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# Quantum transport through 3D Dirac materials

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ABSTRACT

Bismuth and its alloys provide a paradigm to realize three dimensional materials whose low-energy effective theory is given by Dirac equation in 3 + 1 dimensions. We study the quantum transport properties of three dimensional Dirac materials within the framework of Landauer–Büttiker formalism. Charge carriers in normal metal satisfying the Schrödinger equation, can be split into four-component with appropriate matching conditions at the boundary with the three dimensional Dirac material (3DDM). We calculate the conductance and the Fano factor of an interface separating 3DDM from a normal metal, as well as the conductance through a slab of 3DDM. Under certain circumstances the 3DDM appears transparent to electrons hitting the 3DDM. We find that electrons hitting the metal-3DDM interface from metallic side can enter 3DDM in a reversed spin state as soon as their angle of incidence deviates from the direction perpendicular to interface. However the presence of a second interface completely cancels this effect.



## 1. Introduction

After discovery of graphene [1], the concept of Dirac fermions became a live and daily-life concept to condensed matter physicists. In the regime of low-energy excitations, the single-particle excitations

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in graphene obey an effective Hamiltonian that is identical to two dimensional Dirac equation [2]. Some of the intriguing properties inherited from the relativistic-like form of the underlying Dirac equation are, Klein tunneling [3], unconventional Hall effect [4,5], bipolar super-current [6] and so on. Parallel to the developments in graphene physics, inspired by original proposal of Haldane [7] based on the honeycomb lattice structure of graphene, Kane and Mele constructed a model for two-dimensional topological insulator (TI) [8]. Later on other models of TIs carrying edge modes due to their non-trivial topology were theoretically constructed [9] and experimentally verified [10]. Three dimensional counterparts of the TIs displaying gap in the bulk, and massless Dirac fermions on their surface [11] were all based on the Bismuth element.

The elemental Bismuth was studied since a long time ago and the low-energy effective theory around the L point of Brillouin zone was proposed by Wolff [12] based on two-band approximation of Cohen [13]. It was found that effective theory describing the spin–orbit coupled bands of Bismuth is indeed a three dimensional (3D) massive Dirac theory. Later, this picture of 3D Dirac fermions was confirmed experimentally [14–17]. For a recent review on Dirac fermions in Bismuth see Ref. [18]. More recently, massless 3D Dirac fermions were observed at the $\Gamma$ point of Brillouin zone of the $Na_3Bi$ compound [19]. This provides us with condensed matter realization of both massive and massless Dirac fermions in three spatial dimensions. Therefore it is timely to study the transport properties of 3D Dirac electrons in various settings.

In this paper, we investigate the ballistic transport of 3D Dirac fermions across a boundary separating the 3D Dirac material (3DDM) from the normal metal, as well as the quantum transport through a segment of 3DDM sandwiched between two metallic leads as depicted in Fig. 1. The dynamics of charge carriers inside the 3DDM is described by the 3D Dirac equation, while the electronic states inside the normal metallic leads are governed by the scalar Schrödinger equation. Due to such a difference in the governing equations in the two sides of the interface, the boundary condition matching the electronic states will be tricky and one has to choose the wave-functions so as to give identical current density in both sides of the interfaces separating 3DDM and the normal metals. In the following sections we will formulate this problem and will calculate the transport properties in the ballistic regime within the Landauer–Büttiker formalism.

## 2. Formulation of the problem

The structure of junctions that we consider in this work is depicted in Fig. 1. In metallic region the carriers obey the Schrödinger equation that means the wave functions $\phi$ is a one-component function; whereas in 3DDM the wave-function $\psi$ describing the charge carrier is a four component spinor satisfying the 3D Dirac equation. An important question is how to construct a boundary condition for matching these two different types of wave-functions across the boundary?

For a typical 3DDM we use the isotropic form of the effective Hamiltonian which is given by [20]:

$$H = \begin{pmatrix} \Delta & 0 & iv_D q_z & iv_D(q_x - iq_y) \\ 0 & \Delta & iv_D(q_x + iq_y) & -iv_D q_z \\ -iv_D q_z & iv_D(-q_x + iq_y) & -\Delta & 0 \\ -iv_D(q_x + iq_y) & iv_D q_z & 0 & -\Delta \end{pmatrix}, \tag{1}$$

where $\Delta$ is energy gap, $v_D$ is velocity of carriers and $q_i, i = x, y, z$ denotes the Cartesian components of the wave-vector $\mathbf{q}$. The above explicit form corresponds to the following choice of $4 \times 4$ Dirac matrices:

$$\alpha_i = \begin{pmatrix} 0 & i\sigma_i \\ -i\sigma_i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix} \tag{2}$$

where $\sigma_i$ are Pauli matrices and $\sigma_0$ is $2 \times 2$ unit matrix. The $\gamma_0 = \beta$ and other $\gamma_i$ matrices are defined as

$$\gamma_i = v_D \beta \alpha_i = v_D \begin{pmatrix} 0 & i\sigma_i \\ i\sigma_i & 0 \end{pmatrix}. \tag{3}$$