Hot and Cold Spots of the Electron Relaxation Time in Quasi-One-Dimensional Organic Conductors and Cuprates

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1. **Hot spots in quasi-one-dimensional organic metals**

   (a) Singularities in the distribution of electron scattering rate over the Fermi surface:
   Zheleznyak and Yakovenko, *Synthetic Metals* **70**, 1005 (1995)

   (b) Temperature dependence of the Hall effect and resistivity in $(TMTSF)_2PF_6$: Yakovenko and Zheleznyak, *Eur. Phys. J. B* **11** 385 (1999); *Synth. Metals* **103**, 2202 (1999); **120**, 1083 (2001)

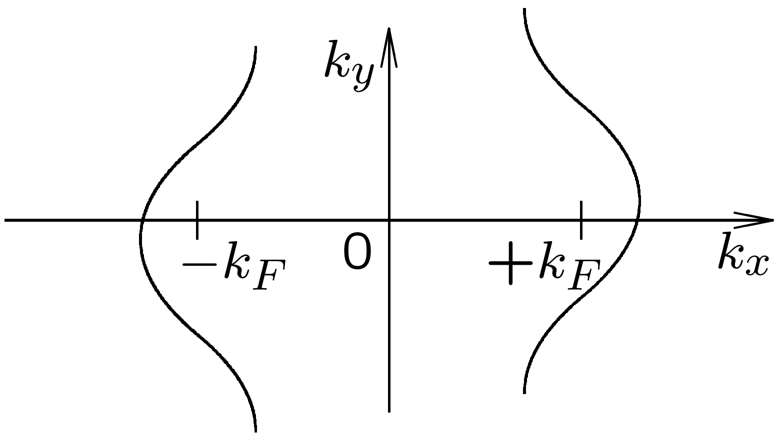
2. **Cold spots in cuprates** — Two-τ interpretation of the ac Hall effect in $YBa_2Cu_3O_7$: Zheleznyak, Yakovenko, Drew, and Mazin, *Phys. Rev. B* **57**, 3089 (1998); **59**, 207 (1999)

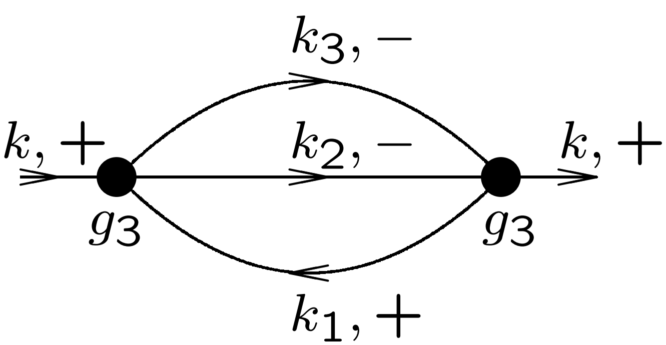
Umklapp Scattering in Q1D Conductors

Electron dispersion law in a Q1D conductor can be approximated as

$$\varepsilon_{\mathbf{k}}^{\pm} = \pm v_F(k_x \mp k_F) + 2t_b \cos(k_y \pm \varphi).$$

The Fermi surface consists of two disconnected, warped sheets:





The electron-electron umklapp scattering rate is

$$\frac{1}{\tau(\mathbf{k})} = g_3^2 \int \frac{d^2k_1\, d^2k_2\, d^2k_3}{(2\pi)^6}\, \delta[\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3]\, \delta[\varepsilon_{\mathbf{k}}^{+} + \varepsilon_{\mathbf{k}_1}^{+} - \varepsilon_{\mathbf{k}_2}^{-} - \varepsilon_{\mathbf{k}_3}^{-}]$$
$$n(\varepsilon_{\mathbf{k}}^{+})\, n(\varepsilon_{\mathbf{k}_1}^{+})\, [1 - n(\varepsilon_{\mathbf{k}_2}^{-})]\, [1 - n(\varepsilon_{\mathbf{k}_3}^{-})].$$

The scattering rate can be written as

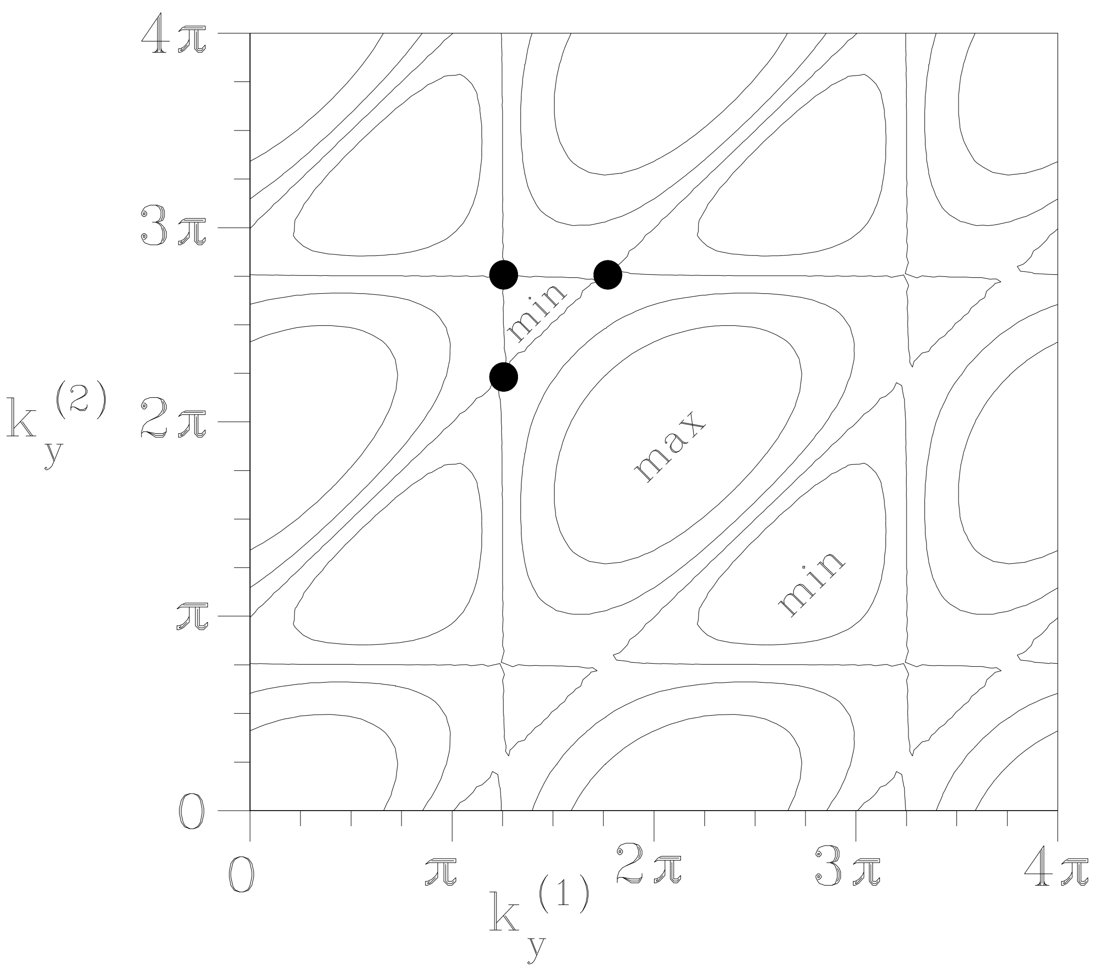
$$1/\tau(k_y, T) = \mathrm{const}\, T^2\, B(k_y),$$

where $B(k_y)$ reflects the phase space available for scattering.

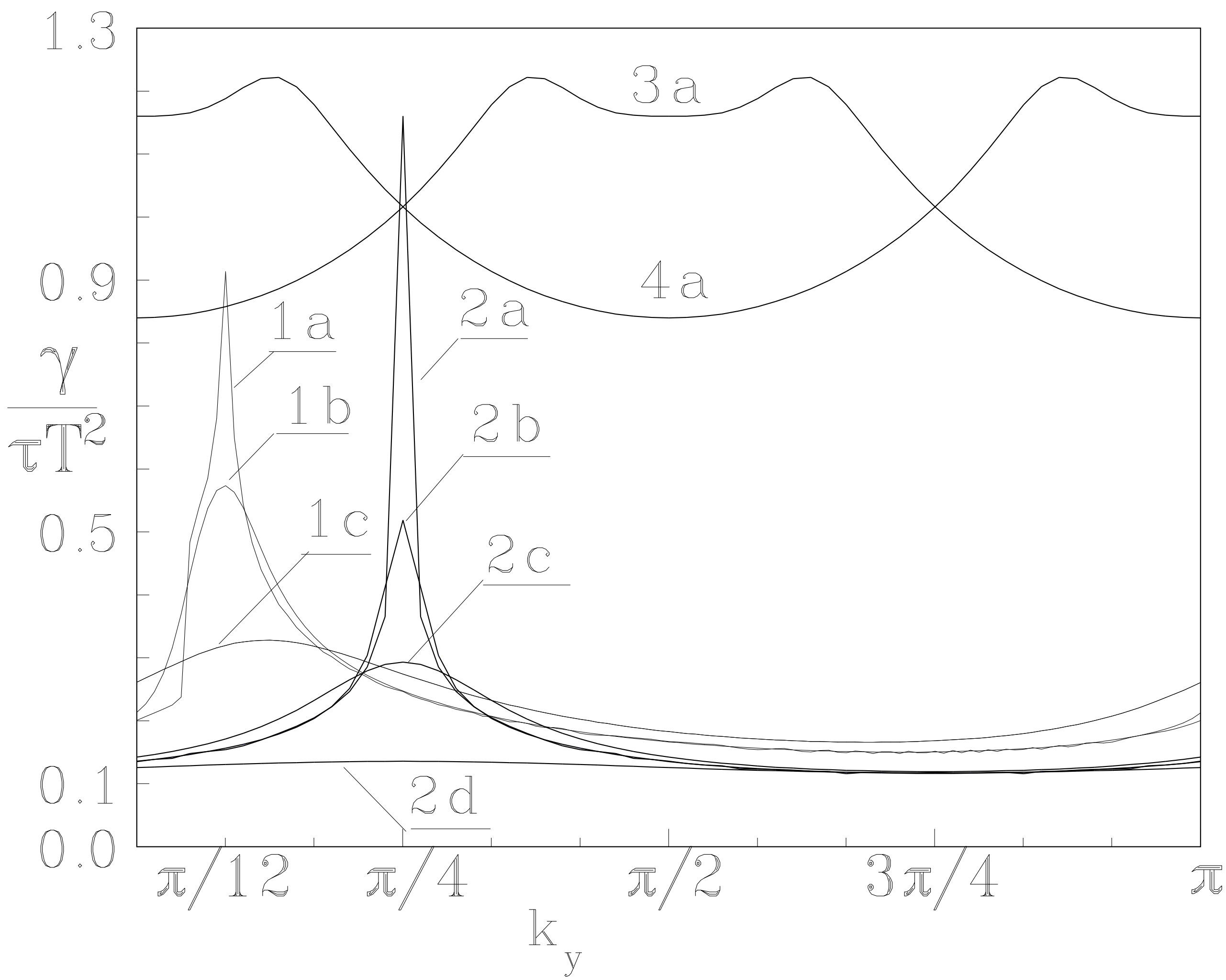
The function $B(k_y) = \int \frac{dk_y^{(1)} dk_y^{(2)}}{(2\pi)^2}\, \delta[t_b F(k_y, \varphi; k_y^{(1)}, k_y^{(2)})]$ has singularities at certain values of k_y, which are determined by the saddle points of the function $F(k_1, k_2)$ and are analogous to the van Hove singularities:

$$F(k, \varphi; k_1, k_2) = \cos(k + \varphi) + \cos(k_1) + \cos(k_2) + \cos(k + k_1 - k_2 - 3\varphi).$$

The contour plot of $F(k_1, k_2)$ is shown below:

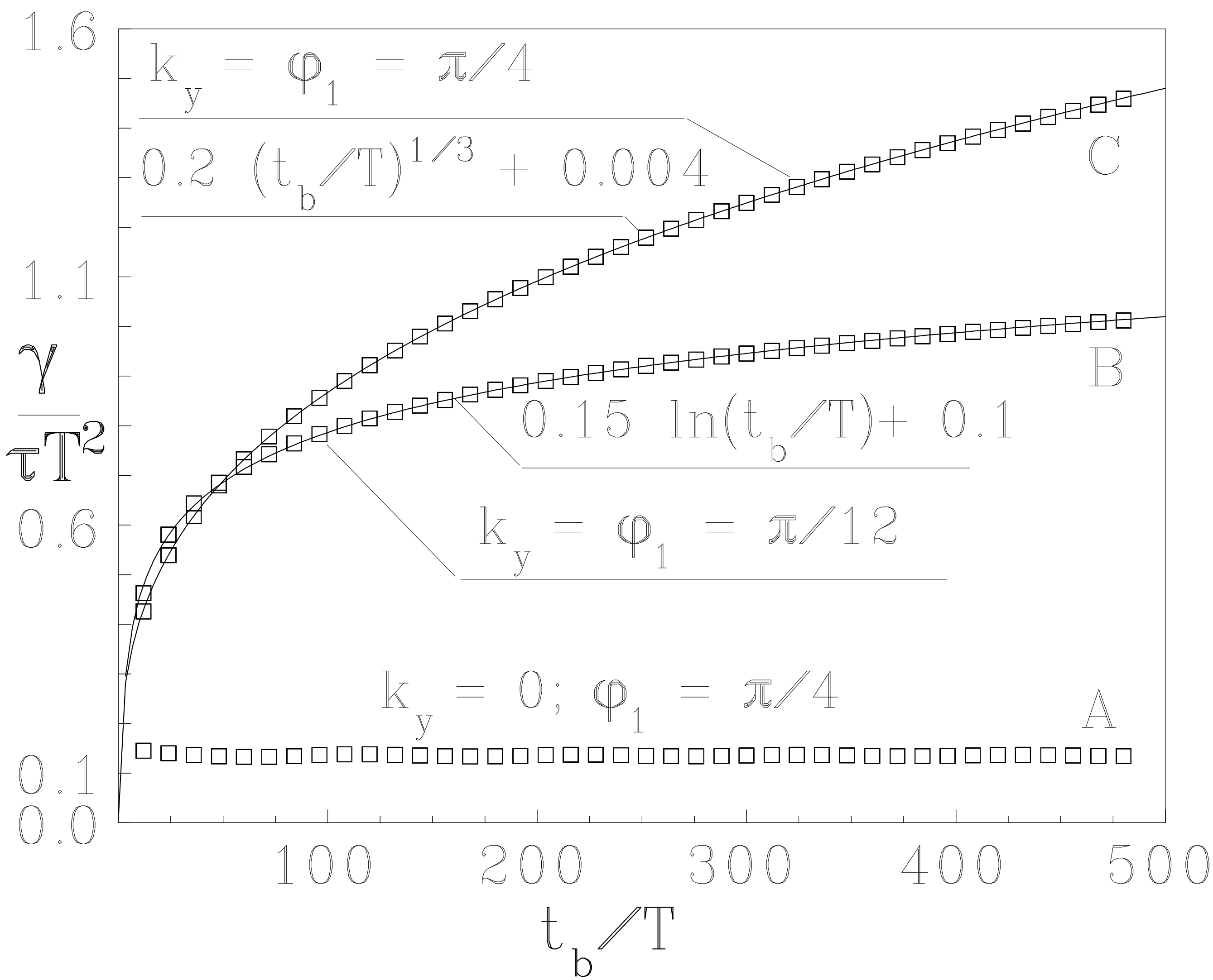


Calculated variation of $1/\tau$ along the Fermi surface



Numbers 1, 2, 3, and 4 correspond to the phases $\varphi = \pi/12$, $\pi/4$, 0, and $\pi/2$; letters a, b, c, and d define the temperature $T = t_b/240$, $t_b/24$, $t_b/5$, and t_b. The normalizing coefficient γ is equal to $(2\pi)^4 t_b v_F^2/60 g_4^2$.

Temperature dependences of $1/\tau$ at different points on the Fermi surface



Squares represent the results of numerical calculations, and the solid lines are curve fits.

Hall effect in Quasi-One-Dimensional Conductors

For weak magnetic fields $\omega_c \tau \ll 1$, according to Ong's formula [PRB **43**, 193 (1991)], the Hall conductivity is proportional to the area enclosed by the mean-free-path curve

$$\sigma_{xy} \propto \oint \mathbf{l} \times d\mathbf{l},$$

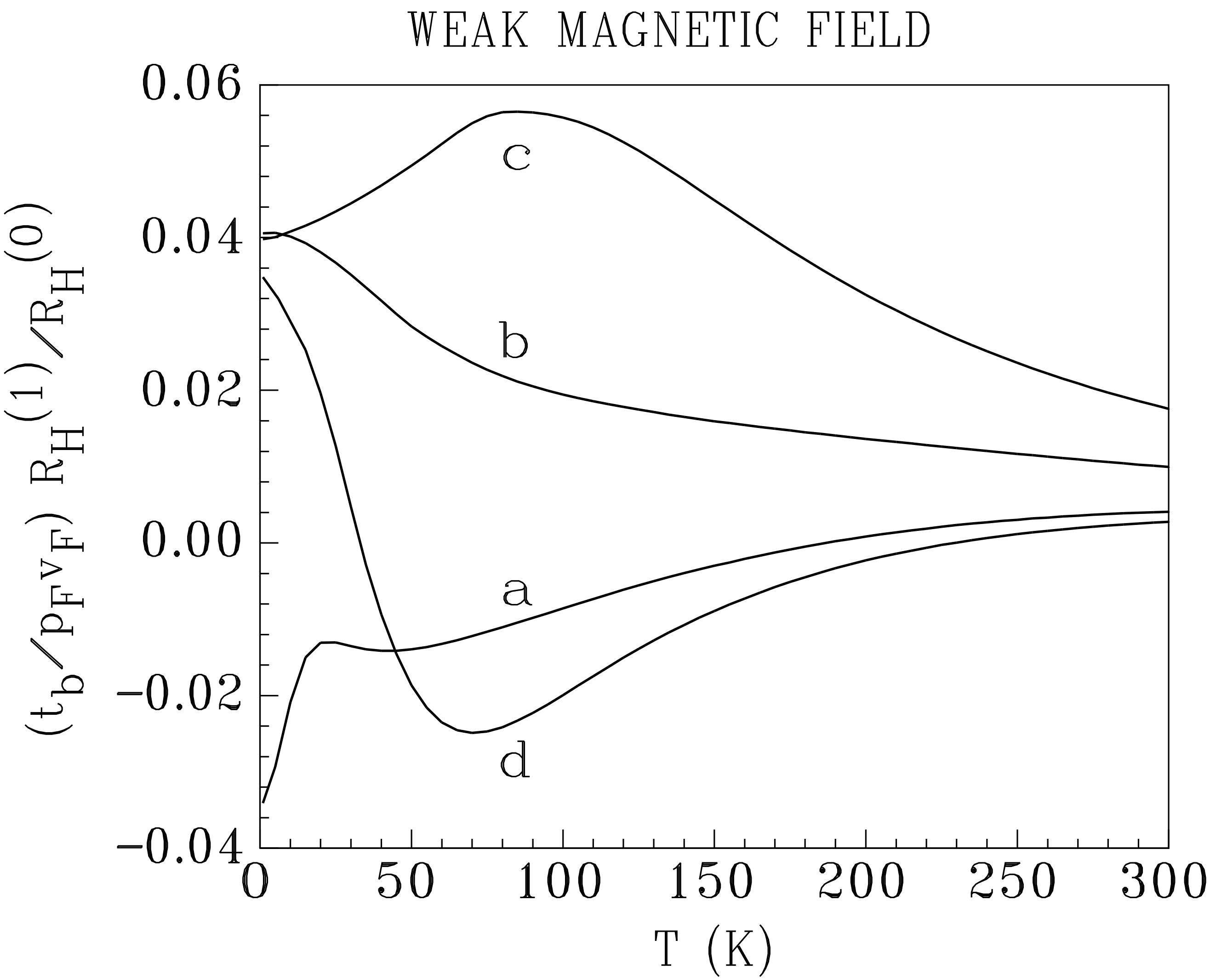
where $\mathbf{l}(k_t) = \tau(k_t)\mathbf{v}(k_t)$ is the local mean-free path at a given point k_t of the Fermi surface. For a Q1D conductor, this formula gives

$$\sigma_{xy} = -\frac{2e^3 H}{(2\pi\hbar)^2 c} \int dk_y \, v_y(k_y)\tau(k_y) \, \frac{d[v_x(k_y)\tau(k_y)]}{dk_y}.$$

Non-zero contributions to the Hall conductivity have two origins:

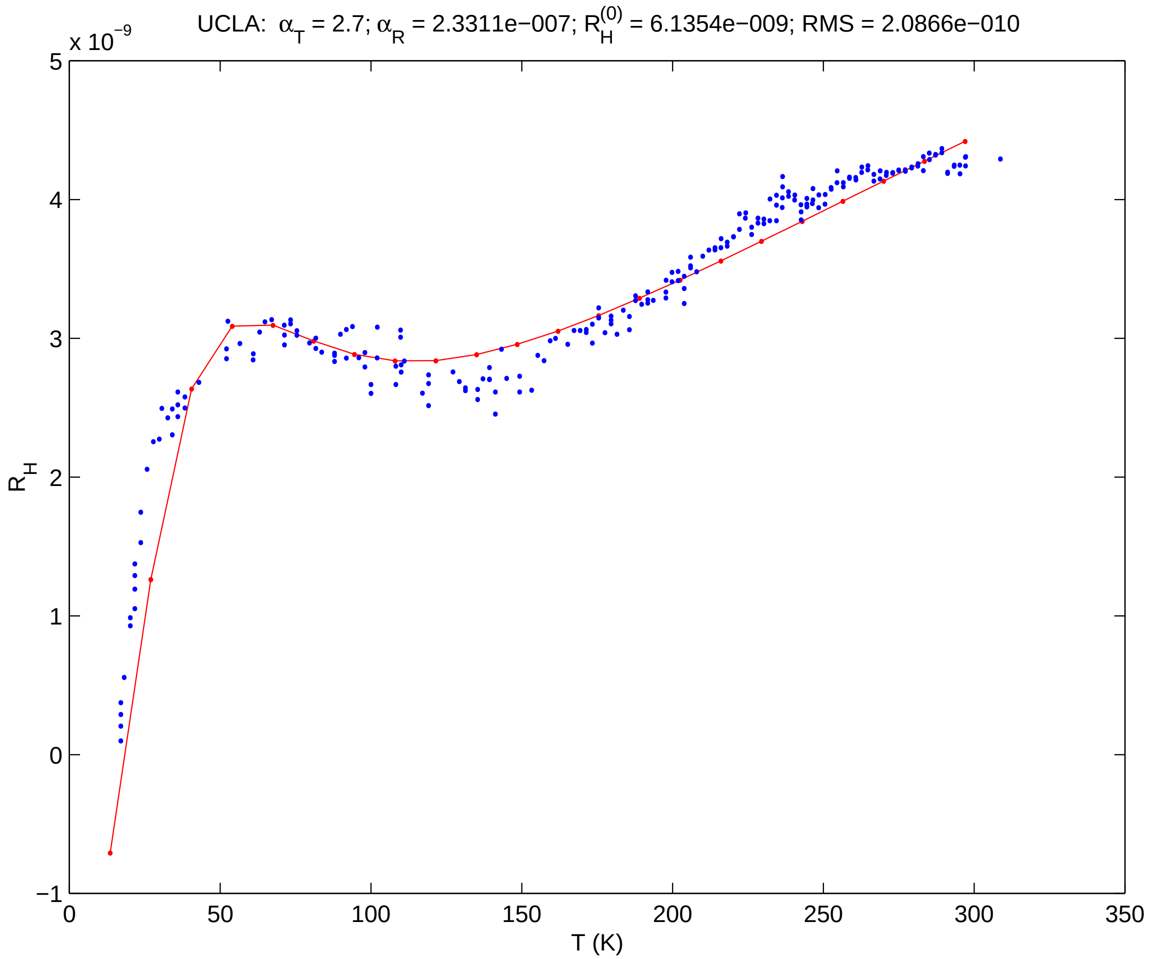
- Dependence of v_x on k_y. This produces conventional temperature-independent expression for the Hall coefficient $R_H = \frac{\sigma_{xy}}{\sigma_{xx}\,\sigma_{yy}} = \frac{1}{nec}$.
- Dependence of τ on k_y. This term is very sensitive to the presence of hot spots and produces strong temperature dependence.

Temperature dependence of the contribution to the Hall coefficient due to hot spots in $1/\tau$



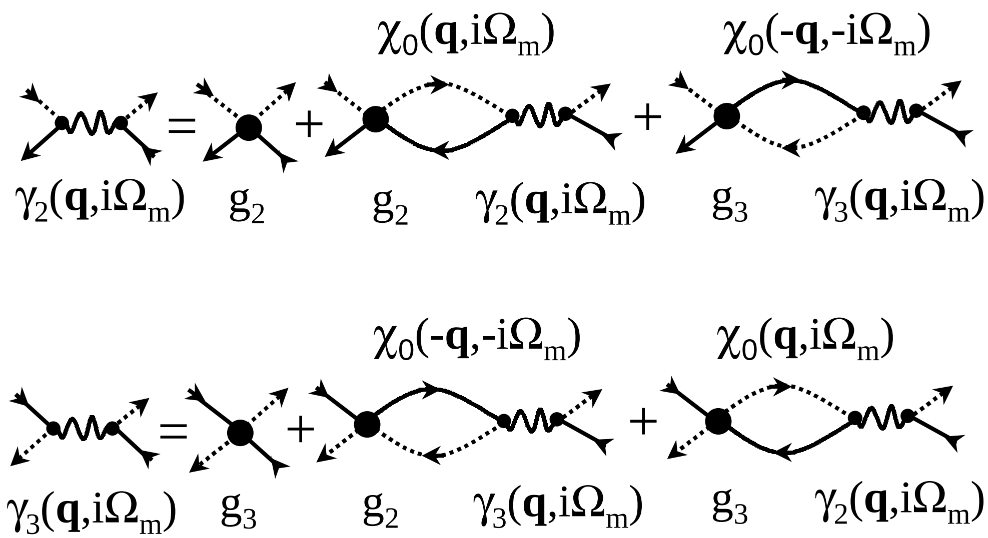
(a) $\varphi = \varphi' = 0$, (b) $\varphi = \frac{\varphi'}{2} = \frac{\pi}{8}$, (c) $\varphi = \frac{\varphi'}{2} = \frac{\pi}{4}$, (d) $\varphi = \frac{\pi}{12}$ and $\varphi' = 0$.

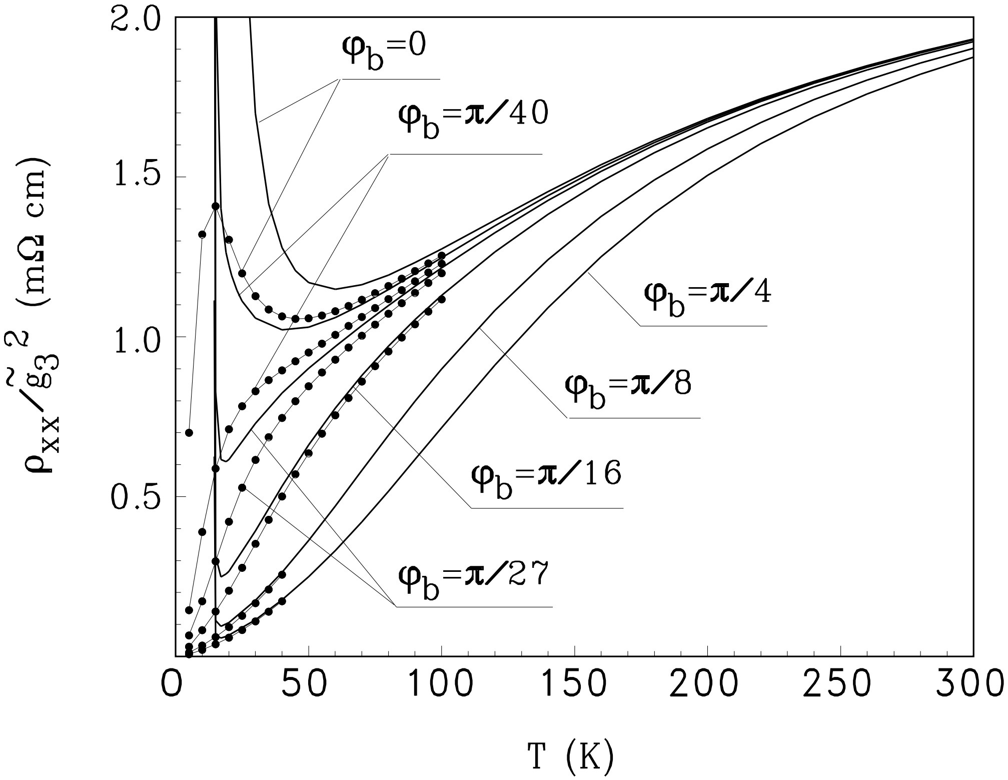
Comparison between theory and experiment for the temperature dependence of the Hall coefficient in $(TMTSF)_2PF_6$



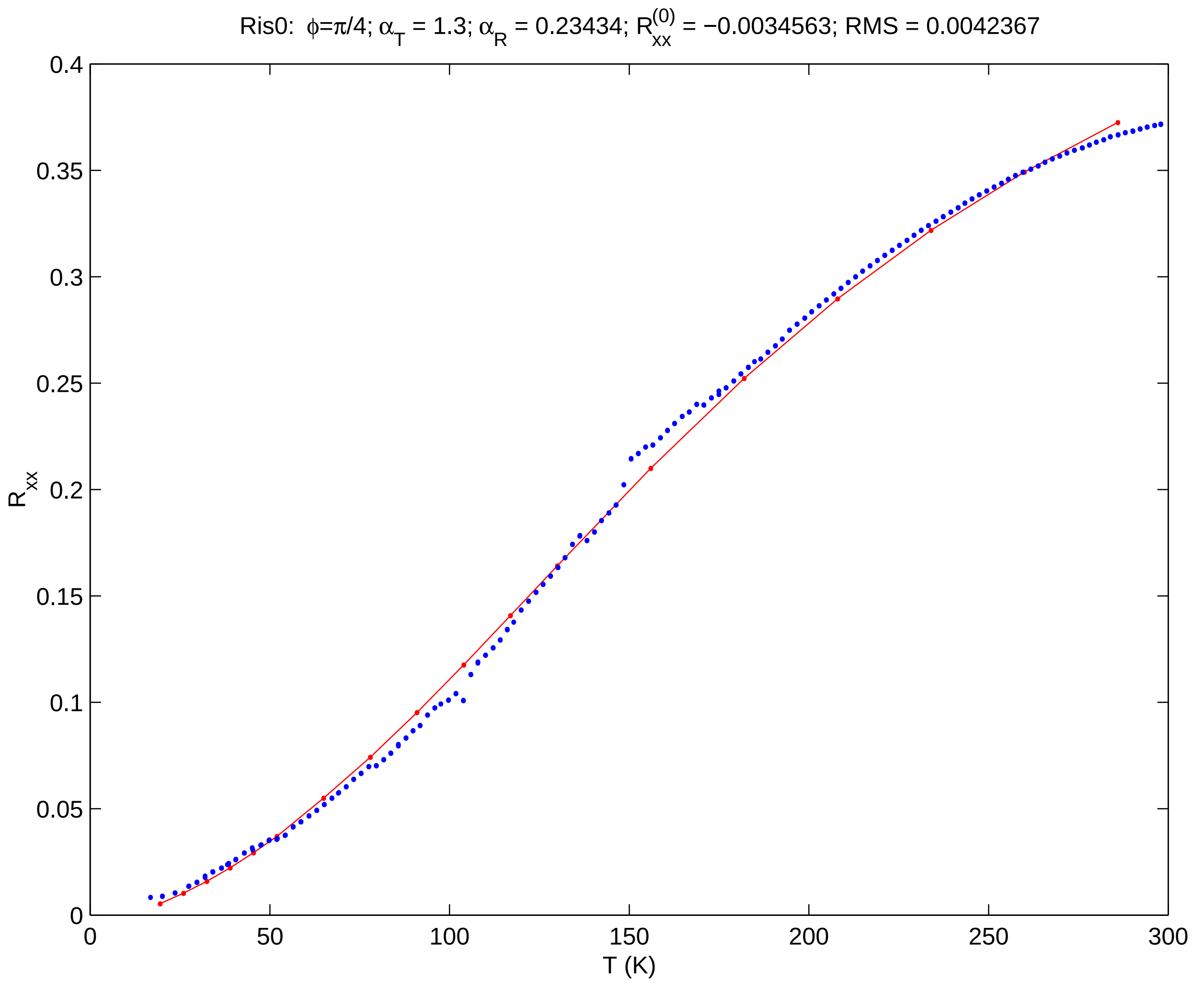
Experimental points are the data from Jérome's group [Phys. Rev. Lett. **84**, 2674 (2000)], and the solid line is our theoretical curve (a).

Renormalization of umklapp scattering amplitude γ_3 and temperature dependence of resistivity ρ_{xx}



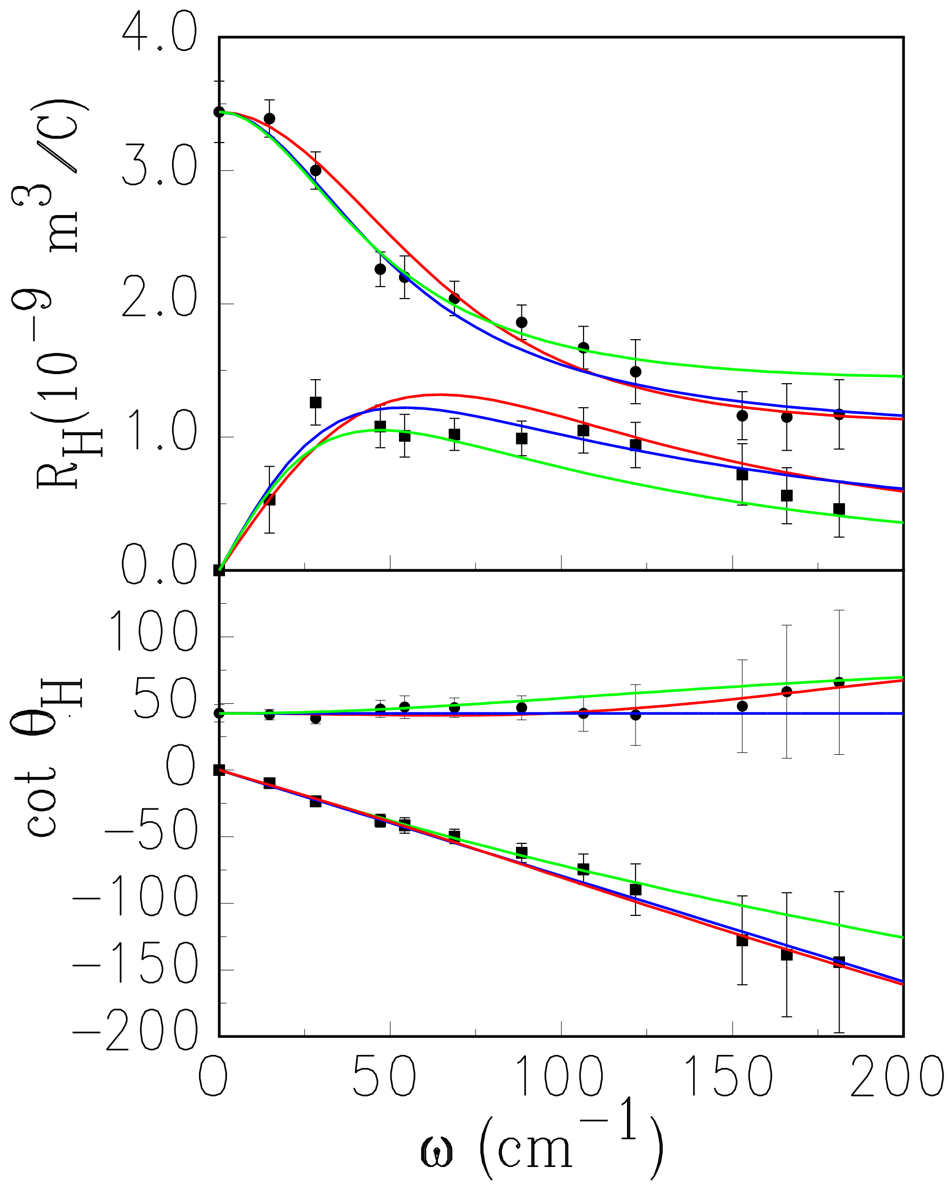


Temperature dependence of resistivity in $(TMTSF)_2PF_6$: theory vs. experiment



Experimental points are Jérome's group data [PRL **84**, 2674 (2000)], and the solid line is our theoretical curve with $\varphi = \frac{\pi}{4}$, $t_b' = 20$ K .

AC Hall effect in $YBa_2Cu_3O_7$ does not follow a simple Drude model



Experimental points are from Drew's group [Phys. Rev. Lett. **76**, 696 (1996)]. Red curve represents the cold spots model.

$$\begin{matrix}\sigma_{xx}(\omega)\\ \sigma_{xy}(\omega)\end{matrix} \to \begin{matrix}\cot\theta_H(\omega) = \sigma_{xx}(\omega)/\sigma_{xy}(\omega)\\ R_H(\omega) = \sigma_{xy}(\omega)/H\sigma_{xx}^2(\omega)\end{matrix}$$

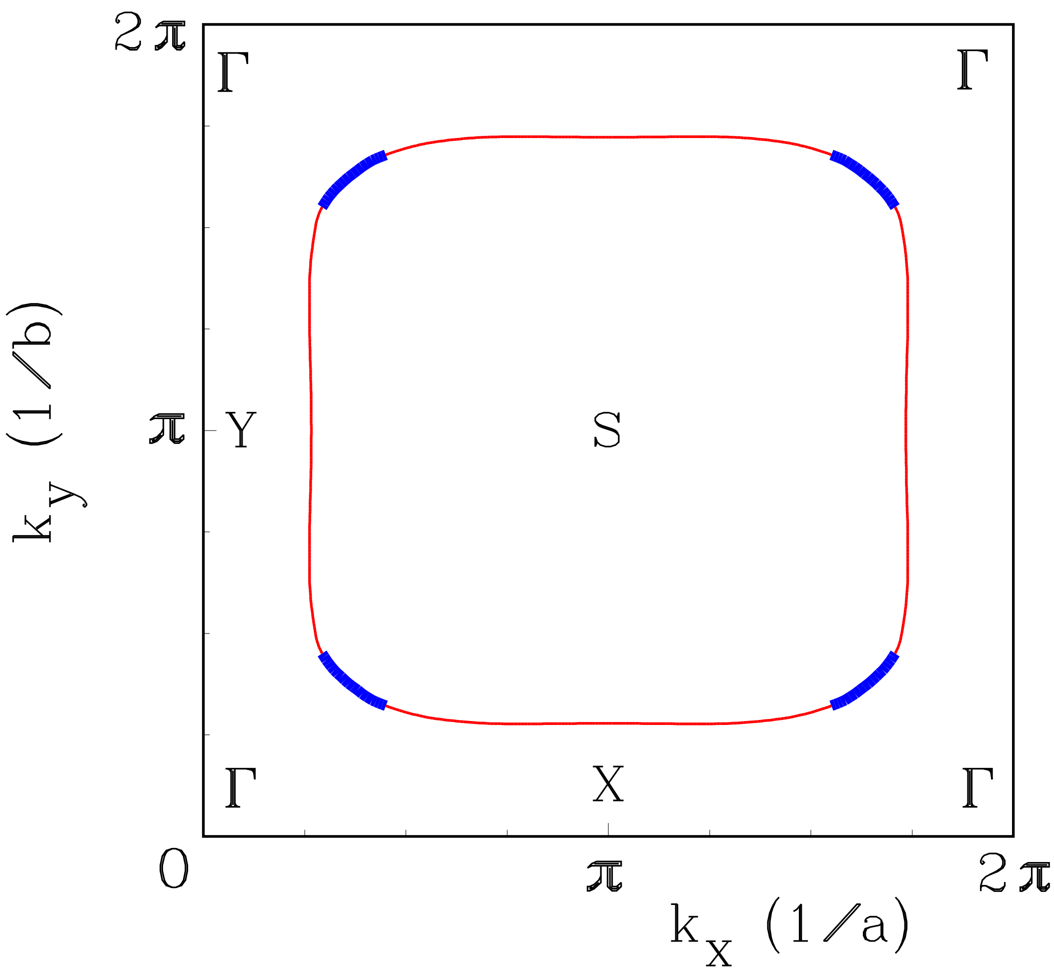
In a simple Drude model:

$$\begin{matrix}\sigma_{xx}(\omega) \propto \tilde{\tau}(\omega)\\ \sigma_{xy}(\omega) \propto \tilde{\tau}^2(\omega)\end{matrix}, \quad \frac{1}{\tilde{\tau}(\omega)} = \frac{1}{\tau} - i\omega.$$

$\cot\theta_H(\omega) = \frac{1}{\tilde{\tau}(\omega)} = \frac{1}{\tau} - i\omega$ agrees with experiment.

$R_H(\omega) = \text{const}(\omega, T)$ does not agree with experiment

Two-τ model with cold spots on the Fermi surface of $YBa_2Cu_3O_7$, at the Brillouin zone diagonals



$$\sigma_{xx}(\omega) = A_1\tilde{\tau}_1(\omega) + A_2\tilde{\tau}_2(\omega)$$

$$\sigma_{xy}(\omega) = B_1\tilde{\tau}_1^2(\omega) + B_2\tilde{\tau}_2^2(\omega)$$

$$1/\tilde{\tau}_{1,2}(\omega) = 1/\tau_{1,2} - i\omega$$

$$\tau_2/\tau_1 = 4$$

$$A_{1,2} \propto \int_{1,2} v(k_t)\, dk_t$$

$$A_1 : A_2 = 9 : 1$$

$$B_{1,2} \propto \int_{1,2} \mathbf{v}(k_t) \times d\mathbf{v}(k_t),$$

$$B_1 : B_2 = 7 : 3$$

Further developments of the cold spots model

Ioffe and Millis, PRB **58**, 11631 (1998): $1/\tau(k_t) \approx 1/\tau_0 + \Gamma k_t^2$, where $1/\tau_0 \propto T^2$ is the relaxation rate at the cold spot, and Γ is temperature-independent.

van der Marel, PRB **60**, R765 (1999): $1/\tau(k_t) = 1/\tau_0 + \Gamma \sin^2(2\theta)$

Possible origins of the cold spots

- Geometry of the Fermi surface: the sides of the square vs. the corners, flat regions vs rounded, 1D vs 2D.
- Fluctuations of a d-wave order parameter (superconducting or insulating): connection to the pseudogap.
- Antiferromagnetic fluctuations at the wave vector (π, π), via merger of the eight hot spots.

Conclusions

- Strong variations of electronic properties, such as relaxation time, along the Fermi surface are common in metals and play important role in electron transport.

- For Q1D conductors, we found hot spots resulting from singularities of the phase space available for scattering. The calculated temperature dependences of resistivity and the Hall coefficient are in semiquantitative agreement with the experiment on the organic conductor $(TMTSF)_2PF_6$.

- For cuprates, the phenomenological model of the cold spots at the Brillouin zone diagonals has certain success in describing dc and ac transport and magnetotransport.