Negative transport times due to anisotropic interband scattering

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Negative transport times can arise due to anisotropic single-particle scattering in multiband systems. Specifically, we show within a semiclassical Boltzmann approach beyond the relaxation-time approximation that anisotropic scattering between electronlike and holelike Fermi surfaces generically leads to negative transport times for the minority carriers. The anisotropy required for this to occur decreases with increasing mismatch between the Fermi-surface radii. We obtain expressions for the resistivity, Hall coefficient, and magnetoresistance and identify the signatures of negative transport times, of which the most dramatic and unambiguous is negative magnetoresistance.

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Introduction.—In basic transport theory, the acceleration of carriers by an applied electric field is balanced by scattering, leading to a steady state with constant drift current [1]. The direction of the drift current is trivially determined by the charge of the carriers and relaxes over a characteristic transport time (TT). Deviations from this picture are remarkable and tend to generate a lot of interest. A striking example are negative TTs: Some fraction of the carriers may drift in the direction opposite of what one would expect based on their charge. Negative TTs of minority carriers were predicted for systems with electron- and holelike Fermi surfaces (FSs) [2], based on strong electron-hole (two-particle) scattering. This carrier drag was first observed in semiconductor quantum wells [3]. It has so far not been appreciated that negative TTs can also arise due to anisotropic single-particle scattering in multiband systems. This can be realized in materials close to an excitonic instability, e.g., the iron pnictides [4–6], chromium and its alloys [7, 8], and the transition-metal dichalcogenides [9, 10]. In these materials, nesting of electron and hole FSs strongly enhances interband spin or charge fluctuations with wavevector close to the nesting vector Q. These fluctuations are expected to promote highly anisotropic scattering between the nested FSs.

Theoretical studies of transport affected by anisotropic scattering have mainly focused on single-band models [11]. The discovery of the iron-pnictide superconductors has shifted attention to the role of spin fluctuations in multiband transport [12–15]. Fanfarillo et al. [15] demonstrated that vertex corrections can lead to negative TTs of the minority carriers when scattering by spin fluctuations dominates. This effect is accompanied by an enhancement of the Hall coefficient, which could explain its pronounced temperature dependence in the pnictides [16, 17].

In this Letter we demonstrate that negative TTs generically appear in partially compensated multiband systems with anisotropic single-particle interband scattering, hence revealing the general principle behind the results of Ref. [15]. Working within a Boltzmann approach beyond the relaxation-time approximation, we consider two FSs and include an interband scattering rate with arbitrary dependence on the scattering angle. When one FS is electronlike and the other holelike, anisotropic scattering naturally leads to a negative TT for the minority carriers. We then explore the implications of the anisotropic scattering for transport.

Model and method.—We consider 2D and 3D metals with two isotropic FSs labelled by $s = 1, 2$. The center of one FS is displaced with respect to the other by a wave vector $Q$, see Fig. 1(a). One of the FSs may be electronlike and the other holelike (e-h case) or both may be of the same type (e-e/h-h case). We employ a semiclassical description in terms of the distribution function $f_{s,k} = f_0(\varepsilon_{s,k}) + g_{s,k}$, with the equilibrium Fermi-Dirac distribution $f_0(\varepsilon_{s,k})$, where $\varepsilon_{s,k}$ is the band energy, and a deviation $g_{s,k}$. In a weak uniform electric field $E$, the stationary state is described by the linearized Boltzmann equation [1]

$$cE \cdot v_{s,k} [-f_0'(\varepsilon_{s,k})] = \sum_{s',k'} W_{s,k}^{s',k'} (g_{s,k} - g_{s',k'}),$$

where $v_{s,k} = \hbar^{-1} \nabla_k \varepsilon_{s,k}$ is the velocity, and $W_{s,k}^{s',k'}$ is the scattering rate from state $s, k$ to state $s', k'$. The scattering term contains an in-scattering contribution proportional to $g_{s',k'}$, which is equivalent to vertex corrections.

Specifically, we consider elastic scattering with an isotropic intraband contribution $W_\epsilon$ and an anisotropic interband contribution $W_\alpha(\theta_{k,k'})$.

$$W_{s,k}^{s',k'} = \delta(\varepsilon_{s',k'} - \varepsilon_{s,k}) \left[ \delta_{s's} W_\alpha(\theta_{k,k'}) + \delta_{s's} W_\epsilon \right],$$

where $s = 2$ (1) for $s = 1$ (2). The interband scattering rate $W_\alpha$ in general depends on $k$ and $k'$. Since we consider a weak electric field $E$, we assume the displacements of the Fermi seas to be small compared to the Fermi momenta $k_{F,s}$. Then the range of relevant absolute values $|k|, |k'|$ is small compared to the range of relevant polar angles, and we can ignore the dependence of $W_\alpha$ on the former. By symmetry, $W_\alpha$ can then only depend on the
\[ \theta = \theta_{k,k'} \text{ spanned by } k \text{ and } k', \text{ see Fig. 1(a)}, \] and is an even function of \( \theta \).

The deviations \( g_{s,k} \) solving the Boltzmann equation \( (1) \) are linear in \( E \) and can thus be written as \( g_{s,k} = eE \cdot \Lambda_{s,k} [-f'_{0}(\varepsilon_{s,k})] \). Since the scattering rate \( W_{s,k}' \) is an even function of \( \theta \), the scattering does not break rotational symmetry and does not introduce a preferred direction of rotation. Therefore, \( \Lambda_{s,k} \) must be parallel to the only vector appearing in the equation, namely the velocity \( v_{s,k} \). Due to rotational symmetry, the prefactor cannot depend on \( k \). Thus we can write

\[ g_{s,k} = \tau_{s} eE \cdot v_{s,k} [-f'_{0}(\varepsilon_{s,k})], \]

where \( \tau_{s} \) is the TT for FS \( s \), to be determined below.

In the Boltzmann equation \( (1) \), there is an essential difference between the out- and in-scattering terms. Factorizing out \( g_{s,k} \), inserting Eq. \( (3) \), and using that the scattering rate \( W_{s,k}' \) only depends on \( \theta \), we can write the right-hand side of Eq. \( (1) \) as

\[ g_{s,k} \sum_{s'} N_{s'} \left[ \delta_{s,s'} W_{a}(\theta) + \delta_{s,s'} W_{i} \right] \times \left( 1 - \eta_{s,s'} \frac{\tau_{s'} v_{F,s'}}{\tau_{s} v_{F,s}} \cos \theta \right)_{\theta}, \]

where \( v_{F,s} > 0 \) is the Fermi velocity and \( N_{s} \) the density of states for FS \( s \), \( \eta_{s,s'} = +1 \) (\( \eta_{s,s'} = -1 \)) if the FSs \( s \) and \( s' \) are of the same (different) type, and the average over \( \theta \) is denoted by \( \langle \ldots \rangle_{\theta} = \frac{1}{\pi} \int d\theta \ldots \) for 2D and \( \langle \ldots \rangle_{\theta} = \frac{1}{\pi} \int d\theta \sin \theta \ldots \) for 3D. Thus, Eq. \( (1) \) implies

\[ \frac{1}{\tau_{s}} = N_{s} W_{i} + N_{s} \langle W_{a}(\theta) \rangle_{\theta} - \eta_{s} N_{s} \frac{\tau_{s} v_{F,s}}{\tau_{s} v_{F,s}} \langle W_{a}(\theta) \cos \theta \rangle_{\theta}. \]

It is useful to define the *anisotropy parameter*

\[ \epsilon \equiv 1 + \eta_{12} \frac{\langle W_{a}(\theta) \cos \theta \rangle_{\theta}}{\langle W_{a}(\theta) \rangle_{\theta}}. \]

as a measure of the anisotropy of \( W_{a}(\theta) \). The limit \( \epsilon = 0 \) (\( \epsilon = 2 \)) corresponds to \( W_{a}(\theta) \) having a \( \delta \)-function peak at \( \theta = 0 \) (\( \theta = \pi \)) for the e-h case, and vice versa for the e-e/h-h case. \( \epsilon = 1 \) always corresponds to \( \langle W_{a}(\theta) \cos \theta \rangle_{\theta} = 0 \), which includes the case of isotropic interband scattering. Figure 1(b) illustrates the connection between \( \epsilon \) and the anisotropic scattering rate for the case of a single maximum. We focus on the situation where the maximum is at \( \theta = 0 \) \([18]\). This naturally occurs for the e-h case close to an excitonic instability, due to the scattering by the enhanced spin or charge fluctuations, allowing \( \epsilon \in [0, 1] \) to be tuned by doping or temperature. Although there is no excitonic instability for the e-e/h-h case, \( \epsilon \in [1, 2] \), collective fluctuations can still be enhanced due to the proximity of nesting.

Transport times.—We first consider pure interband scattering. Solving Eq. \( (5) \) for the TTs, we obtain

\[ \tau_{s} = \tau_{0,s} + \frac{1 + \frac{\epsilon}{1 - \epsilon}}{2 - \epsilon}, \]

where \( \tau_{0,s} = N_{s}^{-1} \langle W_{a}(\theta) \rangle_{\theta}^{-1} \) is the bare lifetime for FS \( s \), and \( \gamma_{s} = v_{F,s} \tau_{0,s}/v_{F,s} \tau_{0,s} = (k_{F,s}/E_{F,s})^{-1} \), where \( d \) is the dimension of the system. Note that only the surface areas of the FSs matter and not their densities of states.

The TT is plotted in Fig. 2. We first focus on the e-h case, \( 0 \leq \epsilon \leq 1 \), cf. Fig. 1(b). The smaller FS has a negative TT for

\[ \epsilon < \epsilon^{*} \equiv 1 - \gamma_{<} \]

where \( \gamma_{<} = \min \gamma_{s} \leq 1 \). In the anisotropic limit, \( \epsilon \to 0 \), the TT of the smaller (larger) FS diverges to negative (positive) values, while their ratio remains finite and negative, \( (\tau_{s}/\tau_{0,s})/(\tau_{s}/\tau_{0,s} \to -\gamma_{s} = -1/\gamma_{s} \). This can be understood as follows. For \( \epsilon \to 0 \), the scattering rate \( W_{a}(\theta) \) becomes a \( \delta \)-function and, therefore, a particle in the state \( s,k \) can only scatter to the state \( s',k' \), where \( k \) is determined by \( \varepsilon_{s,k} = \varepsilon_{s,k} \) and \( \theta_{k,k'} = 0 \), see Fig. 1(a). Thus the system decouples into pairs of states, \( s,k \) and \( s',k' \). Scattering between the two states cannot relax their joint occupation \( F_{s,k} = f_{s,k} + f_{s',k'} \), which therefore accelerates freely, \( F_{s,k}(t) = F_{s,k} - eE_{0}(0) \), so that the TTs diverge.

For small \( \epsilon > 0 \), the scattering between \( s,k \) and \( s',k' \) still dominates and scattering to other states can be treated as a weak perturbation. This additional scattering leads to weak relaxation of \( F_{s,k} \) and thus stabilizes a steady state. Still, the difference \( f_{s,k} - f_{s',k'} \) relaxes much more rapidly than the sum \( f_{s,k} + f_{s',k'} = F_{s,k} \). Hence, in the steady state the former is much smaller in absolute value than the latter so that \( g_{s,k} \approx g_{s,k} \approx F_{s,k}/2 - f_{0}(\varepsilon_{s,k}) \). The occupation numbers on the same side of the two FSs are both either enhanced or reduced in comparison to the equilibrium state. In the e-h case, the electrons at these points have opposite velocities so that the electrons on one of the FSs...
have to drift in the “wrong” direction. As Fig. 2 shows, the direction of the drift and thus the signs of the TTs are set by the majority carriers.

On the other hand, for weak anisotropy, \( \epsilon \approx 1 \), Fig. 2 shows that \( \tau_s/\tau_{0,s} \) decreases with decreasing \( \epsilon \) regardless of the FS sizes. Increasing anisotropy favors small-\( \theta \) scattering. For the e-h case, this enhances backscattering since the velocities \( v_{s,k} \) and \( v_{s,k}^* \) are opposite and is therefore more efficient in relaxing the current. For the compensated case, \( \gamma_s = 1 \), this mechanism is effective at all anisotropy levels, \( 0 \leq \epsilon \leq 1 \), since the mechanism discussed above relies on FSs of unequal size.

In the e-e/h-h case, the carriers from both FSs always drift in the same direction, as expected. The TTs increase monotonically with \( \epsilon \), and diverge in the extreme anisotropic limit \( \epsilon \rightarrow 2 \). The increasing anisotropy favors small-\( \theta \) scattering, which for the e-e/h-h case corresponds to forward scattering, and is thus increasingly inefficient at relaxing the current.

As we show in the Supplemental Material, the inclusion of isotropic intraband scattering essentially leads to a renormalization of the anisotropy parameter \( \epsilon \). We hence ignore intraband scattering in the following discussion of the implications of negative transport times.

**Resistivity.**—The resistivity can be obtained from the TTs \( \tau_s \) \cite{1}. We present the resistivity relative to its isotropic limit, \( \rho_0 \equiv \rho|_{\epsilon=1} \), which coincides with the result one would obtain by approximating the TTs by bare lifetimes. We obtain

\[
\frac{\rho}{\rho_0} = \frac{v_{F,1}k_{F,1}^{d-1}\tau_{0,1} + v_{F,2}k_{F,2}^{d-1}\tau_{1,2}}{v_{F,1}k_{F,1}^{d-1}\tau_1 + v_{F,2}k_{F,2}^{d-1}\tau_2} = \frac{2 - \epsilon}{1 + \frac{1}{\epsilon} \left( 1 - \frac{2}{\gamma_1 + \gamma_2} \right)}. \tag{9}
\]

Figure 3 shows that the anisotropy has a large effect on the resistivity, especially in the e-h case. Although minority carriers give a negative contribution to the current for \( \epsilon < \epsilon^* \), the total current in the direction of \( \mathbf{E} \) is always positive. However, the competition between the two anisotropy effects, the usual enhancement of the resistivity due to backscattering and the reduction due to anisotropic scattering, causes a maximum of \( \rho/\rho_0 \). We find that this maximum occurs at \( \epsilon = \epsilon^* \), which means that the reduction of \( \rho/\rho_0 \) due to anisotropic scattering dominates for small \( \epsilon \).

**Hall coefficient.**—The Hall coefficient of a two-band system with isotropic dispersion obeys \cite{11}

\[
R_H = \pm \frac{1}{e c} \frac{n_s \mu_s^2 + \eta_s n_s \mu_s^2}{(\eta_s n_s \mu_s + \eta_s n_s \mu_s)^2}, \tag{10}
\]

where \( \mu_s = e\tau_s v_{F,s}/k_{F,s} \) and \( n_s \propto k_{F,s}^2 \) are the mobility and particle number of FS \( s \), respectively, and the upper (lower) overall sign pertains to a holelike (electronlike) FS \( s \). With Eq. (7) we obtain

\[
\frac{R_H}{R_{H,s}} = \frac{1 + \gamma_s \frac{1 - 3d}{4}}{1 + \frac{1}{\gamma_s - \frac{1 - \gamma_s}{1 - \gamma_s}} \frac{(1 - \gamma_s)(1 - \gamma_s^*)}{(1 - \gamma_s^*)(1 - \gamma_s)^2}}, \tag{11}
\]

where \( R_{H,s} \propto 1/n_s \) is the Hall coefficient of FS \( s \). In the e-h case, the electrons and holes contribute with different signs to the Hall coefficient, irrespective of the signs of the TTs, which enter squared. Figure 4 shows that \( R_H/R_{H,s} \) is strongly affected by the anisotropy, implying that approximating the TT by the lifetime \cite{13} is not sufficient. In particular, we find a maximum at

\[
\epsilon^* = \frac{(\gamma_s - 1)(1 - \gamma_s^*)^{\frac{1}{2d-1}}}{\gamma_s^{\frac{1}{2d-1}} + \gamma_s}, \tag{12}
\]

which corresponds to equal magnitude but opposite sign of the electron and hole mobilities, \( \mu_e = -\mu_h \). At the maximum the Hall coefficient assumes the value \( R_H/R_{H,s} = 1/[1 - \gamma_s^{-d/(d-1)}] \), which diverges for \( \gamma_s \rightarrow 1 \) so that for nearly compensated e-h systems anisotropic scattering can cause a huge enhancement of the Hall effect, as found in Ref. \cite{15}. 

Figure 2. (Color online) Transport time \( \tau_s \) in units of the bare lifetime \( \tau_{0,s} \) at FS \( s \) as a function of the anisotropy parameter \( \epsilon \) and \( \gamma_s = (k_{F,s}/k_{F,s})^{d-1} \). The corresponding plot of \( \tau_s/\tau_{0,s} \) would be the mirror image with respect to \( \gamma_s = 1 \).

Figure 3. (Color online) Resistivity in terms of its isotropic limit, \( \rho_0 \equiv \rho|_{\epsilon=1} \), as a function of \( \epsilon \) and \( \gamma_s = (k_{F,s}/k_{F,s})^{d-1} \).
$F, \bar{k} = F,s, \bar{k}$

10
10
10
10
0
0.5
1
1.5
2

$\gamma_s = k_F,s/k_F,\bar{s}$

1.05
1.1
1.2
1.4

A particular microscopic origin for the anisotropic scattering is related to the maximum at $\epsilon^*$, as these materials have rather poor nesting, i.e., $\gamma_s$ should differ significantly from unity. However, the most stringent test of negative TTs would be a measurement of the magnetoresistance.

Some general conclusions may be drawn. Close to perfect nesting, negative TTs are restricted to the limit of extreme scattering anisotropy and thus should only become evident in the transport just above the excitonic instability. Significant doping may therefore be required to observe the most striking effects such as negative magnetoresistance or the maximum in the Hall coefficient.

The magnetoresistance is negative if the TT of minority carriers is restricted to the limit of $\epsilon^*$, where one TT becomes negative, for the following reason. If the TT of the minority carriers is negative (positive), the current contributions $j_<$ and $j_>$ of minority and majority carriers, respectively, point in opposite directions (the same direction) for $B = 0$. If a magnetic field is applied, the contributions $j_<$ and $j_>$ are rotated due to the Lorentz force, under the constraint that the total current in the transverse direction vanishes. However, as long as $j_<$ and $j_>$ are not rotated by the same angle, they are no longer parallel and their vector sum is thus larger (smaller) in absolute value than for $B = 0$. Hence, the magnetoresistance is negative (positive). A special point is $\epsilon = \epsilon^*$, where the two angles are equal, the total current is unchanged, and the magnetoresistance vanishes.

Conclusions.—Anisotropic single-particle scattering between electron and hole FSs causes the TT to differ dramatically from the bare carrier lifetime and can lead to negative TTs for the minority carriers. The degree of anisotropy required for this decreases for increasing ratio between the FS areas. This effect does not depend on a particular microscopic origin for the anisotropic scattering and is distinct from carrier drag due to the two-particle electron-hole interaction [2]. Negative TTs have clear signatures in transport; most notably the magnetoresistance is negative if the TT of minority carriers is negative.

Some general conclusions may be drawn. Close to perfect nesting, negative TTs are restricted to the limit of extreme scattering anisotropy and thus should only become evident in the transport just above the excitonic instability. Significant doping may therefore be required to observe the most striking effects such as negative magnetoresistance or the maximum in the Hall coefficient. It is however encouraging that in the pnictides the Hall coefficient is strongly enhanced close to the spin-density-wave transition, in particular in the case of good nesting [16] [17], consistent with our predictions. We further speculate that the broad maximum [19] [20] in the Hall coefficient in LiFeAs and LiFeP as a function of temperature is related to the maximum at $\epsilon^*$, as these materials have rather poor nesting, i.e., $\gamma_s$ should differ significantly from unity. However, the most stringent test of negative TTs would be a measurement of the magnetoresistance.

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For the sake of clarity, we discuss all our results with reference to an anisotropic scattering rate $W_a(\theta)$ with a single maximum at $\theta = 0$, see Fig. 1(b). However, our results hold for a general function $W_a(\theta)$. 

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SUPPLEMENTAL MATERIAL

Inclusion of intraband scattering

We here discuss the consequences of including isotropic intraband scattering. If we include \( W_i \) in Eq. (2), the TTs become

\[
\tau_s = \tau_{0,s} \frac{1 - \frac{1}{\gamma_s} \frac{1 - \epsilon}{1 + \epsilon}}{1 - \frac{1}{\gamma_s} \frac{1 - \epsilon}{1 + \epsilon}},
\]

(S1)

where the bare lifetimes now consist of intra- and interband contributions,

\[
\frac{1}{\tau_{0,s}} = \frac{1}{\tau_{0,s}^{(a)}} + \frac{1}{\tau_{0,s}^{(i)}} \equiv N_s \langle W_a(\theta) \rangle_\theta + N_s W_i,
\]

(S2)

and \( x_s \equiv \tau_{0,s}^{(a)} / \tau_{0,s}^{(i)} \) is the ratio of the lifetimes due to inter- and intraband scattering. If we assume equal densities of states at the two FSs for simplicitly we recover the previous expression (7) for the TTs with a renormalized anisotropy parameter

\[
\epsilon \to \epsilon + x \frac{1}{1 + x},
\]

(S3)

where \( x = W_i / \langle W_a(\theta) \rangle_\theta \). Thus in this case the only effect of isotropic intraband scattering is to reduce the range of the anisotropy parameter to \( x/(1 + x) \leq \epsilon \leq 2 - x/(1 + x) \), and negative TTs still occur provided that \( x < \gamma_\epsilon - 1 \).

Hall coefficient and magnetoresistance in 3D

In the main part of our Letter, we have presented the Hall coefficient and the magnetoresistance coefficient for a 2D model. Here, these quantities are presented for a 3D system. Figure S1 shows the Hall coefficient, while Fig. S2 presents the magnetoresistance. As can be seen, there are only minor quantitative differences between the 2D and 3D results, e.g., the maximum in the Hall coefficient at fixed \( \gamma_s \) is somewhat broader in 3D. The conclusions drawn above thus hold equally for the 2D and 3D cases.

Figure S1. (a) Hall coefficient \( R_H \) for a 3D system as a function of \( \epsilon \) and \( \gamma_s \), in units of the Hall coefficient \( R_{H,s} \) of FS \( s \). (b) The same quantity as a function of \( \epsilon \) on a logarithmic scale for various \( \gamma_s \). The characteristic anisotropy level \( \epsilon^* \) where the TT of the minority carriers changes sign is indicated by a dashed line. The dotted line marked by \( \epsilon^{**} \) indicates the maximum of \( R_H / R_{H,s} \) as a function of \( \epsilon \).
Figure S2. Magnetoresistance coefficient for the 3D system in units of $(\mu_0,s/c)^2$ (a) as a function of $\epsilon$ and $\gamma_s$ and (b) as a function of $\epsilon$ for two values of $\gamma_s$. At $\epsilon = \epsilon^*$ (dashed) and $\epsilon^{**}$ (dotted) the magnetoresistance is zero.