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Temperature Evolution of the Quantum Hall Effect in Quasi-One-Dimensional Organic Conductors

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Abstract

The Hall conductivity in the magnetic-field-induced spin-density-wave (FISDW) state of the quasi-one-dimensional organic conductors $(TMTSF)_2X$ at a finite temperature is calculated. The temperature dependence of the Hall conductivity is found to be the same as the temperature dependence of the Fröhlich current of a regular charge/spin-density wave. Predicted dependence $\sigma_{xy}(T)$ can be verified experimentally in the $(TMTSF)_2X$ compounds if all components of the resistivity tensor are measured and the conductivity tensor is reconstructed.

Keywords: Many-body and quasiparticle theories; Transport measurements, conductivity, Hall effect, magneto-transport; Magnetic phase transitions; Organic conductors based on radical cation and/or anion salts; Organic superconductors.

Organic metals of the $(TMTSF)_2X$ family, where TMTSF is tetramethyltetraselenafulvalene and X represents an inorganic anion, are highly anisotropic, quasi-one-dimensional crystals that consist of parallel conducting chains. The overlap of the electron wave functions and the electric conductivity are the highest in the direction of the chains (the **a** direction) and are much smaller in the **b** direction perpendicular to the chains. In this paper, we neglect the coupling between the chains in the third, **c** direction, which is weaker than in the **b** direction, and study the properties of a single layer (the **a**-**b** plane), modeling $(TMTSF)_2X$ as a system of the uncoupled two-dimensional layers.

When a strong magnetic field is applied perpendicular to the **a**-**b** plane, the magnetic-field-induced spin-density-wave (FISDW) appears in the system (see Ref. [1] for a review). In the FISDW phase, the Hall conductivity per one layer, σ_{xy}, is quantized at zero temperature as

$$\sigma_{xy} = 2Ne^2/h, \tag{1}$$

where e is the electron charge, $h = 2\pi\hbar$ is the Planck constant, and N is an integer that characterizes the FISDW. However, at a finite temperature, because electrons are thermally excited above the FISDW energy gap, the Hall conductivity is not quantized. In this paper, we calculate temperature dependence of the Hall conductivity in the FISDW state.

To model $(TMTSF)_2X$, let us consider a 2D system that consists of many chains, parallel to the x axis and equally spaced along the y-axis with the distance b.[1)] The chains are coupled through the electron tunneling of the amplitude t_b. To calculate the Hall conductivity, suppose that a magnetic field H is applied along the z axis perpendicular to the (x, y) plane, and an electric field E_y is applied perpendicular to the chains. The electron Hamiltonian in the FISDW state is:[2)]

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + 2\Delta\cos(Q_x x) + 2t_b\cos[k_y b - G(x - v_{E_y}t)], \tag{2}$$

where m is the electron mass, Q_x and Δ are the wave vector and the amplitude of the FISDW potential, k_y is the electron wave vector across the chains, t is the time,

$$G = ebH/\hbar c \tag{3}$$

is the wave vector of the magnetic field,

$$v_{E_y} = cE_y/H \tag{4}$$

is the drift velocity in the crossed electric and magnetic fields, and c is the velocity of light. Hamiltonian (2) is written in the mixed representation, where an electron wave function depends on the coordinate x along the chains and the momentum k_y across the chains. For simplicity, we set the FISDW wave vector across the chains, Q_y, to zero, and neglect the next-nearest-neighbor hopping term $2t'_b\cos(2k_y b)$ in Hamiltonian (2). The electric and magnetic fields are intro-

[1)] The x and y axes correspond to the **a** and **b** axes of $(TMTSF)_2X$.

[2)] We pay no attention to the spin indices, because they are not important for our purposes.

duced in Hamiltonian (2) via the Peierls–Onsager substitution, $k_y \to k_y - eA_y/c\hbar$, in the gauge

$$A_x = A_z = 0, \quad A_y = Hx - E_y ct. \tag{5}$$

It follows from Eq. (2) that, in the presence of the magnetic field, the hopping *across* the chains becomes a periodic potential *along* the chains with the wave vector G (3) proportional to the magnetic field. We will refer to this periodic potential as the "hopping potential". Due to the presence of the electric field E_y, the hopping potential moves along the chains with the velocity v_{E_y} (4), whereas the FISDW potential is assumed to be pinned and does not move.

Let us linearize the longitudinal dispersion in Hamiltonian (2) near the Fermi energy and focus on the electrons whose momenta are close to the Fermi momenta $+k_{\rm F}$ and $-k_{\rm F}$. Let us count their momenta from $+k_{\rm F}$ and $-k_{\rm F}$ and denote their wave functions as u and w. In this representation, a complete electron wave function is a spinor (u, w), and the Hamiltonian is a 2×2 matrix, which can be expanded over the Pauli matrices $\hat\tau_1$, $\hat\tau_2$, $\hat\tau_3$, and the unity matrix $\hat 1$ (which we will not write explicitly in the following formulas). It is well known [1, 2, 3] that the FISDW wave vector depends on the magnetic field in the following manner:

$$Q_x = 2k_{\rm F} - NG = 2k_{\rm F} - NebH/\hbar c, \tag{6}$$

where N is an integer that characterizes the FISDW. Taking into account Eq. (6), Hamiltonian (2) can be rewritten in the spinor representation as

$$\hat{\mathcal{H}} = -i\hbar v_{\rm F}\hat\tau_3\frac{\partial}{\partial x} + \Delta\hat\tau_1 e^{i\hat\tau_3 NGx} + 2t_b\cos[k_y b - G(x - v_{E_y}t)], \tag{7}$$

where $v_{\rm F} = k_{\rm F}/m$ is the Fermi velocity. The last term in Eq. (7) can be eliminated by chiral transformation of the electron wave function:[3)]

$$\begin{pmatrix} u \\ w \end{pmatrix} \to \exp\left\{ i\hat\tau_3 \frac{2t_b}{\hbar\omega_c}\sin[k_y b - G(x - v_{E_y}t)]\right\}\begin{pmatrix} u \\ w \end{pmatrix}, \tag{8}$$

where

$$\hbar\omega_c = \hbar v_{\rm F} G = ebHv_{\rm F}/c \tag{9}$$

is the characteristic energy of the magnetic field (the cyclotron frequency). In representation (8), Hamiltonian (7) becomes

$$\hat{\mathcal{H}} = -i\hbar v_{\rm F}\hat\tau_3\frac{\partial}{\partial x} + \Delta\hat\tau_1\exp(i\hat\tau_3 NGx) \times \exp\left\{ i\hat\tau_3\frac{4t_b}{\hbar\omega_c}\sin[k_y b - G(x - v_{E_y}t)]\right\}. \tag{10}$$

Expanding the periodic function in the last term of Eq. (10) into the Fourier series, we get the following expression:

$$\hat{\mathcal{H}} = -i\hbar v_{\rm F}\hat\tau_3\frac{\partial}{\partial x} + \Delta\hat\tau_1 e^{i\hat\tau_3[N(k_y b + Gv_{E_y}t)]} \times \sum_n a_{n+N} e^{i\hat\tau_3 n[k_y b - G(x - v_{E_y}t)]}, \tag{11}$$

where the coefficients of the expansion, a_n, are the Bessel functions: $a_n = J_n(4t_b/\hbar\omega_c)$.[4)] The last term in Eq. (11) is the sum of many sinusoidal potentials whose wave vectors are the integer multiples of the magnetic wave vector G. Each of these periodic potentials mixes the $+k_{\rm F}$ and $-k_{\rm F}$ electrons and opens an energy gap at the electron wave vector k_x shifted from $\pm k_{\rm F}$ by an integer multiple of $G/2$. The distance in energy between the gaps is equal to $\hbar\omega_c$ (9).

The term with $n = 0$ in the sum in Eq. (11) does not depend on x and opens the gap right at the Fermi level.[5)] When the temperature T is much lower than the distance between the energy gaps $\hbar\omega_c$:

$$T \ll \hbar\omega_c, \tag{12}$$

only the gap at the Fermi level is important, whereas the other gaps may be neglected. Condition (12) is always satisfied in the relevant temperature range $0 \le T \le T_c$ (where T_c is the FISDW transition temperature) in the weak coupling theory of the FISDW, where $T_c \ll \hbar\omega_c$. Thus, let us omit all the terms in the sum in Eq. (11), except the term with $n = 0$:

$$\hat{\mathcal{H}} = -i\hbar v_{\rm F}\hat\tau_3\frac{\partial}{\partial x} + \Delta_{\rm eff}\hat\tau_1 e^{i\hat\tau_3[N(k_y b + Gv_{E_y}t)]}, \tag{13}$$

$$\Delta_{\rm eff} = a_N\Delta. \tag{14}$$

This is the so-called single-gap approximation [5]. It was shown explicitly in Ref. [6] that omission of the gaps located deeply below the Fermi energy does not change the value of the Hall conductivity, at least at zero temperature.

By the above sequence of manipulations, we have combined the two periodic potentials in Eq. (2) into the single effective potential (13) that opens a gap at the Fermi level. It follows from Eq. (13) that the phase φ of this effective potential changes in time:

$$\dot\varphi = -NGv_{E_y}, \tag{15}$$

which means that the effective potential moves along the chains. Since, at zero temperature, all electrons are confined under the energy gap opened by this potential, the motion of the potential induces the Fröhlich current [7] along the chains:

$$j_x = -\frac{e}{\pi b}\dot\varphi. \tag{16}$$

Substituting Eqs. (15), (3), and (4) into Eq. (16), we find the quantum Hall effect (QHE) in agreement with Eq. (1):

$$j_x = \frac{2Ne^2}{h}E_y. \tag{17}$$

[3)] This kind of transformation was first introduced in Ref. [4] that started development of the FISDW theory.

[4)] General expression (11) is valid even when the FISDW has a nonzero transverse wave vector and the transverse dispersion law of the electrons is more complicated, but the expression for the expansion coefficients a_n would be different in that case.

[5)] Since, by introducing the $\pm$ electrons, we have already subtracted the wave vectors $\pm k_{\rm F}$, the actual wave vector that corresponds to this term is $2k_{\rm F}$.

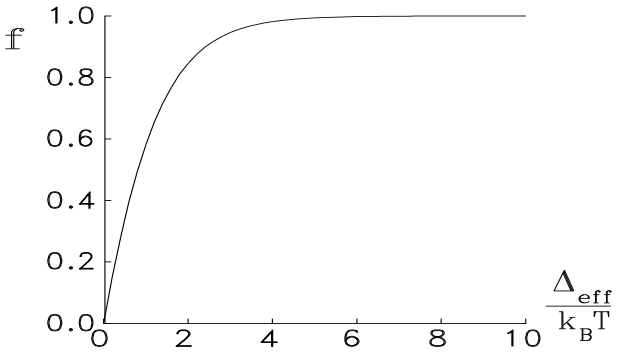

Figure 1: The reduction factor f of the Hall conductivity as a function of the ratio of the energy gap at the Fermi level $\Delta_{\rm eff}$ to the temperature T, as given by Eq. (20).

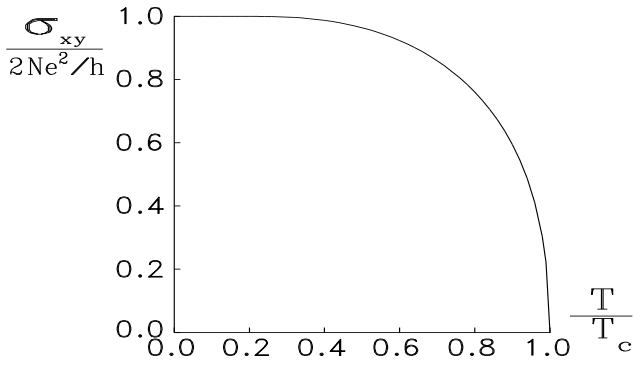

Figure 2: Hall conductivity in the FISDW state as a function of the temperature T normalized to the FISDW transition temperature T_c.

To avoid confusion, we wish to emphasize that here the FISDW is assumed to be immobile, unlike in Ref. [8] where the influence of the FISDW motion on the QHE was studied. The effective potential (13) moves, because it is a combination of the stationary FISDW potential and the moving hopping potential (2).

Eq. (16) is a good starting point to discuss the temperature dependence of the QHE. According to the above consideration, the Hall conductivity is the Fröhlich conductivity of the effective periodic potential (13). Thus, the temperature dependence of the QHE must be the same as the temperature dependence of the Fröhlich conductivity. The latter issue was studied in the theory of a regular charge/spin density wave (CDW/SDW) [9, 10]. At a finite temperature T, the electric current carried by the CDW/SDW condensate is reduced with respect to the zero-temperature value (16) by a factor $f(T)$. The same factor reduces the condensate Hall effect at a finite temperature:

$$\sigma_{xy}(T) = f(T)\, 2Ne^2/h, \tag{18}$$

$$f(T) = 1 - \int_{-\infty}^{\infty} \frac{dk_x}{\hbar v_{\rm F}} \left(\frac{\partial E}{\partial k_x}\right)^2 \left[-\frac{\partial n_{\rm F}(E/k_{\rm B}T)}{\partial E}\right], \tag{19}$$

where $E = \sqrt{(\hbar v_{\rm F} k_x)^2 + \Delta_{\rm eff}^2}$ is the electron dispersion law in the FISDW phase, $k_{\rm B}$ is the Boltzmann constant, and $n_{\rm F}(\epsilon) = (e^{\epsilon}+1)^{-1}$ is the Fermi distribution function. The last term in Eq. (19) reflects the fact that normal quasiparticles, thermally excited above the energy gap, equilibrate with the immobile crystal lattice; thus, only a fraction of all electrons is carried along the chains by the moving periodic potential, which reduces the Hall/Fröhlich current. Derivation of Eq. (19) is given in Appendix.

The function f (19) depends only on the ratio of the energy gap at the Fermi level, $\Delta_{\rm eff}$ (14), and the temperature T and can be written as [10, 11]

$$f\left(\frac{\Delta_{\rm eff}}{k_{\rm B}T}\right) = \int_0^{\infty} d\zeta\, \tanh\left(\frac{\Delta_{\rm eff}}{2k_{\rm B}T}\cosh\zeta\right) / \cosh^2\zeta. \tag{20}$$

The function $f(\Delta_{\rm eff}/k_{\rm B}T)$ is plotted in Fig. 1. It is equal to 1 at zero temperature, where Eq. (18) gives the QHE, gradually decreases with increasing T, and vanishes when $T \gg \Delta_{\rm eff}$. Taking into account that the FISDW order parameter Δ itself depends on T and vanishes at the FISDW transition temperature T_c, it is clear that $f(T)$ and $\sigma_{xy}(T)$ vanish at $T \to T_c$, where $\sigma_{xy}(T) \propto f(T) \propto \Delta(T) \propto \sqrt{T_c - T}$. Assuming that the temperature dependence $\Delta_{\rm eff}(T)$ is given by the BCS theory [5], we plot the temperature dependence of the Hall conductivity, $\sigma_{xy}(T)$, in Fig. 2.

The function $f(T)$ (19) is qualitatively similar to the function $f_{\rm s}(T)$ that describes the temperature reduction of the superconducting condensate density in the London case. Both functions approach 1 at zero temperature, but near T_c the superconducting function behaves differently: $f_{\rm s}(T) \propto \Delta^2(T) \propto T_c - T$. As explained in Appendix, this is due to the difference between the static and dynamic limits of the response function.

The QHE in the FISDW state at zero temperature was derived theoretically in Refs. [2, 6, 12]. An attempt to calculate the Hall conductivity in the FISDW state at a finite temperature was made in Ref. [11], but it failed to produce the QHE at zero temperature. Various aspects of the QHE in $(TMTSF)_2X$ were reviewed in Ref. [13]. Temperature dependence of the Hall resistance in $(TMTSF)_2X$ was measured in experiments [14]. However, to compare the experimental results with our theory, it is necessary to convert the Hall resistivity into the Hall conductivity, which requires experimental knowledge of all components of the resistivity tensor.

We conclude that, at zero temperature, a FISDW

system exhibits the QHE (1) with the same integer number N that characterizes the wave vector (6) of the FISDW. As the temperature increases, the Hall conductivity decreases, vanishing at the FISDW transition temperature T_c. The function $f(T)$ that describes the reduction of the Hall effect with the temperature is the same as the temperature reduction function of the Fröhlich current of a regular charge/spin-density wave.

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Appendix

We derived Eqs. (18) and (19) by calculating the single-loop Feynman diagram that represents the electromagnetic response of the electrons in the FISDW state to the electric field E_y. The expression for the diagram is sensitive to the ratio of the frequency ω and the wave vector q of the field E_y when both ω and q approach zero. Eqs. (19) and (20) correspond to the so-called dynamic limit where $q/\omega = 0$ [10]. This limit is appropriate in our case, because the electric field is, supposedly, strictly homogeneous in space ($q = 0$), but may be time-dependent ($\omega \neq 0$). The effective periodic potential (13) is also time-dependent. In the opposite, static limit $\omega/q = 0$, we obtain the function

$$f_{\rm s}(T) = 1 - \hbar v_{\rm F} \int_{-\infty}^{\infty} dk_x \left[-\frac{\partial n_{\rm F}(E/k_{\rm B}T)}{\partial E} \right], \qquad (21)$$

which describes the charge-density response to a static deformation of the CDW phase, $\partial\varphi/\partial x$, as well as the superconducting condensate density in London superconductors [9, 10]. In the latter cases, the CDW phase or magnetic field in the Meissner effect are stationary ($\omega = 0$), but vary in space ($q \neq 0$). Comparing Eqs. (19) and (21), one can see that $f(T)$ and $f_{\rm s}(T)$ are different. We obtain Eqs. (19) and (21) by summing over the internal frequency of the loop first. Different, but equivalent expressions for $f(T)$ and $f_{\rm s}(T)$ were obtained in Ref. [10] by integrating over the internal momentum of the loop first.

The diagrammatic derivation is not very transparent physically, so below we offer another derivation of Eq. (19), based on the ideas of Refs. [9, 15]. Let us consider a one-dimensional electron system subject to a CDW/SDW of the amplitude Δ_0, which moves with a small velocity $v_{\rm DW}$. Let us calculate the Fröhlich current proportional to $v_{\rm DW}$ at a finite temperature T. We find the electron wave functions in the reference frame moving with the density wave and then Galileo-transform them to the laboratory frame [15]:

$$\psi_k^{\pm}(x,t) = u_k^{\pm} e^{i(k_{\rm F}+k+mv_{\rm DW})x - i(k_{\rm F}+k)v_{\rm DW}t \mp iE_k t/\hbar} + w_k^{\pm} e^{i(-k_{\rm F}+k+mv_{\rm DW})x - i(-k_{\rm F}+k)v_{\rm DW}t \mp iE_k t/\hbar} \qquad (22)$$

where we denote $k = k_x$ and keep only the terms linear in $v_{\rm DW}$. In Eq. (22) and below, the index $\pm$ refers to the states above and below the CDW/SDW energy gap, *not* to the states near $\pm k_{\rm F}$. The coefficients of superposition, u_k and w_k, are given by the following expressions:

$$|u_k^+|^2 = |w_k^-|^2 = \frac{\Delta_0^2}{2E_k(E_k - \xi_k)}, \qquad (23)$$

$$|w_k^+|^2 = |u_k^-|^2 = \frac{E_k - \xi_k}{2E_k}, \qquad (24)$$

where $\xi_k = \hbar v_{\rm F} k$ and $E_k = \sqrt{\xi_k^2 + \Delta_0^2}$ are the electron dispersion laws in the absence and in the presence of the CDW/SDW gap.

By analogy with the standard derivation of the superfluid density [16], let us assume that, because of interaction with impurities, phonons, etc., the electron quasiparticles are in thermal equilibrium with the crystal in the laboratory reference frame, so their distribution function is the equilibrium Fermi function $n_{\rm F}$. However, it is not straightforward to apply the Fermi function, because the two components of the eigenfunction (22), which have the same energy in the reference frame of the moving CDW/SDW, have different energies in the laboratory frame. Let us make a reasonable assumption that a state (22) is populated according to its *average* energy $\bar{E}_k^{\pm}$:

$$\bar{E}_k^{\pm} = |u_k^{\pm}|^2(\pm E_k + \hbar(k_{\rm F}+k)v_{\rm DW}) + |w_k^{\pm}|^2(\pm E_k + \hbar(-k_{\rm F}+k)v_{\rm DW}). \qquad (25)$$

The electric current I carried by the electrons is equal to

$$I = 2e\hbar \sum_{\pm} \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, n_{\rm F}\left(\frac{\bar{E}_k^{\pm}}{k_{\rm B}T}\right) \times \left[|u_k^{\pm}|^2 \left(\frac{k_{\rm F}+k}{m} + \frac{v_{\rm DW}}{\hbar} \right) + |w_k^{\pm}|^2 \left(\frac{-k_{\rm F}+k}{m} + \frac{v_{\rm DW}}{\hbar} \right) \right], \qquad (26)$$

where the factor 2 comes from the spin. Substituting Eq. (25) into Eq. (26) and keeping the terms linear in $v_{\rm DW}$, we find two contributions to I. The first contribution, I_1, is obtained by replacing $\bar{E}_k^{\pm}$ by $\pm E_k$ in Eq. (26), that is, by omitting $v_{\rm DW}$ in Eq. (25). This term represents the current produced by all electrons moving with the velocity $v_{\rm DW}$:

$$I_1 = 2ev_{\rm DW}2k_{\rm F}/2\pi. \qquad (27)$$

The second contribution, I_2, comes from expansion of the Fermi function in Eq. (26) in $v_{\rm DW}$ and represents reduction of the current due to thermally excited quasiparticles staying behind the collective motion:

$$I_2 = 2emv_{\rm DW} \sum_{\pm} \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \frac{\partial n_{\rm F}(\pm E_k/k_{\rm B}T)}{\partial E_k} \times \left[v_{\rm F}(|u_k^{\pm}|^2 - |w_k^{\pm}|^2) + \frac{\hbar k}{m}(|u_k^{\pm}|^2 + |w_k^{\pm}|^2) \right]^2. \qquad (28)$$

The second term in the brackets in Eq. (28) is small compared to the first term and may be neglected. Substituting Eqs. (23) and (24) into Eq. (28) and expressing the CDW/SDW velocity in terms of the CDW/SDW phase derivative in time, $v_{\rm DW} = -\dot{\varphi}/2k_{\rm F}$, we find the temperature-dependent expression for the Fröhlich current:

$$I = I_1 + I_2 = -ef(T)\dot{\varphi}/\pi, \tag{29}$$

$$f(T) = 1 - \int_{-\infty}^{\infty} d\xi_k \left(\frac{\xi_k}{E_k}\right)^2 \left[-\frac{\partial n_{\rm F}(E_k/k_{\rm B}T)}{\partial E_k}\right]. \tag{30}$$

Eq. (30) is the same as Eq. (19). Dividing the current per one chain, I (29), by the interchain distance b, we get the density of current per unit length, j_x (16).

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