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Longitudinal negative magnetoresistance and magneto-transport phenomena in conventional and topological conductors

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Recently a large negative longitudinal (parallel to the magnetic field) magnetoresistance was observed in Weyl and Dirac semimetals. It is believed to be related to the chiral anomaly associated with topological electron band structure of these materials. We show that in a certain range of parameters such a phenomenon can also exist in conventional centrosymmetric and time reversal conductors, lacking topological protection of the electron spectrum and the chiral anomaly. We also discuss the magnetic field enhancement of the longitudinal components of the thermal conductivity and thermoelectric tensors.

One can distinguish two types of magnetoresistance depending on the mutual orientation of the current and the magnetic field: transverse and longitudinal. If the magnetic field is sufficiently small, the magnetoresistance can be described by the quasiclassical Boltzmann kinetic equation (see for example [1–5]). A change in the transverse resistance due to a magnetic field can be related to the fact that electrons experience Lorentz force in that direction. Since there is no Lorentz force in the direction parallel to the magnetic field, the origin of the longitudinal magnetoresistance is more complicated. Moreover, the longitudinal magnetoresistance is absent in the approximation of a spherical Fermi surface, and in the relaxation time approximation [1]. Although no theorem was proven, so far all results based on the conventional Boltzmann kinetic equation correspond to positive longitudinal magnetoresistance, (see for example Refs. 5 and 6 and references therein). Nielsen and Ninomiya [7] suggested a chiral anomaly-related [8, 9] mechanism of negative longitudinal magnetoresistance (NLMR) in materials with massless Dirac and Weyl electronic spectra, which recently attracted great theoretical interest [10– 13]. The calculations of Ref. 7 were done in the ultraquantum limit at zero temperature, and in the case where the chemical potential is at the Dirac point. However, in most of existing Dirac and Weyl semimetals the chemical potential is located away from the Dirac points. In this case a quasiclassical description of the chiral anomalyrelated NLMR was developed in Refs. 14 and 15. It was shown that the existence of strong NLMR requires a large ratio between the chirality and transport relaxation times. Recently large NLMR was observed both in Weyl and in Dirac materials (see for example Refs. 13, 16–20).

In Weyl semimetals the gapless character of the electron spectrum is protected by topology. In Dirac metals the massless Dirac points are protected only by the crystalline symmetry. Therefore a small lattice distortion of a Dirac semimetal can open a gap in the electronic spectrum making it non-topological. Below we consider magnetoresistance in Dirac-type materials in which the electron spectrum is either massless or has a small gap. Existence of a small gap in a Dirac semimetal was reported already in the first observation of NLMR in these materials [16]. Furthermore, NLMR was observed in Weyl

materials in which the Weyl valleys merge into a single electron pocket with zero net topological charge [21]. This implies that existence of massless Dirac points in the spectrum, their topological protection and the chiral anomaly are not necessary ingredients of large NLMR.

In this article we show that a negative contribution to the longitudinal magnetoresistance and other longitudinal magnetotransport phenomena exists even in conventional centrosymmetric and time-reversal symmetric semiconductors and metals. However, for this contribution to dominate the effect a certain hierarchy of relaxation times should take place.

To illustrate the origin of the effect we consider a model [22] where the energy gap E_g between between the conduction and the valence bands is significantly smaller than the energy separation from other bands, and the external potential $V(\mathbf{r})$ is smooth on the interatomic scale. In this case the electron dynamics may be described by the Dirac Hamiltonian (for a recent review see Ref. 23)

$$\hat{H} = u \, \mathbf{p} \cdot \boldsymbol{\sigma} \, \tau_3 + E_q \tau_1 + V(\mathbf{r}). \tag{1}$$

Here, $\mathbf{p} = -i\hbar \nabla - \frac{e}{c} \mathbf{A}(\mathbf{r})$ (with $\mathbf{A}(\mathbf{r})$ being the vector potential) is the kinematic momentum, E_g is half the band gap, and σ_i and τ_i denote the Pauli matrices that act in the spin and chirality subspaces respectively.

We focus on the typical situation in which the electron chemical potential μ is larger than the gap E_g . In this regime electron transport my be described by two equivalent approaches. The first one is based on the quasiclassical kinetic equation, while in the second one the free electron motion is described in terms of the Landau levels. Here we will use the latter approach. In a uniform magnetic field ${\bf B}$ directed along z-direction the energy spectrum of Eq. (1) has the form (see for example § 32 of Ref. 24)

$$\epsilon_n^2(p_z) = E_g^2 + u^2 p_z^2 + \frac{u^2 \hbar^2}{l_B^2} (2n + 1 + \sigma).$$
(2)

Here p_z is the electron momentum along the magnetic field, $l_B = \sqrt{\hbar c/|eB|}$ is the magnetic length, n=0,1,2... labels Landau levels, and $\sigma=\pm 1$ is a spin index.

At $E_g = 0$ the Hamiltonian (1) decouples into a sum of Weyl Hamiltonians describing right- and left-handed

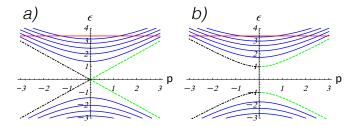


FIG. 1: Landau level spectrum of the Dirac equation in the gapless case, $E_g=0$ [panel a)] and gapped case [panel b)]. All Landau levels except the lowest one are degenerate in helicity and are shown by solid blue lines. The lowest Landau level is nondegenerate. The helicity of electronic states in it is indicated by the line style: Positive helicity states are shown by the green dashed line, and negative helicity states – by the black dash-dotted line. The red horizontal line indicates the location of the chemical potential.

chiral fermions. As a result, the electronic states can be classified by chirality (R and L), $\tau_3 \Psi_R = \Psi_R$, $\tau_3 \Psi_L =$ $-\Psi_L$. All Landau levels except the lowest one (n = $0, \sigma = -1$) are double degenerate. The electron states in these levels consist of opposite chirality pairs. The spectrum of the lowest Landau level consists of two nondegenerate linear branches, $\epsilon_0 = \pm up_z$, formed by the states with opposite chirality. As a result, in the presence of electric field the system exhibits the chiral anomaly [7–9]. Acceleration of the electrons by the electric field creates a population imbalance of electrons with different chirality. Since the Hamiltonian Eq. (1) decouples into a pair of chiral (L and R) Wevl Hamiltonians in the presence of an arbitrary potential $V(\mathbf{r})$, scattering by disorder does not relax the chirality imbalance. Therefore, even at full momentum relaxation of the electron distribution with a given chirality there is an a finite electric current proportional to the chirality imbalance (chiral magnetic effect) [25, 26]. In this approximation the electrical conductivity is infinite.

At $E_q \neq 0$ chirality is no longer conserved as the second term in Eq. (1), $E_g \tau_1$, couples the Weyl fermions with opposite chirality. However, the helicity operator $\hat{\alpha} = \mathbf{p} \cdot \boldsymbol{\sigma}/p$ still commutes with the Hamiltonian of the free electron motion described by the first two terms in Eq. (1). Thus, the states of the free electron motion may be classified by the helicity eigenvalues, $\alpha = \pm 1$ (at $E_q = 0$ helicity of free electron states coincides with chirality up to the sign of the electron energy). Note that this classification applies even in the presence of a magnetic field since the operator $\boldsymbol{p} \cdot \boldsymbol{\sigma}$ is still diagonal in the basis of energy eigenstates. The quantity p in the definition of helicity should be understood as the modulus of the eigenvalue of this operator. The helicity content of Landau level states is shown in Fig. 1. The states in the doubly degenerate Landau levels come in opposite helicity pairs, while the helicity of states in the non-degenerate lowest Landau level is given by $\alpha = \text{sign}(p_z)$.

Although at $E_g \neq 0$ there is no chiral anomaly, the mechanism of longitudinal magnetoresistance is quite

similar to that due to the chiral anomaly. Namely, the acceleration of electrons by the electric field directed along ${\bf B}$ produces helicity imbalance. The helicity imbalance in turn produces an electric current even at full momentum relaxation within a population of electrons with the same helicity. In contrast to chirality, helicity is not conserved by disorder scattering. Nevertheless, if the Fermi energy E_F strongly exceeds the gap E_g the helicity relaxation rate is parametrically small. As is shown in the supplementary materials (SM), in this regime the helicity relaxation time $\tau_h(\varepsilon)$ may be expressed in terms of the transport mean free time $\tau_{tr}(\varepsilon)$ as

$$\frac{\tau_h(\varepsilon)}{\tau_{tr}(\varepsilon)} = \xi \, \frac{4\varepsilon^2}{E_q^2} \gg 1. \tag{3}$$

Here ξ is a numerical coefficient of order unity which depends on the angular dependence of the impurity scattering cross-section. In the Born approximation it is given by Eq. (A7) in the Appendix. Below we develop a theory of electron magnetotransport phenomena in the leading approximation in τ_{tr}/τ_h .

In the regime $\tau_{tr}/\tau_h \ll 1$, during a short time τ_{tr} the electron distribution becomes isotropic in momentum and becomes dependent only on the electron energy ε and helicity $\alpha = \pm 1$, i. e. takes the form $n_{\alpha}(\varepsilon)$. Then the total electron density n is given by

$$n = \sum_{\alpha} \int d\epsilon \nu(\epsilon) n_{\alpha}(\epsilon), \tag{4}$$

where $\nu_{\alpha}(\epsilon)$ is the density of states with helicity α . In the leading approximation in τ_{tr}/τ_h the equations describing electronic transport have the form, see Appendix B,

$$\partial_{t} n_{\alpha}(\varepsilon) = -\frac{\nabla \cdot \mathbf{j}_{\alpha}(\varepsilon)}{\nu_{\alpha}(\varepsilon)} - \frac{k_{\alpha}}{\nu_{\alpha}(\varepsilon)} \frac{e^{2} \mathbf{E} \cdot \mathbf{B}}{h^{2} c} \, \partial_{\varepsilon} n_{\alpha}^{(0)}(\varepsilon) \\ - \frac{n_{\alpha}(\varepsilon) - n_{-\alpha}(\varepsilon)}{\tau_{h}(\varepsilon)} + I_{\alpha}^{in} \{ n_{\alpha}(\varepsilon) \}, \tag{5}$$

where $h = 2\pi\hbar$ and $k_{\alpha} = \alpha$. The collision integral due to inelastic electron-electron and electron-phonon scattering processes, is denoted by $I_{\alpha}^{in}\{n_{\alpha}(\varepsilon)\}$, and we expressed the collision integral due to impurity scattering in terms of the helicity relaxation time, see Eq. (A4). Finally,

$$\mathbf{j}_{\alpha}(\varepsilon) = \frac{ek_{\alpha}n_{\alpha}(\varepsilon)}{h^{2}c}\mathbf{B} \tag{6}$$

denotes the density of particle current with helicity α per unit energy [25, 26]. The electric current \mathbf{j} and the heat flux \mathbf{j}_q may be expressed as

$$\mathbf{j} = e \sum_{\alpha} \int d\varepsilon \, \mathbf{j}_{\alpha}(\varepsilon), \quad \mathbf{j}_{q} = \sum_{\alpha} \int d\varepsilon (\varepsilon - \mu) \, \mathbf{j}_{\alpha}(\varepsilon), \quad (7)$$

where μ is the chemical potential.

Note that in the limit $\tau_{tr}(\varepsilon)/\tau_h(\varepsilon) \to 0$ both the current $\mathbf{j}_{\alpha}(\varepsilon)$ and the helicity pumping are associated

only with the lowest Landau level. Accordingly, the second term in the right hand side of Eq. (5) can be written as $\frac{dp_z}{dt} \frac{\nu_L(\varepsilon)}{\nu(\epsilon)} \frac{d\epsilon_0(p_z)}{dp_z} \frac{\partial n(\epsilon)}{\partial \epsilon}$, where $\frac{dp_z}{dt} = eE_z$, and $\nu_L(\varepsilon) = \frac{1}{2\pi h l_B^2} \frac{dp_z}{d\epsilon_0(p_z)}$ is the density of states of the chiral Landau level (here the derivative $\frac{d\epsilon_0(p_z)}{dp_z}$ is evaluated at $\epsilon_0(p_z) = \varepsilon$). Then elastic scattering redistributes the helicity imbalance created by the electric field between the electron states with a given energy in all Landau levels. This is the reason why there is a density of states in the denominator in the first and the second terms in the right hand side of Eq. (5).

Equations (5)-(7) coincide with those obtained in Refs. 14 and 15 for Weyl semimetals with topologically protected gapless electron spectrum. In Weyl semimetals $k_{\alpha} = \pm 1$ is given by the quantized monopole charge of the Berry curvature flux and Eq. (5) describes the chiral anomaly. The above consideration shows that both generation of helicity imbalance due to the acceleration of electrons by the electric field described by Eq. (5), and the current proportional to helicity imbalance, Eq. (6), exist in generic conductors with no topological protection of the electron spectrum.

Below we discuss longitudinal magnetotransport phenomena: NLMR, enhancement of thermal conductivity and the thermoelectric effect by a magnetic field. Generally speaking, linear response phenomena are characterized by tensor transport coefficients. Equations (5)-(7), on the other hand, describe only the "anomalous" contributions to the transport coefficients which affect only the zz components of the tensors. Here \hat{z} is the direction of the magnetic field.

Using Eq. (5) and assuming that $n_{\alpha}(\varepsilon) = n_F(\varepsilon) + \delta n_{\alpha}(\varepsilon)$, where $n_F(\varepsilon) = [e^{(\varepsilon-\mu)/T(\mathbf{r})} + 1]^{-1}$ is the locally-equilibrium Fermi distribution function, we get

$$I_{\alpha}^{in}\{n_{\alpha}(\varepsilon)\} = \frac{\delta n_{\alpha}(\varepsilon) - \delta n_{-\alpha}(\varepsilon)}{\tau_{h}(\varepsilon)} + \frac{ek_{\alpha}\left(e\mathbf{E} - \frac{\varepsilon - \mu}{T}\mathbf{\nabla}T\right) \cdot \mathbf{B}}{\nu_{\alpha}(\varepsilon)h^{2}c} \,\partial_{\varepsilon}n_{F}(\varepsilon). \quad (8)$$

Note that although both terms in the right hand side are odd in k_{α} their effect on the nonequilibrium distribution function is drastically different. Only the first term creates the helicity imbalance whereas the second term creates an energy imbalance between the electron populations with different helicities. The inelastic collisions relax this energy imbalance but not the helicity imbalance. As a result the nonequilibrium distribution function may be written in the form

$$\delta n_{\alpha}(\varepsilon) = \frac{ek_{\alpha} \left(\tau_{eff} \frac{\varepsilon - \mu}{T} \nabla T - \tau_{h}(\varepsilon) e \mathbf{E} \right) \cdot \mathbf{B}}{2\nu_{\alpha}(\varepsilon) h^{2} c} \frac{dn_{F}(\varepsilon)}{d\varepsilon}.$$
(9)

Here $1/\tau_{eff}$ is the effective rate of energy transfer between the electron populations with opposite helicity. Treating the inelastic collision integral in the relaxation time approximation we may express it as

$$1/\tau_{eff} = 1/\tau_h + 1/\tau_{\epsilon},\tag{10}$$

where $1/\tau_{\epsilon}$ is the inelastic relaxation rate.

Substituting Eq. (9) into Eqs. (6) and (7) and expressing the electric current and energy flux densities in the form

$$\begin{pmatrix} \mathbf{j} \\ \mathbf{j}_q \end{pmatrix} = \begin{pmatrix} \hat{\sigma} & \hat{\beta} \\ \hat{\gamma} & \hat{\zeta} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{\nabla}T \end{pmatrix}$$
 (11)

we obtain the following expressions for the zz components of the transport tensors

$$\sigma_{zz} = \left(\frac{e^2 B}{h^2 c}\right)^2 \int d\varepsilon \left(-\frac{dn_F(\varepsilon)}{d\varepsilon}\right) \frac{\tau_h(\varepsilon)}{\nu_\alpha(\varepsilon)}, \quad (12a)$$

$$\beta_{zz} = \left(\frac{eB}{h^2c}\right)^2 \int d\varepsilon \, \frac{e(\varepsilon - \mu)}{T} \, \frac{dn_F(\varepsilon)}{d\varepsilon} \frac{\tau_{eff}(\varepsilon)}{\nu_{\alpha}(\varepsilon)}, (12b)$$

$$\zeta_{zz} = \left(\frac{eB}{h^2c}\right)^2 \int d\varepsilon \frac{(\epsilon - \mu)^2}{T} \frac{dn_F(\varepsilon)}{d\varepsilon} \frac{\tau_{eff}(\varepsilon)}{\nu_\alpha(\varepsilon)}. \quad (12c)$$

By the Onsager symmetry principle $\gamma_{zz}=-\beta_{zz}T$. The electronic contribution to thermal conductivity κ_{zz} may be expressed in terms of the electrical conductivity σ_{zz} and other transport coefficients in Eq. (12) as [1] $\kappa_{zz}=-\zeta_{zz}-T\beta_{zz}^2/\sigma_{zz}$. Since at high temperatures the considered effects are small we concentrate on the low temperature regime $T\ll\mu$. In this case Eqs. (12) simplify to

$$\sigma_{zz}(\mu) = \left(\frac{e^2 B}{h^2 c}\right)^2 \frac{\tau_h(\mu)}{\nu(\mu)},\tag{13a}$$

$$\zeta_{zz}(\mu) = -\frac{\pi^2 T}{3e^2} \frac{\tau_{eff}(\mu)}{\tau_h(\mu)} \, \sigma_{zz}(\mu), \tag{13b}$$

$$\beta_{zz}(\mu) = e \frac{d\zeta_{zz}(\mu)}{d\mu}.$$
 (13c)

Under the conditions specified above, the results in Eq. (13) are valid not only for Weyl and Dirac materials, but also for conventional conductors. In the case of Weyl and Dirac semimetals these equations reproduce results obtained in Refs. [14, 15]. The difference between the conventional time- and centrosymmetric materials and Weyl semimetals is in value of the helicity relaxation time τ_h . In non-centrosymmetric Weyl semimetals with spinnondegenerate electron spectrum the large value of τ_h/τ_{tr} may be associated with the fact that for smooth disorder potential their inter-valley transitions associated with large momentum transfer are suppressed. In conventional conductors the large value of τ_h/τ_{tr} arises from the large ratio of the Fermi energy to the band gap $E_g \ll \mu$, as described by Eq. (3). Taking $\nu(\mu) = \mu^2/\hbar^3 u^3$ we get

$$\frac{\sigma_{zz}}{\sigma_D} \sim \left(\frac{\hbar u e B}{c \mu E_g}\right)^2 \sim \left(\frac{\hbar \omega_c}{E_g}\right)^2.$$
 (14)

Here $\sigma_D = 2e^2\nu D$, with $D = u^2\tau_{tr}/3$ being the intravalley diffusion coefficient, is the Drude conductivity, and $\omega_c \sim eBu/c\mu$ is the cyclotron frequency. Equation (14) may be considered as an upper bound estimate for the magnitude of NLMR. The presence in the material of

short range impurities, which can not be described by Eq. (1), decreases the magnitude of the effect.

Of course there are other, "conventional" contributions to the longitudinal magnetoresistance associated with the Fermi surface anisotropy (see for example Ref. 6 and references therein). Typically at small magnetic field these contributions to magnetoconductivity scale as $(\sigma_{zz}(B) - \sigma(0)) \sim \chi \sigma(0)(\omega_c \tau_{tr})^2$, and saturate at $\omega_c \tau_{tr} \sim 1$. Here $\chi < 1$ is a parameter characterizing the Fermi surface anisotropy. Thus, the condition for Eq. (14) to dominate the LMR is

$$\chi (E_q \tau_{tr}/\hbar)^2 < 1. \tag{15}$$

Even if this condition is not satisfied the negative contribution to the magnetoresistance, Eq. (14) can dominate at high magnetic fields where the conventional contribution saturates. In this case the longitudinal magnetoresistance is a non-monotonic function of the magnetic field. We note that a non-monotonic B-dependence of σ_{zz} at low magnetic field was observed in most of experiments on Dirac and Weyl metals.

In experiments on Dirac semimetals the observed magnetoconductance was a few times greater than the Drude value of the conductivity at $\mathbf{B} = 0$. According to Eq. (14) this may happen if $\hbar \omega_c / E_g > 1$. Note that in the quasiclassical limit $\hbar \omega_c \ll \mu$. Then to have a big effect one should have $\mu \gg E_g$.

We would like to point out an important physical difference between the expressions for the magnetoconductivity σ_{zz} in Eq. (12a) on the one hand, and κ_{zz} and the thermoelectric α_{zz} in Eqs. (12b) and (12c) on the other hand. The magnetoconductance in Eq. (12a) is controlled by the helicity relaxation time τ_h , while the magnetic field dependence of the thermoelectric coefficient and thermal conductivity are controlled by τ_{eff} , which is a combination of the helicity relaxation time τ_h and the inelastic relaxation time τ_{ϵ} . Thus, according to Eq. (13b) the Wiedemann-Franz law is violated at high temperatures where $\tau_{eff} \ll \tau$. Furthermore, despite the conventional form of Eq. (13c) the Mott relation also does not hold, $\beta_{zz}(\mu) \neq -\pi^2 T/(3e)\partial_{\mu}\sigma_{zz}(\mu)$. The aforementioned difference and, consequently, the violation of the Wiedemann-Franz and Mott relations, can be traced to the difference in the physical processes which determine magnetoconductance $\sigma_{zz}(B)$, and the magnetic field dependence of $\zeta_{zz}(B)$, and $\beta_{zz}(B)$. The magnetoconductance is controlled by the long relaxation time τ_h of helicity imbalance at the Fermi level, which is created by the acceleration of the electrons in the lowest Landau level in the presence of the electric field. This is similar to the chiral anomaly. As long as $T \ll \mu$ and τ_h slowly depends of the electron energy, the temperature dependence of the negative longitudinal magnetoresistance is weak. This explains why NLMR was observed up to relatively high temperatures. In contrast, the temperature gradient does not create helicity imbalance, but only produces an energy imbalance between the electron populations with opposite helicity. The relaxation of the energy

imbalance is governed by the time τ_{eff} , which at $\tau_h > \tau_\epsilon$ coincides with the inelastic relaxation time, $\tau_{eff} \approx \tau_\epsilon$. As a result, the thermal conductivity and the thermoelectric coefficient exhibit a strong temperature dependence. In the "hydrodynamic" regime where $\tau_{tr} \gg \tau_\epsilon$ the described above contributions $\kappa_{zz}(B)$ and $\alpha_{zz}(B)$ become negligible compared to the conventional contributions. Thus the dependence thermal conductivity and the thermoelectric coefficient on the magnetic field is unrelated to the chiral anomaly.

In conclusion, we have shown that positive contributions to the parallel magneto-conductance $\sigma_{zz}(B)$, the magnetic field dependent parallel thermal conductivity and the thermoelectric coefficient $\beta_{zz}(B)$ can exist not only in Weyl and Dirac semimetals, but also in conventional cento-symmetric conductors as well. We also would like to mention that the magnetic field dependence of the sound absorption coefficient exhibits similar properties [15]. We also expect that, similarly to the negative magnetoresistance of pn-junctions in Weyl semimetals [27], the magnetoresistance of pn-junctions in Dirac semimetals with a sufficiently small gap E_g will also be negative.

Our consideration focused on the quasiclassical regime $\hbar u/l_B \ll \mu$. In the ultra-quantum limit, $\hbar u/l_B \gg \mu$, when only the zeroth Landau level is occupied the situation is more complicated. In Weyl semimetals in the single particle approximation an expression for conductivity in this regime was obtained in Ref. 7, $\sigma_{zz} \propto \frac{e^2 u}{4\pi \hbar l_R^2} \tau_h$. A similar result can be obtained for degenerate Dirac metals in the ultra-quantum regime. The magnetic field dependence of the longitudinal magnetoresistance in this regime is controlled by the corresponding magnetic field dependence of the helicity relaxation rate. The latter depends on the type of impurities. Its evaluation is not essentially different from the calculation of the backscattering rate in conventional semiconductors in the ultraquantum limit. In the context of conventional semiconductors in quantized magnetic field there is also a strongly anisotropic contribution to magnetoresistance, unrelated to the chiral anomaly, which may become negative in the longitudinal direction (see for example Refs. 28–32). It is related to the fact that in the presence of smooth potential in quantized magnetic field the small angle scattering is suppressed. An additional difficulty in interpreting magnetotransport measurements in the ultra-quantum regime is associated with the instability of the electron liquid with respect to charge density wave formation, which drives the system to the insulating state. In contrast, in the semiclassical limit, the theoretical consideration of electron transport is free of the aforementioned complications.

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