Field-induced spin density wave state of the quasi-one-dimensional organic conductors under the anion ordering

K Kishigi\(^1\), H Kaneyasu\(^2\) and Y Haseagwa\(^2\)

\(^1\) Faculty of Education, Kumamoto University, Kurokami 2-40-1, Kumamoto, 860-8555, Japan
\(^2\) Department of Material Science, Graduate School of Material Science, University of Hyogo, Hyogo, 678-1297, Japan

E-mail: kishigi@educ.kumamoto-u.ac.jp

Abstract. The periodical oscillation of the Hall resistance as a function of the magnetic field \(B\) has been observed in the field-induced spin density wave (FISDW) state of \((TMTSF)_{2}\)ClO\(_4\) in strong magnetic field [Uji \textit{et al}. Phys. Rev. Lett. \textbf{94}, 077206 (2005)]. The mechanism of this interesting phenomenon has not been explained. It is known that the periodic potential due to the ordering of the anion plays important role in the FISDW and the Hall conductivity. Although some properties such as the suppression of the FISDW state with even index are explained in the perturbative treatment of the periodic potential, the non-perturbative calculation is indispensable to this system because the periodic potential is thought to be not small. We calculate the susceptibility in the system to obtain the wave vector of the FISDW at strong fields. We also discuss the Hall resistance in the strong periodic potential case.

1. Introduction

\((TMTSF)_{2}\)ClO\(_4\), which is known as the quasi-one-dimensional organic conductor, has a pair of the open sheet-like Fermi surfaces[1]. The energy band of \((TMTSF)_{2}\)ClO\(_4\) is given by

\[\epsilon(k_x, k_y, k_z) = -2t_a \cos a k_x - 2t_b \cos b k_y - 2t_c \cos c k_z,\]

where \(t_a : t_b : t_c \simeq 1 : 0.1 : 0.03 \simeq 3000\) K: 300 K: 10 K and we neglect \(t_c\) in this paper. In this material, the field-induced spin density wave (FISDW) transition [1] is observed when the magnetic field \((B)\) is applied to the conductive plane \((a-b)\) plane), whose transition is caused by the quasi-one-dimensionality of the Fermi surface of \((TMTSF)_{2}\)ClO\(_4\). The FISDW transition is the successive phase transition characterized by changing \(N\) values of the SDW wave number \(Q_x = 2k_F + NG\), \(k_F = \pi/4a\) the Fermi wave number, \(N\); integer and \(G = eaB/\hbar c\). The low field region \((B < 10\) T\) is divided into the subphases which have different \(N\) values of \(Q_x\). In the high field \((B > 10\) T\), the SDW state is the \(N = 0\) phase with \(Q_x = 2k_F\) and \(Q_y = \pi/b\).

When \((TMTSF)_{2}\)ClO\(_4\) is cooled very slowly, the anion ordering occurs at \(T_{AO} = 24\) K having the ordering vector \(Q_{AO} = (0, \pi/b)\). In this case, the periodic potential by the anion ordering is written by \(H_V = V \cos(\frac{\pi}{b} y)\), where \(V\) is the strength of the periodic potential. The Fermi surface is reconstructed, and the energy band structure becomes

\[\epsilon^\pm(k_x, k_y) = -2t_a \cos a k_x \pm \sqrt{4t_b^2 \cos^2 b k_y + V^2}.\]
The successive transitions are observed even in this case but a new $B$-$T$ phase diagram[4, 5] is shown experimentally. The different points from the FISDW phase diagram[6] without the anion ordering are mainly:

(A) The high field region is occupied by new kinds of SDW subphases: SDW$_1$ ($20\, T < B < 28\, T$) and SDW$_2$ ($B > 28\, T$).

(B) There is a first-order transition line between the SDW$_1$ phase and the SDW$_2$ phase.

Lebed' and Bak[2] and Osada et al.[3] introduced perturbationally the effect of $V$ into the usual FISDW theory. Osada et al assume $V/t_b = 0.05$ from $2V/k_B \sim T_{\text{AO}}$ and show from the spin susceptibility ($\chi(Q)$) in the non-interacting state that the stable wave vector is $Q_{\text{SDW}}^+ = (2k_F^+, \pi/b)$ ($2k_F^+ = 2k_F \pm 2\Delta_0/hv_F$, $\Delta_0 = VJ_0(4t_b/v_F G)$, $v_F = 2t_a \sin(\pi/\hbar)$ and $J_0(x)$ is the Bessel function). However, the new points ((A) and (B)) cannot be explained by their perturbative theory[2, 3] for $V$, because $V$ is actually too large to justify the perturbative calculation. Recently, Yoshino et al.[7] estimate that $V/t_b$ is 0.3.

The new points have been almost explained by the non-perturbative calculation[8, 9, 10, 11, 12, 13, 14, 15, 16]. It has been shown that the FISDW state of $N = 0$ with $Q_{\text{SDW}} = (2k_F^+, \pi/b)$ is stabilized for higher field, which corresponds to SDW$_2$ state. On the contrary, for lower fields the FISDW state of $N = 0$ is realized, where $Q_{\text{SDW}}^+ = (2k_F + 2V/hv_F, \pi/2b)$ and $Q_{\text{SDW}}^- = (2k_F - 2V/hv_F, \pi/2b)$ coexist, which is considered as SDW$_1$ state.

Recently, Uji et al.[17] find the periodic oscillation with sign reversal of the Hall resistance for (TMTSF)$_2$ClO$_4$ under the anion ordering at high fields (from 26 T to 45 T) which is corresponding to the SDW$_2$ state. It has been shown that the peak of $\chi(Q)$ periodically oscillates with 260 T from both of the perturbative[3] and non-perturbative[10] calculations. Therefore, it seems to correspond to the oscillating Hall resistance by Uji et al.[17]. However, the sign reversal cannot be explained by the perturbative calculation[3], where the peak of $\chi(Q)$ at $q_x = 2k_F + 2\Delta_0/hv_F > 2k_F$ is the same as that at $q_x = 2k_F - 2\Delta_0/hv_F < 2k_F$. If both FISDW states with $q_x < 2k_F$ and $q_x > 2k_F$ are realized periodically as a function of $1/B$, the electron and hole bands appear alternatively, which becomes the origin of the sign reversal. Since in our previous non-perturbative calculation[10] we show the peak of $\chi(Q)$ only for $q_x \geq 2k_F$, we cannot examine the sign reversal of the Hall resistance. Therefore, in this study, we non-perturbatively calculate the peaks of $\chi(Q)$ for $q_x \leq 2k_F$ in addition to $q_x \geq 2k_F$ and show the stable FISDW state.

2. Calculation of Susceptibility

When the magnetic field is applied perpendicular to $x$-$y$ plane, we use the following linearized dispersion in the absence of the anion ordering:

$$\mathcal{H}_0 = hv_F (\mp i \partial_{k_x} - k_F) + t_\perp (-ib \partial_{k_y} + Gx),$$

$$t_\perp (k_y) = -2t_b \cos(bk_y) - 2t'_b \cos(2bk_y).$$

In this paper, we set $t_b/t_a = 0.1$ and $t'_b/t_a = 0.01$ as the band parameters of (TMTSF)$_2$ClO$_4$.

When the anion ordering exits, we introduce the periodic potential given by $\mathcal{H}_F$. The eigen value, which are obtained by the non-perturbative calculation[10], for the left ($l$) and right ($r$) Fermi surface and upper (+) and lower (−) energy bands becomes as followings:

$$E_{K_x+nG}^{l(r)(\pm)} = -hv_F (K_x + nG) \pm (-1)^n \Delta,$$

where $\Delta$ is the splitting of the energy band and $n$ is integer. The eigen state for the left ($l$) and right ($r$) Fermi surface and upper (+) and lower (−) energy bands is given by $|\Psi_n^{l(r)(\pm)}(K)\rangle$.

In the perturbative calculation, Osada et al.[3] show that $\Delta = \Delta_0 = VJ_0(\theta_0/B)$, where
$B_0 = 4t_b/(v_F be)$ is a unit of the magnetic field strength. When we set quarter-filled ($k_F = \pi/4a$), $t_b/t_a = 0.1$ and $a \approx b \approx 0.7$ nm, we get $B_0 \sim 400$ T.

We have shown that the susceptibility of $\mathcal{H}_0 + \mathcal{H}_V$ is given by[10]

$$\chi_0(q) = \frac{\sum_n \sum_{K} \sum_{\gamma = \pm} |\Psi_{n'}^{(\gamma)}(K + q - 2k_F)|^2}{\sum_n \sum_{K} \sum_{\gamma = \pm} |\Psi_{n}^{(\gamma)}(K)|^2} \times \left| f(E_{K_x+nG}^{(\gamma)} - f(E_{K_x+q_x-2k_F+n'G}^{(\gamma)}) \right| 

(5)

We find the maximum $\chi_0(q)$ for $q_x = 2k_F \pm 2\Delta/hv_F$ and $q_x = 2k_F + NG$ ($N = 1$) at $k_B T/t_a = 0.0001$ by changing $q_y$ from the perturbative and non-perturbative calculations.

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{perturbative_calculation}
\caption{For the perturbative calculation, the maximum of $\chi_0(q)$, where labeled $0\pm$ and 1 mean $q_x = 2k_F \pm 2\Delta/hv_F$ and $q_x = 2k_F + G$, respectively.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{non-perturbative_calculation}
\caption{The maximum of $\chi_0(q)$ for the non-perturbative calculation.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{perturbative_calculation_2}
\caption{The maximum of $\chi_0(q)$ for the perturbative calculation.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{non-perturbative_calculation_2}
\caption{The maximum of $\chi_0(q)$ for the non-perturbative calculation}
\end{figure}

3. Results and Discussions

When $V$ is small ($V/t_b = 0.05$), it can be seen from the perturbative calculation (Fig. 1) that the peak of $\chi(Q)$ at $q_x = 2k_F + 2\Delta/hv_F$ is the same as that at $q_x = 2k_F - 2\Delta/hv_F$. We can see almost the same situation for the non-perturbative calculation (Fig. 2).
In the case of $V/t_b = 0.2$, the peak of $\chi(Q)$ at $q_x = 2k_F + 2\Delta/\hbar v_F$ is the same as that at $q_x = 2k_F - 2\Delta/\hbar v_F$ for perturbative calculation (Fig. 3). However, these peaks become biggest alternatively at higher field ($B_0/B < 15$) for non-perturbative calculation (Fig. 4). We find that the optimized wave vector along $k_x$-axis at higher field ($B_0/B < 15$) is always $q_x = 2k_F + |2\Delta/\hbar v_F|$ by checking the sign of $\Delta$ as a function of $1/B$. Thus, the system at the high field is stabilized by the FISDW state with the nesting vector larger than $2k_F$.

4. Conclusion
We find the new FISDW states at strong magnetic field. However, we could not explain the sign reversal and oscillation of the Hall resistance at strong magnetic field, which has been observed recently in (TMTSF)$_2$ClO$_4$. The other mechanisms such as 3rd and 4th nearest transfer integrals may be taken into account in order to explain the experiments.

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