**Minimal Conductivity of Topological Surface States with Magnetic Impurities**

Liang Chen and Shaolong Wan

*Corresponding author; Electronic address: slwan@ustc.edu.cn*

**Institute for Theoretical Physics and Department of Modern Physics**

**University of Science and Technology of China, Hefei, 230026, P. R. China**

(Dated: May 25, 2010)

In this paper we use the semiclassical Boltzmann equation to investigate the transport properties of Dirac fermion on the surface of topological insulator with magnetic impurities. The results obtained show that there is also a minimal conductivity in this system as in graphene. We also argue the low temperature transport property, and find that there is no low temperature anomaly known as Kondo effect when the temperature is $T > 10^{-6}$ K.

PACS numbers: 72.10.Fk, 73.20.Hb, 73.25.+i

1. INTRODUCTION

Recently topological insulator has been theoretically predicted and experimentally observed in HgTe quantum wells[1, 2], in Bi$_{1-x}$Sb$_x$ alloys[3, 4], and in Bi$_2$Se$_3$ and Bi$_2$Te$_3$ bulk crystals[5-8]. The topological insulator is a new discovered novel material with gapped bulk phase and robust gapless surface(edge) state. And novel properties of topological insulator have been predicted, for instance, effective monopole and topological magnetoelectric effect[9], superconductor proximity effect induced Majorana fermion states[10] etc. Sb$_{1-x}$Te$_x$ is the first material has been reported to be topological insulator[4], and Bi$_2$Se$_3$, Bi$_2$Te$_3$, Sb$_2$Te$_3$ have been predicted to be topological insulator[5] with single Dirac cone on the surface. This material has potential applications in spintronics, topological quantum computation, etc[11].

Recently, nanoribbons of Bi$_2$Se$_3$ have been fabricated[12], and transport properties of magnetic doped nanoribbons have been measured[13] with conductivity Kondo effect. However, the experiment can’t distinct the conductivity anomaly from Kondo effect induced by bulk defect conductance. In this paper, we use the semi-classical Boltzmann equation to investigated the transport properties of topological insulator surface state with surface magnetic impurity doped.

The paper is organized as follows: In Sec. II, we construct an effective interaction between topological insulator surface state and magnetic impurities, and give the corresponding Boltzmann equation with coherent distribution function. In Sec. III, we analyze the incoherent case and give an exact solution for the Boltzmann equation. We also take into account the conductivity correction from electron-hole coherent terms in Sec. IV. In Sec. V, we consider the high-order correction of coupling constant, and give the renormalization group equation of the the interaction between TISS and magnetic impurities. We make a conclusion in Sec. VI.

2. HAMILTONIAN AND BOLTZMANN EQUATION

At first we take Sb$_2$Te$_3$ as an example to construct the Hamiltonian and make some assumptions: (i) The chemical potential has been tune to seat at the Dirac point, which has been realized by D.Hsieh et al.[14] (ii) The interaction between topological insulator surface state(TISS) and magnetic impurities take the form of spin-spin interaction. (iii) The effective couplings are short-range rotational symmetric potential, which can be simulated by $J_{\mu}(r) = J_{\mu} e^{-r/R}/r$, where exchange parameters $J_{\mu}$ are estimated to the order 0.1eV $\sim$ 0.5eV[15, 16], and the range R of interaction has been assume to about 13Å[15]. (iv) Due to the effective RKKY interaction between magnetic impurities, all of the impurities have been ranged in the same direction[15]. (v)The concentration of magnetic impurity is very small, so we can take the single impurity approximation. According to above, the Hamiltonian of this system can be described
by:

\[ H_0 = \hbar v_F \int d^2r C^\dagger(r) i\sigma^\alpha \partial_\alpha C(r), \]  

\[ H_{\text{int}} = \int d^2r J_\mu(r) \hat{S}_\mu C^\dagger(r) \hat{\sigma}^\mu C(r), \]  

where \( C(r), C^\dagger(r) \) are annihilation, creation operators of TISS respectively, \( \sigma^\alpha (\alpha = x, y) \) are the Pauli matrices in spin space of TISS, \( \hat{S}_\mu (\mu = x, y, z) \) is the spin operators of impurities and \( \hbar v_F \simeq 3.7\text{eV}\cdot\text{Å} \) is Fermi velocity. The eigenstates of free Hamiltonian take:

\[ |\psi_+(k)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta} \\ 1 \end{pmatrix}, \quad |\psi_-(k)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta} \\ -1 \end{pmatrix}, \]  

with corresponding eigenvalues \( \epsilon_\pm(k) = \pm \hbar v_F k \) and \( \theta \) is the azimuth angle \( \arctan k_y/k_x \). Under these basis, the scattering of TISS by magnetic impurity can be expressed as:

\[ H_{\text{int}}(k_1, k_2) = \frac{1}{2} \sum_{\mu, \nu = \pm 1} \left[ J_\mu(e^{i(\theta_1 - \theta_2)} - \mu \nu)\hat{S}^z + \nu J_\mu e^{i\theta_1}\hat{S}^- + \mu J_\mu e^{-i\theta_2}\hat{S}^+ \right] C^\dagger_\mu(k_1) C_\nu(k_2), \]  

where \( J_\mu \) is the short-written of \( |k_1 - k_2|^2 + \frac{1}{2\mu^2} \)^{-1/2}, and we assume \( J_x = J_y = J_z \). \( \theta_1, \theta_2 \) are the azimuth angle of \( k_1 \) and \( k_2 \).

Electrical current of this system reads:

\[ J = \int \frac{d^2k}{(2\pi)^2} \text{tr} \left[ e\hat{v}\hat{f}(k) \right], \]  

where \( \hat{f}(k) \) is particle number distribution, and the velocity operator \( \hat{v} \) is a 2 \times 2 matrix in the space expand by \( \{ \psi_+, \psi_- \} \):

\[ \hat{v} = \frac{\hbar}{v_F} \begin{pmatrix} e_x \cos \theta + e_y \sin \theta & -i(e_x \sin \theta - e_y \cos \theta) \\ i(e_x \sin \theta - e_y \cos \theta) & -e_x \cos \theta - e_y \sin \theta \end{pmatrix}, \]

\[ (\hat{v}/v_F) = \begin{pmatrix} e_x \cos \theta + e_y \sin \theta & -i(e_x \sin \theta - e_y \cos \theta) \\ i(e_x \sin \theta - e_y \cos \theta) & -e_x \cos \theta - e_y \sin \theta \end{pmatrix}, \]  

here \( \theta \) is the azimuth angle of \( v \).

The Boltzmann equation, up to linear order of homogeneous electric field, of a similar system in graphene has been derived in reference [17]:

\[ \left( \frac{d\hat{f}}{dt} \right)^{\text{coll}} = \frac{i}{\hbar} \begin{pmatrix} 0 & f^+(-\langle k \rangle) - f^-(-\langle k \rangle) \\ f^-(-\langle k \rangle) + f^+(-\langle k \rangle) & 0 \end{pmatrix} + \frac{e}{\hbar} E \cdot \begin{pmatrix} \frac{\hbar v_{11}}{2} \frac{\partial f_i^{++}}{\partial \epsilon_i} & \frac{1}{2} \frac{\hbar v_{12}}{\epsilon_i} \left( f_i^{++} - f_i^{--} \right) \\ \frac{1}{2} \frac{\hbar v_{21}}{\epsilon_i} \left( f_i^{--} - f_i^{++} \right) & \frac{\hbar v_{22}}{2} \frac{\partial f_i^{--}}{\partial \epsilon_i} \end{pmatrix}, \]  

and the elastic collision term can be expressed by[18]:

\[ \left( \frac{d\hat{f}}{dt} \right)^{\text{coll}} = \frac{1}{2} \sum_{\alpha, \beta = \pm 1} \int \frac{d^2k'}{(2\pi)^2} \left\{ \delta(\epsilon_i - \epsilon_\alpha) + \delta(\epsilon_i - \epsilon_\beta) \right\} K_\alpha^{\mu\nu} f_{\alpha\beta}(k') \]  

\[ -\delta(\epsilon_\alpha - \epsilon_\beta) \left( K_\beta^{\mu\nu} f_{\alpha.}(k) + K_\alpha^{\mu\nu} f_{\beta.}(k) \right). \]  

where \( f_{\mu\nu} (\mu, \nu = \pm) \) are the four components of \( \hat{f}(k) \), \( f_{\mu\nu}^{0} \) are equilibrium distribution function without external electrical field, \( E \) is the homogeneous external electrical field, and \( v_{ij} \) (\( i,j=1,2 \)) are the four elements of velocity matrix.
3. INCOHERENT CASE

In equation (7) and (8), by setting the coherent terms \( f^{--}(\mathbf{k}), f^{+-}(\mathbf{k}) \) to be zero, we can get a more familiar Boltzmann transport equation of the form:

\[
e\mathbf{E} \cdot v_\mu = \int \frac{d^2k'}{(2\pi)^2} \left( \frac{2\pi}{\hbar} \right) \delta(\epsilon_\mu(\mathbf{k}) - \epsilon_\mu(\mathbf{k}')) |\langle \psi_\mu(\mathbf{k})|\hat{T}|\psi_\mu(\mathbf{k}')\rangle|^2 (f_\mu(\mathbf{k}') - f_\mu(\mathbf{k})),
\]

where \( \mu = \pm \) for \( \psi_\pm(\mathbf{k}) \) states, \( \hat{T} \) is the transition matrix, \( \mathbf{E} \) is the homogeneous external electric field. Under the first order of coupling constant \( \hat{T} \)-Matrix can be expressed as:

\[
\langle u(\mathbf{k}_1)|\hat{T}|u(\mathbf{k}_2)\rangle = \frac{1}{2} \left[ J_z(e^{i(\theta_1-\theta_2)} - 1)\hat{S}_z + J_x e^{i\theta_1} \hat{S}^- + J_y e^{-i\theta_2} \hat{S}^+ \right],
\]

and under the relaxation time approximation up to linear order of external homogeneous electric field, we have

\[
f_\mu(\mathbf{k}) = f_\mu^0(\mathbf{k}) + e\mathbf{E} \cdot v_\mu(\mathbf{k}) \frac{\partial f_\mu^0(\mathbf{k})}{\partial \epsilon_\mu(\mathbf{k})}.
\]

According to equation (9), (10) and (11), we can find an exact analytical solution for relaxation time:

\[
\frac{1}{\tau_\pm(\mathbf{k})} = \frac{kR^2N}{2\hbar^2v_F \sqrt{1 + 4R^2k^2}} \left\{ J_z^2S^zS^z \left[ 1 - \left( 3 + \frac{1}{2R^2k^2} \right) \frac{\sqrt{1 + 4R^2k^2} - (1 + 2R^2k^2)}{2R^2k^2} \right] 
+ J_x^2(S(S + 1) - S^zS^z) \left[ 1 - \frac{\sqrt{1 + 4R^2k^2} - (1 + 2R^2k^2)}{2R^2k^2} \right] \right\},
\]

here \( N \) is the concentration of magnetic impurities on topological insulator surface. In the short-range limit \( Rk \ll 1 \), relaxation time takes:

\[
\tau_\pm(\mathbf{k}) = \frac{1}{k} \frac{2\hbar^2v_F}{R^2N} \frac{1}{4J_z^2S^zS^z + J_x^2(S(S + 1) - S^zS^z)}.
\]

4. COHERENT TERMS INCLUDED

In this section, we take into account contributions of coherent terms in equation (7) and (8), the non-equilibrium part of the contribution function in these equations can be written as:

\[
\begin{align*}
 f_{++}^1(k) &= eE v_F [\cos(\theta - \phi) \tau_{11}(k) + \sin(\theta - \phi) \lambda_{11}(k)], \\
 f_{+-}^1(k) &= eE v_F [-i \sin(\theta - \phi) \tau_{12}(k) - i \cos(\theta - \phi) \lambda_{12}(k)], \\
 f_{--}^1(k) &= eE v_F [i \sin(\theta - \phi) \tau_{21}(k) + i \cos(\theta - \phi) \lambda_{21}(k)], \\
 f_{-+}^1(k) &= eE v_F [-\cos(\theta - \phi) \tau_{22}(k) - \sin(\theta - \phi) \lambda_{22}(k)],
\end{align*}
\]

here \( \theta \) is the azimuth angle \( \arctan(k_y/k_x) \) and \( \phi \) determines the direction of electric field \( \mathbf{E} = E(\cos \phi, \sin \phi) \). It can be verified that longitudinal current is proportional to the terms contain \( \tau_{ij}(k) \) and transverse current is proportional to the terms contain \( \lambda_{ij}(k) \). And we will show that the transverse current induced by magnetic impurities vanishes.

We calculated all of the matrix elements \( K_{\alpha\beta}^\gamma \):

\[
K_{\gamma\delta}^{\alpha\beta} = \frac{\pi}{R} \langle \left( \psi_\alpha(\mathbf{k})|\hat{T}|\psi_\gamma(\mathbf{k}')\right) \langle \psi_\beta(\mathbf{k})|\hat{T}|\psi_\delta(\mathbf{k}') \rangle^*,
\]
replaced non-equilibrium terms of $f_{\mu
u}(k)$ with equation (14), and took some tedious calculations from equations (7) and (8), then we found that $\tau_{ij}(k)$ and $\lambda_{ij}(k)$ satisfy the following equations (in the short-range limit $Rk \ll 1$):

$$
\begin{align*}
-2(\alpha + \xi)\tau_{11} - \alpha(\tau_{12} + \tau_{21}) + i\zeta(\lambda_{12} - \lambda_{21}) &= \frac{\hbar^2 v_F}{k} \frac{\partial f_{11}^0}{\partial \epsilon_1}, \\
-2(\alpha + \xi)\lambda_{11} - \alpha(\lambda_{12} + \lambda_{21}) + i\zeta(\tau_{12} - \tau_{21}) &= 0, \\
-\zeta(\tau_{11} - \tau_{22}) - i\alpha(\lambda_{11} + \lambda_{22} - \lambda_{21}) + i(2\xi + \alpha)\lambda_{12} &= \frac{\hbar^2 v_F}{\hbar} \left( \frac{\epsilon_1 - \epsilon_2}{\hbar} \right) \lambda_{12}, \\
-\zeta(\Lambda_{11} - \lambda_{22}) + i\alpha(\tau_{11} + \tau_{22} + \tau_{21}) + i(2\xi + \alpha)\tau_{12} &= \frac{\hbar^2 v_F}{k} \left( \frac{\epsilon_1 - \epsilon_2}{\hbar} \right) \tau_{12} - \frac{i}{2} \frac{f_{11}^0 - f_{22}^0}{\epsilon_1},
\end{align*}
$$

(1 \leftrightarrow 2)

where $\alpha$, $\xi$ and $\zeta$ are three parameters: $\alpha = \frac{N}{8} R^2 J_z^2 S^z S^z$, $\xi = \frac{N}{8} R^2 [2J_z^2 S^z S^z + 2J_z^2 (S(S+1) - S^z S^z)]$, $\zeta = -\frac{N}{8} R^2 J_z^2 S^z$.

(1 $\leftrightarrow$ 2) means exchange indexes 1 and 2 to get another four equations. By solving Eq.(15), we find a solution to equations (7) and (8) in the short-range limit, which are:

$$
\begin{align*}
\frac{f_{11}^0(k)}{\tau} &= e Ev_F \cdot \tau(k) \left\{ \cos(\theta - \phi) \left[ 1 + \frac{1}{F} \right] \left( \frac{\partial f_{11}^0}{\partial \epsilon_1} \right) + \frac{\alpha}{\alpha + \xi} \frac{1}{F} \left( \frac{f_{11}^0 - f_{22}^0}{2\epsilon_1} \right) \right\}, \\
\frac{f_{22}^0(k)}{\tau} &= -e Ev_F \cdot \tau(k) \left\{ \cos(\theta - \phi) \left[ 1 + \frac{1}{F} \right] \left( \frac{\partial f_{22}^0}{\partial \epsilon_2} \right) + \frac{\alpha}{\alpha + \xi} \frac{1}{F} \left( \frac{f_{22}^0 - f_{11}^0}{2\epsilon_2} \right) \right\}, \\
\frac{f_{12}^0(k)}{\tau} &= i\epsilon Ev_F \cdot \tau(k) \left\{ \sin(\theta - \phi) \left[ \frac{1}{F} - i \frac{1}{G} \right] \left( \frac{\alpha}{\alpha + \xi} \left( \frac{\partial f_{11}^0}{\partial \epsilon_1} \right) + \left( \frac{f_{11}^0 - f_{22}^0}{2\epsilon_1} \right) \right) \right\}, \\
\frac{f_{21}^0(k)}{\tau} &= -i\epsilon Ev_F \cdot \tau(k) \left\{ \sin(\theta - \phi) \left[ \frac{1}{F} + i \frac{1}{G} \right] \left( \frac{\alpha}{\alpha + \xi} \left( \frac{\partial f_{22}^0}{\partial \epsilon_2} \right) + \left( \frac{f_{22}^0 - f_{11}^0}{2\epsilon_2} \right) \right) \right\},
\end{align*}
$$

(16)

here we define:

$$
\frac{1}{F} = \frac{\xi(\alpha + \xi) - \zeta^2}{\hbar^2 v_F^4}, \quad \frac{1}{G} = \frac{\alpha + \xi}{\hbar^2 v_F^4}, \quad \frac{1}{H} = \frac{\zeta}{\hbar^2 v_F^4}.
$$

And the new relaxation time with coherent term correction is determined by

$$
\tau(k) \cdot |\epsilon(k)| = \frac{\hbar G/2}{1 + \frac{\zeta(\alpha + \xi)}{\hbar^2 v_F^4}}.
$$

(17)

The conductivity of this system can be deduced from equation (5) straightforwardly, while the longitudinal conductivity reads:

$$
\sigma = \frac{e^2 v_F^2}{2\pi} \int_0^\infty k dk \tau(k) \left[ -\frac{\partial f_{11}^0}{\partial \epsilon_1} + \frac{1}{F} \left( \frac{2\alpha + \xi}{\epsilon_1} \right) \left( \frac{\partial f_{11}^0}{\partial \epsilon_1} + \left( \frac{f_{11}^0 - f_{22}^0}{2\epsilon_1} \right) \right) \right],
$$

(18)

and the contribution to transverse current from terms in $f_{11}^0(k)$ and $f_{22}^0(k)$ proportional to $1/H$ have been canceled to each other.

5. HIGH ORDER CORRECTIONS

Assuming the correction from coherent terms is small $\frac{1}{H} \ll 1$, so the conductivity correction from high order terms of transition matrix may be taken into considered only in the incoherent case. In the short-range regime, Poorman's...
The integration over $k'$ has been limited in a finite regime, because these conductivity correction is induced by a virtual state $|\psi_\mu(k')\rangle$ while $|\psi_\mu(k)\rangle$ was propagating, and the uncertainty principle needs $|\epsilon_\mu(k') - \epsilon_\mu(k)|/|\tau(k')| < h$. Then according to equation (17), the boundary of $\epsilon_\mu(k')$ takes the form $\epsilon_\mu(k') = \epsilon_\mu(k)/(1 \pm \frac{h}{\Delta k'})$. The conductivity correction can be rewritten as:

$$\delta \sigma = -\frac{e^2TNR}{h} \frac{R^3J_zJ_zS(S+1)}{(4\pi\hbar v_F)^3} \left( \frac{2}{G} \right)^{-2} \kappa(2/G),$$

$$\kappa(2/G) = \int_0^{2/G} dx \frac{x e^{x}}{(e^{x} + 1)^2} \int_{-2/G}^{2/G} dx \left( 1 + \frac{1}{\lambda} \right) \frac{1 - e^{-x(1+\lambda)}}{1 + e^{-x(1+\lambda)}}.$$

where $\kappa(2/G)$ ($0 < 2/G < 1$) is a nondimensional function of $2/G$. So the high-order conductivity correction $\delta \sigma$ proportional to temperature. In the low temperature limit, coupling constants flow into a strong coupled regime $2/G \to \infty$, this semi-classical Boltzmann equation method is invalid because equation (17) is not consistent with uncertainty principle. For this reason, it is necessary to discuss the validity of our results obtained furthermore. According to equation(19), we estimate the Kondo temperature of this system and obtain $T_K = \frac{D}{\exp\left(-\frac{4\pi\hbar v_F^2 J_z}{k_B T_K}\right)}$, where D take the value of bulk energy gap which is about 0.1eV for $\text{Sb}_2\text{Te}_3$, R is about 13Å[15], and antiferromagnetic coupling is assumed to be isotropy with value 3.5eV. We get Kondo temperature is about $10^{-6}$K. So we obtain that surface magnetic dropped $\text{Sb}_2\text{Te}_3$ doesn’t reveal low temperature conductivity anomaly when temperature is not very low and hope be observed in future.
6. CONCLUSION

In this paper we investigate the transport properties of Dirac fermion on the surface of topological insulator with magnetic impurities. We find that there is also a minimal conductivity in the system studied as in graphene and there is no low temperature anomaly known as Kondo effect when the temperature $T > 10^{-6}K$.

Acknowledgement

This work is supported by NSFC Grant No.10675108.

[1] B. A. Bernevig, T. L. Hughes, and S.C. Zhang, *Science* **314**, 1757(2006).
[2] M. König, *et al. Science* **318**, 766(2007).
[3] L. Fu and C. L. Kane, *Phys. Rev. B* **76**, 045302(2007).
[4] D. Hsieh, *et al. Nature* **452**, 970(2008).
[5] H. Zhang, *et al. Nat. Phys.* **5**, 438(2009).
[6] Y. Xia, *et al. Science*, **323**, 919(2009).
[7] Y.L. Chen, *et al. Science* **325**, 178(2009).
[8] D. Hsieh, *et al. Phys. Rev. Lett.* **103**, 146401(2009).
[9] X-L. Qi, T.L. Hughes, S-C. Zhang, *Phys. Rev. B* **78**, 195424(2008).
[10] L. Fu and C.L. Kane, *Phys. Rev. B* **100**, 096407(2008).
[11] J.E. Moore, *Nature* **464**, 194-198(2010).
[12] H-L. Peng, *et al. nature materials* **9**, 225-229(2010).
[13] J.J. Cha, *et al. Nano Lett.* **10**, 1076-1081(2010).
[14] D. Hsieh, *et al. Nature* **460**, 1101-1105(2009).
[15] Q.Liu, C-X. Liu, C. Xu, X-L. Qi, S-C. Zhang, *Phys. Rev. Lett.* **102**, 156603(2009).
[16] J.S. Dyck, *et al. Phys. Rev. B* **65**, 115212(2002).
[17] M. Trushin and J. Schliemann, *Phys. Rev. Lett.* **99**, 216602 (2007).
[18] M.I. Dyakonov and A.V. Khaetskii, *Zh. Eksp. Teor. Fiz.* **86**, 1843 (1984) [Sov. Phys. JETP **59**, 1072 (1984)].
[19] A.C. Hewson, *The Kondo problem to heavy Fermions*, Cambridge University press, (2003).