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Hydrodynamic Electron Transport and Terahertz Plasma-Wave in Topological Insulator FETs (TI-FETs)

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***Abstract*—The peculiar matrix form of the distribution function as the solution to the spinor Boltzmann Transport Equation (S-BTE) has been constructed to address the spin-momentum locking in topological insulators (TIs). Further the hydrodynamic equations with the potential of including spin scattering is derived by taking the momentum moments of the Boltzmann-Vlasov (BV) equation, and is further solved analytically under the ballistic transport assumption. We obtained similar results for TIs as in graphene that the Dyakonov-Shur (D-S) instability [1] can be sustained and the plasma-wave frequency can be tuned into Terahertz frequency range by changing the channel length in TI-FETs. Computational results are presented for the case of Bi_2Se_3.**

***Keywords*—spinor Boltzmann equation; topological insulator; spin-momentum locking; plasma-wave instability; terahertz**

I. Introduction

The feasibility of realizing terahertz signal emitters at room-temperature has long been established by Dyakonov and Shur using high-electron mobility FETs (HEMTs), and hydrodynamic equation with asymmetric electrical boundary conditions (constant voltage source at the source contact and constant current source at the drain contact) [1]. When the carrier scattering in the channel is taken into consideration, it has been shown by numerical simulation that electron viscosity, as the predominant scattering mechanism for 2-dimensional electron gas (2DEG) , determines the condition for the existence and the strength of the D-S instability [2]. By using the hydrodynamic method, plasma-wave instability in graphene FETs (GFETs) at room-temperature has been analyzed under the ballistic assumption [3] and a viscosity term in the scattering process has been solved numerically [4]. The D-S instability in the channel of a FET is suppressed by scattering mechanisms, hence the channel materials with high carrier mobility are desired to maintain this type of plasma-wave instability at room-temperature.

Topological insulators (TIs) have a natural 2-dimensional conductive surface (for 3-D TIs) much like graphene, but the difference is that the former has one Dirac cone at Γ point, instead of two in graphene's first Brillouin zone (at K and K' points). Also, unlike graphene, due to the time-reversal invariance (TRI) of Hamiltonian and strong spin-orbit coupling (SOC) in TIs, the Kramers degeneracy is removed from the Γ point [5]. Although it is believed that the absence of backscattering [6] in TIs contributes little to the potentially high mobility, the chiral spin-momentum locking (see the Hamiltonian given later) nonetheless makes carriers on TI's surface insensitive to non-magnetic scattering. This is because in a two-body non-magnetic (a carrier and an impurity, for instance) collision, the total spin angular momentum is conserved, and thus the spin of the impurity must be changed to counter-balance the change of the spin and orbital momentum of the carrier if happens. It is this constraint that makes the carrier's momentum of the surface conductive state correlated to its spin in the process of scattering. Even though the specific form of the scattering mechanisms in TIs is still an open problem, a framework is needed to let us take into consideration the effect of spin on orbital momentum.

In this study, we generalize the scalar distribution function to a matrix form, which includes the spin-momentum locking, and is the solution to Boltzmann-Vlasov (BV) equation [7]. The matrix distribution function in TIs gives the spin polarization density explicitly, and spin scattering mechanisms can be accommodated in the BV equation. Hydrodynamic equations with spin can further be derived by applying moment method to BV equation and they can be solved analytically under the ballistic assumption. We obtained a similar exponential increment for the amplitude of plasma-wave as in GFETs, justifying the feasibility of this method to some extent.

II. Method

For the spin-momentum locking in TIs be taken into consideration, we adopt a matrix form of a so-called pseudo-distribution function, which is derived from the density matrix based on the eigenfunctions of spin states by Wigner transformation: $F = \frac{1}{2}\left(f_0\sigma_0 + \boldsymbol{f}\cdot\boldsymbol{\sigma}\right)$, where σ_0 and $\boldsymbol{\sigma}$ are 2×2 identity matrix and the Pauli basis set, respectively, and $\boldsymbol{f}$ is a 3D-vector, hence F is a 2×2 complex matrix. According to the Wigner transform relation given in [8] and the property of density matrix

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$$F(\boldsymbol{x},\boldsymbol{p})=\frac{1}{(2\pi\hbar)^3}\int\left\langle \boldsymbol{x}+\frac{\boldsymbol{x}'}{2}\middle|\hat{\rho}\middle|\boldsymbol{x}-\frac{\boldsymbol{x}'}{2}\right\rangle \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}'/\hbar}\mathrm{d}^3x' \quad (1)$$

$\mathrm{tr}(F)=f_0$ is the classical electron (assuming the carriers are electrons) distribution function while $\mathrm{tr}\left(\frac{\hbar}{2}\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}F\right)=\frac{\hbar}{2}\hat{\boldsymbol{n}}\cdot\boldsymbol{f}$ is the projection of spin on the direction of $\hat{\boldsymbol{n}}$, thus $\boldsymbol{f}$ represents the distribution of vector spin polarization. Although the physical meanings of the traces on F are clear, the equations of these variables are too complex to solve both analytically and numerically [8]. Here we do not get the traces of the Wigner quasi-distribution function at the beginning but extract the information about the spin component from the hydrodynamic equation afterwards. The form of the BV equation obtained from the Wigner transformed quantum Liouville equation by taking the classical limit is relatively simple [9]:

$$\frac{\partial}{\partial t}F+\frac{1}{2}\{\boldsymbol{v},\nabla_xF\}+e\nabla_x\varphi\cdot\nabla_pF+\frac{\mathrm{i}}{\hbar}[H,F]=\mathcal{Q} \quad (2)$$

where the second term on the left is introduced to eliminate the imaginary part, and the forth term describes the spin precession, while in our case they are $\boldsymbol{v}\cdot\nabla_xF$ and 0, respectively. $\mathcal{Q}$ is the collision integral.

In Bi_2Se_3 the effective surface Hamiltonian is $H_{\mathrm{surf}}(k_x,k_y)=\hbar v_F(\boldsymbol{k}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma}$ [6], from which the velocity can be obtained by $\boldsymbol{v}=\partial H/\partial(\hbar\boldsymbol{k})=v_F\hat{\boldsymbol{s}}\times\hat{\boldsymbol{z}}$, where $\hat{\boldsymbol{s}}$ is the unit vector of spin polarization of an electron, $\hat{\boldsymbol{z}}$ is the unit vector in the direction of positive z axis (the x-y axes are on the surface of Bi_2Se_3) and $\boldsymbol{\sigma}$ is the Pauli operator. Thus, since the spin polarization is perpendicular to the momentum, which can be expressed as $\boldsymbol{s}=\frac{\hbar}{2}\hat{\boldsymbol{p}}\times\hat{\boldsymbol{z}}$, the matrix distribution function has a peculiar form of $\frac{1}{2}f_0(\sigma_0+(\hat{\boldsymbol{p}}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma})$. In the absence of external magnetic field, which will break the time-reversal invariance in TIs, decoupled Boltzmann transport equation (3) and spin polarization equation (4) are obtained immediately by substituting F into the rigorous form of BV equation (2).

$$\frac{\partial}{\partial t}f_0+v_F\hat{\boldsymbol{p}}\cdot\nabla_xf_0+e\nabla_x\varphi\cdot\nabla_pf_0=0 \quad (3)$$

$$\begin{aligned}\frac{\partial}{\partial t}\left(f_0(\hat{\boldsymbol{p}}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma}\right)+v_F(\hat{\boldsymbol{p}}\cdot\nabla_xf_0)(\hat{\boldsymbol{p}}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma}&\\+e\nabla_x\varphi\cdot\nabla_p\left(f_0(\hat{\boldsymbol{p}}\times\hat{\boldsymbol{z}})\cdot\boldsymbol{\sigma}\right)=0&\end{aligned} \quad (4)$$

Here we represent the spin polarization in terms of $\hat{\boldsymbol{p}}\times\hat{\boldsymbol{z}}$ instead of $\boldsymbol{s}$, in that our purpose of deriving this model is to consider the effects of spin scattering on momentum transport. The set of corresponding hydrodynamic equations is an infinite hierarchy and some further condition, especially the approximate form of the distribution function, is necessary to truncate the infinite series of equations. This is equivalent to finding an approximate solution of the distribution function in a fixed functional subspace. The displaced Fermi-Dirac distribution is chosen as the nonequilibrium distribution, as in [3]:

$$f_0(\boldsymbol{x},\boldsymbol{p},t)=\left\{1+\exp\left[\frac{1}{k_BT}\left(\frac{pv_F-\boldsymbol{p}\cdot\boldsymbol{u}(t)}{\left(1-u^2(t)/v_F^2\right)^{3/4}}-\epsilon_F(t)\right)\right]\right\}^{-1} \quad (5)$$

where $v_F\simeq 6.2\times10^5\mathrm{m/s}$ [6], ϵ_F is the Fermi level which is assumed to be above the Dirac point (i.e., n-type), $\boldsymbol{u}(t)$ is the collective drift velocity assumed to be in x direction only. This form of distribution assumes that apart from the energy arising from the collective motion $\boldsymbol{u}$, which can be included in the quasi-Fermi level, electrons still obey Fermi-Dirac distribution as a result of the maximum entropy principle. The term $\left(1-u^2/v_F^2\right)^{3/4}$ is introduced to eliminate the unreasonable dependence of the electron concentration on the drift velocity.

After the zeroth- and first-order moments in momentum for the nonequilibrium distribution function are taken, (3) leads to the continuity equation and the Euler equation; (4) leads to the equations on spin polarization (6) and spin-momentum tensor (7). In the following, we restrict the derivation in 2-D case.

$$\frac{\partial}{\partial t}(0,-n\gamma)+\left(\frac{\partial}{\partial y}\left(\frac{v_F}{2}n\left(1-\gamma^2\right)\right),\frac{\partial}{\partial x}\left(-\frac{v_F}{2}n\right)\right)=0 \quad (6)$$

$$\begin{aligned}&\frac{\partial}{\partial t}\begin{bmatrix}0 & -\frac{\varepsilon_0}{v_F}\left(\frac{1+2\gamma^2}{2-\frac{1}{2}\gamma^2}\right)\\ \frac{\varepsilon_0}{2v_F}\left(1-\frac{3}{4}\gamma^2\right) & 0\end{bmatrix}\\&+\begin{bmatrix}\frac{\partial}{\partial y}\frac{\varepsilon_0}{2}\left(1-\frac{3}{4}\gamma^2\right)\frac{3}{4}\gamma & -\frac{\partial}{\partial x}\varepsilon_0\frac{6\gamma}{2-\frac{1}{2}\gamma^2}\\ \frac{\partial}{\partial x}\frac{\varepsilon_0}{2}\left(1-\frac{3}{4}\gamma^2\right)\frac{3}{4}\gamma & -\frac{\partial}{\partial y}\frac{\varepsilon_0}{2}\left(1-\frac{3}{4}\gamma^2\right)\frac{3}{4}\gamma\end{bmatrix}\\&+e\begin{bmatrix}0 & \frac{\partial\varphi}{\partial x}n\gamma\\ 0 & \frac{\partial\varphi}{\partial y}n\gamma\end{bmatrix}=0\end{aligned} \quad (7)$$

where γ is a relativistic factor defined by u/v_F, and the electron density $n=\frac{1}{(2\pi\hbar)^2}\int f_0\mathrm{d}^2p$, energy density $\varepsilon=\frac{1}{(2\pi\hbar)^2}\int pv_Ff_0\mathrm{d}^2p\approx\varepsilon_0\left[\left(2+\gamma^2\right)/\left(2-\frac{1}{2}\gamma^2\right)\right]$. During the derivation all the terms of γ higher than fourth order have been neglected. Equation (6) represents the change of spin polarization density in time resulting from the gradient of electron concentration and drift velocity. It contains no more information than the continuity equation does, and since the drift velocity and its time dependence both are small, some information about it has been ignored via approximation. Thus we solve (7) analytically by incorporating the carrier continuity equation $\partial_tn+\nabla_x(n\boldsymbol{u})=0$ instead. The spin-momentum tensor represents the momentum density along a certain direction of spin, and its diagonal elements are zero due to the spin-momentum locking. The space derivative of the electric potential can be associated with the electron concentration through the Poisson's equation for two-dimensional charge system [3], and in TI-FETs this relation is $\partial(e\varphi)/\partial x\approx-4\pi e^2/(\kappa_2/d_2+\kappa_1/d_1)\partial n/\partial x$. Also the derivatives of ε_0 are simplified in a similar way as in [3]: $\partial\varepsilon_0/\partial\epsilon_F=2n$ while $\partial n/\partial\epsilon_F=\ln\left(1+\exp(\beta\epsilon_F)\right)/\left(2\pi\beta v_F^2\hbar^2\right)$, then $\partial\varepsilon_0/\partial t=2n\left(1-\gamma^2\right)^{1/4}/\langle\varepsilon^{-1}\rangle\partial n/\partial t$ and $\partial\varepsilon_0/\partial x=2n\left(1-\gamma^2\right)^{1/4}/\langle\varepsilon^{-1}\rangle\partial n/\partial x$ where $\langle\varepsilon^{-1}\rangle=\frac{1}{(2\pi\hbar)^2}\int(pv_F)^{-1}f_0\mathrm{d}^2p=\left(1-\gamma^2\right)^{1/4}\frac{\ln(1+\exp(\beta\epsilon_F))}{\left(2\pi\beta v_F^2\hbar^2\right)}$. Thus, the set of the continuity equation and the Euler equation, and the set of the equations about spin are closed, respectively.

The boundary conditions, $\partial_t n|_{x=0} = 0$ at constant voltage source and $\partial_t (nu)|_{x=L} = 0$ (L is the channel length) at constant current source, are sustained. In the case of one-dimensional motion, assuming that all of the variables are uniform in y (i.e., width) direction, we restrict the equations to x direction, and concentrate on the spin component in y direction:

$$\frac{9}{4v_F}\gamma\frac{\partial\gamma}{\partial t} + \left[(3-\xi) + \left(\frac{9}{4} - 2\xi\right)\gamma^2\right]\frac{\partial\gamma}{\partial x} + \left[5 - 2\gamma^2 + \frac{4\pi e^2}{\kappa_2/d_2 + \kappa_1/d_1}\left\langle\varepsilon^{-1}\right\rangle\right]\xi\frac{\gamma}{n}\frac{\partial n}{\partial x} = 0 \tag{8}$$

where $\xi = n^2/\left(\varepsilon_0\left\langle\varepsilon^{-1}\right\rangle\right)$. The solution process is simplified through the decomposition of solutions to the sum of steady-state part and time-harmonic perturbation part, i.e. $n(x,t) = n_0 + \delta n(x)\,\mathrm{e}^{-\mathrm{i}\omega t}$; $\gamma(x,t) = \gamma_0 + \delta\gamma(x)\,\mathrm{e}^{-\mathrm{i}\omega t}$ where ω has both real and imaginary parts, i.e., a complex number [1, 3].

III. Results and Discussion

The analytical solution for the frequency of the plasma-wave is shown in (9) and (10) where $A = \gamma_0\left[6\xi_0 - 3 - 9\gamma_0^2/4 + 4\pi e^2/(\kappa_2/d_2 + \kappa_1/d_1)\xi_0\left\langle\varepsilon^{-1}\right\rangle\right]$, $B = \left[(3-\xi_0) + (9/2 - 2\xi_0)\gamma_0^2\right]/v_F$ and $C = 9\gamma_0^2/\left(4v_F^2\right)$ are introduced for simplicity.

$$\omega_r = \frac{A\pi}{\sqrt{B^2 + 4AC}L} \tag{9}$$

$$\omega_i = \frac{A}{\sqrt{B^2 + 4AC}L}\ln\left|\frac{\sqrt{B^2+4AC}+B}{\sqrt{B^2+4AC}-B}\right| \tag{10}$$

As we can see, in order to sustain the D-S instability, the increment of the wave amplitude (the imaginary part ω_i) must be positive, thus A and B must be both positive. Knowing from the expressions, ε_0, n and $\left\langle\varepsilon^{-1}\right\rangle$ can be written out in terms of Fermi-Dirac integration $F_j(x)$ explicitly: $\varepsilon_0 = \frac{\Gamma(3)}{2\pi\beta^3 v_F^2\hbar^2}F_2(\beta\epsilon_F)$, $n = \frac{\Gamma(2)}{2\pi\beta^2 v_F^2\hbar^2}F_1(\beta\epsilon_F)$ and $\left\langle\varepsilon^{-1}\right\rangle \approx \frac{\Gamma(1)}{2\pi\beta v_F^2\hbar^2}F_0(\beta\epsilon_F)$. In the condition of a strongly degenerate system ($\beta\epsilon_F \gg 1$), there are asymptotic relations: $F_0(\beta\epsilon_F) \to \beta\epsilon_F$, $F_1(\beta\epsilon_F) \to \frac{(\beta\epsilon_F)^2}{2}$ and $F_2(\beta\epsilon_F) \to \frac{(\beta\epsilon_F)^3}{6}$. Further, ξ and $\left\langle\varepsilon^{-1}\right\rangle$ which appear in A, B and C can be presented as $\xi = 3/4 - 3n_T/(2n)$ and $\left\langle\varepsilon^{-1}\right\rangle = \sqrt{n}/(\sqrt{\pi}v_F\hbar)$, where n_T is the thermo-electron concentration when $\epsilon_F = 0$ and has a typical order of $10^{11}\mathrm{cm}^{-2}$ [3]. Therefore, the condition that A and B are positive can be met easily only if the system is strongly degenerate and the drift velocity is sufficiently small. The oscillation frequency (the real part ω_r) can be tuned by changing the channel length.

Assuming that the gate dielectric is SiO_2 and the thicknesses of SiO_2 and Bi_2Se_3 are both 20 nm, we use the following parameters: $\kappa_1 = 3.4$, $\kappa_2 = 29$, $d_1 = d_2 = 20\,\mathrm{nm}$. The surface electron density varies from 0.1×10^{13} to $10\times10^{13}\,\mathrm{cm}^{-2}$ [10]. When the channel length is 40 nm (smaller than the typical value in graphene), the oscillation frequency is generally about 1 THz, and the increment of the wave amplitude is larger than that in graphene [3] in a wide range of γ.

However, in terms of the physical picture, there should be no difference between the 2-D surface conductive states of TIs and graphene except for the degeneracy in the absence of spin scattering (this can also be accepted in that the equations of the charge transport have the same form with those in graphene). The differences of the analytical solutions between TIs and graphene stem from the framework itself. As discussed above, in general the approximate solutions we obtain in the fixed functional subspace differ considerably from the exact solution because the distribution functions always hold complex forms (see the examples in [11]). Furthermore, after the form of distribution function has been fixed, any variable in hydrodynamic equations can be presented in terms of the variables in the distribution function, thus any two equations in this infinite hierarchy are closed. Our principles for selecting from these equations are the physical meaning and the variables on which we are concentrating. In the study of the transport

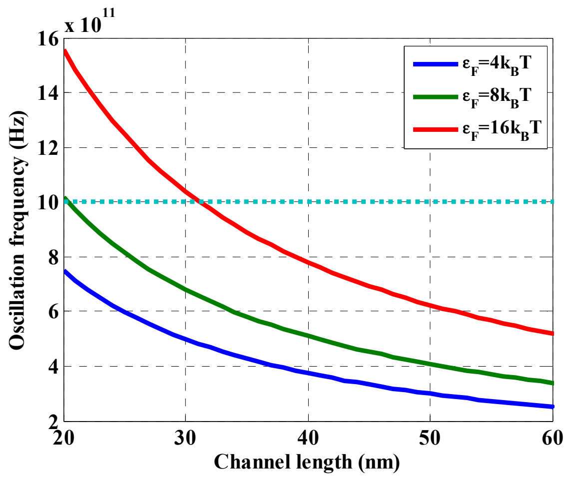

Fig. 1. The dependence between oscillation frequency (the real part of ω) and channel length. The dashed line shows the 1 THz frequency. The drift velocity is fixed at $0.05v_F$ and the surface electron density is fixed at 10^{13} cm^{-2}.

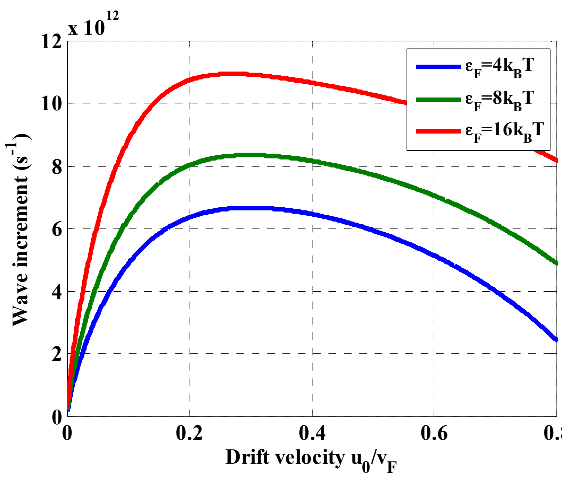

Fig. 2. The increment of the wave amplitude (the imaginary part of ω) as function of the electron drift velocity. The electron density is chosen to be 3×10^{12} cm^{-2}. The wave increment will be negative if the drift velocity is close to v_F, typically larger than $0.9v_F$, so the curves in that range are not shown here.

properties in graphene, the continuity equation and the Euler equation are the zeroth- and the first-order moments of the Boltzmann equation, respectively, while the spin-momentum equation in our work is higher than first order.

It might be noted that the effect of the spin-orbit coupling in TIs doesn't appear in the $\partial \boldsymbol{p}/\partial t$ term in the BV equation. This is natural, since this term is replaced by $-\nabla_x V$ in the common method to deal with it but the spin-orbit coupling cannot be represented by a conservative potential. However, the effect of the spin-orbit coupling is to make the direction of spin perpendicular to momentum, which has already been taken into consideration in the spin polarization part of the distribution function.

IV. Conclusions

Due to the linear spectrum of the carrier energy on the surface and the spin-momentum locking, TI-FETs are considered as potential candidates for room-temperature THz emitter. We propose the hydrodynamic framework based on spinor Boltzmann transport equation in order to include the spin scattering mechanisms in future work. The spin-momentum locking in TIs is considered in the matrix Wigner distribution function. It gives similar analytical results as with our results in graphene [4], illustrating that the D-S instability and the possibility of THz oscillation can be sustained on the surface of TIs, which proves the feasibility of this framework. Further research on the scattering mechanisms in TIs is needed to handle the spin scattering in our hydrodynamic framework.

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