativistic quantum hydrodynamic equations for Dirac electrons on a surface of a three dimensional-topological insulator are presented and numerically simulated. The surface of the topological insulator is modulated by a perpendicular magnetic field and a pulsed exchange field provided by an array of ferromagnetic insulating (FI) stripes. The collective polarization of the hydrodynamic density and the induced potential in the Dirac electron system are simulated and analyzed. It is shown that the influence of the spin quantum effects on the collective motion of the Dirac electrons is obvious under a laboratory condition.

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Plasmons are the quantized collective oscillations of electrons in metals and semiconductors. There has been much interest in the excitation of plasmons in quantum plasmas, including plasmons of Schrödinger electrons which has been a long time research priorities, as well as plasmons of Dirac electrons since which has been observed in the edge state of topological insulators (TIs) has received great attention, especially in the field of nano-scale electro-mechanical systems. As such plasmons could be of appearance under external modulations in bulk metals, semiconductor heterostructures, quantum-wells, and the surface of three dimensional (3D) TIs. The both experimentally and theoretically treatments of collective motion of plasmons in Dirac electron systems, have received important results, conductive to understand the dynamics of Dirac electrons and develop more efficient plasmonic designs in the intriguing topological materials. Pietro et al. have used infrared spectroscopy to report the first examination of collective excitations of Dirac plasmons in thin films on $\text{Bi}_2\text{Se}_3$ TI surface. Some theoretical works based on the Bernevig-Hughes-Zhang model, have studied plasmon excitation dispersion of topological edge states within random-phase approximation (RPA) dielectric theory, in which the collective motion between Schrödinger electrons and Dirac electrons is compared. While in a two-dimensional (2D) Dirac system, the dispersion relation of surface plasmons at the interface between a TI and a dielectric, has been achieved within the framework of classical electrodynamics.

Despite the large number of studies performed on plasmon dynamics in a Schrödinger electron system or Dirac electrons on an edge state of a TI, the unique properties and physics in the collective motion of plasmons are still far from understood. One possible approach to collective motion in Schrödinger plasmas is represented by the quantum hydrodynamic model (QHD), a useful tool for describing the dynamics of the quantum plasmons, by solving the nonlinear Schrödinger-Poisson or the Wigner-Poisson kinetic models. Compared to the Wigner-Poisson system, the QHD model is more simple for numerical studies and has a straightforward interpretation in terms of fluid quantities that are employed in classical physics. The hydrodynamic study of collective motion in Schrödinger quantum plasmas has received much interests in high energy density physics and plasma physics. However, there have also been interests in hydrodynamic study of collective excitation modes of spin systems, for example, hydrodynamic models including non-relativistic spin and relativistic spin effects have been presented. This non-relativistic spin quantum effects are obvious in dispersion relation and the linear response of the quantum plasmas. Felipe has studied electromagnetic wave propagation with relativistic QHD model, in which the relativistic effects increase the fluid opacity to electromagnetic waves while the spin
quantum effects could make the fluid more transparent. In addition, the magnetization dynamics of a thin ferromagnetic film exchange coupled with a surface of a 3D-TI has been studied and shown that the ferromagnetic strip could cut the TI surface into two gapless regions.\(^\text{13}\)

However, the spin hydrodynamic study of Dirac plasmons have not been examined up until now due to the peculiar band structures and electronic properties of the Dirac electrons, also because it is difficult to solve the nonlinear equations of relativistic hydrodynamic. It is expected that new features could appear in research of Dirac plasmons on a 3D TI surface with describing their spin hydrodynamic properties. The 3D TIs are expected to show several unique properties when the time reversal symmetry is broken.\(^\text{14}\) The latter can be achieved directly by a ferromagnetic insulating (FI) layer attached to the 3D TI surface, such that the TI surface states are exchange coupled to the collective magnetization of the FI. The collective motion of the Dirac electrons (relativistic spin electrons) are influenced mainly by the magnetization of the FI layer rather than its stray field. This is in contrast to the Schrödinger electrons in modulated by nanomagnets.

In this work, we are interested in collective excitations of Dirac electrons on Bi$_2$Se$_3$ TI surface with FI strips and a perpendicular magnetic field. The Bi$_2$Se$_3$ material has been verified to have a bulk gap of 0.3 eV and a single Dirac cone of surface states. The collective motion under electromagnetic modulation and spin effect of the Dirac electrons can behave as a tool of surface modification of the TI, or as a useful probe to characterize the average electromagnetic properties of the 2D Dirac electron system. Gauss units will be adopted throughout the paper except in specific definitions.

We consider a 2D semi-infinite Dirac electrons on an identified surface of a 3D TI like Bi$_2$Se$_3$ material ($v_F = 5 \times 10^7$ cm/s) with initial density of $n_0 = 3 \times 10^{14}$ cm$^{-2}$, in which $n_0 = 3k_F^2/2\pi$ and $k_F = m_e v_F/\hbar$. Here $v_F$ is the Fermi velocity, $k_F$ is the Fermi wave number, $m_e$ is the electron mass, $\hbar$ is the Planck constant divided by $2\pi$. Take a cartesian coordinate system $\{z, x\}$ in the surface and the 2D surface electrons are in the region $z \geq 0$. The in-plane FI stripes are deposited periodically on top of the surface along the $x$ axis, as sketched in Fig. 1. Their initial magnetizations are along the $z$ axis in the $\{z, x\}$ plane. All FI stripes take the same width $d/2$ and magnetization strength $m_0$, the smallest distance between them is $d/2$ and the periodic length is $d = 5$ nm.

In addition, an external perpendicular-plane magnetic field $\mathbf{B} = B_y(x, t)\mathbf{e}_y$ is applied to the surface that is a plane wave propagating long the $x$ axis and directed along the $y$ axis, we consider
the magnetic vector potential $\mathbf{A} = (0, 0, A_z)$ and $\mathbf{B} = (0, B_y, 0)$ with,

$$
B_y(x, t) = -B_0 k \cos(k_x x) \cos(kct) / k_x
$$

$$
A_z(x, t) = B_0 k \sin(k_x x) \sin(kct) / k_x^2.
$$

(1)

In the simulation domain the electromagnetic fields $\mathbf{E} = (E_x, 0, E_z)$ and $\mathbf{B}$ in space vector form can be identified by the Maxwell equations. The boundary condition at $x = 0$ can be expressed as a perfectly conducting wall. It is possible to solve analytically the Maxwell equations inside this physical system. The analytical solution of the electric field considered here can be expressed as

$$
E_x(x, t) = B_0 \cos(k_x x)
$$

$$
E_z(x, t) = B_0 \sin(k_x x) \sin(kct) / k_x^2
$$

(2)

with $k^2 = k_x^2$.

In the presence of the perpendicular-plane magnetic field and in-plane FI strips, the motion of surface electrons that take collective polarization can be regarded as relativistic surface plasmons. The plasmons which are regarded as charged fluids with 2D average density field $n_e(z, x, t)$ and velocity field $u_e(z, x, t)$ can be described by the relativistic QHD equations. Thus we will here focus on the collective properties of the surface electrons. Now comes the crucial point: by introducing the decomposition of the spinors according to $\psi = \sqrt{\gamma n} \exp(iS/\hbar) \varphi$ with the relation $m_e u_e = \nabla S + eA/c$, it is possible to derive relativistic quantum continuity and momentum equations from the EOM of relativistic fluid and the Dirac equation

$$
i\hbar \frac{\partial \psi}{\partial t} = v_F \sigma \cdot (p - \frac{e}{c} A) \psi - e\varphi \psi + \sigma \cdot \mathbf{M} \psi.
$$

(3)

Here $\gamma = 1/\sqrt{1 - u_e^2/c^2}$ is the relativistic factor, $e$ is the elementary charge and $c$ is the light speed, $p = (p_z, p_x)$ is the electron momentum, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices, and $\varphi$ is the 2-spinor with $\varphi \varphi^+ = 1$. In particular, $\mathbf{M} = m_z(x) e_z$ is the effective exchange field induced from the FI strips, and $m_z(x)$ takes a constant value $m_0$ in the stripe regions with magnetization aligned to the $z$ axis and zero otherwise. Moreover, the last term in the right side of Eq. (3) is induced by the spin quantum effects where the magnitude of $\mathbf{M}$, $m_0$ (can also be defined as the value of the exchange field), represents the strength of the spin quantum effects. Thus, the collective motions of the surface Dirac electrons can be described by the continuity equation

$$
\frac{\partial \gamma n_e}{\partial t} + \nabla \cdot (\gamma n_e \mathbf{u}_e) = 0,
$$

(4)
and the momentum-balance equation

$$\frac{\partial u_e}{\partial t} + (u_e \cdot \nabla) u_e = \frac{e}{\gamma m_e} (\nabla \Phi_{ext} + \nabla \Phi_{ind} + \frac{1}{e} \frac{\partial A}{\partial t} - \frac{u_e \times B}{c}) \mp \frac{1}{\gamma m_e} \nabla m_z. \quad (5)$$

Here, “−” represents spin-up and “+” represents spin-down in the last term on the right side of Eq. (5), \( \nabla = \frac{\partial}{\partial z} e_z + \frac{\partial}{\partial x} e_x \), and \( \Phi_{ext} \) is external electric potential. \( \Phi_{ind} \) is the induced potential that satisfies the Poisson equation

$$\nabla^2 \Phi_{ind} = 4\pi e (n_e - n_0). \quad (6)$$

The Poisson equation (6) is solved by the successive over relaxation (SOR) method. Flux-corrected transport (FCT) method\(^{16} \) is adopted to numerically solve the Eqs. (4) and (5) by time integration from the initial time \( t = 0 \) when the values of all quantities are known.

For convenience we introduce the length of a basic unit \( a = 5 \times 10^{-8} \) cm. Note that we examine the collective polarization of 2D Dirac electrons on the surface of \( \text{Bi}_2\text{Se}_3 \) TI material by considering the electromagnetic modulation and spin quantum effects in the following results. In our simulations, we take several period length of both \( B_y \) and \( m_z \) in \( x \) direction \((x/a = 0 – 32)\) as simulation region, the initial electron density \( n_0 = 3 \times 10^{14} \text{ cm}^{-2} \) and velocity \( u_e = 0 \) are treated as given parameters, while the values of \( m_0, B_0 \) and the wave number \( k \) are varied in order to examine the electromagnetic modulation and the spin quantum influences on the collective polarization of Dirac electrons.

The spin quantum effects on the collective density oscillation are illustrated in Fig. 2 without spin effects \( m_0 = 0 \) (solid line) and with spin effects \( m_0 = 1 \text{ meV} \sim (17 \text{ T}) \) (spin-up: dashed line, spin-down: dotted line). Laboratory magnetic fields are at most several tens of T. Here \( B_0 = 0.1 \) T for \( ka = \pi/8 \) (a), \( ka = \pi/4 \) (b), \( ka = \pi/2 \) (c) and \( ka = \pi \) (d). It is found from Fig. 2 that the collective oscillations with spin effects are larger than that without spin effects. We can note that the contribution from the spin term is significant in particular for large values of the wave number \( k \). In addition, it is interesting to see that the spin-up effects are more significant when \( ka = \pi/2 \) than spin-down effects. However, for most plasmas, the strength of magnetization is very small while the temperature is high, the spins mainly randomly orient, and the spin quantum effects are negligible. On the other hand, when there exist strongly magnetic modulations (larger than several T) in a quantum plasma, the spin vectors are essentially modulated and the spin effects can be significant. Thus, in our calculation, when the exchange fields induced by the FI strips take a strength of several meV or several tens of T, spin effects are significant, which can meet the most of the experimental conditions. That is, the spin quantum effects are evident on the collective
motion of Dirac electrons, leading to the increase of the density oscillation. The spin-up effects on the density oscillation in a 2D spectrum with different wave number is illustrated in Fig. 3, with \( m_0 = 1 \, \text{meV} \). Here \( B_0 = 0.1 \, \text{T} \) for \( ka = \pi/8 \) (a), \( ka = \pi/4 \) (b), \( ka = \pi/2 \) (c) and \( ka = \pi \) (d).

As demonstrated above, the collective polarization features with \((m_0 = 1 \, \text{meV})\) and without \((m_0 = 0)\) spin quantum effects are quite distinct. Such a difference is also exhibited when the strength of the spin quantum effects are varied. In Fig. 4 the hydrodynamic density of the Dirac electrons (a-b) with (a) \( B_0 = 0.1 \, \text{T} \) and (b) \( B_0 = 0.5 \, \text{T} \), and the induced potential \( \phi_{\text{ind}}/\phi_0 \) (\( \phi_0 = e/a \)) (c-d) with (c) \( B_0 = 0.1 \, \text{T} \) and (d) \( B_0 = 0.5 \, \text{T} \), are plotted as a function of \( x \) for different spin-up quantum effects \( m_0 = 1 \, \text{meV} \) (solid line), \( m_0 = 2 \, \text{meV} \) (dashed line) and \( m_0 = 3 \, \text{meV} \) (dotted line). Here \( ka = \pi/2 \). For a larger \( B_0 \) (\( B_0 = 0.5 \, \text{T} \)) there exist small differences in the three curves for three exchange field values (see Figs. 4(b) and 4(d)), while with the decreasing of \( B_0 \) (\( B_0 = 0.1 \, \text{T} \)) the differences become more obvious (see Figs. 4(a) and 4(c)). That is, a perpendicular-magnetic field of a few T, compared to an in-plane exchange field of several meV between the FI strips and the TI surface electrons, might dominate the collective oscillations. When \( B_0 = 0.1 \, \text{T} \), the collective oscillations become larger with increasing \( m_0 \).

In summary, we have studied the collective excitation and induced potential of Dirac electrons on the surface of a 3D-TI subject to a perpendicular magnetic field and a periodic exchange field which is provided by a series of equally spaced FI stripes attached to the TI surface. In many plasmas spin effects can be neglected due to its random orientations. In our simulation, however, in a relativistic plasma such as the surface electron gas of a 3D-TI, the spin quantum effects are included naturally and the spin effects are significant under the FI strips modulation with a laboratory condition. The simulation results presented in this paper will likely find its experimental application in relativistic quantum plasmas including Dirac electron plasmas and solid density plasmas, especially in the research of the surface states of 3D-TIs. Here we should emphasis that it was generally believed that the spin QHD related effects can be never be observed in experiments\(^{11}\), as it may require the external magnetic field as high as several thousand T in 3D bulk materials, like in a neutral star, as it is well known. However, this work shows that in a reduced 2D Dirac electron system on the surface of a topological insulator, the spin QHD can be observed with only around 20 T.

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Figure Captions

FIG. 1: Schematic illustration of the device: the 2D Dirac electrons in the surface of a TI is modulated by a pulsed exchange field. The latter is generated by an array of FI stripes. The magnetization directions of FI stripes are parallel to the z. Both the FI regions and the spacing regions have the same length $d/2 (d = 5$ nm). A perpendicular plane wave $B_y$ propagating in the surface of the TI along the $x$ direction.

FIG. 2: (Color online) The hydrodynamic density ($n_{e1} = n_e - n_0$) of Dirac electrons versus $x$ for (a-d) $B_0 = 0.1$ T with (a) $ka = \pi/8$, (b) $ka = \pi/4$, (c) $ka = \pi/2$ and (d) $ka = \pi$, without spin effects $m_0 = 0$ (solid line) and with spin effects $m_0 = 1$ meV (spin-up: dashed line) and (spin-down: dotted line).

FIG. 3: (Color online) The spin-up effects on the hydrodynamic density ($n_{e1} = n_e - n_0$) of Dirac electrons in 2D spectrums for (a-d) $B_0 = 0.1$ T with (a) $ka = \pi/8$, (b) $ka = \pi/4$, (c) $ka = \pi/2$ and (d) $ka = \pi$. Here $m_0 = 1$ meV.
FIG. 4: (Color online) The spin-up effects on the hydrodynamic density \( (n_{e1} = n_e - n_0) \) of Dirac electrons versus \( x \) for (a) \( B_0 = 0.1 \) T and (b) \( B_0 = 0.5 \) T, and the induced potential \( \phi_{\text{ind}} / \phi_0 \) versus \( x \) for (c) \( B_0 = 0.1 \) T, (d) \( B_0 = 0.5 \) T, with \( m_0 = 1 \) meV (solid line), \( m_0 = 2 \) meV (dashed line) and \( m_0 = 3 \) meV (dotted line). \( k \alpha = \pi/2 \) and \( \phi_0 = e/a \).
