Current-Voltage Characteristics of Weyl Semimetal Semiconducting Devices, Veselago Lenses and Hyperbolic Dirac Phase

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1 Supplementary Information

Here we present supplementary information for the paper titled "Current-Voltage Characteristics of Weyl Semimetal Transistors". The information here provides additional derivation for the calculations in the main text, which may be of interest to the reader.

1.1 Conservation of Probability Current

For the potential step the initial and final mediums are different. To allow for this the expression for transmission can be checked with the current continuity equation:

$$\frac{d}{dt}|\psi|^2 + \nabla \cdot \mathbf{j} = 0 \tag{1}$$

as the system here is time independent only the probability current;

$$\mathbf{j} = \psi^* \sigma \psi \tag{2}$$

needs to be considered. From the continuity equation; the probability current into the system must equal the probability current out of the system.

$$j_i = j_t + j_r \qquad 1 = \frac{j_t}{j_i} + \frac{j_r}{j_i} \tag{3}$$

By calculating the probability current both sides of the step the ratios of the transmitted and reflected current can be calculated. Using the eigenvectors derived previously the wave-functions on the left the step can be stated as:

$$\psi_a = \begin{bmatrix} \psi_{a1} \\ \psi_{a2} \end{bmatrix} = \begin{bmatrix} \left(e^{iq_a x} + re^{-iq_a x}\right) e^{ik_y y} e^{ik_z z} \\ \left(\alpha_a e^{iq_a x + i\theta_a} - r\alpha_a e^{-iq_a x - i\theta_a}\right) e^{ik_y y} e^{ik_z z} \end{bmatrix} \tag{4}$$

where the incident and reflected components have been included. The subscript a corresponds to region a in Figure 1. The wave-functions on the right of the step (corresponding to region b in Figure 1) only contain a transmitted component and is therefore given as:

$$\psi_b = \begin{bmatrix} \psi_{b1} \\ \psi_{b2} \end{bmatrix} = \begin{bmatrix} te^{iq_b x} e^{ik_y y} e^{ik_z z} \\ t\alpha_b e^{iq_b x + i\theta_b} e^{ik_y y} e^{ik_z z} \end{bmatrix} \tag{5}$$

The groups of constants have been given the regional subscripts a and b to allow for different potentials in each region. For clarity these are defined as:

$$q_a = \sqrt{\frac{(E-V_a)^2}{\hbar^2 v_f^2} - k_z^2 - k_y^2} \qquad q_b = \sqrt{\frac{(E-V_b)^2}{\hbar^2 v_f^2} - k_z^2 - k_y^2} \tag{6}$$

$$\alpha_a = \frac{|E-V_a| sin\left(\phi_a\right)}{E - V_a + |E-V_a| cos\left(\phi_a\right)} \qquad \alpha_b = \frac{|E-V_b| sin\left(\phi_b\right)}{E - V_b + |E-V_b| cos\left(\phi_b\right)} \tag{7}$$

$$\phi_a = arccos\left(\frac{\hbar v_f k_z}{|E-V_a|}\right) \qquad \phi_b = arccos\left(\frac{\hbar v_f k_z}{|E-V_b|}\right) \tag{8}$$

$$\theta_a = arcsin\left(\frac{\hbar v_f k_y}{|E-V_a| sin\phi_a}\right) \qquad \theta_b = arcsin\left(\frac{\hbar v_f k_y}{|E-V_b| sin\phi_b}\right) \tag{9}$$

The probability current on the left of the step in the x-direction is then:

$$\psi_a^* \sigma_{\mathbf{x}} \psi_a = \begin{bmatrix} e^{-iq_a x} + r^* e^{iq_a x} & \alpha_a e^{-iq_a x - i\theta_a} - r^* \alpha_a e^{iq_a x + i\theta_a} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} e^{iq_a x} + r e^{-iq_a x} \\ \alpha_a e^{iq_a x + i\theta_a} - r \alpha_a e^{-iq_a x - i\theta_a} \end{bmatrix} \tag{10}$$

$$= \begin{bmatrix} \alpha_a e^{-iq_a x - i\theta_a} - r^* \alpha_a e^{iq_a x + i\theta_a} & e^{-iq_a x} + r^* e^{iq_a x} \end{bmatrix} \begin{bmatrix} e^{iq_a x} + r e^{-iq_a x} \\ \alpha_a e^{iq_a x + i\theta_a} - r \alpha_a e^{-iq_a x - i\theta_a} \end{bmatrix} \tag{11}$$

$$= 2\alpha_a cos\left(\theta_a\right) - 2|r|^2 \alpha_a cos\left(\theta_a\right) \tag{12}$$

and on the right side:

$$\psi_b^* \sigma_{\mathbf{x}} \psi_b = \begin{bmatrix} t^* e^{-iq_b x} & t^* \alpha_b e^{-iq_b x - i\theta_b} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} t e^{iq_b x} \\ t \alpha_b e^{iq_b x + i\theta_b} \end{bmatrix} \tag{13}$$

$$= 2|t|^2 \alpha_b cos\left(\theta_b\right) \tag{14}$$

Current on the left side of the step must then equal current on the right of the step. Equating Equation (12) and Equation (14) produces:

$$1 = |t|^2 \frac{\alpha_b cos\left(\theta_b\right)}{\alpha_a cos\left(\theta_a\right)} + |r|^2 \tag{15}$$

Showing that the normal method of using $|t|^2$ as the transmission probability does not hold for asymmetrical systems. With this modification the transmission can now be found by:

$$T = 1 - R \qquad T = |t|^2 \frac{\alpha_b cos\left(\theta_b\right)}{\alpha_a cos\left(\theta_a\right)} \tag{16}$$

However if α_a and θ_a are equal to α_b and θ_b, as with the symmetrical barrier case, the current conservation produces $1 = |t|^2 + |r|^2$ and transmission can be calculated normally.

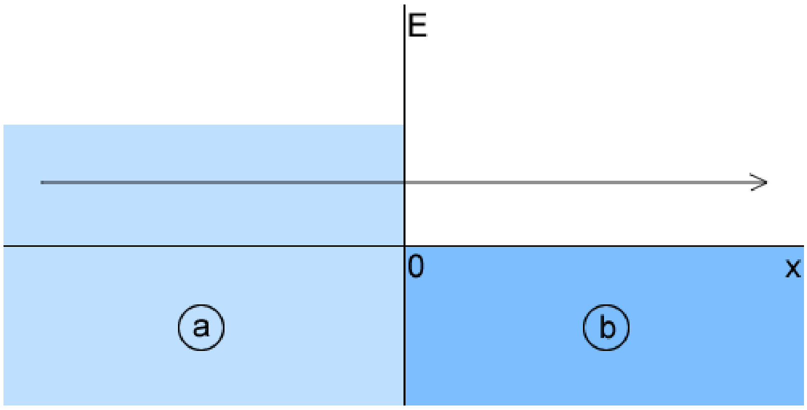

Figure 1: The potential step centered at $x = 0$ with $V_a \neq 0$ and $V_b = 0$.

1.2 The Potential Step

The system in Figure 1 can be described with the previously derived wave-functions as a set of simultaneous equations. Continuity at the barrier interface causes the wave-functions on the left and right of the step to be equal:

$$e^{ik_z z} e^{ik_y y} \left(e^{iq_a x} + r e^{-iq_a x} \right) = t e^{iq_b x} e^{ik_y y} e^{ik_z z} \tag{17}$$

$$e^{ik_z z} e^{ik_y y} \left(\alpha_a e^{iq_a x + i\theta_a} - r\alpha_a e^{-iq_a x - i\theta_a} \right) = t\alpha_b e^{iq_b x + i\theta_b} e^{ik_y y} e^{ik_z z} \tag{18}$$

The subscripts a and b represent constants for the corresponding region in Figure 1. By setting the boundary between the two regions as $x = 0$:

$$1 + r = t \tag{19}$$

$$\alpha_a e^{i\theta_a} - r\alpha_a e^{-i\theta_a} = t\alpha_b e^{i\theta_b} \tag{20}$$

and solving for t:

$$t = \frac{2\alpha_a cos\left(\theta_a\right)}{\alpha_a e^{-i\theta_a} + \alpha_b e^{i\theta_b}} \tag{21}$$

an expression for $|t|^2$ is then:

$$|t|^2 = \frac{4\alpha_a^2 cos^2\left(\theta_a\right)}{\alpha_a^2 + \alpha_b^2 + 2\alpha_a\alpha_b cos\left(\theta_a + \theta_b\right)} \tag{22}$$

However, from Section 1.1, it is known that the transmission through the step is not simply $|t|^2$. With Equation (16); the expression for transmission from the conservation of current calculation the transmission through the step becomes:

$$T = \frac{4\alpha_a\alpha_b cos\left(\theta_a\right) cos\left(\theta_b\right)}{\alpha_a^2 + \alpha_b^2 + 2\alpha_a\alpha_b cos\left(\theta_a + \theta_b\right)} \tag{23}$$

1.3 The Potential Barrier

The wave-functions previously derived can then be used in the scattering problem described in Figure 2. Here regional subscripts will be added to groups of constants. For the transfer matrix method [1] left and right travelling waves are considered in all regions

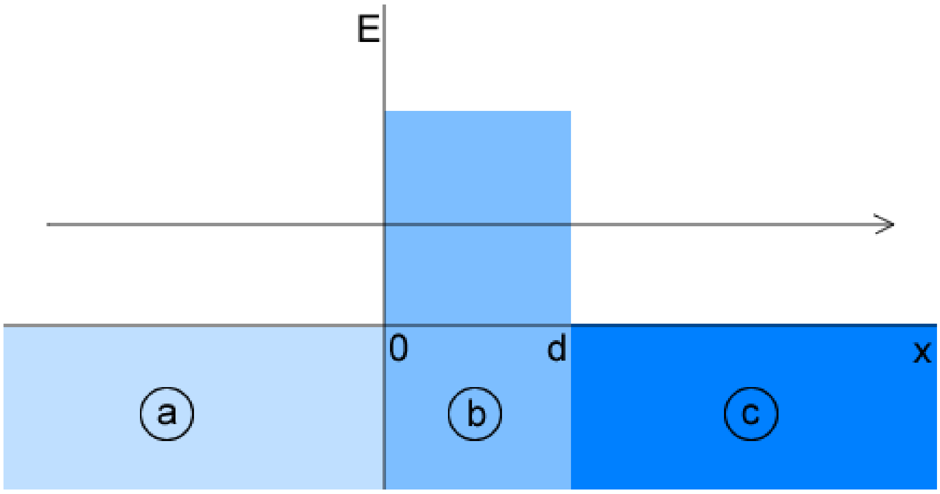

Figure 2: The potential barrier problem. A potential barrier is placed in the x-direction with a height V_b and a width d. The shaded region shows where hole transport is present. The three independent regions have been labled as a, b and c.

so that the wave-functions in each region can be defined as:

$$\psi_a = \begin{bmatrix} \psi_{a1} \\ \psi_{a2} \end{bmatrix} = \begin{bmatrix} \left(a_1 e^{iq_a x} + a_2 e^{-iq_a x}\right) e^{ik_y y} e^{ik_z z} \\ \left(a_1 \alpha_a e^{iq_a x + i\theta_a} - a_2 \alpha_a e^{-iq_a x - i\theta_a}\right) e^{ik_y y} e^{ik_z z} \end{bmatrix} \tag{24}$$

$$\psi_b = \begin{bmatrix} \psi_{b1} \\ \psi_{b2} \end{bmatrix} = \begin{bmatrix} \left(a_3 e^{iq_b x} + a_4 e^{-iq_b x}\right) e^{ik_y y} e^{ik_z z} \\ \left(a_3 \alpha_b e^{iq_b x + i\theta_b} - a_4 \alpha_b e^{-iq_b x - i\theta_b}\right) e^{ik_y y} e^{ik_z z} \end{bmatrix} \tag{25}$$

$$\psi_c = \begin{bmatrix} \psi_{c1} \\ \psi_{c2} \end{bmatrix} = \begin{bmatrix} \left(a_5 e^{iq_a x} + a_6 e^{-iq_a x}\right) e^{ik_y y} e^{ik_z z} \\ \left(a_5 \alpha_a e^{iq_a x + i\theta_a} - a_6 \alpha_a e^{-iq_a x - i\theta_a}\right) e^{ik_y y} e^{ik_z z} \end{bmatrix} \tag{26}$$

Continuity of the wave-functions requires that at the first barrier interface $\psi_a = \psi_b$. As the barrier interface is located at $x = 0$ the wave-functions reduce to:

$$\begin{bmatrix} 1 & 1 \\ \alpha_a e^{i\theta_a} & -\alpha_a e^{-i\theta_a} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \alpha_b e^{i\theta_b} & -\alpha_b e^{-i\theta_b} \end{bmatrix} \begin{bmatrix} a_3 \\ a_4 \end{bmatrix} \tag{27}$$

$$m_1 \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = m_2 \begin{bmatrix} a_3 \\ a_4 \end{bmatrix} \tag{28}$$

For convenience the matrices m_1, m_2, m_3, m_4 have been introduced as the corresponding wave-function in matrix form. At the second boundary $x = d$ the continuity requires that $\psi_b = \psi_c$ resulting in:

$$\begin{bmatrix} e^{iq_b d} & e^{-iq_b d} \\ \alpha_b e^{iq_b d + i\theta_b} & -\alpha_b e^{-iq_b d - i\theta_b} \end{bmatrix} \begin{bmatrix} a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} e^{iq_a d} & e^{-iq_a d} \\ \alpha_a e^{iq_a d + i\theta_a} & -\alpha_a e^{-iq_c d - i\theta_a} \end{bmatrix} \begin{bmatrix} a_5 \\ a_6 \end{bmatrix} \tag{29}$$

$$m_3 \begin{bmatrix} a_3 \\ a_4 \end{bmatrix} = m_4 \begin{bmatrix} a_5 \\ a_6 \end{bmatrix} \tag{30}$$

The transfer matrix M can then be obtained by eliminating constants a_3 and a_4 so that:

$$\begin{bmatrix} a_5 \\ a_6 \end{bmatrix} = M \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \qquad M = m_4^{-1} m_3 m_2^{-1} m_1 \tag{31}$$

Evaluating the transfer matrix allows the transmission coefficient and the total transmission to be obtained. From transfer matrix theory $t = 1/M_{2,2}$ and $T = |t|^2$ resulting in:

$$t = \frac{2\alpha_a\alpha_b e^{-idq_a} cos\left(\theta_a\right) cos\left(\theta_b\right)}{2\alpha_a\alpha_b\left(cos\left(dq_b\right) cos\left(\theta_a\right) cos\left(\theta_b\right) + isin\left(dq_b\right) sin\left(\theta_a\right) sin\left(\theta_b\right)\right) - isin\left(dq_b\right)\left(\alpha_a^2 + \alpha_b^2\right)} \tag{32}$$

$$T = \frac{4\alpha_a^2\alpha_b^2 cos^2\left(\theta_a\right) cos^2\left(\theta_b\right)}{4\alpha_a^2\alpha_b^2 cos^2\left(dq_b\right) cos^2\left(\theta_a\right) cos^2\left(\theta_b\right) + sin^2\left(dq_b\right)\left(2\alpha_a\alpha_b sin\left(\theta_a\right) sin\left(\theta_b\right) - \alpha_a^2 - \alpha_b^2\right)^2} \tag{33}$$

This equation can then be reduced to produce the transmission results for two-dimensional systems. To remove k_z the angles $\phi_{a,b}$ can be set to $\pi/2$ resulting in:

$$T = \frac{4s_a^2 s_b^2 cos^2\left(\theta_a\right) cos^2\left(\theta_b\right)}{4s_a^2 s_b^2 cos^2\left(dq_b\right) cos^2\left(\theta_a\right) cos^2\left(\theta_b\right) + sin^2\left(dq_b\right)\left(2s_a s_b sin\left(\theta_a\right) sin\left(\theta_b\right) - s_a^2 - s_b^2\right)^2} \tag{34}$$

where $s_{a,b} = sgn\left(E - V_{a,b}\right)$. Similarly the k_y dependence can be removed from Equation (35) by setting the angles $\theta_{a,b} = 0$. Therefore the result for a two-dimensional material in the $x - z$ plane takes the form:

$$T = \frac{4\alpha_a^2\alpha_b^2}{4\alpha_a^2\alpha_b^2 cos^2\left(dq_b\right) + sin^2\left(dq_b\right)\left(\alpha_a^2 + \alpha_b^2\right)^2} \tag{35}$$

1.4 Transfer Matrix in Optics

In optics an electromagnetic wave can be expressed as:

$$\psi = c_1 e^{ikx} + c_2 e^{-ikx} \tag{36}$$

where k is the wave number equivalent to $2\pi/\lambda$. When incident on a boundary the wave and the spacial derivitive must be continuous.

$$\frac{d}{dx}\psi = c_1 ike^{ikx} - c_2 ike^{-ikx} \tag{37}$$

When the boundary separates mediums; the wave must change within the medium so that:

$$\psi = c_3 e^{iqx} + c_4 e^{-iqx} \tag{38}$$

where $q = nk$ and n is the refractive index of the new medium. The transfer matrix for the wave passing through some medium can now be constructed. The waves in matrix form for each region are defined as:

$$\psi_a = \begin{bmatrix} e^{ikx} & e^{-ikx} \\ ike^{ikx} & -ike^{-ikx} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{39}$$

$$\psi_b = \begin{bmatrix} e^{iqx} & e^{-iqx} \\ iqe^{iqx} & -iqe^{-iqx} \end{bmatrix} \begin{bmatrix} c_3 \\ c_4 \end{bmatrix} \tag{40}$$

$$\psi_c = \begin{bmatrix} e^{ikx} & e^{-ikx} \\ ike^{ikx} & -ike^{-ikx} \end{bmatrix} \begin{bmatrix} c_5 \\ c_6 \end{bmatrix} \tag{41}$$

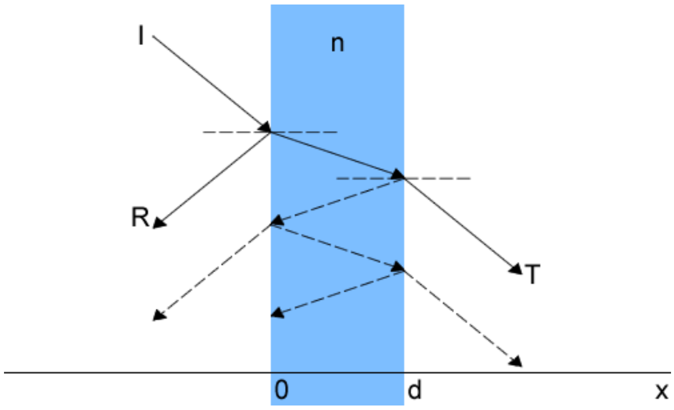

Figure 3: Diagram of an electromagnetic wave entering a region with refractive index n. The incident (I), reflected (R) and transmitted (T) probabilties are shown for a region of width d.

At the first boundary at $x = 0$ the waves ψ_a and ψ_b must be continuous and therefore $\psi_a = \psi_b$, which may be written as:

$$\begin{aligned}
\begin{bmatrix} c_3 \\ c_4 \end{bmatrix} &= \begin{bmatrix} 1 & 1 \\ iq & -iq \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ ik & -ik \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} && (42) \\
&= \frac{1}{2q} \begin{bmatrix} q+k & q-k \\ q-k & q+k \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} && (43) \\
&= m_1 \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} && (44)
\end{aligned}$$

At the second boundary at $x = d$ the wave ψ_b must be continuous with ψ_c and therefore $\psi_b = \psi_c$. This will be expressed as:

$$\begin{aligned}
\begin{bmatrix} c_5 \\ c_6 \end{bmatrix} &= \begin{bmatrix} e^{ikd} & e^{-ikd} \\ ike^{ikd} & -ike^{-ikd} \end{bmatrix}^{-1} \begin{bmatrix} e^{iqd} & e^{-iqd} \\ iqe^{iqd} & -iqe^{-iqd} \end{bmatrix} \begin{bmatrix} c_3 \\ c_4 \end{bmatrix} && (45) \\
&= \frac{1}{2k} \begin{bmatrix} (k+q)\, e^{-ikd+iqd} & (k-q)\, e^{-ikd-iqd} \\ (k-q)\, e^{ikd+iqd} & (k+q)\, e^{ikd-iqd} \end{bmatrix} \begin{bmatrix} c_3 \\ c_4 \end{bmatrix} && (46) \\
&= m_2 \begin{bmatrix} c_3 \\ c_4 \end{bmatrix} && (47)
\end{aligned}$$

The transfer matrix relating the final wave amplitudes to the incident wave amplitudes can finally be expressed as:

$$\begin{bmatrix} c_3 \\ c_4 \end{bmatrix} = m_2 m_1 \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{48}$$

Here the transfer matrix M is defined as:

$$\begin{aligned}
M &= m_2 m_1 && (49) \\
&= \frac{1}{4kq} \begin{bmatrix} (k+q)\, e^{-ikd+iqd} & (k-q)\, e^{-ikd-iqd} \\ (k-q)\, e^{ikd+iqd} & (k+q)\, e^{ikd-iqd} \end{bmatrix} \begin{bmatrix} q+k & q-k \\ q-k & q+k \end{bmatrix} && (50) \\
&= \frac{1}{2kq} \begin{bmatrix} \left(2kqcos\,(qd) + i\,(k^2+q^2)\, sin\,(qd)\right) e^{-ikd} & \left(i\,(q^2-k^2)\, sin\,(qd)\right) e^{-ikd} \\ \left(i\,(k^2-q^2)\, sin\,(qd)\right) e^{ikd} & \left(2kqcos\,(qd) - i\,(k^2+q^2)\, sin\,(qd)\right) e^{ikd} \end{bmatrix} && (51)
\end{aligned}$$

The transmission probability though the intermediate medium is then taken as:

$$T = \frac{1}{|M_{22}|^2} = \frac{4k^2q^2}{4k^2q^2cos^2\left(qd\right) + \left(k^2+q^2\right)^2 sin^2\left(qd\right)} \tag{52}$$

With the resonance condition of $T = 1$ occuring when:

$$dq = n\pi \tag{53}$$

With the equations for electromagnetic waves:

$$k = \frac{2\pi}{\lambda} \qquad c = f\lambda \qquad E = hf \tag{54}$$

where c is the speed of light in a vacuum, h is the plank constant, f is the frequency of the wave and λ is the wavelength. With these definitions the wave number can be expressed in terms of the energy E:

$$k = \frac{E}{\hbar c} \tag{55}$$

The transmission probability can also be expressed in terms of energy:

$$T = \frac{4n^2}{4n^2cos^2\left(\frac{dnE}{\hbar c}\right) + \left(1+n^2\right)^2 sin^2\left(\frac{dnE}{\hbar c}\right)} \tag{56}$$

with the resonance condition:

$$\frac{dnE}{\hbar c} = n_r\pi \tag{57}$$

2 Landauer Formalism in Weyl Semimetals

In this section the Landauer formalism is derived for a Weyl semimetal scattering device. For a single channel system at non-zero temperatures the current through the system shown in Figure 4 can be found []. The system in Figure 4 consists of 2 incoherent

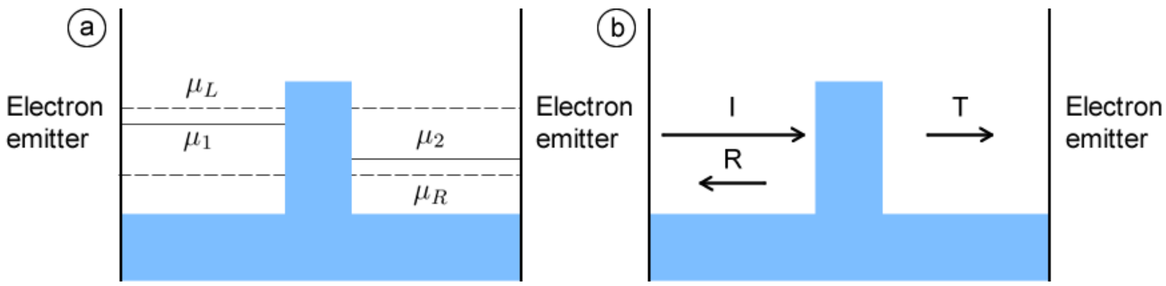

Figure 4: (Colour Online) (a) Diagram showing quasi-Fermi-energies and chemical potentials of the perfectly conducting wires. Here the left emitter injects electrons up to the quasi-Fermi-energy μ_L and the right emitter injects electrons up the the quasi-Fermi-energy μ_R. μ_1 and μ_2 are the chemical potentials of the perfectly conducting wires to the left and right of the scattering device. (b) A scattering device between two electron emitters. Charge carriers from the left emitter are scattered with a probability R of being reflected and probability T or transmitting through the scattering device.

electron reservoirs, which emit charge carriers up to the quasi-Fermi-energy $\mu_{L,R}$, where the subscript L and R represent the reservoir at left or right side of the system respectivly. These reservoirs are then connected to a scattering device via perfect and identical one dimensional conductors. These conductors have chemical potentials μ_1 and μ_2. The current leaving the left reservoir is then:

$$I = ev_f \frac{dn}{dE} \left(\mu_L - \mu_R\right) \tag{58}$$

where e is the electron charge, v_f is the Fermi velocity and dn/dE is the density of states. The current that is transmitted through the sample is then:

$$I = ev_f \frac{dn}{dE} T \left(\mu_R - \mu_R\right) \tag{59}$$

where T is the transmission probability through the scattering device. The density of states for Weyl semimetals at a Dirac point is given by:

$$\rho\left(E\right) = \frac{L_x L_y L_z}{\pi \hbar^3 v_f^3} E^2 \tag{60}$$

Where L_x, L_y is the size of the sample in the respective dimension. As only the x-direction current will be considered here, the current in the x-direction will be the same in each cell, therefore only size of the system in the y-direction will affect the x-directional current. This way the quantity L_x can be set to one and removed from the calculation. The current through the sample from equation (59) in the x-direction becomes:

$$I_x = e \frac{L_y L_z}{\pi \hbar^3 v_f^2} T\left(E, \theta, \phi\right) \left(\mu_L - \mu_R\right) E^2 cos\left(\theta\right) sin\left(\psi\right) \tag{61}$$

The energy and angular dependence for T has been included here to allow for the Weyl semimetal transmission probability. At non-zero temperatures the states are instead filled according to the corresponding Fermi-Dirac distribution.

$$f_{L,R} = f\left(E - \mu_{L,R}\right) = \frac{1}{e^{\frac{E-\mu_{L,R}}{k_b t}} + 1} \tag{62}$$

The current must then be integrated over all energies and incident angles to account for all states in the Fermi-Dirac distributions.

$$I_x = I_0 \int_{-\infty}^{\infty} \int_{-\pi/2}^{\pi/2} \int_0^{\pi} T\left(E, \theta, \phi\right) \left[f_L - f_R\right] E^2 cos\left(\theta\right) sin\left(\phi\right) dE d\theta d\phi \tag{63}$$

with the constant $I_0 = e\frac{2L_y L_z}{\pi \hbar^3 v_f^2}$.

3 References

[1] Wave Propagation: From Electrons to Photonic Crystals and Left-Handed Materials, P. Markos and C. M. Soukoulis, Princeton University Press, 1 Apr 2008