Hall effect in quasi-one-dimensional metals in the presence of anisotropic scattering

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(Received 2 April 2012; published 11 June 2012)

We apply Boltzmann transport theory to investigate the possible effect of an anisotropic scattering time τ on the temperature dependence of the Hall coefficient R_H in quasi-one-dimensional (q1D) conductors. Specifically we show that the measured R_H in two candidate materials $(TMTSF)_2PF_6$ and $PrBa_2Cu_4O_8$ can be accounted for almost entirely by using a model that assumes only weak sinusoidal variation of τ along the Fermi surface. While the temperature dependence of R_H is markedly different in the two cases, the variations in τ are found to be almost identical. This work highlights the importance of considering the anisotropy of the electrical resistivity in any analysis of $R_H(T)$ in q1D systems and hints that the momentum dependence of the inelastic scattering rate, and thus its origin, are rather generic in both organic and inorganic q1D metals.

DOI: 10.1103/PhysRevB.85.235117 PACS number(s): 72.10.−d, 72.15.Gd

I. INTRODUCTION

Quasi-one-dimensional (q1D) metallic systems possess a highly anisotropic electronic state characterized by weakly corrugated sheets of open Fermi surface (FS). As a result, their Fermi-liquid (FL) ground state is extremely fragile, prone both to competing instabilities such as superconductivity[1,2] and spin[3] and charge[4] density waves, as well as to the possible emergence of the Tomonaga-Luttinger liquid (TLL) state with its distinct, collective excitations of spin and charge.[5] Since the TLL state is predicted to occur strictly in one dimension, the inevitable coupling that exists between individual conducting chains in real solids ought to inhibit manifestations of TLL physics, at least at low energies or at low temperatures.[5] As an example of an easy-to-measure low-energy probe, the Hall effect has the potential to address the nature of the electronic state in q1D conductors and its evolution with temperature.[6] Interpretation of existing results, however, has so far proved controversial.[7–10]

In conventional metallic systems, the Hall coefficient R_H depends only on the size of the FS and the sign of the charge carriers. A marked T dependence of $R_H(T)$ is often the first indicator of a change in state, as found, for example, in underdoped high-T_c cuprates near the 1/8-doping anomaly.[11,12] In quasi-two-dimensional (q2D) metals with a single band or a single carrier type, the magnitude and sign of R_H can also be dependent on the FS curvature whenever the mean free path ℓ is anisotropic,[13–15] and can be T dependent whenever the anisotropy in ℓ changes.

Here, we investigate to what extent the Hall effect of real q1D metals can be explained within a conventional band picture by developing a version of the Boltzmann transport equation that incorporates sinusoidal variation of both the Fermi velocity v_F and scattering time τ. We then use this approach to model $R_H(T)$ in $PrBa_2Cu_4O_8$ (Pr124) and $(TMTSF)_2PF_6$, whose Hall coefficients both exhibit strong, distinct temperature dependencies.[8,16] We find that $R_H(T)$ is extremely sensitive, both to small variations in τ (as found previously[17]) and to the T-dependent anisotropy of the electrical resistivity $\rho(T)$. We also find that the measured $R_H(T)$ in both compounds can be explained by a quantitatively similar evolution of their τ anisotropy, save for the sharp drop in $R_H(T)$ in $(TMTSF)_2PF_6$ at low T. In the important high-T regime, where one might expect a crossover to TLL behavior,[8] an anisotropic FL description is found to be sufficient to explain the magnitude and T dependence of R_H. Moreover, the form (and, by inference, the origin) of the inelastic scattering rate in both the organic and inorganic systems appears to the same.

II. ANISOTROPIC SCATTERING MODEL

Using the Jones-Zener expansion of the linearized Boltzmann equation within the relaxation time approximation, we obtain an expression for $\sigma_{ij}^{(n)}$, the nth order term of the ij component of the conductivity tensor,

$$\sigma_{ij}^{(n)} = \frac{-e^{2+n}}{4\pi^3\hbar^n}\int \mathbf{v}_i\tau\left([\mathbf{v_k}\times\mathbf{B}]\frac{\partial}{\partial\mathbf{k}}\right)^n\mathbf{v}_j\tau\left(-\frac{\partial f_k^0}{\partial\epsilon_k}\right)d^3k, \tag{1}$$

where $\mathbf{B}$ is the applied field, $\mathbf{v}_i$ the electron velocity in the i direction, f_k^0 the density of carriers occupying momentum state k in equilibrium, and ϵ_k the energy of the electron in state k. For a q1D system with an open FS, it is most convenient to use Cartesian coordinates, the energy integral being performed along the reciprocal axis parallel to the conducting chain (i.e., k_x). This introduces a factor $1/(\hbar v_x|_{k=k_F})$ in the denominator of Eq. (1), which for $\mathbf{B}||z$ (the crystal axis of lowest conductivity), current $\mathbf{J}||x$, and Hall voltage $V_H||y$ now reads

$$\sigma_{xy} = \frac{e^3B}{4\hbar^2\pi^3}\iint\left(l_x\frac{\partial l_y}{\partial k_y} - l_y\frac{\partial l_y}{\partial k_x}\right)dk_ydk_z, \tag{2}$$

where l_x (l_y) is the mean free path in the x (y) direction. Usually, v_y does not depend on k_x. For the simple q1D tight-binding FS shown in Fig. 1, for example, the energy dispersion is given by $\epsilon = -2t_x\cos(k_xa) - 2t_y\cos(k_yb) + \epsilon_z$. Here $t_y \ll t_x$ is the y-axis (interchain) hopping parameter, t_x the intrachain hopping parameter, a and b the x- and y-axis lattice parameters, and ϵ_z the energy dispersion in the z direction. Thus, for isotropic scattering, or for a scattering function that only depends on k_y, Eq. (3) reduces to

$$\sigma_{xy} = \frac{e^3B}{4\hbar^2\pi^3}\iint l_x(k_y)\frac{\partial l_y(k_y)}{\partial k_y}dk_ydk_z. \tag{3}$$

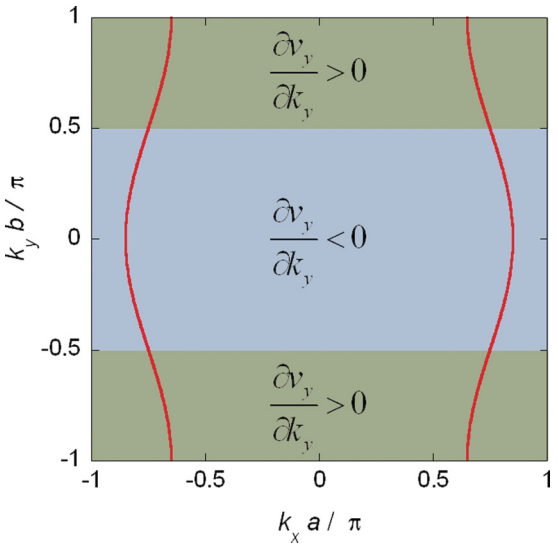

FIG. 1. (Color online) Typical Fermi surface of a q1D conductor. In the case of isotropic scattering, the green (blue) shaded sections give negative (positive) contributions to R_H, respectively.

Ong[13] showed that in q2D metals, this expression could be interpreted using a geometrical picture of the "Stokes area" swept out by the vector $\mathbf{l}_k$ as $\mathbf{k}$ moves around the FS. A similar geometric picture can also be considered for q1D metals,[18] though it is illuminating to consider separately the effect of the anisotropy of v and τ, as we do here.

Let us consider first the case of isotropic scattering at a doping level equivalent to half-filling, at which point v_x is constant everywhere on the FS [see Eq. (4)]. In the green shaded regions, $\frac{\partial v_y}{\partial k_y}$ is positive, whereas it is negative elsewhere. Since v_x is constant, the contributions to σ_{xy} from the green and blue sections cancel out and $R_H = \frac{\sigma_{xy}}{\sigma_{xx}\sigma_{yy}} = 0$. For a band filling greater (smaller) than 0.5, v_x (and correspondingly l_x) will be less (more) at $k_y = 0$ than at $k_y = \pi/2b$ due to the dispersion of the band. Therefore the contribution from the blue shaded region will be less (more) than that of the green region and R_H will be finite and positive (negative), even in the case of an isotropic τ. Assuming constant charge carrier density, this gives a temperature-independent Hall coefficient, since the (T-dependent) isotropic scattering time has canceled in the equation for R_H. This is in agreement with earlier work[17,19] but is contrary to the claims of Fortune *et al.*[18]

Equation (3) shows that there may also be contributions to R_H due to anisotropic scattering, i.e., to a variation of τ with k_y. Since scattering time anisotropy is likely to be T dependent, this should give rise to a T-dependent Hall effect. More formally, for the FS depicted in Fig. 1, the variation of v_x with k_y can be shown[20] to be

$$v_x = v_x^0 + \frac{2t_y a}{\hbar \tan(k_F a)} \cos(k_y b) = v_x^0 + \delta v_x, \tag{4}$$

where k_F is the Fermi wave vector. Going forward, we assume that the scattering rate has the simple form

$$\frac{1}{\tau(k_y)} = \frac{1}{\tau_0}[1 + \gamma \cos(k_y b)], \tag{5}$$

where γ is a dimensionless variable that quantifies the scattering rate anisotropy. For $\gamma \ll 1$, we can reexpress this, via a Taylors series, as an equivalent scattering time

$$\tau(k_y) \sim \tau_0[1 - \gamma \cos(k_y b)] = \tau_0 + \delta\tau \tag{6}$$

which makes the calculations easier to handle. Substituting Eqs. (6) and (4) into Eq. (3) gives

$$\sigma_{xy} \propto \int \delta v_x \tau_0^2 \frac{\partial v_y}{\partial k_y} + \tau_0 v_x^0 \delta\tau \frac{\partial v_y}{\partial k_y} + \delta\tau \delta v_x \frac{\partial (v_y \delta\tau)}{\partial k_y} dk_y. \tag{7}$$

The first term in Eq. (7), of order t_y^2, describes the contribution to R_H from the variation in v_x alone and leads to the usual expression $R_H = \frac{1}{ne} \frac{k_F a}{\tan k_F a}$, where n is the carrier density.[19] The second term comes from the variation in τ and, being of order $t_x t_y$, can have a much greater influence on the magnitude (and sign) of σ_{xy} and thus $R_H(T)$. The third term is a small correction that comes from both the variation in τ and in v_x. Note that in general there may be another small correction term which appears upon expansion of Eq. (3), $\delta\tau v_x^0 \frac{\partial (v_y \delta\tau)}{\partial k_y}$, which is zero for this particular FS. Equation (7) then enables us to model the measured $R_H(T)$ in our candidate q1D systems within a Boltzmann approach and to estimate the level of anisotropy in τ that is required to account for any departures from the isotropic band value.[19]

III. RESULTS AND DISCUSSION

A. $PrBa_2Cu_4O_8$

Pr124, the nonsuperconducting structural analog of the underdoped cuprate $YBa_2Cu_4O_8$, is a q1D conductor with two 1/4-filled zigzag chains of corner-sharing CuO_4 units oriented along the b axis. It has a large resistivity anisotropy, $\rho_b : \rho_a \approx 1 : 1000$, with $\rho_c \gg \rho_a$.[21] The T dependence of $\rho_b(T)$ is approximately quadratic at low T and T linear above ~150 K,[22] consistent with expectations for a q1D FL with dominant electron-electron scattering.[23] Optical measurements on Pr124, on the other hand, have been interpreted in terms of TLL physics.[24]

In the absence of published band-structure calculations, we assume here that its FS takes the form shown in Fig. 1. In order to obtain a value for the hopping parameters which are self-consistent with the data used in fitting $R_H(T)$, we first take $v_F = 2.5 \times 10^5$ ms^{-1}, as inferred from photoemission spectroscopy,[25] then use the equation $t_x = t_b = \hbar v_F / 2b \sin(k_F b)$ to calculate t_b. From $\rho_a/\rho_b = (t_x/t_y)^2 \sim 1000$ at low T, we thus obtain $t_y = t_a = 9.7$ meV, which compares with 1.5 meV estimated from dimensional crossover studies.[21] This discrepancy is significant and is likely to arise from a combination of factors. First, the value for v_F is taken from data more than 20 meV away from the Fermi level, and any further band renormalization below this energy scale, e.g., due to the electron-phonon interaction, would only act to reduce v_F. Second, the interchain hopping parameter determined from the dimensional crossovers is an *effective* hopping parameter, which may be reduced further, relative to that measured from ρ_a/ρ_b, through interactions.[5]

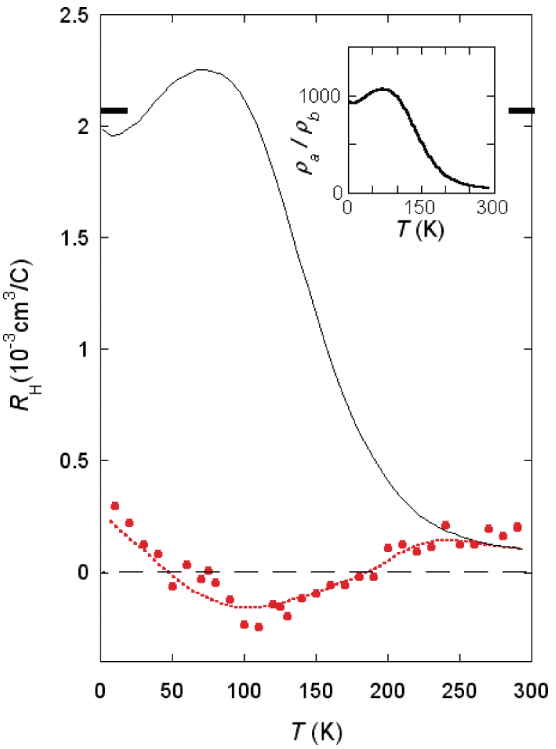

FIG. 2. (Color online) $R_H(T)$ for Pr124. Solid circles represent measured data; the thin black line, the band estimate assuming isotropic scattering; and the dashed red line, the fitted curve assuming an anisotropic τ. The thick black lines indicate the band value for R_H assuming isotropic scattering and $\rho_a \propto \rho_b$. Inset: Corresponding resistivity anisotropy $\rho_a/\rho_b(T)$. Note its similarity to the solid line in the main panel.

While the intrachain resistivity $\rho_b(T)$ in Pr124 is metallic and monotonic, the interchain resistivity $\rho_a(T)$ goes through maximum around 130 K.[21] Since $R_H \propto \sigma_{xy}/\sigma_{xx}\sigma_{yy}$, this difference in the two $\rho(T)$ curves has a dramatic effect on $R_H(T)$. As an illustration, the solid black line in Fig. 2 represents $R_H(T)$ calculated using the published resistivity data[21] and assuming strictly isotropic scattering. As one can see from comparison with the inset to Fig. 2, the T dependence of $R_H(T)$ precisely mimics that of $\rho_a/\rho_b(T)$. Were $\rho_{xx} \propto \rho_{yy}$, R_H would simply be a constant, as indicated by the short thick lines on either side of the ordinate axis.

The $R_H(T)$ data, plotted as solid circles in Fig. 2, were measured using the four-point ac lock-in technique and agree with previously published work.[16] While the measured data overlap with the isotropic fit at high T, below around 250 K, the two curves separate, with the measured $R_H(T)$ curve changing sign at intermediate temperatures before becoming positive again as $T \to 0$. Within the Boltzmann picture, this separation of the two curves indicates the development of anisotropy in τ with decreasing T. The solid red line is the corresponding fit to the data obtained by allowing γ, the strength of the anisotropy in τ, to vary with temperature. The resultant $\gamma(T)$ is plotted in Fig. 4. It is striking to note that this marked departure in the as-measured $R_H(T)$ results from a very small (<10%) change in τ across the entire FS. We shall return to this point later, after we first consider the case of $(TMTSF)_2PF_6$.

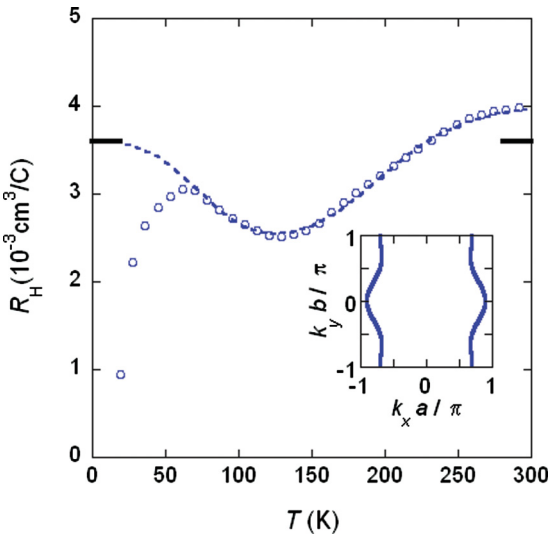

FIG. 3. (Color online) $R_H(T)$ for $(TMTSF)_2PF_6$. Open circles represent measured data (Ref. 7); the solid black lines, the band estimate (Ref. 7) assuming isotropic scattering; and the dashed blue line, the fitted curve for anisotropic scattering. The inset shows an exaggerated Fermi surface of $(TMTSF)_2PF_6$.

B. $(TMTSF)_2PF_6$

$(TMTSF)_2PF_6$ is one of several q1D organic metals which have been the subject of intense interest with regard to the possible realization of a TLL ground state. As Pr124, it too has a large resistive anisotropy ratio, with $\rho_a : \rho_b \approx 1 : 100$ and $\rho_c \gg \rho_b$.[7] The T dependence of $\rho_a(T)$ (taking into account the large thermal expansion coefficient) varies approximately as T^2 below ~130 K and, as Pr124, it has a lower temperature exponent at higher T.[8] Its Hall effect, meanwhile, has been analyzed both in terms of TLL physics[8] and within a q1D FL picture with an anisotropic τ.[26] Hence it is an ideal compound with which to compare our analysis.

The dispersion relation of $(TMTSF)_2PF_6$ is taken to be $\epsilon = -2t_a \cos(k_x a) - 2t_b \cos(k_y b) - 2t'_b \cos(2k_y b) + \epsilon_z$, where $t_a(t_b)$ are the intrachain (interchain) hopping parameters, and $2t'_b = t_b^2 \cos(k_F a)/t_a \sin^2(k_F a)$.[27] The inclusion of phase factors in the above cosine terms[17] is found to have a minimal impact on our results. The FS takes the form shown (greatly exaggerated) in the inset of Fig. 3. Using the method outlined above for Pr124 and the literature value of $v_F = 4.0 \times 10^5$ ms^{-1} for $(TMTSF)_2PF_6$,[27] we estimate $t_b = 24$ meV, in reasonable agreement with previous analysis[27,28] (taking $t_a/t_b = t_x/t_y \approx 10$). The t'_b term constitutes ~3% of the total warping and thus its inclusion has a negligible impact on the magnitude and T dependence of R_H.

As with Pr124, we can estimate $\gamma(T)$ from the as-measured $R_H(T)$ curve,[7] plotted as open circles in Fig. 3. Here we have scaled the expected band value at 1/4 filling [the thick black lines in Fig. 3 (Ref. 7)] by ~10% (within the experimental uncertainty) to allow the calculated, isotropic, R_H to be equal to the measured R_H at $T = 300$ K. The solid blue line in Fig. 3 represents the anisotropic-τ fit and the corresponding anisotropy parameter $\gamma(T)$ is plotted in Fig. 4. The dramatic change in $R_H(T)$ around $T = 60$ K is at too high a temperature to be associated with any known FS reconstruction. The sharp

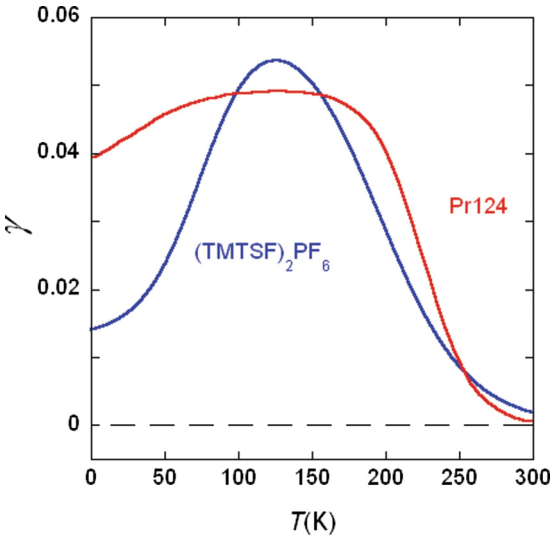

FIG. 4. (Color online) Scattering time anisotropy parameter γ extracted from fits to $R_H(T)$ in $(TMTSF)_2PF_6$ and Pr124.

reduction in R_H is reminiscent of what occurs in hole-doped cuprates at 1/8 doping where it was attributed to a possible confinement of carriers to individual stripes.[11] However, in the absence of any reconstruction, such confinement is expected to arise only once $k_BT > 2t_b$,[5] and hence should occur at higher T, rather than at lower T. Within our anisotropic-τ model, the drop in $R_H(T)$ corresponds to an increase in $\gamma(T)$ from ~0.02 at $T = 50$ K to around 0.14 at $T = 15$ K [i.e., just above the spin density wave (SDW) transition]. Hence, the more likely explanation for the sudden drop in R_H is the development of "hot spots,"[26] regions of intense scattering (e.g., due to SDW fluctuations[7] or umklapp scattering[29]) that we have not tried to capture here.

IV. CONCLUSIONS

The results presented above highlight several key points. First, it confirms the finding of Yakovenko and Zheleznyak[17] that $R_H(T)$ in q1D systems is highly sensitive to anisotropy in $\tau(k_y)$. We can see in Fig. 4 that in the two cases considered here, a variation of at most 10% ($\gamma < 0.05$) is sufficient to recover the measured $R_H(T)$ in Pr124, including the change of sign, and in $(TMTSF)_2PF_6$ above $T = 50$ K. We have also demonstrated the importance of taking into account the T dependence of the resistivity anisotropy. An interesting finding of this work is the remarkable similarity in the magnitude, sign, and T dependence of γ in Pr124 and $(TMTSF)_2PF_6$ (above 50 K). The reduction in $\gamma(T)$ toward zero as $T \to 300$ K presumably reflects the mixing of states at high T due to an increase in scattering, while the small residual anisotropy at low T in both systems can be attributed to small-angle impurity scattering (i.e., scattering off defects located outside the conducting chains[30]). Given the similarity in $\gamma(T)$ in both systems, it is tempting to assign the same origin for the dominant scattering process in each compound. In the future, it will be illuminating to apply this model to a range of q1D systems to determine how generic this form of $\gamma(T)$ actually is. Then we may turn our attention to other q1D conductors, such as $(TMTTF)_2AF_6$ (Ref. 10) and $Li_{0.9}Mo_6O_{17}$,[31] where the Hall effect cannot easily be explained within this anisotropic framework and consider Hall effect anomalies arising from more exotic (e.g., TLL) electronic states.[32]

Finally, the small magnitude of the τ anisotropy in Pr124 and $(TMTSF)_2PF_6$ contrasts markedly with that found in the q2D cuprates, for example, where even far from the Mott insulating state, τ anisotropy can peak at over 100% (at $T = 100$ K).[33] In the cuprates, this anisotropic scattering is associated with an anomalous scattering rate, of as yet unknown origin, that varies linearly in T down to the lowest temperatures studied.[34] From this perspective, it would be interesting to explore the possibility that the rapidly developing τ anisotropy inferred from $R_H(T)$ in $(TMTSF)_2PF_6$ might also be associated with a similar T-linear term observed in the low-T resistivity.[35]

ACKNOWLEDGMENTS

We thank J. R. Cooper and R. H. McKenzie for invaluable comments and discussions. This work was supported by EPSRC (EP/G031460) and by a Royal Society Wolfson Research Merit Award (NEH).

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