Sign reversal of the quantum Hall coefficient in the field-induced spin density wave states of quasi-one-dimensional system with periodic potential

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Abstract. The magnetic susceptibility of the quasi-one-dimensional system with the periodic potential such as slow cooled (TMTSF)\textsubscript{2}ClO\textsubscript{4} is studied numerically. The magnitude of the periodic potential is given by $V$. The imperfect nesting on the Fermi surface originates from higher harmonics ($t'_4$, $t_3$, $t_4$) of the tight-binding model. We have found that $q_x$ of \( Q = (2k_F + q_x, \pi/b + q_y) \) which gives a maximum of $\chi_0(Q)$ has a negative value at $t_4/t_b \geq 0.007$, $t_4/t_b \geq 0.0001$, and $V < 2t'_4 - 2t_4$, where $t'_4/t_b$ is fixed to be 0.1. It means that the negative quantum Hall coefficient is possible in these parameters. Since the sign reversal of the quantum Hall coefficient is observed in (TMTSF)\textsubscript{2}ClO\textsubscript{4}, $t_3$, $t_4$ and $V$ should satisfy the above conditions. We also discuss the periodic oscillation of Hall resistance with sign reversal which has been observed by Uji \textit{et al}.

1. Introduction

(TMTSF)\textsubscript{2}X ($X$=ClO\textsubscript{4} or PF\textsubscript{4}) has a two-piece sheet-like Fermi surface\textsuperscript{[1]}. By neglecting the very small transfer integrals between layers, the energy band becomes

$$\epsilon(k) = \hbar v_F(|k_x| - k_F) - 2t_b \cos(bk_y) - 2t'_4 \cos(2bk_y) - 2t_4 \cos(4bk_y) - 2t_4 \cos(4bk_y), \quad (1)$$

where the dispersion in $k_x$ is linearized, i.e., $v_F = 2t_a a \sin(ak_F)$, $t_a$ and $t_b$ are transfer integrals, and $t'_4$, $t_3$ and $t_4$ are the higher harmonic terms. We take $t_a$, $t_b$, $t'_4$, $t_3$ and $t_4$ as positive. The field-induced spin density wave (FISDW) transition \cite{1, 2, 3, 4, 5} has been observed when the magnetic field ($B$) is applied perpendicular to the conductive plane ($a$-$b$ plane). It has been known\textsuperscript{[6, 7, 8, 9, 10, 11]} that the FISDW is characterized by an integer $N$ of the SDW wave number $Q_x = 2k_F + NG$, where $k_F = \frac{\pi}{2b}$ is the Fermi wave number and $G = \frac{\hbar \omega}{eB}$. The quantized Hall effect in FISDW states and the sign change of the Hall voltage in some range of the magnetic field are found in (TMTSF)\textsubscript{2}X, $X$=ClO\textsubscript{4}\textsuperscript{[2, 12]} and PF\textsubscript{6}\textsuperscript{[13]}. Theoretically, it has been shown that the Hall conductivity is quantized as $\sigma_{xy} = 2Ne^2/h$ with the quantum number $N$ of the nesting vector\textsuperscript{[14, 15]} and the sign change of the Hall coefficient is explained\textsuperscript{[16, 17, 18]}.

When (TMTSF)\textsubscript{2}ClO\textsubscript{4} is cooled slowly, ClO\textsubscript{4} anion orders at $T_{AO} = 24K$. It makes the periodic potential along $b$-axis as $\mathcal{H}_V = V \cos(\frac{\pi}{4}y)$, where we take $V$ as positive. In this case,
the state $|k\rangle$ and $|k + Q_A\rangle$ are mixed, where $Q_A = (0, \pi/b)$. The Hamiltonian is written as[19]

$$\hat{H} = \left( \begin{array}{cc} \epsilon(k) & V \\ V & \epsilon(k + Q_A) \end{array} \right).$$

(2)

By the anion ordering, it is known that the $B$ and temperature phase diagram in $(\text{TMTSF})_2\text{PF}_6$[2] is different from that in $(\text{TMTSF})_2\text{ClO}_4\text{[3, 4, 5]}$. Some features of the difference have been explained theoretically[19, 20, 21, 22, 23, 24, 25, 26, 27, 28]. In slow cooled $(\text{TMTSF})_2\text{ClO}_4$, a negative phase ($N = -2$) appears in some region of the magnetic field and $0 < V/t'_b < 2$ by taking $t'_b/t_b = 0.1$, $t_3/t'_b = 0.02$, and $t_4/t'_b = 0.002$.

Recently, from the numerical study[29, 30] in the nesting vector ($Q$) and the magnetic susceptibility ($\chi_0(Q)$) in the quasi-one-dimensional system with the periodic potential, it is found that $\chi_0(Q)$ has the plateau-like maximum in sweptback region in the momentum space. It has been analytically[30] shown that the sweptback region is surrounded by $q_1$, $q_3$ and $q_4$ ($q_2$, $q_3$ and $q_1$), as seen in Figs. 1, 2 and 3, where $Q = (2k_F, \pi/b) + q_i$ ($i = 1, 2, 3, 4$) and

$$q_1 = \left( \frac{1}{\hbar v_F}(-4t'_b + 4t_4), 0 \right), \quad q_2 = \left( \frac{1}{\hbar v_F}(-4t'_b + 4t_4 + 2V), 0 \right), \quad q_3 = \left( \frac{1}{\hbar v_F}(4t'_b + 4t_4), 0 \right),$$

$$q_4 = \left( \frac{1}{\hbar v_F} \frac{24t'_b}{\sqrt{1 + 128(\frac{t'_b}{t_b})^2 + 1}}, \pm \frac{2}{b} \sin^{-1} \left( \frac{8(\frac{t'_b}{t_b})}{\sqrt{1 + 128(\frac{t'_b}{t_b})^2 + 1}} \right) \right).$$

\textbf{Figure 1.} The sweptback region is enclosed by $q_1$, $q_3$ and $q_4$, where we set $\hbar = b = 1$.

\textbf{Figure 2.} The same figure as Fig. 1 with $V/t'_b = 1$. The sweptback region is enclosed by $q_2$, $q_3$ and $q_4$.

\textbf{Figure 3.} The same figure as Fig. 1 with $V/t'_b = 2$.

In the parameters of $t_3/t_b = 10$, $t'_b/t_b = 0.1$, $t_3/t_b = 0.02$ and $t_4/t_b = 0.002$, we found that a maximum of $\chi_0(Q)$ appears at $q_2$ for $0 < V < 4t'_b - 4t_4$[30]. When $t_3$ and $t_4$ are neglected, a maximum is located near $q_4$. However, its maximum is suppressed due to $t_3$ and the degeneracy of peaks of $\chi_0(Q)$ at $q_2$ and at $q_3$ is released by $t_4$. For $V = 0$, Zanchi and Montambaux[17] have found that a maximum of $\chi_0(Q)$ appears at $q_1$ owing to $t_3$ and $t_4$. As the $x$-component of $q_2$ is negative when $V < 2t'_b - 2t_4$, we have concluded[30] that $V$ should be smaller than $2t'_b - 2t_4$ in $(\text{TMTSF})_2\text{ClO}_4$, because the sign reversal of the quantum Hall effect has been observed. If the conventionally used $t'_b/t_b = 0.1$ and $t_4/t_b = 0.001$ are supposed in $V < 2t'_b - 2t_4$, we obtain $V/t_b < 0.198$. It gives the limitation for the value of $V$. The experimentally estimated $V/t_b$ has a upper limit value as $V/t_b = 0.23$[31] or a little larger value as $V/t_b = 0.34$[32].

In this paper, we examine whether $q_4$ of $q$ which gives a maximum of $\chi_0(Q)$ is positive or negative in the wide parameter region such as $0 \leq t_3/t_b \leq 0.02$, $0 \leq t_4/t_b \leq 0.002$ and $0 \leq V/t'_b \leq 4$. For other band parameters, we set $t_{a}/t_b = 10$, $t'_b/t_b = 0.1$ and $k_B T/t_b = 0.001$. 
2. Susceptibility

We can diagonalize Eq. (2) by the unitary transformation,

$$U \hat{H} U^{-1} = \begin{pmatrix} e^+ & 0 \\ 0 & e^- \end{pmatrix},$$

$$U^{-1} = \begin{pmatrix} u^* & -u \\ v^* & u \end{pmatrix},$$

$$u = \frac{1}{\sqrt{2}} \left[ 1 + \frac{d}{\sqrt{d^2 + V^2}} \right], v = \left[ 1 - \frac{d}{\sqrt{d^2 + V^2}} \right],$$

$$d = \frac{1}{2} \left( \epsilon(k) - \epsilon(k + Q_A) \right).$$

By using Eq. (4), the eigenvectors ($|k^+\rangle$ and $|k^-\rangle$) are given by

$$\begin{pmatrix} |k^+\rangle \\ |k^-\rangle \end{pmatrix} = U \begin{pmatrix} |k\rangle \\ |k + Q_A\rangle \end{pmatrix}.$$  

The eigenvalues ($\epsilon^\pm$) are obtained as

$$\epsilon^\pm(k) = \frac{1}{2} \left[ (\epsilon(k) + \epsilon(k + Q_A)) \pm \sqrt{(\epsilon(k) - \epsilon(k + Q_A))^2 + 4V^2} \right].$$

The generalized susceptibility is given by

$$\chi_0(Q) = \frac{1}{\Omega} \sum_{k,k',\gamma,\gamma'} \left| \langle k'| e^{iQr} | k' \rangle \right|^2 \frac{f(\epsilon^\gamma(k')) - f(\epsilon^\gamma(k))}{\epsilon^\gamma(k) - \epsilon^\gamma(k')}.$$  

where $\Omega$ is the volume of the system. By using the unitary matrix, Eq. (8) becomes[19]

$$\chi_0(Q) = \frac{1}{\Omega} \sum_k \left[ (u_{k+Q}u_k + v_{k+Q}v_k)^2 \frac{f(\epsilon^+(k)) - f(\epsilon^+(k + Q))}{\epsilon^+(k + Q) - \epsilon^+(k)} + \frac{f(\epsilon^-(k)) - f(\epsilon^-(k + Q))}{\epsilon^-(k + Q) - \epsilon^-(k)} \right]$$

$$\left. + \left. (u_{k+Q}u_k + v_{k+Q}v_k)^2 \frac{f(\epsilon^-(k)) - f(\epsilon^+(k + Q))}{\epsilon^+(k + Q) - \epsilon^-(k)} + \frac{f(\epsilon^+(k)) - f(\epsilon^-(k + Q))}{\epsilon^-(k + Q) - \epsilon^+(k)} \right].$$

### Figures

**Figure 4.** Sign of $q_x$ which gives the maximum of $\chi_0(Q)$ in the plain of $V$ and $t_4$. Open circles (blue closed circles) mean positive (negative) $q_x$.

**Figure 5.** The same as Fig. 4 with $t_3/t_b = 0.02$. A red dotted line represents $V/t_b' = 2 - 2t_4/t_b'$.

**Figure 6.** Sign of $q_x$ in the parameter plain of $V$ and $t_3$ with $t_4/t_b = 0.0003$. 

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3. Results and Discussions

We investigate a maximum of $\chi_0(Q)$ by changing nesting vectors. When $t_3$ is zero, $q_x$ of $q$ which gives a maximum of $\chi_0(Q)$ is positive at $0 \leq t_4/t_b \leq 0.002$ and $0 \leq V/t_b \leq 4$, as seen in Fig. 4. When we set $t_3/t_b = 0.02$, the region where $q_x$ is negative appears at $t_4/t_b \geq 0.0001$, as seen in Fig. 5. When $t_4/t_b$ is fixed to be $0.0003$, $q_x$ is negative at $t_3/t_b \geq 0.007$, as seen in Fig. 6. These negative regions are limited in the region of $V < 2t_b^3 - 2t_4$.

4. Conclusion

Even in the case of $V \neq 0$, both of $t_3$ and $t_4$ are needed to the occurrence of the negative quantum Hall resistance. In particular, we consider that $t_3/t_b \geq 0.007, t_4/t_b \geq 0.0001$ and $V < 2t_b^3 - 2t_4$ are realized in (TMTSF)$_2$ClO$_4$.

Uji et al. [33] found the periodic oscillation with sign reversal of the Hall resistance at 26 T $< B < 45$ T. The value of $q_x$ of $q_2$ maximized $\chi_0(Q)$ is near zero when $V/t_b^3 \simeq 2$. Therefore, $q_2$ may be the origin of the sign reversal periodical Hall resistance in (TMTSF)$_2$ClO$_4$ with $V/t_b^3 \simeq 2$. The magnitude of $V$ is thought to be small when cooling rate is fast. The amplitude of the sign reversal oscillation of the Hall resistance may be changed by the cooling rate.

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