Transport in multiband systems with strong spin fluctuations: forward-scattering corrections

Maxim Breitkreiz, P. M. R. Brydon, and Carsten Timm

1 Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany
2 Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, USA 20742

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Transport in materials with strong spin fluctuations is dominated by highly momentum-dependent scattering. We show that for multiband systems this anisotropic scattering can lead to transport anomalies that are missed by a simple relaxation-time approximation, which neglects forward-scattering corrections. Most notably, the concept of hot and cold regions of the Fermi surfaces breaks down: Hot regions with strong scattering show correspondingly short lifetimes but can nevertheless contribute significantly to transport. We discuss the underlying physics on the basis of the Boltzmann transport equation, taking forward-scattering corrections into account. We also calculate the resistivity and the Hall, Seebeck, and Nernst coefficients for a two-band model relevant for the iron pnictides and discuss their temperature and doping dependence.

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I. INTRODUCTION

Many materials of high current interest for condensed matter physics are metals with strong spin fluctuations, for example doped cuprates and iron pnictides. In both classes, spin fluctuations are thought to mediate the superconducting pairing at relatively high temperatures. However, spin fluctuations are also crucial in the normal state, where they provide an important scattering mechanism and thus strongly affect transport. The transport properties of the pnictides are quite distinct from the cuprates and show unusual temperature dependences. The main ingredients needed for the description of transport in these systems have been controversially discussed.

The scattering of electrons off spin fluctuations is governed by the spin susceptibility. Close to an antiferromagnetic instability, the susceptibility is strongly peaked in momentum space in the vicinity of the possible order- ing vectors \( Q \). Transport in such systems can thus often be understood based on the concept of hot and cold regions of the Fermi surfaces. The hot regions are the parts of the Fermi surfaces that are connected by the possible ordering vectors \( Q \). The scattering is particularly strong in these regions. Conversely, in the cold regions not connected by ordering vectors the scattering rate is lower. If the difference in the scattering rate is large, i.e., close to the instability, transport is thus dominated by the cold regions with high conductivity.

The concept of hot and cold regions generally explains the experimental observations for cuprates and was implicitly assumed to hold also for the pnictides. An analysis of the lifetimes of excited electrons close to the Fermi surfaces seems to support this picture. The pnictides indeed show hot and cold regions with short and long lifetimes, respectively. Hence, one is led to assume that the states with short lifetimes do not significantly contribute to the transport. We show in this paper that this expectation is unfounded. conductors and

The crucial difference between cuprates and pnictides is that the physics of the former can be understood within a one-band model, whereas the latter are multiband systems with electronlike and holelike Fermi pockets. As we will show, this undermines the relaxation-time approximation (RTA), which consists of replacing the transport times entering the transport coefficients by the lifetimes of the electronic states. For the pnictides, calculations of transport coefficients within the RTA have not been able to reproduce the experiments, even using multiband models. The study of two-band models with circular Fermi pockets has shown that forward-scattering corrections to the RTA are huge close to the antiferromagnetic instability and that they give rise to transport anomalies such as a large enhancement of the Hall coefficient and negative magnetoresistance. The minority carriers, i.e., the carriers on the smaller Fermi pocket, were found to exhibit negative transport times, indicating a drift in the direction opposite of what one would expect based on their charge. However, in the simplified models with circular Fermi pockets all states on a given Fermi pocket are equivalent because of rotational symmetry. They are thus unable to address the concept of hot and cold regions, which relies on noncircular Fermi pockets.

In this article we present a semiclassical Boltzmann theory of transport for a two-band model relevant for the iron pnictides. Going beyond the RTA, we take the forward-scattering corrections into account, which are equivalent to vertex corrections in the Kubo formalism. We show that the hot-spot picture fails for the pnictides even for very strong spin fluctuations and highly elliptical electron pockets. Moreover, we calculate the temperature dependence of transport coefficients and compare the full results with the RTA, finding that the RTA makes qualitatively incorrect predictions. For strongly momentum-dependent scattering, we find large transport anomalies.
of the Brillouin zone, while the band to a nearly circular holelike Fermi pocket at the center where

$\varepsilon_e = 3 t_h, \varepsilon_{e,2} = 4 t_h$ and $t_{e,2} = t_h$.

We assume that the transport behavior is dominated by the scattering from spin fluctuations, which we model by the phenomenological susceptibility proposed by Millis, Monien, and Pines with temperature-dependent parameters based on neutron-scattering experiments. Although this ignores the anisotropy of the magnetic excitations in the pnictides caused by the ellipticity of the electronlike Fermi pockets we shall see that the precise form of the susceptibility is less important for the transport than the anisotropy of the scattering rate. Together with momentum-independent impurity scattering, the scattering rate from a single-electron state $(b, \mathbf{k})$ to a state $(b', \mathbf{k}')$, where $b = e$, $h$ denotes the band, can be written as:

$$W_{b\mathbf{k} \rightarrow b'\mathbf{k}'} = (1 - \delta_{bb'}) W_{sf} \frac{p_T(\varepsilon_{b\mathbf{k}} - \varepsilon_{b'\mathbf{k}'})}{(\varepsilon_{b\mathbf{k}} - \varepsilon_{b'\mathbf{k}'})^2 + \omega_{b\mathbf{k}'}^2} + \delta(\varepsilon_{b\mathbf{k}} - \varepsilon_{b'\mathbf{k}'}) W_{\text{imp}},$$

(3)

where $W_{sf}$ and $W_{\text{imp}}$ represent the overall strength of the scattering off spin fluctuations and impurities, respectively, $p_T(x) \equiv x (\cosh x/2k_B T - \tanh x/2k_B T)$, and

$$\omega_{b\mathbf{k}'} = \Gamma_T \left(1 + \frac{x^2}{4} \min\{(k - k' \mathbf{Q})^2\right),$$

(4)

where the four possible values for $\mathbf{Q}$ are $\pm \mathbf{Q}_{e,1}$ and $\pm \mathbf{Q}_{e,2}$. With the Curie-Weiss temperature $-\theta_{CW} < 0$, the frequency scale and the correlation length are given by $\Gamma_T = \Gamma_0 (T + \theta_{CW})/\theta_{CW}$ and $\xi_T = \xi_0 \sqrt{|\theta_{CW} (T + \theta_{CW})|} \exp(-T/T_0)$, respectively. Following Ref. we here introduce an additional exponential decay of $\xi_T$ to account for the high-temperature behavior and choose $T_0 = 200$ K. Following Ref. we take $\xi_0 = 10 a, \theta_{CW} = 30$ K and $\Gamma_0 = 4.2$ meV. The resulting form of $\omega_{b\mathbf{k}'}$ and thus $W_{b\mathbf{k} \rightarrow b'\mathbf{k}'}$ is only valid as long as the system does not order antiferromagnetically or becomes superconducting.

The transport is governed by states on the Fermi pockets, denoted by $(s, \theta)$, where $s = h, e, e$ is the pocket index and $\theta$ is the polar angle along the pocket, see Fig. 1. From Eq. (3) we see that in the low-temperature regime, $k_B T \ll \varepsilon_F$, the scattering rate is sharply peaked at $\varepsilon_{b\mathbf{k}} = \varepsilon_{b'\mathbf{k}'}$ so that scattering is nearly elastic. We exploit this fact by writing

$$W_{b\mathbf{k} \rightarrow b'\mathbf{k}'} \approx \delta(\varepsilon_{b'\mathbf{k}'}) W_{s'\theta'},$$

(5)

where

$$W_{s'\theta'} \equiv (1 - \delta_{bb'}) W_{sf} \int d\varepsilon \frac{p(\varepsilon)}{\varepsilon^2 + \omega_{b\mathbf{k}'}^2} + W_{\text{imp}}$$

(6)

is the effective elastic scattering rate between states on the Fermi pockets $s, s'$ belonging to the bands $b, b'$. Since
the spin susceptibility and thus $W_{s' \theta'}^{sk}$ is strongly momentum dependent, the elastic scattering rate $W_{s' \theta'}^{sk}$ strongly depends on the angles $\theta$ and $\theta'$, in particular on the change in angle, $\theta' - \theta$. This is what we call anisotropic scattering in the following.

More specifically, the anisotropy stems from the spin-susceptibility peaks at the wave vectors $\pm Q_{e,1}$ and $\pm Q_{e,2}$. For an initial state $|h, \theta\rangle$ with wave vector $k$, the scattering rate has maxima for the final states $|e_1, \theta_1\rangle$ and $|e_2, \theta_2\rangle$, defined as the states on the Fermi pockets $e_1$, $e_2$ with wave vectors closest to $k + Q_{e,1}$ and $k + Q_{e,2}$, respectively, see Fig. 1. Similarly, for an initial state $|e_1, \theta\rangle$ with wave vector $k$, the scattering rate has a maximum for the final state $|h, \theta_h\rangle$ with wave vector closest to $k - Q_{e,1}$ ($k - Q_{e,2}$), where $\theta_h \approx \theta$ since the hole pocket is nearly circular.

The scattering rate summed over all final states determines the characteristic lifetime of the state $|s, \theta\rangle$,

$$
\tau_{s\theta} = \left( \frac{1}{2\pi} \sum_{s'} \int d\theta' N_{s' \theta'} W_{s' \theta'}^{sk} \right)^{-1},
$$

where $N_{s\theta} = k'_{F,s}(\theta)/\pi \hbar v_{F,s}(\theta)$ is the density of states, with the spin degeneracy included, of pocket $s$ at the polar angle $\theta$ and $k'_{F,s}(\theta)$ and $v_{F,s}(\theta)$ are the Fermi momentum and the Fermi velocity, respectively.

**III. BOLTZMANN FORMALISM**

Our starting point is the semiclassical Boltzmann transport equation for a multiband system,

$$
-f_0'(\varepsilon_{b\theta}) \mathbf{E} \cdot \mathbf{v}_{b\theta} - \frac{e}{\hbar} \mathbf{B} \cdot (\mathbf{v}_{b\theta} \times \nabla_{k}) g_{b\theta} = \sum_{b'k'} W_{b'b\theta}^{bk'} (g_{b'b\theta} - g_{b'k'}),
$$

where $\mathbf{E} = (E_x, E_y, 0)$ and $\mathbf{B} = (0, 0, B)$ are weak uniform electric and magnetic fields, respectively, $\mathbf{v}_{b\theta} \equiv \hbar^{-1} \nabla_{k} \varepsilon_{b\theta}$ is the velocity and $g_{b\theta} \equiv f_0(\varepsilon_{b\theta})$ is the difference between the non-equilibrium distribution function $f_{b\theta}$ and the Fermi-Dirac distribution $f_0(\varepsilon_{b\theta})$. This difference is of the general form:

$$
g_{b\theta} = -f_0'(\varepsilon_{b\theta}) \mathbf{E} \cdot (\mathbf{A}_{b\theta} + \delta \mathbf{A}_{b\theta}),
$$

with the as yet unknown vector mean free path $\mathbf{A}_{b\theta}$ and $\delta \mathbf{A}_{b\theta}$. Here, $\mathbf{A}_{b\theta}$ ($\delta \mathbf{A}_{b\theta}$) is of zero (first) order in the magnetic field $\mathbf{B}$. For states on the Fermi pockets we write $\mathbf{A}_{s\theta}$, $\delta \mathbf{A}_{s\theta}$ with obvious definitions.

Inserting Eqs. (5), (6), and (9) into the Boltzmann equation (8) and using

$$
\sum_{b'k'} = \sum_{s'} \int \frac{d\theta'}{2\pi} N_{s' \theta'} \int d\varepsilon_{b'k'},
$$

one finds for states at the Fermi energy,$^{25}

$$
\mathbf{A}_{s\theta} = \tau_{s\theta} \mathbf{v}_{s\theta} + \tau_{s\theta} \sum_{s'} \int \frac{d\theta'}{2\pi} N_{s' \theta'} W_{s' \theta'}^{s\theta} \mathbf{A}_{s' \theta'},
$$

$$
\delta \mathbf{A}_{s\theta} = \tau_{s\theta} \eta_s \frac{eB}{\pi \hbar^2} \frac{1}{N_{s\theta}} \frac{\partial \mathbf{A}_{s\theta}}{\partial \theta} + \tau_{s\theta} \sum_{s'} \int \frac{d\theta'}{2\pi} N_{s' \theta'} W_{s' \theta'}^{s\theta} \delta \mathbf{A}_{s' \theta'},
$$

where $\eta_1 = 1$ and $\eta_1 = \eta_2 = -1$. The RTA consists of neglecting the forward-scattering corrections in Eqs. (10) and (11), i.e., the second terms on the right-hand sides. Thus in the RTA one obtains

$$
\mathbf{A}_{s\theta} = \mathbf{A}_{s\theta}^{(0)} \equiv \tau_{s\theta} \mathbf{v}_{s\theta},
$$

$$
\delta \mathbf{A}_{s\theta} = \delta \mathbf{A}_{s\theta}^{(0)} \equiv \tau_{s\theta} \eta_s \frac{eB}{\pi \hbar^2} \frac{1}{N_{s\theta}} \frac{\partial \mathbf{A}_{s\theta}^{(0)}}{\partial \theta}.
$$

Evidently, within the RTA the solution is determined by the bare lifetimes $\tau_{s\theta}$ given in Eq. (7). The RTA becomes exact if the scattering rate is isotropic around the Fermi pockets so that the forward-scattering corrections average out. For a nonzero anisotropy, however, the result may differ significantly from the RTA.$^{15}$

The charge current $\mathbf{J} = \sigma \mathbf{E}$ is controlled by the conductivity tensor $\sigma$, which is in turn determined by the vector mean free path,$^{25}$

$$
\sigma_{ij} = e^2 \sum_s \int \frac{d\theta}{2\pi} N_{s\theta} v_{s\theta}^i (\mathbf{A}_{s\theta}^j + \delta \mathbf{A}_{s\theta}^j) = \sum_s \int \frac{d\theta}{2\pi} \sigma_{ij}^{s\theta}.
$$

Writing $\mathbf{E} = E (\cos \phi, \sin \phi, 0)$, we find the current parallel to the electric field as

$$
\mathbf{J} \cdot \mathbf{E} = \sum_s \int \frac{d\theta}{2\pi} \left( \sigma_{xx}^{s\theta} \cos^2 \phi + \sigma_{yy}^{s\theta} \sin^2 \phi \right) + \sigma_{xy}^{s\theta} \cos \phi \sin \phi + \sigma_{yx}^{s\theta} \cos \phi \sin \phi \right)
$$

$$
= \sum_s \int \frac{d\theta}{2\pi} J_{s\theta},
$$

where $J_{s\theta}$ is the contribution of the state $|s, \theta\rangle$ to the current.

**IV. ANALYTICAL RESULTS**

To gain insight into transport beyond the RTA, we now construct an approximate analytical solution of Eqs. (10) and (11) that fully accounts for the anisotropic scattering. We will first discuss a few reasonable assumptions that make an analytical solution feasible. The full numerical solution is discussed in Sec. [V].

As illustrated in Fig. 1, the scattering rate $W_{s' \theta'}$ understood as a function of $\theta'$ has a maximum at $\theta' = \theta_s$, which of course depends on $\theta$. The small difference between $\theta$ and $\theta_s$ stems from the ellipticity of the electron pockets. We now make two simplifying assumptions: (i)
The Fermi pocket cuss the states appearing in this series. The zero-order power series in the anisotropy parameter. We now dis-
recovered. a
intersection of the Fermi pocket $\vec{\tau}_s$ to the limit of strong anisotropy, $W_s^{\theta} \rightarrow 0$ such that
is approached. In the opposite limit of isotropic scatter-
peaked spin susceptibility, i.e., as the magnetic instability
(18) ensure that
The Kronecker symbols $\delta_{s,s'}$ is of course $s' = 0$ and that $a_s' \rightarrow 1$ corresponds to the limit of strong anisotropy, $W_s^{\theta} \propto \delta(\theta' - \theta_s)$, while $a_s' \rightarrow 0$ gives the isotropic case, where the RTA result is recovered.

Iterating Eq. (17), we obtain $A$ in terms of $A^{(0)}$ as a power series in the anisotropy parameter. We now discuss the states appearing in this series. The zero-order contribution to $A_{s'\theta}$ is of course $A_{s\theta}^{(0)}$, the RTA result for the same state $|s, \theta\rangle$. The first-order term involves $A_{s'\theta}^{(0)}$, for the state $|s', \theta_s\rangle$. This is the final state on the Fermi pocket $s' \neq s$ to which the initial state $|s, \theta\rangle$ has the largest scattering rate. Due to the ellipticity of the electron pockets, the shift of the angle, $\theta_s \rightarrow \theta$, is always directed towards the closest hot spot, i.e., the intersection of the Fermi pocket $s$ with pocket $s'$ shifted by the appropriate vector $Q$. The state appearing in the second-order term is the one reached from $|s', \theta_s\rangle$ with the largest scattering rate, again shifted towards the closest hot spot. The states appearing in all higher-order terms are obtained in the same way. The whole process can be interpreted as an effective hopping of the electron along a sequence of states, as illustrated by Fig. 2.

The contribution to $A_{s'\theta}$ from $A_{s'\theta}^{(1)}$ of the state $|s', \theta_s\rangle$ reached after $\nu$ hopping events involves the product of $\nu$ anisotropy parameters at $\theta, \theta_1, \ldots, \theta_{\nu-1}$. Since the angular shift between successive hopping events is due to the ellipticity of the electron pockets, and vanishes for a purely circular pocket, it is small for small ellipticities. Indeed, in the appendix we show that for a circular hole pocket and a single elliptical electron pocket the error in the vector mean free path is of fourth order in the eccentricity of the electron pocket. If we henceforth neglect this shift, i.e., let $\theta_s \approx \theta_{\nu-1}$ for all $\nu$, we incur an error that is small for the moderate ellipticities of the electronlike Fermi pockets of the pnictides. In the following section we shall see that this convenient approximation generally compares well with the full numerical solution of Eqs. (10) and (11).

Accordingly setting $\theta_s = \theta$ in Eq. (17), the vector mean free paths for different $\theta$ decouple and we obtain

$$A_{s\theta} = A_{s\theta}^{(0)} + \left(1 - \frac{1}{2} \delta_{s,h}\right) \sum_{s'} a_s' a_s^{s'} \Lambda_{s'\theta_s}^{(0)} \Lambda_{s'\theta_s},$$

(16)

with the anisotropy parameter

$$a_s' = (1 + \delta_{s,h}) \tau_{s,h} \int \frac{d\theta'}{2\pi} N_{s'} W_{s'\theta_s}^{\theta'} \cos(\theta' - \theta_s).$$

(18)

The Kronecker symbols $\delta_{s,h}$ appearing in Eqs. (17) and (18) ensure that $a_s' \in [0, 1]$ and that $a_s' \rightarrow 1$ corresponds to the limit of strong anisotropy, $W_{s'\theta_s}^{\theta'} \propto \delta(\theta' - \theta_s)$, while $a_s' \rightarrow 0$ gives the isotropic case, where the RTA result is recovered.

Iterating Eq. (17), we obtain $A$ in terms of $A^{(0)}$ as a power series in the anisotropy parameter. We now discuss the states appearing in this series. The zero-order contribution to $A_{s\theta}$ is of course $A_{s\theta}^{(0)}$, the RTA result for the same state $|s, \theta\rangle$. The first-order term involves $A_{s'\theta}^{(0)}$, for the state $|s', \theta_s\rangle$. This is the final state on the Fermi pocket $s' \neq s$ to which the initial state $|s, \theta\rangle$ has the largest scattering rate. Due to the ellipticity of the electron pockets, the shift of the angle, $\theta_s \rightarrow \theta$, is always directed towards the closest hot spot, i.e., the intersection of the Fermi pocket $s$ with pocket $s'$ shifted by the appropriate vector $Q$. The state appearing in the second-order term is the one reached from $|s', \theta_s\rangle$ with the largest scattering rate, again shifted towards the closest hot spot. The states appearing in all higher-order terms are obtained in the same way. The whole process can be interpreted as an effective hopping of the electron along a sequence of states, as illustrated by Fig. 2.

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Accordingly setting $\theta_s = \theta$ in Eq. (17), the vector mean free paths for different $\theta$ decouple and we obtain

$$A_{\theta} = A_{0\theta}^{(0)} + \frac{1}{2} \left(a_{10}^{s} A_{10}^{s} + a_{20}^{s} A_{20}^{s}\right),$$

(19)

$$A_{\theta} = A_{0\theta}^{(0)} + a_{10}^{s} A_{10}^{s},$$

(20)

$$A_{\theta} = A_{0\theta}^{(0)} + a_{20}^{s} A_{20}^{s}.$$ 

(21)

Results for the magnetic part $\delta A_{\theta}$ can be found analogously by replacing $A$ by $\delta A$ and $A^{(0)}$ by $\tau_{\theta} \eta_s \frac{eB}{\pi n} \frac{1}{N_{s\theta}} \partial A_{\theta} / \partial \theta,$

(22)

cf. Eq. (11). Since the anisotropy parameters $a^{s'}_s$ are the only parameters in the solution, apart from the RTA vector mean free paths, we will refer to these expressions as the anisotropy approximation (AA). Clearly, for $a^{s'}_s \neq 0$ the vector mean free paths involve the RTA solutions of all three Fermi pockets. This coupling between the pockets becomes stronger for larger anisotropy parameters. Additionally, the denominator in Eq. (19), which appears in all results, provides a factor that is larger than unity. In the anisotropic limit, $a^{s'}_s \rightarrow 1$, the vector mean free paths $A_{\theta}$ of all three pockets at a certain angle $\theta$ become equal and diverge. Thus, for strong anisotropy the vector mean free path of the minority carriers must be inverted relative to the RTA result $A_{\theta}^{(0)} \propto v_{s\theta}$.

Semiclassically, we can interpret our results as follows. The solution to the Boltzmann equation describes a non-equilibrium stationary state in which the acceleration of the electrons due to external forces is balanced by scattering. The vector mean free path of state $|s, \theta\rangle$ can be understood as the displacement that an electron suffers until its velocity $v_{s\theta}$ is randomised by scattering. The lifetime $\tau_{\theta}$ is the mean time between two scattering events.
If the scattering is isotropic the velocity is randomised after a single scattering event and the vector mean free path thus reads \( \tau_{\text{sf}} v_{\text{sf}} \equiv \Lambda_{\text{sf}}^{(0)} \). On the other hand, anisotropic scattering only partially randomises the velocity so that the effective relaxation time exceeds the lifetime \( \tau_{\text{sf}} \), giving rise to multiple scattering during the relaxation, see Fig. 2. The enhancement by denominator in Eq. (19) accounts for this fact. In the extreme limit of \( a_{\text{sf}} \rightarrow 1 \), the factor diverges, indicating that the velocities cannot relax at all and the vector mean free paths become infinite.

This physical picture also applies to the case of two circular Fermi pockets considered in Ref. 15. Because of rotational symmetry, the vector mean free path is parallel to the velocity in that case. This permits a simple description in terms of transport times. However, we are here concerned with noncircular Fermi pockets, which means that the vector mean free path is generally not parallel to the velocity. The common feature is that strong anisotropic scattering forces the vector mean free path of electron and hole pockets at \( \theta \) to point in the same direction, which is set by the majority carriers. In the relevant parameter range for our model, we will find that the direction is set by the electrons since there are two electron pockets. A change of the dominant carrier type can only be achieved by strong hole doping.

V. NUMERICAL RESULTS

To obtain quantitative results without further approximations beyond the choice of the model and the semiclassical transport theory, we calculate the scattering rate given in Eq. (4) by numerical integration. Furthermore, we discretize the polar angle \( \theta \), choosing 160 sites on each Fermi pocket. We have checked that taking more points does not significantly change the results. The lifetimes, Eq. (7), and the anisotropy parameters, Eq. (18), are obtained by summation over the discrete sites. Finally, Eqs. (10) and (11) are solved numerically by matrix inversion. The numerical results will be compared to the AA, which is given by inserting the lifetimes and the anisotropy parameters into Eqs. (19)–(21).

A. Scattering rate

Figure 3(a) shows the temperature dependence of the scattering rate for \( \xi = 1 \) in Eq. (2) and \( W_{\text{imp}}/W_{\text{sf}} = 10^{-3} \). At high temperatures the scattering rate is flat and the anisotropy therefore vanishes. At lower temperatures a peak due to spin fluctuations develops corresponding to scattering vectors close to \( Q_{01} \) or \( Q_{02} \). The peak becomes sharper as the temperature is lowered so that the anisotropy increases. At very low temperatures spin fluctuations freeze out and only the isotropic impurity scattering remains so that the anisotropy vanishes again. Recall that our model spin susceptibility assumes that the system is neither antiferromagnetically ordered nor superconducting. In real pnictides, this low-temperature behavior will in most cases be preempted by antiferromagnetic or superconducting order.

In Fig. 3(b) we plot the anisotropy parameter corresponding to the scattering rate shown in Fig. 3(a), averaged over the Fermi pocket. It clearly exhibits the increase for decreasing temperature and the final sharp downturn at very low temperatures.

B. Current contributions, hot-spot picture

In this subsection we explore how different parts of the Fermi pockets contribute to the transport. In particular, we want to find out to what extent the concept of hot and cold regions is applicable. Choosing \( T = 1 \) K and \( W_{\text{imp}}/W_{\text{sf}} = 0 \), we focus on the regime of strong spin fluctuations with strong anisotropy, where the difference between the RTA and the full result is the most striking.

The current parallel to the electric field is given by Eq. (15). The state-resolved current contributions \( J_{\text{sf}} \) depend on the direction of the electric field due to the noncircular Fermi pockets but we are here not interested in this dependence and therefore average \( J_{\theta} \) over all directions of the electric field in the \( xy \)-plane. For \( B = 0 \) this gives

\[
J_{\theta} = e^2 N_{\text{sf}} v^x_{\text{sf}} A^x_{\theta} + v^y_{\text{sf}} A^y_{\theta} E. \tag{23}
\]

Figure 4 shows the contributions \( J_{\theta} \) resulting from the RTA as well as from the full numerical calculation. The two are completely different. Most prominently, the holes
Figure 4. (Color online) Contributions to the current of states on the Fermi surface. Panels (a) and (b) show the RTA result as a color map and as a line plot along a quarter of the Fermi pockets, respectively. Note the reduction of the current contributions in the hot regions. Panels (c) and (d) show the same for the full numerical results. The large anisotropy leads to negative current contributions from the hole pocket. No signatures of hot spots are apparent. The parameters are $\xi = 2.5$, $n = 2.08$, $T = 1$ K, and $W_{\text{imp}} / W_{\text{sf}} = 0$.

Contribute negatively to the total current in the full calculation. In the semiclassical picture, this means that the holes drift in the same direction as the electrons. The insights gained in section V illuminate this behavior: For the set of parameters chosen in Fig. 4, the scattering anisotropy averaged over all Fermi states is close to unity, $\langle a \rangle_\theta = 0.96$. As discussed in section V, such a huge anisotropy leads to an effective relaxation time that is much longer than the lifetime. In effect, during the relaxation, an electron initially on the holonlike Fermi pocket scatters multiple times between states on the holonike pocket and states on the electronlike Fermi pockets, which have nearly opposite velocity. Since there are more states on the electronlike pockets than on the holonike pocket, the electron spends the larger part of the time on the electronlike pockets. The electron thus on average drifts in the opposite direction to what one would get if it stayed on the holonike pocket. The RTA is not sensitive to the inversion of the velocity upon interpocket scattering and thus cannot account for this effect.

Figure 4 also shows that the hot-spot picture is no longer valid if forward-scattering corrections are taken into account. As discussed above, the scattering off spin fluctuations is strongest in the hot regions since the spin susceptibility is peaked at $Q_e1$, $Q_e2$, see Fig. 1. Thus the lifetimes are shorter and the RTA vector mean free paths are smaller. This is indeed reflected by the suppressed current contributions in the hot regions shown in Figs. 4(a) and 4(b). However, no signatures of hot regions are seen in the full results in Figs. 4(c) and 4(d). This is due to the anisotropy of the scattering rate. In the hot regions, the anisotropy $a^\prime_s \theta$ is enhanced and, according to Eqs. (19)–(21), this leads to an enhancement of the vector mean free path. Thus the reduction of the lifetimes is compensated by the enhanced anisotropy and the contribution of the hot regions to the current is comparable to that of other parts of the Fermi pockets.

C. Transport coefficients

The transport coefficients can be obtained from the vector mean free paths. The conductivity tensor is given in Eq. (14), while the thermoelectric tensor reads

$$\alpha_{ij} = -\frac{\pi^2 k_B^2 T}{3e} \frac{\partial \sigma_{ij}}{\partial \mu}.$$  

We will focus on the resistivity

$$\rho = \frac{1}{\sigma_{xx}},$$

the Hall coefficient,

$$R_H = \frac{\sigma_{xy}}{(\sigma_{xx})^2 B},$$

the Seebeck coefficient (thermopower),

$$S = -\frac{\alpha_{xx}}{\sigma_{xx}}.$$
and the Nernst coefficient,
\[ N = \frac{\sigma^{xy} \alpha^{xx} - \sigma^{xx} \alpha^{xy}}{(\sigma^{xx})^2 B}. \] (28)

We give the resistivity in units of
\[ \rho_0 = \frac{\hbar}{e^2} \frac{\hbar W_{sf}}{V_0} \times 10^{-2} \text{(eV)}^2, \] (29)

where \( V_0 \) is the volume of the unit cell, and the Nernst coefficient in units of
\[ N_0 = \frac{V_0}{e \rho_0} \times 10^{-5} \text{V/K}. \] (30)

For the scattering strength ratio we choose in the following
\[ W_{imp}/W_{sf} = 10^{-3}. \]

1. Comparison of approximations

Figure 5 shows the temperature dependence of the transport coefficients, comparing the full numerical result with the RTA and the AA. We see that the RTA results tend to coincide with the full calculation only at very high and very low temperatures, where the scattering is nearly isotropic, see Fig. [3]. In the temperature range with strong anisotropy (20–150 K) the deviations from the RTA are huge. On the other hand, the AA shows qualitative agreement with the full results over all temperatures and for both ellipticities. The agreement is even quantitative for the resistivity. It is the worst for the Nernst coefficient \( N \) but even here the positive and negative extrema in \( N \) are predicted by the AA close to the correct temperatures. For \( \xi = 1 \) the AA is slightly better than for \( \xi = 2 \) since the former value leads to less eccentric electron pockets. The close agreement between the AA and the full numerical results shows that the transport behavior does not sensitively depend on the precise details of the anisotropic scattering, and thus justifies our use of the approximate susceptibility in Eq. [3].

Both the RTA and the full results show strong temperature dependence. For the RTA, this can be traced back to the nontrivial geometry of the Fermi pockets leading to the hot-spot structure for high scattering anisotropies. However, as discussed in subsection [10] forward-scattering corrections invalidate the hot-spot picture for strong anisotropies. The temperature dependence of the RTA results thus stems from the wrong origin. The true temperature dependence can be understood on the basis of the AA, which gives qualitatively correct results. Here, it is due to the strong temperature dependence of the anisotropy parameters \( a_{sf} \) shown in Fig. [3(b)], i.e., it relies on the corrections to the RTA in Eqs. [10] and [11] as well as [19]–[21].

The differences between the RTA and the full results for the resistivity and the Hall coefficient are consistent with the predictions of Ref. [15] for two circular Fermi pockets. In the resistivity, we note that the expected enhancement and reduction for high and low anisotropies, respectively, lead to a more pronounced change of slope compared to the RTA. The predicted enhancement of the Hall coefficient is also present. However, the extremum of the Hall coefficient in Fig. 5 is due to the maximum in the anisotropy (cf. Fig. [3]) and is thus of different origin than in Ref. [15]. In the Hall coefficient was predicted for the case that the anisotropy crosses a characteristic anisotropy level at which the mobilities of holes and electrons are of equal magnitude but opposite sign. We do not see any signatures of such a crossing in the present results. For the thermoelectric effects, Fig. 5 shows that the RTA results are even qualitatively incorrect, with the Seebeck and Nernst coefficients showing the wrong sign in the temperature range with strong anisotropy. According to Eqs. [24] and [27], the Seebeck coefficient \( S \) is proportional to \( \partial \ln \sigma^{xx}/\partial \mu = -\partial \ln \rho/\partial \mu \). In the RTA, it stems from the shift of the hot spots with the chemical potential, i.e., with doping. In the full results and the AA, it is instead due to the change in the anisotropy parameters \( a_{sf} \) with the chemical potential. Figure 5 shows that for the chosen parameters, the two effects contribute to \( S \) with opposite sign. The full results for the Nernst coefficient \( N \) change sign between the ellipticities \( \xi = 1 \) and \( \xi = 2 \). This effect is missed by the RTA. We return to the Nernst coefficient below.

Qualitative differences between the RTA and the full solution of the Boltzmann equation have also been reported for a single-band cuprate model with strongly anisotropic scattering. The physics discussed here, including the inverted vector mean free path of minority carriers, rely on the presence of multiple bands and Fermi pockets, though.

2. Doping dependence

We now turn to the doping dependence of the transport coefficients. Figures [3(a)–3(d)] show the full solutions at different fillings, while Fig. 6(e) shows the current contributions of states on the Fermi surfaces at the two temperatures \( T = 100 \text{K} \) and \( T = 400 \text{K} \) with strong and weak anisotropy, respectively. Note that the current contributions from the hole pocket are negative for \( T = 100 \text{K} \) and \( n \gtrsim 1.99 \), i.e., towards the electron-doped side. On the hole-doped side, the scattering is more isotropic due to the large discrepancy in size between the electron and hole pockets.

At high temperatures, the transport coefficients all show a smooth doping dependence resulting from the change in the Fermi surfaces and velocities in the presence of mostly isotropic scattering. In the intermediate temperature range, where anisotropic scattering is strong, this is overlaid by nontrivial doping dependence due to the forward-scattering corrections.

The resistivity around \( T \approx 100 \text{K} \) is largest for inter-
mediate fillings, for which the Fermi pockets are well nested. This is because the narrow peaks in the spin susceptibilities at $Q_{e1}$ and $Q_{e2}$ lead to efficient scattering only for nested Fermi pockets. The inefficiency of anisotropic scattering for small and large $n$ causes a rapid decrease in the resistivity with doping, as shown in the inset in Fig. 5(a). Note that the relative change in $\rho$ with doping is much larger here than at high temperatures. Since the Seebeck coefficient $S$ is proportional to $\partial \ln \sigma^{xx}/\partial \mu = -\partial \ln \rho/\partial \mu = -\rho^{-1} \partial \rho/\partial \mu$, it is sensitive to this relative change in $\rho$ with $\mu$ or $n$ and is, therefore, strongly enhanced in the intermediate temperature range with strong anisotropy, as Fig. 5(c) clearly shows.

For the Hall coefficient $R_H$, Fig. 5(b), one would naively expect the largest and smallest values for the most strongly hole-doped and electron-doped cases, respectively, since electrons and holes contribute with opposite signs. This is indeed the case at $T \approx 400$ K, where the scattering is nearly isotropic and no negative current contributions occur. At $T \approx 100$ K, however, Fig. 5(b) shows a strong negative enhancement of $R_H$ for intermediate filling. According to Fig. 5(e), the contribution of the holes to the total current is negative in this range. In the semiclassical picture this means that the holes drift in the same direction as the electrons, reducing the charge current. Irrespective of that, the magnetic field deflects the holes and the electrons in the same direction. Hence, the inverted sign of the hole contribution reduces the charge current without changing the Hall voltage. This gives rise to an enhancement of the Hall coefficient defined as the Hall voltage relative to the charge current.

The Nernst coefficient $\mathcal{N}$ plotted in Fig. 5(d) is highly sensitive to small doping changes and also, as is evident from Fig. 5, to changes in the band parameters. Equations (24)–(26) and (28) show that

$$\mathcal{N} = \frac{3e}{\pi^2 k_B T} \frac{\partial}{\partial \mu} \frac{R_H}{\rho} = \frac{3e}{\pi^2 k_B T} \frac{\partial n}{\partial \mu} \frac{\partial}{\partial n} \frac{R_H}{\rho}. \quad (31)$$

The Nernst coefficient is thus sensitive to the nonmonotonic doping dependence of both $\rho$ and $R_H$. For the cases we have considered, the contributions from $\rho$ and $R_H$ usually counteract each other. The complicated behavior of $\mathcal{N}$, for example the different sign of $\mathcal{N}$ for $n = 2.05$ compared to the other fillings, is thus due to the quantitative competition of the doping dependences of $\rho$ and $R_H$ and not to any clear qualitative features in the Fermi surfaces or the scattering. This suggests that the other coefficients might be more advantageous as probes of the electronic system. However, the detailed comparison of experimental transport coefficients and calculations for realistic models remains work for the future.

VI. CONCLUSIONS

We have studied transport in a two-band model relevant for the iron pnictides, using the semiclassical Boltzmann equation. Forward-scattering corrections due to anisotropic interband scattering off spin fluctuations have been included. Spin fluctuations have been described by a phenomenological Millis-Monien-Pines susceptibility, with temperature-dependent parameters chosen based on neutron-scattering results for the pnictides. Our analytical and numerical investigations show that the anisotropic scattering gives rise to unusual transport behavior. Specifically, we have considered the resistivity and the Hall, Seebeck, and Nernst coefficients as functions of temperature and doping. Consistent with predictions for circular Fermi pockets, we have obtained
inverted vector mean free paths and negative current contributions from minority carriers in the regime of highly anisotropic scattering. These lead to strong signatures in particular in the Hall and Nernst coefficients. Negative current contributions can also lead to a negative magnetoresistance. However, the present model with two electron pockets and one hole pocket does not show negative magnetoresistance in the considered parameter range. Calculations of transport coefficients for more realistic pnictide models are desirable to allow quantitative predictions.

Most surprisingly, the ellipticity of the electron pockets does not lead to the short-circuiting of the hot spots by the cold regions of the Fermi pockets even for very strong scattering. The enhanced scattering rate in the hot regions indeed leads to a short lifetime there, but this effect is balanced by the enhanced vector mean free path due to the anisotropic scattering. Hot and cold regions are thus found to contribute similarly to the transport. This breakdown of the concept of hot and cold regions is not found in a simple RTA neglecting forward-scattering corrections. Moreover, the predictions of the RTA for the transport coefficients are even qualitatively incorrect.

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APPENDIX: DISCUSSION OF THE ANGULAR SHIFT

As discussed in the main text, the vector mean free path of a state \( |s, \theta \rangle \) can be written as a power series in the anisotropy parameter, where the term of order \( n \) contains the RTA vector mean free path of a state reached by \( n \) hopping events towards the closest hot spot. We have argued that the angular shift towards the hot spot is a small effect for the vector mean free path for realistic ellipticities of the electron pockets and have therefore ignored it above. We here explore this effect analytically within a simple model. To get an estimate for the upper limit of the correction to the vector mean free path, it is sufficient to consider only a single electron pocket. Our simple model consists of a circular holelike Fermi pocket with the Fermi wave number \( k \) and an elliptical electronlike Fermi pocket described by the semi-major and semi-minor axis \( k_a = k(1 - \epsilon^2)^{-1/4} \) and \( k_b = k(1 - \epsilon^2)^{1/4} \), respectively, where \( \epsilon \) is the eccentricity of the ellipse. To focus on the shift effect we assume constant anisotropy, \( \alpha_{\epsilon \theta} = \alpha \). For two Fermi pockets and constant anisotropy, Eq. \( (17) \) takes the form

\[
\Lambda_{s \theta} = \Lambda_{s \theta}^{(0)} + a \Lambda_{z \delta}, \tag{32}
\]

where \( \bar{h} = e, \bar{e} = h \), and the RTA solution \( \Lambda^{(0)} \) is given by Eq. \( (12) \). Using simple trigonometry, we find that for the given geometry, the difference between \( \bar{\theta} \) and \( \theta \) to leading order in the eccentricity \( \epsilon \) reads \( \sqrt{16} \sin 4\theta \). Iterating Eq. \( (32) \), we obtain the solution for the electron pocket as

\[
\Lambda_{e \theta} = \sum_{n=0}^{\infty} a^{2n} \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right), \tag{33}
\]

with

\[
\theta_n = \theta_{n-1} + \frac{\epsilon^4}{16} \sin 4\theta_{n-1} \quad \text{and} \quad \theta_0 = \theta. \tag{34}
\]

The solution for the hole pocket follows immediately from Eqs. \( (32) \) and \( (33) \).

Replacing the discrete index \( n \) by a continuous variable, we obtain

\[
\Lambda_{e \theta} = -\frac{2 \ln a}{1 - a^2} \int_0^{\infty} dz \frac{a^{2n}}{a^{2n} \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right)} + R, \tag{35}
\]

with a correction \( R \). By splitting the integration range into intervals \( \left[ m, m + 1 \right] \) with integer \( m \), one can easily show that

\[
|R| \leq \sum_n a^{2n} \left| \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right) - \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right) \right|, \tag{36}
\]

which is obviously of higher order in \( \epsilon^2 \) because of Eq. \( (34) \). Substituting \( n = 4 \ln(1 + z)/\epsilon^4 \) we obtain

\[
\Lambda_{e \theta} = \frac{1}{1 - a^2} \int_0^{\infty} d\gamma \frac{1}{1 + z} \gamma \left( \frac{1}{1 + z} \right)^{\gamma + 1} \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right), \tag{37}
\]

with

\[
\gamma \equiv \frac{8 \ln(1/a)}{\epsilon^4} \tag{38}
\]

and

\[
\theta(z) = \frac{1}{2} \arctan [(z + 1) \tan 2\theta]. \tag{39}
\]

In the integral in Eq. \( (37) \), the factor \( \gamma (1/(1 + z))^{\gamma + 1} \) acts as a distribution function which is normalized to unity and becomes a \( \delta \)-function in the limit of zero ellipticity, i.e., for \( \gamma \to \infty \). Hence, the largest shifts are achieved for small values of \( \gamma \), which, according to Eq. \( (38) \), correspond to large anisotropy and large ellipticity.

The shift also depends on the position on the Fermi pocket. There is no shift at the hot spots, \( \theta = (2n - 1) \pi/4 \), and at the cold spots, \( \theta = n \pi/2 \). The largest shift can be expected to occur between the hot and cold spots, in the vicinity of \( (2n - 1) \pi/8 \).

We can make further analytical progress by expanding the vector \( \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right) \) to linear order in \( \theta(z) \). This is best justified if the total angular shift is small, i.e., if we start with \( \theta \) close to a hot spot. However, the total shift can never be larger than \( \pi/4 \) so that the approximation always gives at least qualitatively correct results for not excessive eccentricities. Equation \( (37) \) can then be written as

\[
\Lambda_{e \theta} = \frac{1}{1 - a^2} \left( \Lambda_{e \theta}^{(0)} + a \Lambda_{h \theta}^{(0)} \right), \tag{40}
\]
with the effective angular shift
\[
\Delta_{\theta, \gamma} = \int_0^{\infty} dz \gamma \left( \frac{1}{1 + z} \right)^{\gamma + 1} \theta(z) - \theta
\]
\[
\approx \frac{\sin 4 \theta}{32} \frac{\epsilon^4}{\ln(1/a)} + \frac{\sin \theta}{512} \left( \frac{\epsilon^4}{\ln(1/a)} \right)^2
\]
\[+ \mathcal{O} \left( \left( \frac{\epsilon^4}{\ln(1/a)} \right)^3 \right). \tag{41}
\]
By neglecting the shift, \( \Delta_{\theta, \gamma} = 0 \), we would obtain the analogue of Eqs. \([19]–[21]\) for the case of constant anisotropy and a single electron pocket.

In Fig. 7 we plot the angular shift at \( \theta = \pi/8 \) for different anisotropies as a function of the eccentricity squared, \( \epsilon^2 \). Realistic anisotropies hardly exceed the value \( a = 0.95 \), for which the shift is small up to \( \epsilon^2 \approx 0.5 \). Stronger ellipticities might, however, lead to significant corrections.

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