Comparison of experimental data and theoretical calculations for electrical resistivity and Hall coefficient in (TMTSF)$_2$PF$_6$

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Abstract

The temperature dependences of the Hall coefficient and electrical resistivity recently measured by Moser et al. [Phys. Rev. Lett. 84, 2674 (2000)] in the quasi-one-dimensional organic conductor (TMTSF)$_2$PF$_6$ are quantitatively compared with our previous theoretical calculations [Synth. Met. 103, 2202 (1999); Eur. Phys. J. B 11, 385 (1999)]. We find a good agreement, albeit not with a fully consistent set of parameters for the two quantities.

Key words: Many-body and quasiparticle theories, Transport measurements, conductivity, Hall effect, magnetotransport, Organic conductors based on radical cation and/or anion salts, Organic superconductors

Recently, the temperature dependences of the Hall coefficient, as well as electrical resistivity, were measured in the quasi-one-dimensional (Q1D) organic conductor (TMTSF)$_2$PF$_6$ by the two groups [1,2]. The results were interpreted using the Luttinger liquid concept in Ref. [1] and the conventional Fermi liquid theory in Ref. [2]. Before the experimental data became known, we had published theoretical calculations of the temperature dependences of the Hall coefficient [3] and electrical resistivity [4]. In the present paper, we quantitatively compare our theoretical predictions and the experimental results. Since we have calculated the Hall coefficient in the (a-b) plane, we compare only with the results of Ref. [1], where the Hall coefficient was measured in that geometry, unlike in Ref. [2], were the (b-c) plane geometry was employed. Electrical resistivity, calculated in Ref. [4] for the direction along the chains, is compared only with the experimental results of Ref. [1], because they correspond to constant volume, unlike the constant-pressure results of Ref. [2].

The Hall coefficient $R_H = \sigma_{xy}/H \sigma_{xx} \sigma_{yy}$, where $\sigma_{ij}$ are the components of the conductivity tensor and $H$ is the magnetic field, is usually a constant, because, in a simple Drude model, $\sigma_{xy} \propto \tau^2$ and $\sigma_{xx,yy} \propto \tau$, so the temperature-dependent relaxation time $\tau$ cancels out in $R_H$. However, the experiment [1] found that $R_H$ in (TMTSF)$_2$PF$_6$ does depend on temperature. The authors invoked the Luttinger liquid concept in order to explain this effect. However, it has been shown theoretically that $R_H$ of weakly coupled one-dimensional Luttinger chains does not depend on frequency and temperature [5], because the power-law dependences of $\sigma_{xy}$ and $\sigma_{yy}$ cancel out.

The Hall coefficient may depend on temperature if the system has relaxation times with different temperature dependences. (See discussion [6] of the “cold spots” for the cuprate high-temperature superconductors, where $R_H$ is also temperature-dependent.) In Ref. [7], we had calculated the distribution of the umklapp scattering rates over the Fermi surface of a Q1D conductor and found that at low temperatures “hot spots” develop with a different temperature dependence. Using this distribution, we have calculated the temperature dependence of $R_H$ in Ref. [3]. Fig. 1 shows our theoretical curve with the experimental points from Ref. [1]. In our calculation, the Hall coefficient consists of two terms: $R_H = R_H^{(0)} + R_H^{(1)}$. The first term is a temperature-independent band-structure contribution. In our fit, it is taken to be $R_H^{(0)} = 6.1 \times 10^{-3} \text{m}^3/\text{C}$, which is 1.7 times greater than the value assumed in Ref. [1]. The second,
The theoretical line is taken from Fig. 4 of Ref. [4]. The temperature scale of Fig. 1 from Ref. [4] is multiplied by the factor $\alpha_T = 1.3$. The curve with $\varphi = \pi/4$ and $t_b' = 20$ K from Fig. 4 of Ref. [4].

The upturn can be suppressed by selecting a small but finite value for the phases (see the other curves in Fig. 4 of Ref. [4]) or by selecting a greater value for $t_b'$ (see Fig. 6 of Ref. [4]). The second problem is the difference in the temperature scales $\alpha_T$ utilized to obtain the fits in Figs. 1 and 2. While the scale 1.3 for $R_{xx}$ is reasonable, the value 2.7 for $R_H$ is too big. However, the scale of $R_H$ is controlled primarily by $t_b'$ (because $R_H^{(1)} = 0$ if $t_b' = 0$ [3]), whereas the scale of $R_{xx}$ is controlled by $t_b$. So the agreement could be achieved by increasing $t_b'$ without increasing $t_b$. The increase of $t_b'$ could suppress the SDW transition, which is present at the ambient pressure, but that could be compensated by an increase in the interaction strength.

The space of model parameters is big, and there are opportunities to achieve better agreement with the experiment by optimizing the choice of parameters. Our first try presented here appears to be promising.

References

[1] J. Moser, J. R. Cooper, D. Jérome, B. Alavi, S. E. Brown, and K. Bechgaard, Phys. Rev. Lett. 84, 2674 (2000).
[2] G. Mihály, I. Kézsmárki, F. Zamborszky, and L. Forró, Phys. Rev. Lett. 84, 2670 (2000).
[3] V. M. Yakovenko and A. T. Zheleznyak, Synth. Met. 103, 2202 (1999).
[4] A. T. Zheleznyak and V. M. Yakovenko, Eur. Phys. J. B 11, 385 (1999).
[5] A. V. Lopatin, Phys. Rev. B 57, 6342 (1998);
A. Lopatin, A. Georges, and T. Giamarchi, cond-mat/0008066.
[6] A. T. Zheleznyak, V. M. Yakovenko, H. D. Drew, and I. Mazin, Phys. Rev. B 57, 3089 (1998); 59, 207 (1999).
[7] A. T. Zheleznyak and V. M. Yakovenko, Synth. Met. 70, 1065 (1995).