Generalized susceptibility of quasi-one dimensional system with periodic potential: model for the organic superconductor (TMTSF)$_2$ClO$_4$

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The nesting vector and the magnetic susceptibility of the quasi-one-dimensional system having imperfectly nested Fermi surface are studied analytically and numerically. The magnetic susceptibility has the plateau-like maximum in “sweptback” region in the momentum space, which is surrounded by $Q = (2k_F, \pi) + q_i$ ($k_F$ is the Fermi wave number, $i = 1, 3, 4$, and $q_1$, $q_3$ and $q_4$ are given in this paper). The best nesting vector, at which the susceptibility $\chi_0(Q)$ has the absolute maximum at $T = 0$, is obtained near but not at the inflection point, $Q = (2k_F, \pi) + q_4$. The effect of the periodic potential $V$ on the susceptibility is studied, which is important for the successive transitions of the field-induced spin density wave in (TMTSF)$_2$ClO$_4$. We obtain that the sweptback region (surrounded by $q_2$, $q_3$ and $q_4$ when $V > 0$) becomes small as $V$ increases and it shrinks to $q_3$ for $V \geq 4t'_4$, where $t'_4$ gives the degree of imperfect nesting of the Fermi surface, i.e. the second harmonics of the warping in the Fermi surface. The occurrence of the sign reversal of the Hall coefficient in the field-induced spin density wave states is discussed to be possible only when $V < 2t'_4 - 4t_4$, where $t_4$ is the amplitude of the fourth harmonics of the warping in the Fermi surface. This gives the novel limitation for the magnitude of $V$.

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I. INTRODUCTION

Various interesting properties, such as field-induced spin density wave (FISDW), quantum Hall effect and superconductivity, have been observed in the quasi-one-dimensional organic conductors, (TMTSF)$_2$X, where X is PF$_6$, ClO$_4$ etc.. The successive transitions between different FISDW phases occur as the magnetic field is increased. The FISDW has been understood as a consequence of the reduction of the dimensionality due to the magnetic field and the quantization of the nesting vector$^{2,3,4,5,6,7,8,9,10,11}$. The FISDW phases are characterized by the integer $N$, by which the wave number of FISDW is given as $Q_x = 2k_F + NG$, where $k_F$ is the Fermi wave number, $G = beB/h$, $b$ is the lattice constant (we take $b = 1$ in this paper), $e$ is the electron charge, $B$ is the magnetic field and $h = h/2\pi$ ($h$ is the Planck constant). We take $h = 1$ hereafter in this paper. The Hall conductivity is quantized as $\sigma_{xy} = 2Ne^2/h$ with the quantum number $N$ of the nesting vector$^{12,13,14}$. The quantization of the $x$ component of the nesting vector, $Q_x$, can be seen as the sharp peaks in the susceptibility for the non-interacting system, $\chi_0(Q)$, at $Q_x = 2k_F + NG$ in the magnetic field.

The peaks of $\chi_0(Q)$ in the magnetic field can be understood to some extent by the peaks of $\chi_0(Q)$ in the absence of the magnetic field. If the nesting of the Fermi surface is perfect, $\chi_0(Q)$ in the absence of the magnetic field diverges at the nesting vector as temperature becomes zero. In that case the successive transitions of FISDW does not happen. If the nesting of the Fermi surface is not perfect, the best nesting vector at $B = 0$, which gives the maximum of $\chi_0(Q)$, is located in the
anisotropic transfer integral elements
study the tight binding model in the square lattice with
and we have to consider the multiple-
the lattice constant to be 1. In the real system the
k susceptibility are studied in detail numerically.

V of
estimated the value as
analytically for the first time in the simple model with
and the nearly flat region in the reciprocal space are given
perfectly nested F ISDW state

V is first estimated to be the order of
T_{AO} = 24 K, i.e. \( V \ll t_b \).\(^{24,25}\) The suppression of the
N = 0 FISDW state\(^{24}\) and even-N FISDW state\(^{25}\) has been shown by the perturbation in \( V \). On the other hand, the magnitude of \( V \) has been estimated to be \( V = 0.83 t_b \) from the angle dependence of the magnetoresistance by Yosshino et al.\(^{26}\). By treating \( V \) not in perturbation, a lot of interesting features, such as existence of several nesting vectors\(^{27,28,29,30}\) and the phase diagram of the FISDW state\(^{31,32}\), has been obtained. Recently, Yoshino et al.\(^{33}\) has estimated the value to be \( V = 0.028 t_a \) (\( V = 0.34 t_b \) with their estimation \( t_a = 12 t_b \)). Lebed et al.\(^{34,35}\) have estimated the value as \( V = 0.2 t_b \). The novel estimation of \( V \) is given in this paper from the existence of the sign reversal of the Hall effect.

In this paper we study the nesting vector and the sus-ceptibility in the quasi-one dimensional system with im-
perfectly nested Fermi surface in the absence of the mag-
netic field. The analytic expression of the susceptibility and the nearly flat region in the reciprocal space are given analytically for the first time in the simple model with
\( V = 0 \). The effect of \( V \) on the nesting vector and the susceptibility are studied in detail numerically.

II. MODEL

We neglect the small dispersion in \( k_z \) direction and study the tight binding model in the square lattice with anisotropic transfer integral elements \( t_a \gg t_b \). We take the lattice constant to be 1. In the real system the crystal is triclinic and we have to consider the multiple-transverse-transfer integrals\(^{36}\) but most of the essential features are obtained by studying the simple model in the square lattice\(^{1}\). The energy dispersion can be linearized with respect to \( k_z \) and we take account of the higher harmonic terms for \( k_y \) as

\[
\epsilon(k) = v_F(\{k_x - k_F\} + t_\perp(k_y)),
\]

where

\[
t_\perp(k_y) = -2 t_b \cos k_y - 2 t'_b \cos(2k_y) + 2 \cos(3k_y) - 4 \cos(4k_y),
\]

and we study the case \( t_b, t'_b, t_3, t_4 \) to be positive. The terms proportional to \( t_3 \) and \( t_4 \) are thought to be essential\(^{15,32}\) to understand the negative \( N \) phase\(^{33,38}\) of FISDW in some region of the magnetic field. The Fermi surface consists of two “Fermi lines” near \( k_z = \pm k_F \), as shown in Fig. 1. The Fermi surface is almost nested, i.e. when we translate the left part of the Fermi line with the vector \( Q \approx Q_0 \), it overlaps with the right part of the Fermi line, but the overlap is not perfect due to the \( t'_b \) and \( t_4 \) terms.

The Brillouin zone is divided into halves in the \( k_y \) direction by the periodic potential. The Hamiltonian is written as a 2 \( \times \) 2 matrix with the anion potential \( V \) as

[\begin{pmatrix} \epsilon(k) & V \\ V & \epsilon(k + Q_A) \end{pmatrix}],

where \( Q_A = (0, \pi) \). The energy \( E(k) \) is given by

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

and the Fermi surface consists of four lines as shown in Fig. 2.

It is known\(^{25}\) that the susceptibility \( \chi_0(Q) \) has max-
imum near \( Q \approx Q_0 \) if \( V \lesssim 1.5 t_b \) when \( t'_b = 0.1 t_b \) (i.e. \( V \lesssim 15 t'_b \)), while the absolute maximum of \( \chi_0(Q) \) is located near \( Q \approx (2k_F \pm 2V/v_F, \pi/2) \) if \( V \gtrsim 1.5 t_b \). The peak of \( \chi_0(Q) \) near \( Q \approx Q_0 \) is caused by the nesting between the outer Fermi surface and the inner Fermi surface \( (k_x^{(R+)} \) and \( k_x^{(L-)} \), i.e., the red and blue arrows in Fig. 2, while the peaks of \( \chi_0(Q) \) near \( Q \approx (2k_F \pm 2V/v_F, \pi/2) \) are caused by the nesting the outer Fermi surfaces \( (k_x^{(R+)} \) and \( k_x^{(L+)} \) or the inner Fermi surfaces \( (k_x^{(R-)} \) and \( k_x^{(L-)} \).\(^{31,39,40}\) The maximum value of \( \chi_0(Q) \) near \( Q \approx Q_0 \) depends weakly on \( v_F \) if \( V \lesssim 0.4 t_b \), and it decreases as \( V \) increases if \( V \gtrsim 0.4 t_b \). Sengupta and Dupuis\(^{37}\) and Zanchi and Bjelis\(^{26}\) obtained the sim-
ilar results.

In this paper we examine in detail the nesting properties of the quasi-one dimensional systems without and with the periodic potential \( V \lesssim 0.5 t_b \). Thus we focus on the nesting condition for only \( Q \approx Q_0 \).

III. NESTING OF THE FERMI SURFACE FOR

\( V = 0 \)

In this section we study the nesting properties of the quasi-one dimensional system described by Eq. (3). The
We translate the left part of the Fermi surface with the nesting vector, \( Q = Q_0 + q \). The translated curve is given by

\[
k_x^{(L)(+)}(k_y) = k_F - \frac{1}{v_F} t_\perp(k_y),
\]

\[
k_x^{(L)(-)}(k_y) = -k_F + \frac{1}{v_F} t_\perp(k_y).
\]

We translate the left part of the Fermi surface with the nesting vector, \( Q = Q_0 + q \). The translated curve is given by

\[
k_x^{(L)(+)}(k_y) = k_F + q_x + \frac{1}{v_F} t_\perp(k_y + q_y + \pi),
\]

\[
k_x^{(L)(-)}(k_y) = -k_F + \frac{1}{v_F} t_\perp(k_y + q_y + \pi).
\]

The difference of the right part of the Fermi surface and the translated left part of the Fermi surface is given by

\[
k_x^{(L)(+)}(k_y) - k_x^{(L)(-)}(k_y) = q_x + \frac{1}{v_F} (t_\perp(k_y) + t_\perp(k_y + q_y + \pi)).
\]

If \( t_b' = t_4 = 0 \), the nesting of the Fermi surface is perfect with \( q_x = q_y = 0 \), i.e. \( k_x^{(L)(+)}(k_y) - k_x^{(L)(-)}(k_y) = 0 \) for all values of \( k_y \). If \( t_b' \neq 0 \) or \( t_4 \neq 0 \), the nesting of the Fermi surface is not perfect. In this case the Fermi surface intersect with the translated one with the nesting vector \( Q_0 + q \), if \( q_x \) and \( q_y \) satisfy

\[
q_x = -\frac{1}{v_F} [t_\perp(k_y) + t_\perp(k_y + q_y + \pi)]
\]

\[
= \frac{4}{v_F} \left[ t_b \sin(K_y) \sin\left(\frac{q_y}{2}\right) + t_{b'} \cos(2K_y) \cos(q_y) + t_3 \sin(3K_y) \sin\left(\frac{3q_y}{2}\right) + t_4 \cos(4K_y) \cos(2q_y) \right],
\]
for some value of $K_y$,

$$K_y = k_y + \frac{q_y}{2}.$$  \(12\)

Eq. 11 is the condition for the nesting vector ($Q = Q_0 + q$) to realize the intersection of the translated left part of the Fermi surface with the right part of the Fermi surface at $k_y$. In Fig. 3 we plot $q_x$ vs $K_y$ for $q_y = 0$. We define two vectors, $q_1$ and $q_3$, as $q_{1y} = q_{3y} = 0$ and $q_{1x}$ and $q_{3x}$ being the minimum and the maximum of $q_x$, as a function of $K_y$ at $q_y = 0$, respectively. When $t_4 \leq t'_b/4$ (in this paper we study only in this case), the maximum of $q_x$ as a function of $K_y$ for $q_y = 0$ is given at $K_y = 0$ and $\pi$, and the minimum of $q_x$ as a function of $K_y$ for $q_y = 0$ is given at $K_y = \pi/2$, as shown in Fig. 3.

$$q_1 = \left( \frac{4}{v_F} (-t_b + t_4), 0 \right),$$

$$q_3 = \left( \frac{4}{v_F} (t'_b + t_4), 0 \right).$$  \(13, 14\)

We define $q_2 = q_1$ for $V = 0$ and we will define $q_2$ for $V \neq 0$ in section IV.

We plot $q_x$ vs. $K_y$ (Eq. 11) for some values of $q_y$ in Fig. 4. As seen in Fig. 4, $q_x$ as a function of $K_y$ has two minimums at $K_y = \pm \pi/2 (q_x^{\text{min}(\pm)}(q_y))$ and one maximum at $0 \leq K_y \leq \pi/2 (q_x^{\text{max}}(q_y))$, if $0 < |q_y| < q_{4y}$ ($q_i$ will be given later). There are one minimum at $K_y = -\pi/2$ and one maximum at $K_y = \pi/2$ if $|q_y| > q_{4y}$. We obtain $q_x^{\text{min}(+)}(q_y)$ and $q_x^{\text{max}(+)}(q_y)$ as

\[
q_x^{\text{min}(+)}(q_y) = \frac{4}{v_F} \left( -t_b \cos q_y + t_b \sin \frac{|q_y|}{2} \right.
- \left. t_3 \sin \frac{3|q_y|}{2} + t_4 \cos 2q_y \right),
\]

\[
q_x^{\text{max}(+)}(q_y) = \frac{4}{v_F} \left( -t_b \cos q_y - t_b \sin \frac{|q_y|}{2} \right.
+ \left. t_3 \sin \frac{3|q_y|}{2} + t_4 \cos 2q_y \right).
\]

If $t_3$ and $t_4$ are finite, we have to solve the fourth-degree equation to obtain the expression of $q_x^{\text{max}}(q_y)$, but it is easy to obtain $q_x^{\text{min}}(q_y)$ numerically. We define $q_1 = (q_{1x}, q_{4y})$ by the equation

$$q_x^{\text{min}(+)}(q_y) = q_x^{\text{max}(+)}(q_y) = q_{4x}.$$  \(17\)

If $t_3 = t_4 = 0$, the simple expressions of $q_x^{\text{min}(+)}(q_y)$ and $q_4$ are obtained as

$$q_x^{\text{max}}(q_y) = \frac{4}{v_F} (t'_b \cos q_y + \frac{t_b^2 \sin^2 q_y}{8 t_b^2 \cos q_y}),$$

$$q_{4x} = \frac{1}{v_F} \frac{24 t'_b}{\sqrt{1 + 128 \left( \frac{t'_b}{t_b} \right)^2} + 1}.\]  \(18, 19\)

We define $q_2 = q_1$ for $V = 0$ and we will define $q_2$ for $V \neq 0$ in section IV.

We plot $q_x$ vs. $K_y$ (Eq. 11) for some values of $q_y$ in Fig. 4. As seen in Fig. 4, $q_x$ as a function of $K_y$ has two minimums at $K_y = \pm \pi/2 (q_x^{\text{min}(\pm)}(q_y))$ and one maximum at $0 \leq K_y \leq \pi/2 (q_x^{\text{max}}(q_y))$, if $0 < |q_y| < q_{4y}$ ($q_i$ will be given later). There are one minimum at $K_y = -\pi/2$ and one maximum at $K_y = \pi/2$ if $|q_y| > q_{4y}$. We obtain $q_x^{\text{min}(+)}(q_y)$ and $q_x^{\text{max}(+)}(q_y)$ as

\[
q_x^{\text{min}(+)}(q_y) = \frac{4}{v_F} \left( -t_b \cos q_y + \frac{t_b^2 \sin^2 q_y}{8 t_b^2 \cos q_y} \right) \right),
\]

\[
q_x^{\text{max}(+)}(q_y) = \frac{4}{v_F} \left( -t_b \cos q_y - \frac{t_b^2 \sin^2 q_y}{8 t_b^2 \cos q_y} \right) \right).
\]

and

$$q_{4y} = \pm 2 \sin^{-1} \left[ \frac{8 t'_b}{\sqrt{1 + 128 \left( \frac{t'_b}{t_b} \right)^2} + 1} \right].$$  \(20\)

Note that $q_x^{\text{max}}(q_y)$ has the physical meaning only if $|q_y| < q_{4y}$, since the analytical form Eq. 15 obtained in the case of $t_3 = t_4 = 0$ and the numerically obtained values at $|q_y| > q_{4y}$ corresponds to the local maximum of $q_x$ as a function of $\sin(K_y/2)$ at $|\sin(K_y/2)| > 1$. We plot $q_x^{\text{max}}(q_y)$, $q_x^{\text{min}(+)}(q_y)$ and $q_i$ ($i = 1, 3, 4$) in Fig. 5. There are large overlap between the Fermi line and the translated one, if $q$ is in the “sweepback” region with the apexes $q_1$ and $q_4$ enclosed by the thick lines in Fig. 5.

IV. SUSCEPTIBILITY IN THE Q1D SYSTEM WITH $V = 0$

The susceptibility

$$\chi_0(Q) = \sum_k f(E_{k+Q}) - f(E_k),$$

where $f(E_k)$ is the Fermi distribution function, is calculated at $T = 0$ as

$$\chi_0(Q) = \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \int_{k_y^{(L)}(k)}^{k_y^{(R)}(k)} \frac{2}{2\pi} \frac{dk_x}{\epsilon(k - Q) - \epsilon(k)}$$

$$= \frac{1}{\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left[ \int_{k_y^{(L)}(k)}^{k_y^{(R)}(k)} \frac{dk_x}{v_F Q_x + t_1(k_y - Q_y) - t_\perp(k_y)} \right.$$  \(21\)

$$+ \left. \int_{k_y^{(L)}(k)}^{k_y^{(R)}(k)} \frac{dk_x}{v_F Q_x - t_1(k_y - Q_y) - t_\perp(k_y)} \right]$$

$$= \frac{1}{\pi v_F} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left[ \frac{v_F Q_x + t_1(k_y - Q_y) + t_\perp(k_y)}{v_F Q_x + t_\perp(k_y - Q_y) - t_\perp(k_y)} \right.$$  \(22\)

$$- \left. \frac{1}{2} \log \left| \frac{v_F Q_x + t_\perp(k_y - Q_y) + t_\perp(k_y)}{v_F Q_x + t_\perp(k_y - Q_y) - t_\perp(k_y)} \right| \right]$$

The susceptibility is finite at $T = 0$ and has the singularity (kinks) as a function of $Q$. The singularity of $\chi_0(Q)$ comes from the integration of the logarithmic term in Eq. 22. For $Q_y = \pi$ (i.e. $q_y = 0$) and $t_3 = t_4 = 0$, the singular part of $\chi_0(Q + Q)$ is calculated as

$$\chi_{0, \text{sing}} = \frac{1}{\pi v_F} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left( \frac{1}{2} \right) \log \left| \frac{v_F Q_x - 4t_b' \cos 2k_y}{2k_F v_F} \right|$$

$$= \left\{ \begin{array}{ll}
- \frac{1}{2 \pi v_F} \log \left| q_{xF} + \sqrt{q_{xF}^2 - 4k_F^2\left( 4t_b' \right)^2} \right| & \text{if } |q_{xF}| > 4t_b' \\
- \frac{1}{2 \pi v_F} \log \left| t'_b \right| & \text{if } |q_{xF}| < 4t_b'
\end{array} \right.$$  \(23\)

\[\]
It is obtained from Eq. (23), that $\chi(Q)$ has a plateau as a function of $q_x$ when $t_3 = t_4 = 0$ and $q_y = 0$. If $t_3 + t_4$ and $q_y$ are not zero, we have to integrate Eq. (22) numerically. In Fig. 6 we plot $\chi_0(Q)$ for several $t_3$ and $t_4$ and $q_y$ as a function of $q_x$. It can be seen that if $t_3 = t_4 = 0$, nearly flat peak at $q_x^{\min}(q_y) < q_x < q_x^{\max}(q_y)$ first increases as $q_y$ increases, and have the absolute maximum before $q_y$ reaches $q_y = 0.2065\pi$ and $v_F q_x/t_b = 0.956$ when $t'_b/t_b = 0.1$ as shown in the top figure in Fig. 6. If $t_3 > 0$, the peaks for $q_y \neq 0$ are suppressed as shown in the middle figure in Fig. 6. If $t_4 > 0$, the degeneracy of $\chi_0(Q_0 + Q)$ at $q_1$ and $q_3$ is lifted and the absolute maximum of $\chi_0(Q_0 + q)$ is obtained at $q_1$ for the sufficiently large values of $t_3$ and $t_4$, as seen in the bottom figure in Fig. 6.

As seen in Fig. 6, $\chi_0(Q_0 + q)$ has plateau-like maximum in the region $q_x^{\min}(q_y) < q_x < q_x^{\max}(q_y)$. The absolute maximum of $\chi_0(Q_0 + q)$ occurs at $q$ close to $q_4$ but not at $q = q_4$, as seen in Figs. 7 and 8 where we plot $\chi_0(Q_0 + q)$ as a function of $q_x$ or $q_y$ on the curves of $q_x = q_x^{\min}(q_y)$ and $q_x = q_x^{\max}(q_y)$, respectively. The three-dimensional plot of $\chi_0(Q_0 + q)$ is shown in Fig. 9. When $t_3 = t_4 = 0$ and $q_y = q_4 y$, eq. (11) becomes

$$q_x = \frac{1}{k_F} \frac{4t'_b}{\pi} \left( \frac{4}{1 + 128} \left( \frac{q_y}{t_b} \right)^2 + 1 \right) \left(6 - 16 \sin^4(K_y - \frac{\pi}{2})\right).$$

Therefore, $q_x$ as a function of $K_y$ has a maximum at $K_y = \pi/2$ as $q_x \propto 6 - 16(K_y - \pi/2)^4$ when $q_y = q_4 y$. With the vector $Q = Q_0 + q_4$ the nesting of the Fermi surface is better than other $Q$s, which will make the expectation of the large $\chi_0(Q_0 + q)$. However, the region of $q_y$ where $\chi_0(Q_0 + q)$ is mainly contributed, is larger at $q_x \approx q_x^{\min}$ and $|q_y| \approx q_y$ than at $q = q_1$. This is the reason why the absolute maximum of $\chi_0(Q_0 + q)$ is not located at the inflection point (Fig. 9).

V. NESTING OF THE FERMI SURFACE FOR $V \neq 0$

In this section we study the effects of periodic potential $V$ on the nesting of the Fermi surface and the susceptibility. When $V \neq 0$, there are two pairs of the Fermi lines in $k_x - k_y$ plane (see Fig. 2), which are given by $k_x$ as a function of $k_y$, i.e., $k_x^{L\pm}(k_y)$ and $k_x^{R\pm}(k_y)$ for the left and the right parts of the Fermi lines, respectively. The nesting vectors are characterized by four types according to the pairs of the left and right parts of the Fermi lines, i.e. $(+, -)$, $(-, +)$, $(+, +)$, and $(-, -)$ as shown in Fig. 2. The left and right parts of the Fermi lines are given by

$$k_x^{L\pm}(k_y) = -k_F - \frac{1}{v_F} \left( -t_\perp(k_y) - t_\perp(k_y + \pi) \pm \sqrt{[t_\perp(k_y) - t_\perp(k_y + \pi)]^2 + 4V^2} \right),$$

and

$$k_x^{L\pm}(k_y) = k_F + \frac{1}{v_F} \left( -t_\perp(k_y) - t_\perp(k_y + \pi) \pm \sqrt{[t_\perp(k_y) - t_\perp(k_y + \pi)]^2 + 4V^2} \right).$$

The condition for the Fermi surface intersect by the translation of the left part (Eq. (11) for $V = 0$) is written

FIG. 6: $\chi_0(Q)$ at $T = 0$ (eq. 23) as a function of $q_x$. We take $t'_b/t_b = 0$ and $t_3 = t_4 = 0$ (the upper figure), $t_3/t_b = 0.02$, $t_4 = 0$ (middle figure), and $t_3/t_b = 0.02$, $t_4/t_b = 0.002$ (lower figure). As obtained by Zanchi and Montambaux 18, $t_4$ reduces the peak height near $q_4$ and $t_3$ lifts the degeneracy at $q_1$ and $q_1$.
as the four equations $(++,+-,-+,$ and $-)$,  
\[
q_x^{(\pm)}(\pm)=\frac{-1}{2V_F}\frac{1}{2V_F}\left[-t_\perp(k_y) - t_\perp(k_y + \pi)\right] \\
- t_\perp(k_y + q_y) - t_\perp(k_y + g_y + \pi) \\
\pm \sqrt{(t_\perp(k_y) - t_\perp(k_y + \pi))^2 + 4V^2} \\
\pm \sqrt{(t_\perp(k_y + q_y) - t_\perp(k_y + q_y + g_y + \pi))^2 + 4V^2}. \\
\]

When $q_y = 0$, we obtain Eq. (27) for $(+,-)$ and $(-,+)$ to be the same as that for $V = 0$ (Eq. (11)),  
\[
q_x^{(+-)} = q_x^{(-+)} = \frac{1}{v_F}[-t_\perp(k_y) - t_\perp(k_y + \pi)]. \\
\]

The condition for the intersect of $(+,+)$ is obtained as  
\[
q_x^{(++)} = \frac{1}{v_F}[-t_\perp(k_y) - t_\perp(k_y + \pi)] \\
+ \frac{1}{v_F} \sqrt{(t_\perp(k_y) - t_\perp(k_y + \pi))^2 + 4V^2}, \\
\]

and the condition for the intersect of $(--)$ is obtained as  
\[
q_x^{(--)} = \frac{1}{v_F}[-t_\perp(k_y) - t_\perp(k_y + \pi)] \\
- \frac{1}{v_F} \sqrt{(t_\perp(k_y) - t_\perp(k_y + \pi))^2 + 4V^2}. \\
\]

We define $q_{0x}$, $q_{1x}$, $q_{2x}$, and $q_{3x}$ as the maximum of $q_x^{(--)}$ (at $K_y = \pm \pi/2$), the minimum of $q_x^{(+-)}$ (at
We define $q_x$ as a function of $K_y$ for $q_y/\pi = 0.1$, $0.3$, and $q_y/\pi = 0.5$. In Figs. 10, 11, 12 and 13 we plot $q_x^{(+)}(q_y)$, $q_x^{max}(q_y)$, and $q_x^{min(+)}(q_y)$ for each $q_y$ in the plane of $q_x$ and $q_y$ for $V/t_b = 0.1, 0.3, 0.4$ and 0.5. As $V$ becomes zero, $q_x^{min(+)}(q_y)$, $q_x^{max}(q_y)$, and $q_x^{min(+)}(q_y)$ approach $q_x^{max}(q_y)$, $q_x^{max}(q_y)$ and $q_x^{min(-)}(q_y)$ at $V = 0$, respectively (cf. Fig. 10). On the other hand $q_x^{min(+)}(q_y)$ has no partner at $V = 0$, since the filled squares in Figs. 10, 11, 12, and 13 become not the minimum but just the crossing points due to the folding in $K_y$ as $V$ becomes zero. We define $q_x$ as the crossing points of $q_x^{min(+)}(q_y)$ and $q_x^{max}(q_y)$, which is the extension of that in $V = 0$.

We plot $\chi_0(\mathbf{q}_0 + \mathbf{q})$ as a function of $q_x$ for several values of $q_y$ in Fig. 15 ($V/t_b = 0.2$) and Fig. 16 ($V/t_b = 0.4$) for the parameters $t'_0/t_b = 0.1$ and some values of $t_3$ and $t_4$. The contour plots of the $\chi_0(\mathbf{q}_0 + \mathbf{q})$ in the $k_x - k_y$ plane are shown in Fig. 20 ($t_3 = t_4 = 0$) and Fig. 21.
The best nesting vector moves to $q_4$ if $t_3 = t_4 = 0$, as shown in Fig. 6. The negative Hall constant is possible, since $q_{1x} < 0$. If $V/t'_b > 0$ and $t_3$ and $t_4$ are the same as above, the best nesting vector is $q_2$ (see the lower figures in Fig. 18). The authors have numerically obtained the phase diagram for the quantum Hall effect as a function of the magnetic field and periodic potential $V$. We have shown that the negative Hall constant ($N = -2$) appears only in the region $0.03 \lesssim V/t_b \lesssim 0.2 (0.3 \lesssim V/t'_b \lesssim 2)$ for the parameters $t'_b/t_b = 0.1$, $t_3/t_b = 0.02$ and $t_4/t_b = 0.002$ (the upper figure of Fig. 12 in Ref. 32). That result can be understood by the fact that for $V > 2t'_b - 2t_4$ the best nesting vector has the positive $x$ component. The existence of the negative Hall constant ($N/2 > 0.3$ is understood by the effect of $V$ that will make $\chi_0(Q_0 + q)$ at $q = q_4$ to be smaller. Experimentally, a negative Hall effect is observed when the system is cooled slowly (less than 0.03K/s) and the external magnetic field region for the negative Hall effect becomes larger as the cooling rate becomes slower (the slowest cooling rate is 0.00009 K/s). It is expected that the magnitude of the periodic potential $V$ becomes larger at the slower colling rate. Therefore, we can conclude from the existence of the negative Hall effect in (TMTSF)$_2$ClO$_4$ that $V < 2t'_b - 2t_4$. The value of $V$ estimated from the magnetic-field-angle dependence of the conductivity is close to the border of this condition.
FIG. 18: $\chi_0(Q)$ at $T = 0$ as a function of $q_x$. The parameters are the same as in Fig. 6 but $V/t_b = 0.2$. 

FIG. 19: The same as Fig. 18 with $V/t_b = 0.4$. 
FIG. 20: The contour plot of $\chi_0(Q_0 + q)$. The filled circles show the location of the maximum (best nesting vector). The diamonds, the open circles, the triangles, and the squares are $q_1$, $q_2$, $q_3$, and $q_4$, respectively. We take $t'_b/t_b = 0.1$, $t_3 = t_4 = 0$.

FIG. 21: The same as Fig. 20 with $t'_b/t_b = 0.1$, $t_3/t_b = 0.02$ and $t_4/t_b = 0.002$. 

$V/t_b = 0$

$V/t_b = 0.2$

$V/t_b = 0.4$

$q_y/\pi$

$t_3 = t_4 = 0$

$t_3/t_b = 0.02$, $t_4/t_b = 0.002$

$t_3/t_b = 0.02$, $t_4/t_b = 0.002$
\[ V_F t = t_4 = 0 \]
\[ V/F_b = 0.4 \]

FIG. 22: Open diamond, open triangle and open squares are \( q_1, q_3 \) and \( q_4 \) for \( V = 0 \), respectively. Open circles and closed circles are \( q_2 \) and the locations of the maximum of \( \chi_0(Q) \) (best nesting vector), respectively, for \( V/t_b = 0, 0.1, 0.2, 0.3 \) and 0.4. We take \( t'_b/t_b = 0.1, t_3 = t_4 = 0. \)
VI. SUMMARY AND DISCUSSIONS

We have studied the nesting vector and $\chi_0(Q)$ in the quasi-one-dimensional systems having the imperfectly nested Fermi surface (the imperfectness is measured by $t'_b$). We have obtained the plateau-like maximum of $\chi_0(Q)$ when $Q$ is in the sweptback region with the apexes $q_1$ and $q_4$. The absolute maximum of $\chi_0(Q)$ is obtained near but not at $Q = Q_0 + q_4$ if $t_3 = t_4 = 0$. When the periodic potential $V$ is finite but not as large as $4t'_b$ (which is thought to be the case in (TMTSF)$_2$ClO$_4$), the “sweptback” region (with apexes $q_2$ and $q_4$) becomes smaller as $V$ increases and shrinks to $q_3$ when $V = 4t'_b$. The best nesting vector moves to $Q \approx Q_0 + q_3$. The absolute maximum of $\chi_0(Q)$ is located at $Q = Q_0 + q_3$ when $V > 4t'_b$. The negative Hall coefficient observed in the field-induced spin density wave states in some region in the region of the magnetic field is shown to be possible only when $V < 2t'_b - 2t_4$, in which case the vectors $q'$s giving the plateau-like maximum of $\chi_0(Q_0 + q'_4)$ (“sweptback” region) can have the negative $x$ component, $(q_{2x} < 0)$. Therefore, we conclude that $V$ should be smaller than $2t'_b - 2t_4$ in (TMTSF)$_2$ClO$_4$, where the sign reversal of the Hall effect has been observed.

Recently, a lot of interest is attracted by the quasi-one-dimensional conductor (Per)$_2M$(mnt)$_2$ (where Per = perylene, mnt = maleonitriledithiolate and $M = Au$ and Pt)$^{11,12,13,14,15}$. The charge density wave (CDW) state is realized in (Per)$_2M$(mnt)$_2$, and the successive transitions of the field-induced CDW has been observed in high magnetic field$^{16,17}$, in contrast to the field-induced SDW in (TMTSF)$_2$ClO$_4$. This material has a similar band structure as (TMTSF)$_2$ClO$_4$, but the origin of the pairs of the quasi-one-dimensional Fermi surface in (Per)$_2M$(mnt)$_2$ is different from that in (TMTSF)$_2$ClO$_4$. The origin of the four pairs of the quasi-one-dimensional Fermi surface in (Per)$_2M$(mnt)$_2$ is the existence of four perylene molecules in the unit cell in the perpendicular plane to the conduction axis$^{18,19}$, while the origin of the two pairs of the quasi-one-dimensional Fermi surface in (TMTSF)$_2$ClO$_4$ is the periodic potential caused by the anion ordering. It will be interesting to study the similarity and the difference between two materials, since the spin susceptibility $\chi_0(Q)$ and the charge susceptibility $\chi_c(Q)$ for the non-interacting system have the same $Q$ dependence caused by the nesting properties of the Fermi surface, except for the effects of the Zeeman splitting of the Fermi surface, which play important role only for CDW.

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