

# Generalized susceptibility of a quasi-one-dimensional system with periodic potential: A model for the organic superconductor (TMTSF)<sub>2</sub>Clo<sub>4</sub>

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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 plateaulike maximum in *sweptback* region in the momentum space, which is surrounded by  $\mathbf{Q}=(2k_F, \pi)+\mathbf{q}_i$  ( $k_F$  is the Fermi wave number  $i=1, 3, 4$  and  $\mathbf{q}_1, \mathbf{q}_3$ , and  $\mathbf{q}_4$  are given in this paper). The best nesting vector, at which the susceptibility  $\chi_0(\mathbf{Q})$  has the absolute maximum at  $T=0$ , is obtained near but not at the inflection point  $\mathbf{Q}=(2k_F, \pi)+\mathbf{q}_4$ . 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)<sub>2</sub>Clo<sub>4</sub>. We obtain that the sweptback region (surrounded by  $\mathbf{q}_2, \mathbf{q}_3$ , and  $\mathbf{q}_4$  when  $V>0$ ) becomes small as  $V$  increases and it shrinks to  $\mathbf{q}_3$  for  $V \geq 4t'_b$ , where  $t'_b$  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  $V < 2t'_b - 2t_4$ , where  $t_4$  is the amplitude of the fourth harmonics of the warping in the Fermi surface. This gives the 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 (Q1D) organic conductors, (TMTSF)<sub>2</sub>X, where X is PF<sub>6</sub>, Clo<sub>4</sub>, etc.<sup>1</sup> The successive transitions between the different FISDW phases occur as the magnetic field is increased. The FISDW has been understood as a consequence of the reduction in the dimensionality due to the magnetic field and the quantization of the nesting vector.<sup>2–11</sup> 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,  $G=beB/\hbar$ ,  $b$  is the lattice constant (we take  $b=1$  in this paper),  $e$  is the electron charge,  $B$  is the magnetic field, and  $\hbar=h/2\pi$  ( $h$  is the Planck constant). We take  $\hbar=1$  hereafter in this paper. The Hall conductivity is quantized as  $\sigma_{xy}=2Ne^2/h$  with the quantum number  $N$  of the nesting vector.<sup>12–14</sup> The quantization of the  $x$  component of the nesting vector  $Q_x$  can be seen as the sharp peaks in the susceptibility for the noninteracting system  $\chi_0(\mathbf{Q})$  at  $Q_x=2k_F+NG$  in the magnetic field.

The peaks of  $\chi_0(\mathbf{Q})$  in the magnetic field can be understood to some extent by the peaks of  $\chi_0(\mathbf{Q})$  in the absence of the magnetic field. If the nesting of the Fermi surface is perfect,  $\chi_0(\mathbf{Q})$  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  $\chi_0(\mathbf{Q})$ , is located in the reciprocal space at

$$\mathbf{Q} = \mathbf{Q}_0 + \mathbf{q}, \quad (1)$$

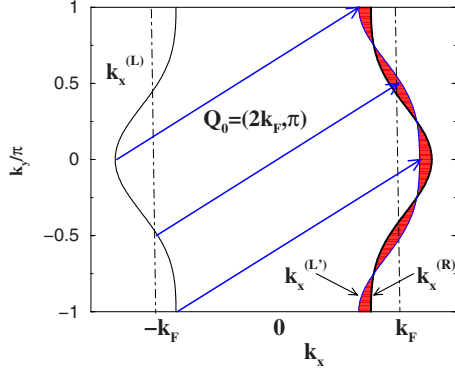
where

$$\mathbf{Q}_0 = (2k_F, \pi), \quad (2)$$

and  $\mathbf{q} \neq 0$ . If  $q_x > 0$ , the quantum number  $N$  of FISDW is positive. If  $q_x < 0$  at the best nesting vector, however, the negative  $N$  is possible in some region of the magnetic field.<sup>15</sup> The umklapp scattering has been proposed as the alternative explanation for the negative  $N$  (Ref. 16). We do not consider the umklapp scattering in this paper.

Although (TMTSF)<sub>2</sub>PF<sub>6</sub> is well understood by the quasi-one-dimensional model, (TMTSF)<sub>2</sub>Clo<sub>4</sub> is a little more complicated. Below  $T_{AO} \approx 24$  K the anion Clo<sub>4</sub> (which has no inversion symmetry) orders alternatively in the  $y$  direction, resulting the periodic potential  $V$  in the electron system. Actually, the magnetic field and temperature phase diagram in (TMTSF)<sub>2</sub>PF<sub>6</sub> (Refs. 17–21) is different from that in (TMTSF)<sub>2</sub>Clo<sub>4</sub> (Refs. 22–24). The origin of the different phase diagrams in (TMTSF)<sub>2</sub>PF<sub>6</sub> and (TMTSF)<sub>2</sub>Clo<sub>4</sub> is caused by the periodic potential  $V$ . The magnitude of  $V$  is first estimated to be of the order of  $T_{AO}=24$  K, i.e.,  $V \ll t_b$  (Refs. 25 and 26). The suppression of the  $N=0$  FISDW state<sup>25</sup> and even- $N$  FISDW states<sup>26</sup> has been shown by the perturbation in  $V$ . On the other hand, the magnitude of  $V$  has been estimated to be  $V=0.83t_b$  from the angle dependence of the magnetoresistance by Yoshino *et al.*<sup>27</sup> By treating  $V$  not in perturbation, a lot of interesting features, such as existence of several nesting vectors<sup>28–31</sup> and the phase diagram of the FISDW states,<sup>32,33</sup> has been obtained. Recently, Yoshino *et al.*<sup>34</sup> has estimated the value to be  $V=0.028t_a$  ( $V=0.34t_b$  with their estimation  $t_a=12t_b$ ). Lebed *et al.*<sup>35,36</sup> have estimated the value as  $V=0.2t_b$ . The 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 susceptibility in the quasi-one-dimensional system with imperfectly nested Fermi surface in the absence of the magnetic field. The analytical expression of the susceptibility and the nearly flat region in the reciprocal space is given analytically in the


 FIG. 1. (Color online) Fermi surface for  $V=0$ .

simple model with  $V=0$ . The effect of  $V$  on the nesting vector and the susceptibility are studied in detail numerically. Although we consider the zero magnetic-field case, we hope that the obtained results are valid in a finite magnetic-field case.

## II. MODEL

We neglect the small dispersion in the  $k_z$  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 one. In the real system, the crystal is triclinic and we have to consider the multiple-transverse-transfer integrals,<sup>37</sup> but most of the essential features are obtained by studying the simple model in the square lattice.<sup>1</sup> The energy dispersion can be linearized with respect to  $k_x$  and we take account the higher harmonic terms for  $k_y$  as

$$\epsilon(\mathbf{k}) = v_F(|k_x| - k_F) + t_\perp(k_y), \quad (3)$$

where

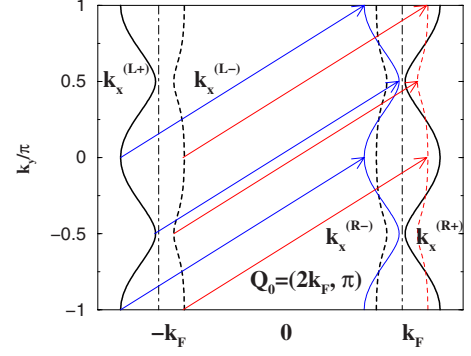
$$t_\perp(k_y) = -2t_b \cos k_y - 2t'_b \cos(2k_y) - 2t_3 \cos(3k_y) - 2t_4 \cos(4k_y) \quad (4)$$

and we study the case  $t_b$ ,  $t'_b$ ,  $t_3$ , and  $t_4$  to be positive. The terms proportional to  $t_3$  and  $t_4$  are thought to be essential<sup>15,33</sup> to understand the negative  $N$  phase<sup>38,39</sup> of FISDW in some region of the magnetic field. The Fermi surface consists of two ‘‘Fermi lines’’ near  $k_x \approx \pm k_F$  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  $\mathbf{Q} \approx \mathbf{Q}_0$ , 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

$$\mathcal{H} = \begin{pmatrix} \epsilon(\mathbf{k}) & V \\ V & \epsilon(\mathbf{k} + \mathbf{Q}_A) \end{pmatrix}, \quad (5)$$

where  $\mathbf{Q}_A = (0, \pi)$ . The energy  $E(\mathbf{k})$  is given by


 FIG. 2. (Color online) Fermi surface for  $V \neq 0$ .

$$E(\mathbf{k}) = \frac{1}{2}(\epsilon(\mathbf{k}) + \epsilon(\mathbf{k} + \mathbf{Q}_A) \pm \sqrt{[\epsilon(\mathbf{k}) - \epsilon(\mathbf{k} + \mathbf{Q}_A)]^2 + 4V^2}), \quad (6)$$

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

It is known<sup>28</sup> that the susceptibility  $\chi_0(\mathbf{Q})$  has the maximum near  $\mathbf{Q} \approx \mathbf{Q}_0$  if  $V \leq 1.5t_b$  when  $t'_b = 0.1t_b$  (i.e.,  $V \leq 15t'_b$ ), while the absolute maximum of  $\chi_0(\mathbf{Q})$  is located near  $\mathbf{Q} \approx (2k_F \pm 2V/v_F, \pi/2)$  if  $V \geq 1.5t_b$ . The peak of  $\chi_0(\mathbf{Q})$  near  $\mathbf{Q} \approx \mathbf{Q}_0$  is caused by the nesting between the outer Fermi surface and the inner Fermi surface ( $\mathbf{k}_x^{(R+)}$  and  $\mathbf{k}_x^{(L-)}$ ), i.e., the red and blue arrows in Fig. 2, while the peaks of  $\chi_0(\mathbf{Q})$  near  $\mathbf{Q} \approx (2k_F \pm 2V/v_F, \pi/2)$  are caused by the nesting of the outer Fermi surfaces [ $\mathbf{k}_x^{(R+)}$  and  $\mathbf{k}_x^{(L+)}$ ] or the inner Fermi surfaces [ $\mathbf{k}_x^{(R-)}$  and  $\mathbf{k}_x^{(L-)}$ ] (Refs. 32, 40, and 41). The maximum value of  $\chi_0(\mathbf{Q})$  near  $\mathbf{Q} \approx \mathbf{Q}_0$  depends weakly on  $V$  if  $V \leq 0.4t_b$ , and it decreases as  $V$  increases if  $V \geq 0.4t_b$ . Sengupta and Dupuis<sup>29</sup> and Zanchi and Bjelis<sup>30</sup> obtained similar results.

In this paper we examine in detail the nesting properties of the quasi-one-dimensional systems without and with the periodic potential ( $V \leq 0.5t_b$ ). Thus we focus on the nesting condition for only  $\mathbf{Q} \approx \mathbf{Q}_0$ .

## 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 Fermi surface consists of two curves (see Fig. 1). The right and left parts of the Fermi surface are given as a function of  $k_y$ ,

$$k_x^{(R)}(k_y) = k_F - \frac{1}{v_F} t_\perp(k_y), \quad (7)$$

$$k_x^{(L)}(k_y) = -k_F + \frac{1}{v_F} t_\perp(k_y). \quad (8)$$

We translate the left part of the Fermi surface with the nesting vector  $\mathbf{Q} = \mathbf{Q}_0 + \mathbf{q}$ . The translated curve is given by

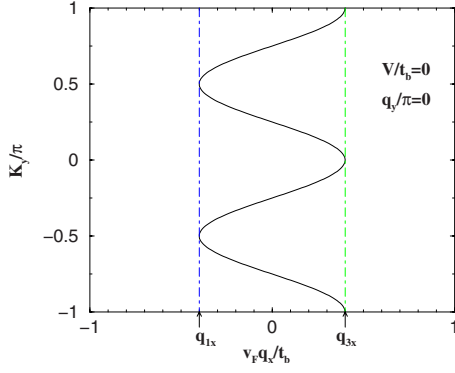


FIG. 3. (Color online)  $q_x$  vs  $K_y$  (Eq. (11)) for  $q_y=0$  and  $q_y=\pi$ .

$$k_x^{(L')}(k_y) = k_F + q_x + \frac{1}{v_F} t_{\perp} (k_y + q_y + \pi). \quad (9)$$

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

$$k_x^{(L')}(k_y) - k_x^{(R)}(k_y) = q_x + \frac{1}{v_F} [t_{\perp}(k_y) + t_{\perp}(k_y + q_y + \pi)]. \quad (10)$$

If  $t'_b = t_4 = 0$ , the nesting of the Fermi surface is perfect with  $q_x = q_y = 0$ , i.e.,  $k_x^{(L')}(k_y) - k_x^{(R)}(k_y) = 0$  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 intersects with the translated one with the nesting vector  $\mathbf{Q}_0 + \mathbf{q}$ , if  $q_x$  and  $q_y$  satisfy

$$\begin{aligned} q_x &= \frac{-1}{v_F} [t_{\perp}(k_y) + t_{\perp}(k_y + q_y + \pi)] \\ &= \frac{4}{v_F} \left[ t_b \sin(K_y) \sin\left(\frac{q_y}{2}\right) + t'_b \cos(2K_y) \cos(q_y) \right. \\ &\quad \left. + t_3 \sin(3K_y) \sin\left(\frac{3q_y}{2}\right) + t_4 \cos(4K_y) \cos(2q_y) \right], \end{aligned} \quad (11)$$

for some value of  $K_y$ , where

$$q_x^{\min(+)}(q_y) = \frac{4}{v_F} \left( -t'_b \cos q_y + t_b \sin \frac{|q_y|}{2} - t_3 \sin \frac{3|q_y|}{2} + t_4 \cos 2q_y \right), \quad (15)$$

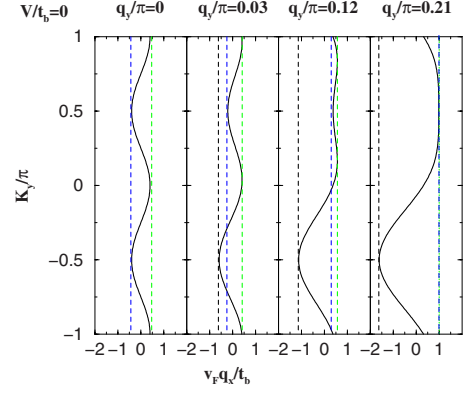


FIG. 4. (Color online)  $q_x$  vs  $K_y$  [Eq. (11)] for some values of  $q_y$ . There are two minimums [ $q_x^{\min(\pm)}(q_y)$ ] and one maximum [ $q_x^{\max}(q_y)$ ] of  $q_x$  as a function of  $K_y$  for each  $0 < |q_y| < q_{4y}$ , while only one minimum and one maximum of  $q_x$  for  $|q_y| > q_{4y}$  as shown by the dotted vertical lines.

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

Equation (11) is the condition for the nesting vector ( $\mathbf{Q} = \mathbf{Q}_0 + \mathbf{q}$ ) 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,  $\mathbf{q}_1$  and  $\mathbf{q}_3$ , 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  $\pm\pi$ , and the minimum of  $q_x$  as a function of  $K_y$  for  $q_y = 0$  is given at  $K_y = \pm\pi/2$  as shown in Fig. 3;

$$\mathbf{q}_1 = \left( \frac{4}{v_F} (-t'_b + t_4), 0 \right), \quad (13)$$

$$\mathbf{q}_3 = \left( \frac{4}{v_F} (t'_b + t_4), 0 \right). \quad (14)$$

We define  $\mathbf{q}_2 = \mathbf{q}_1$  for  $V=0$  and we will define  $\mathbf{q}_2$  for  $V \neq 0$  in Sec. V.

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  $K_y = \pm\pi/2$  [ $q_x^{\min(\pm)}(q_y)$ ] and one maximum at  $0 \leq K_y \leq \pi/2$  [ $q_x^{\max}(q_y)$ ] if  $0 < |q_y| < q_{4y}$  ( $\mathbf{q}_4$  will be given later). There is one minimum at  $K_y = -\pi/2$  and one maximum at  $K_y = \pi/2$  if  $|q_y| > q_{4y}$ . We obtain  $q_x^{\min(+)}(q_y)$  and  $q_x^{\min(-)}(q_y)$  as

$$q_x^{\min(-)}(q_y) = \frac{4}{v_F} \left( -t'_b \cos q_y - t_b \sin \frac{|q_y|}{2} + t_3 \sin \frac{3|q_y|}{2} + t_4 \cos 2q_y \right). \quad (16)$$

If  $t_3$  and  $t_4$  are finite, we have to solve the fourth-degree equation to obtain the expression of  $q_x^{\max}(q_y)$ , but it is easy to obtain  $q_x^{\max}(q_y)$  numerically. We define  $\mathbf{q}_4=(q_{4x}, q_{4y})$  by the equation

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

If  $t_3=t_4=0$ , the simple expressions of  $q_x^{\max}(q_y)$  and  $\mathbf{q}_4$  are obtained as

$$q_x^{\max}(q_y) = \frac{4}{v_F} \left( t'_b \cos q_y + \frac{t_b^2 \sin^2 \frac{q_y}{2}}{8t'_b \cos q_y} \right), \quad (18)$$

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

and

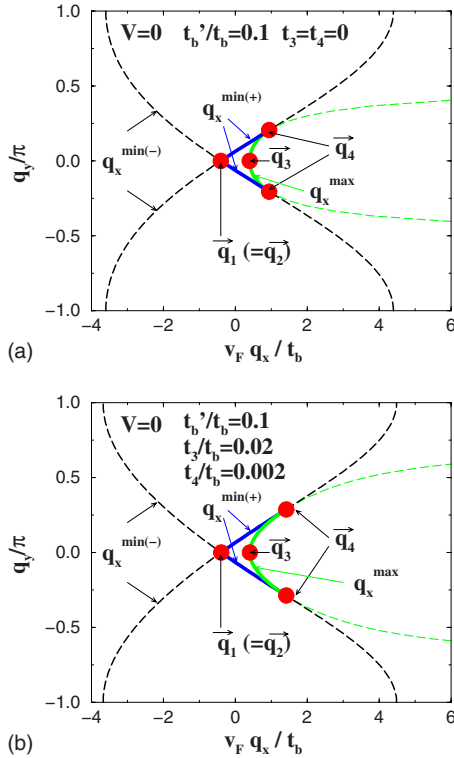


FIG. 5. (Color online)  $q_x^{\min(-)}(q_y)$  (dashed lines in  $q_x < q_{1x}$ ),  $q_x^{\min(+)}(q_y)$  (thick blue lines in  $q_{1x} < q_x < q_{4x}$  and dashed lines in  $q_x > q_{4x}$ ), and  $q_x^{\max}(q_y)$  (thick green lines in  $q_{3x} < q_x < q_{4x}$  and dashed green lines in  $q_x > q_{4x}$ ). We take  $t'_b/t_b=0.1$  and  $t_3=t_4=0$  (upper figure) and  $t_3/t_b=0.02$  and  $t_4/t_b=0.002$  (lower figure). In the sweptback region enclosed by  $\mathbf{q}_1$ ,  $\mathbf{q}_3$ , and  $\mathbf{q}_4$ ,  $\chi_0(\mathbf{Q})$  has large values.

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

Note that  $q_x^{\max}(q_y)$  has the physical meaning only if  $|q_y| \leq q_{4y}$ , since the analytical form [Eq. (18)] obtained from the

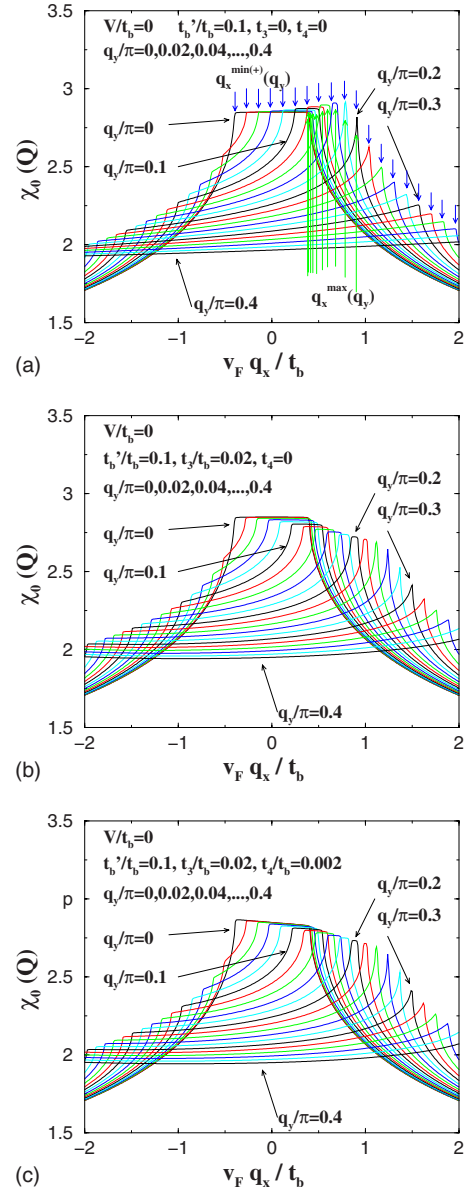


FIG. 6. (Color online)  $\chi_0(\mathbf{Q})$  at  $T=0$  (Eq. (22)) as a function of  $q_x$ . We take  $t'_b/t_b=0$  and  $t_3=t_4=0$  (upper figure);  $t_3/t_b=0.02$  and  $t_4=0$  (middle figure); and  $t_3/t_b=0.02$  and  $t_4/t_b=0.002$  (lower figure). As obtained by Zanchi and Montambaux (Ref. 15),  $t_3$  reduces the peak height near  $\mathbf{q}_4$  and  $t_4$  lifts the degeneracy at  $\mathbf{q}_1$  and  $\mathbf{q}_3$ .

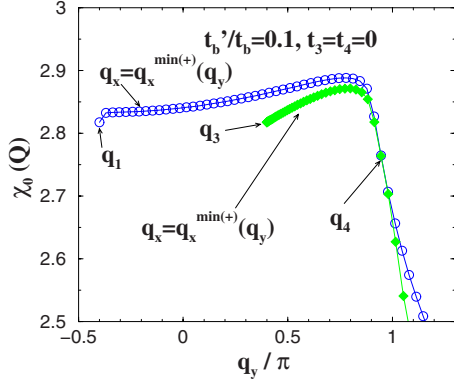


FIG. 7. (Color online)  $\chi_0(\mathbf{Q})$  at  $T=0$  (Eq. (22)) as a function of  $q_x$  for  $(q_x, q_y)$  on the curves  $(q_x^{\min(+)}(q_y), q_y)$  (filled green diamonds) and  $(q_x^{\max}(q_y), q_y)$  (open blue circles) in Fig. 5. For  $q_x > q_{4x}$ , we use Eq. (18), although curves  $(q_x^{\max}, q_y)$  terminate at  $\mathbf{q}=\mathbf{q}_4$ . Note that the absolute maximum is not realized at  $(q_{4x}, q_{4y})$ . We take  $t'_b/t_b = 0.1$  and  $t_3 = t_4 = 0$ .

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  $q_x^{\max}(q_y)$ ,  $q_x^{\min(+)}(q_y)$ , and  $\mathbf{q}_i$  ( $i=1, 3$ , and 4) in Fig. 5. There is a large overlap between the Fermi line and the translated one if  $\mathbf{q}$  is in the *sweptback* region with the apexes  $\mathbf{q}_1$  and  $\mathbf{q}_4$  enclosed by the thick lines in Fig. 5.

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

The susceptibility

$$\chi_0(\mathbf{Q}) = \sum_{\mathbf{k}} \frac{f(E_{\mathbf{k}+\mathbf{Q}}) - f(E_{\mathbf{k}})}{E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{Q}}}, \quad (21)$$

where  $f(E_{\mathbf{k}})$  is the Fermi distribution function, is calculated at  $T=0$  as

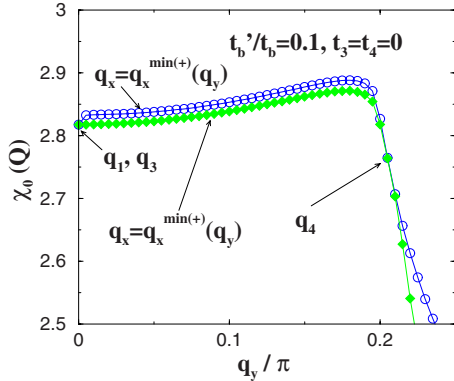


FIG. 8. (Color online)  $\chi_0(\mathbf{Q})$  at  $T=0$  (Eq. (22)) as a function of  $q_y$  for  $(q_x, q_y)$  on the curves  $(q_x^{\min(+)}(q_y), q_y)$  (filled green diamonds) and  $(q_x^{\max}(q_y), q_y)$  (open blue circles) in Fig. 5. We take  $t'_b/t_b = 0.1$  and  $t_3 = t_4 = 0$ .

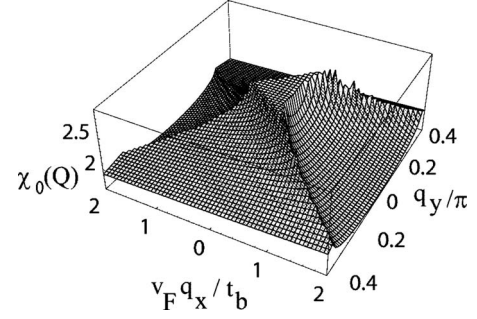


FIG. 9. 3D plot of  $\chi_0(\mathbf{Q})$  at  $T=0$  (Eq. (22)) as a function of  $q_x$  and  $q_y$ . We take  $t'_b/t_b = 0.1$  and  $t_3 = t_4 = 0$ .

$$\begin{aligned} \chi_0(\mathbf{Q}) &= \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \int_{k_x^{(L)}(k_y)}^{k_x^{(R)}(k_y)} \frac{dk_x}{2\pi} \frac{2}{\epsilon(\mathbf{k}-\mathbf{Q}) - \epsilon(\mathbf{k})} \\ &= \frac{1}{\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left[ \int_{k_x^{(L)}(k_y)}^0 \frac{dk_x}{v_F Q_x + t_{\perp}(k_y - Q_y) - t_{\perp}(k_y)} \right. \\ &\quad \left. + \int_0^{k_x^{(R)}(k_y)} \frac{dk_x}{v_F(-2k_x + Q_x) + t_{\perp}(k_y - Q_y) - t_{\perp}(k_y)} \right] \\ &= \frac{1}{2\pi v_F} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left[ \frac{v_F k_F - t_{\perp}(k_y)}{v_F Q_x + t_{\perp}(k_y - Q_y) - t_{\perp}(k_y)} \right. \\ &\quad \left. - \frac{1}{2} \log \left| \frac{v_F(Q_x - 2k_F) + t_{\perp}(k_y - Q_y) + t_{\perp}(k_y)}{v_F Q_x + t_{\perp}(k_y - Q_y) - t_{\perp}(k_y)} \right| \right]. \end{aligned} \quad (22)$$

The susceptibility is finite at  $T=0$  and has the singularity (kinks) as a function of  $\mathbf{Q}$ . The singularity of  $\chi_0(\mathbf{Q})$  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  $\chi_0(\mathbf{Q}_0 + \mathbf{Q})$  is calculated as

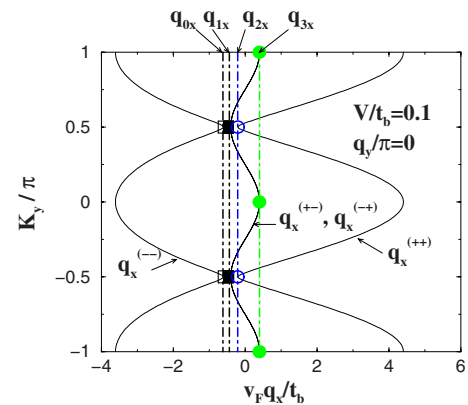
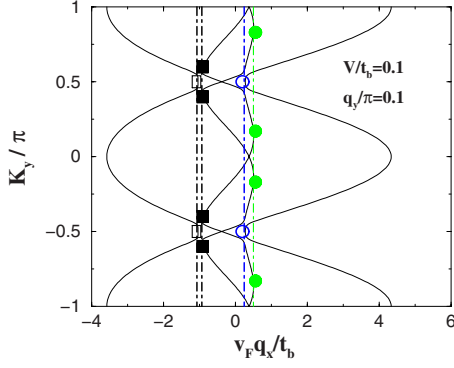


FIG. 10. (Color online)  $q_x$  vs  $K_y$  [Eq. (27)] for  $q_y = 0$  and  $V/t_b = 0.1$ .

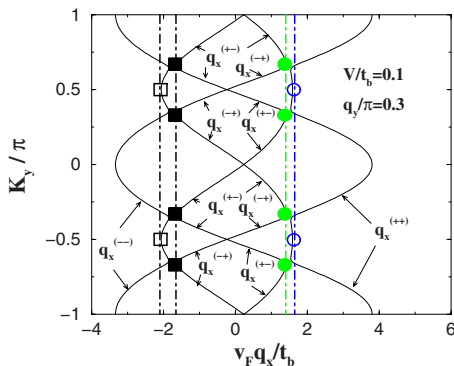
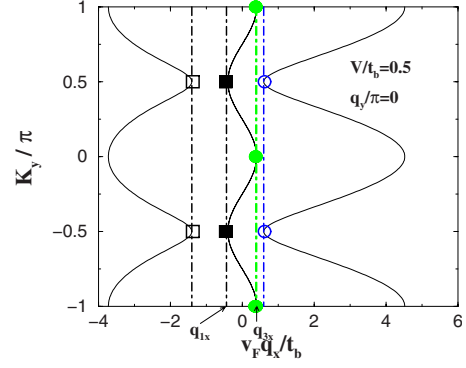

 FIG. 11. (Color online)  $q_x$  as a function of  $K_y$  for  $q_y/\pi=0.1$ .

$$\chi_{0,\text{sing}} = \frac{1}{\pi v_F} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \left( -\frac{1}{2} \right) \log \left| \frac{v_F q_x - 4t'_b \cos 2k_y}{2k_F v_F} \right|$$

$$= \begin{cases} -\frac{1}{2\pi v_F} \log \left| \frac{q_x v_F + \sqrt{(q_x v_F)^2 - (4t'_b)^2}}{4k_F v_F} \right| & \text{if } |q_x v_F| > 4t'_b \\ -\frac{1}{2\pi v_F} \log \left| \frac{t'_b}{k_F v_F} \right| & \text{if } |q_x v_F| < 4t'_b \end{cases} \quad (23)$$

It is obtained from Eq. (23) that  $\chi_0(\mathbf{q})$  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  $\chi_0(\mathbf{Q})$  for several  $t_3$ ,  $t_4$ , 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 it has the absolute maximum before  $q_y$  reaches  $q_{4y}$  ( $=0.2065\pi$  and  $v_F q_{4y}/t_b=0.956$  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  $\chi_0(\mathbf{Q}_0+\mathbf{Q})$  at  $\mathbf{q}_1$  and  $\mathbf{q}_3$  is lifted and the absolute maximum of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  is obtained at  $\mathbf{q}_1$  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,  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  has a plateaulike maximum in the region  $q_x^{\min(+)}(q_y) < q_x < q_x^{\max}(q_y)$ . The absolute maxi-


 FIG. 12. (Color online)  $q_x$  as a function of  $K_y$  for  $q_y/\pi=0.3$ .

 FIG. 13. (Color online)  $q_x$  as a function of  $K_y$  for  $q_y/\pi=0.0$  and  $V/t_b=0.5$ .

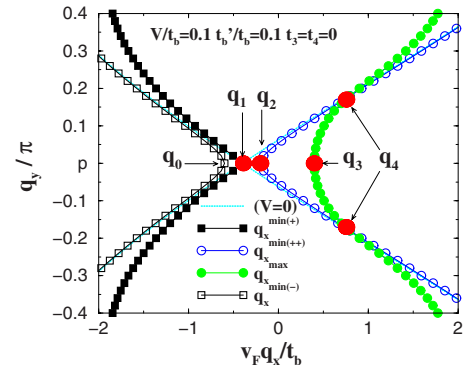
um of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  occurs at  $\mathbf{q}$  close to  $\mathbf{q}_4$  but not at  $\mathbf{q}=\mathbf{q}_4$  as seen in Figs. 7 and 8, where we plot  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  as a function of  $q_x$  or  $q_y$  on the curves of  $q_x=q_x^{\min(+)}(q_y)$  and  $q_x=q_x^{\max}(q_y)$ , respectively. The three-dimensional plot of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  is shown in Fig. 9. When  $t_3=t_4=0$  and  $q_y=q_{4y}$ , Eq. (11) becomes

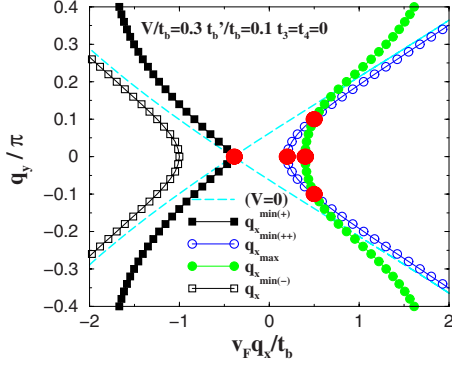
$$q_x = \frac{1}{k_F} \frac{4t'_b [6 - 16 \sin^4(K_y - \frac{\pi}{2})]}{\sqrt{1 + 128 (\frac{t'_b}{t_b})^2 + 1}} \quad (24)$$

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  $q_y=q_{4y}$ . With the vector  $\mathbf{Q}=\mathbf{Q}_0+\mathbf{q}_4$  the nesting of the Fermi surface is better than other  $\mathbf{q}$ 's, which will make the expectation of the large  $\chi_0(\mathbf{Q}_0+\mathbf{q})$ . However, the region of  $q_y$  [where  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  is mainly contributed] is larger at  $q_x \leq q_{4x}$  and  $|q_y| \leq q_{4y}$  than at  $\mathbf{q}=\mathbf{q}_4$ . This is the reason why the absolute maximum of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  is not located at the inflection point ( $\mathbf{q}=\mathbf{q}_4$ ).

## 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.


 FIG. 14. (Color online) The same as Fig. 5 for  $V/t_b=0.1$ .  $q_1$  is given as the minimum of  $q_x^{(+-)}$  as a function of  $K_y$  for each  $q_y$ .  $q_2$  is given as  $q_x^{(++)}$  at  $K_y = \pi/2$  for each  $q_y$ .  $q_3$  is given as the maximum of  $q_x^{(+-)}$  as a function of  $K_y$  for each  $q_y$ .  $q_0$  is given as  $q_x^{(-)}$  at  $K_y = \pi/2$  for each  $q_y$ .


 FIG. 15. (Color online) The same as Fig. 14 for  $V/t_b=0.3$ .

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 into 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

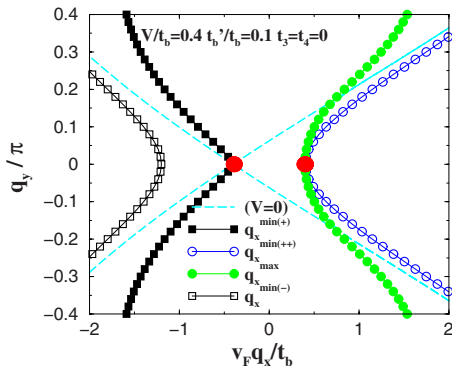
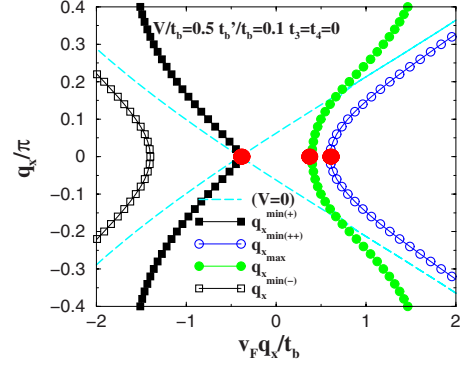
$$k_x^{(L\pm)}(k_y) = -k_F - \frac{1}{v_F} \{-t_{\perp}(k_y) - t_{\perp}(k_y + \pi) \pm \sqrt{[t_{\perp}(k_y) - t_{\perp}(k_y + \pi)]^2 + 4V^2}\}, \quad (25)$$

and

$$k_x^{(R\pm)}(k_y) = k_F + \frac{1}{v_F} \{-t_{\perp}(k_y) - t_{\perp}(k_y + \pi) \pm \sqrt{[t_{\perp}(k_y) - t_{\perp}(k_y + \pi)]^2 + 4V^2}\}. \quad (26)$$

The condition for the Fermi surface intersects by the translation of the left part [Eq. (11) for  $V=0$ ] is written as the four equations  $(++)$ ,  $(+-)$ ,  $(-+)$ , and  $(--)$ ,

$$q_x^{(\pm\pm)} = \frac{1}{2v_F} \{-t_{\perp}(k_y) - t_{\perp}(k_y + \pi) - t_{\perp}(k_y + q_y) - t_{\perp}(k_y + q_y + \pi) \pm \sqrt{[t_{\perp}(k_y) - t_{\perp}(k_y + \pi)]^2 + 4V^2} \pm \sqrt{[t_{\perp}(k_y + q_y) - t_{\perp}(k_y + q_y + \pi)]^2 + 4V^2}\}. \quad (27)$$


 FIG. 16. (Color online) The same as Fig. 14 for  $V/t_b=0.4$ .

 FIG. 17. (Color online) The same as Fig. 14 for  $V/t_b=0.5$ .

When  $q_y=0$ , we obtain Eq. (27) for  $(+, -)$  and  $(-, +)$  to be the same as that for  $V=0$  [Eq. (11)],

$$q_x^{(+,-)} = q_x^{(-,+)} = \frac{1}{v_F} [-t_{\perp}(k_y) - t_{\perp}(k_y + \pi)]. \quad (28)$$

The condition for the intersect of  $(+, +)$  is obtained as

$$q_x^{(++)} = \frac{1}{v_F} [-t_{\perp}(k_y) - t_{\perp}(k_y + \pi) + \frac{1}{v_F} \sqrt{[t_{\perp}(k_y) - t_{\perp}(k_y + \pi)]^2 + 4V^2}], \quad (29)$$

and the condition for the intersect of  $(--)$  is obtained as

$$q_x^{(--)} = \frac{1}{v_F} [-t_{\perp}(k_y) - t_{\perp}(k_y + \pi) - \frac{1}{v_F} \sqrt{[t_{\perp}(k_y) - t_{\perp}(k_y + \pi)]^2 + 4V^2}]. \quad (30)$$

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  $K_y = \pm \pi/2$ ), the minimum of  $q_x^{(+-)}$  (at  $K_y = \pm \pi/2$ ), and the maximum of  $q_x^{(+,-)}$  (at  $K_y = 0$  and  $\pi$ ) as a function of  $K_y$  when  $q_y=0$  ( $q_{0y}=q_{1y}=q_{2y}=q_{3y}=0$ ), respectively (see Fig. 10), i.e.,

$$\mathbf{q}_0 = \left( \frac{1}{v_F} (-4t'_b + 4t_4 - 2V), 0 \right), \quad (31)$$

$$\mathbf{q}_1 = \left( \frac{1}{v_F} (-4t'_b + 4t_4), 0 \right), \quad (32)$$

$$\mathbf{q}_2 = \left( \frac{1}{v_F} (-4t'_b + 4t_4 + 2V), 0 \right), \quad (33)$$

$$\mathbf{q}_3 = \left( \frac{1}{v_F} (4t'_b + 4t_4), 0 \right). \quad (34)$$

When  $q_y$  is given, the maximums and minimums of  $q_x^{(+-)}$  are obtained as a function of  $K_y$  as shown by the filled green circles and the filled squares in Figs. 10–13. We define  $q_x^{\max}(q_y)$  and  $q_x^{\min(+)}(q_y)$  by the maximums (filled green circles) and minimums (filled squares) of  $q_x^{(+-)}$  for each  $q_y$ , respectively. We also define  $q_x^{\min(-)}(q_y)$  by the value of  $q_x^{(-)}$

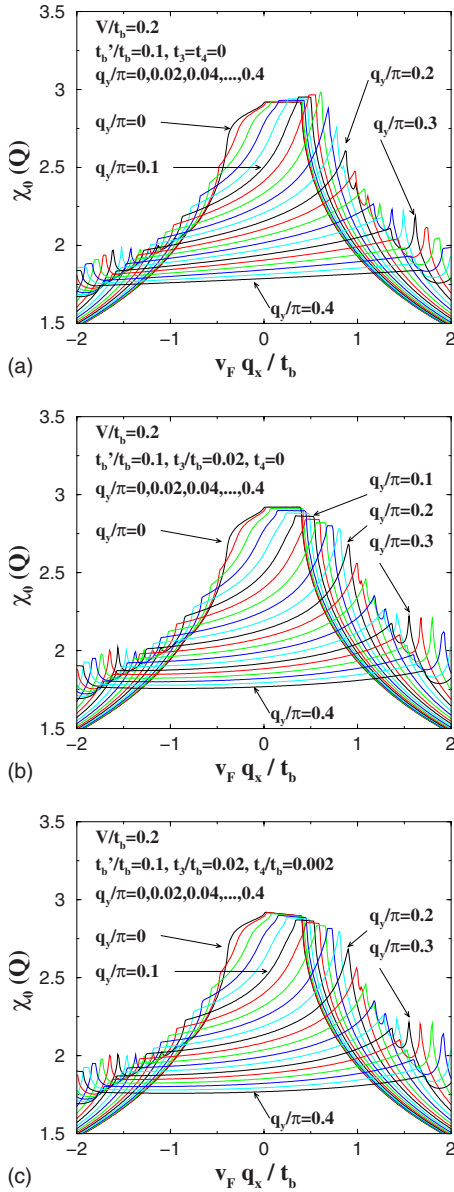


FIG. 18. (Color online)  $\chi_0(\mathbf{Q})$  at  $T=0$  as a function of  $q_x$ . The parameters are the same as in Fig. 6 but  $V/t_b=0.2$ .

at  $K_y = \pm \pi/2$  (open black squares) and  $q_x^{\min(++)}(q_y)$  by the value of  $q_x^{(++)}$  at  $K_y = \pm \pi/2$  (open circles). In Figs. 14–17 we plot  $q_x^{\max}(q_y)$ ,  $q_x^{\min(+)}(q_y)$ ,  $q_x^{\min(-)}(q_y)$ , and  $q_x^{\min(++)}(q_y)$  in the planes 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 to  $q_x^{\min(+)}(q_y)$ ,  $q_x^{\max}(q_y)$ , and  $q_x^{\min(++)}(q_y)$  at  $V=0$ , respectively (cf. Fig. 5). On the other hand,  $q_x^{\min(+)}(q_y)$  has no partner at  $V=0$ , since the filled squares in Figs. 10–13 become not the minimum but just the crossing points due to the folding in  $K_y$  as  $V$  becomes zero. We define  $\mathbf{q}_4$  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. 18 ( $V/t_b=0.2$ ) and Fig. 19 ( $V/t_b=0.4$ ) for the parameters  $t'_b/t_b=0.1$  and some values of  $t_3$  and  $t_4$ . The contour plots of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  in the  $k_x$ - $k_y$  plane are shown in Fig. 20 ( $t_3=t_4=0$ ) and Fig. 21 ( $t_3/t_b=0.02$ ,  $t_4/t_b=0.002$ ) for

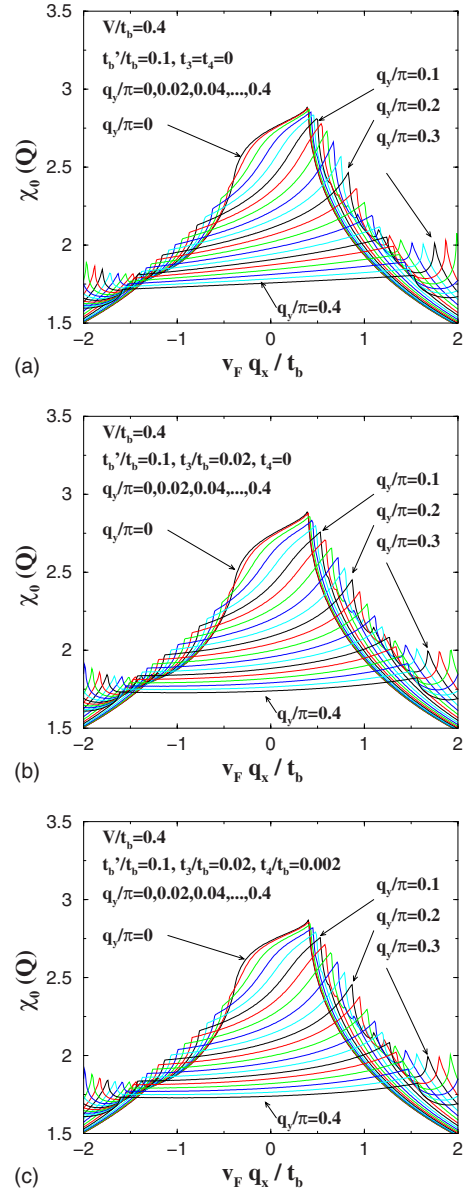


FIG. 19. (Color online) The same as Fig. 18 with  $V/t_b=0.4$ .

$V/t_b=0, 0.2$  ( $V/t'_b=2$ ), and  $0.4$  ( $V/t'_b=4$ ). When  $0 < V < 4t'_b$ ,  $q_{1x} < q_{2x} < q_{3x}$ . In this case  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  has a plateaulike maximum in the *sweptback* region enclosed by  $\mathbf{q}_2$ ,  $\mathbf{q}_4$ , and  $\mathbf{q}_3$  as shown in Figs. 14 and 15. This region shrinks to the point  $\mathbf{q}_3$  when  $V/t'_b=4$  as shown in Fig. 16. The absolute maximum of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  occurs near  $\mathbf{q}_4$  if  $t_3=t_4=0$ . The effects of  $t_3$  and  $t_4$  on  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  are the same as those at  $V=0$ . A finite  $t_3$  suppresses  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  at  $q_y \neq 0$  and  $t_4$  lifts the degeneracy at  $q_{2x} \leq q_x \leq q_{4x}$ . If  $V > 4t'_b$ , we obtain  $q_{1x} < q_{3x} < q_{2x}$  and there is no region where  $\chi_0(\mathbf{Q})$  has a plateaulike maximum as shown in Figs. 16, 17, and 19. In that case, the effects of  $t_3$  and  $t_4$  are small. In Fig. 22,  $\mathbf{q}_2$  and  $\mathbf{q}$  which gives the maximum of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  (i.e., the best nesting vector) are shown for some values of  $V/t_b$  in the case of  $t_3=t_4=0$ . The best nesting vector moves to  $\mathbf{q}_3$  as  $V/t_b$  approaches 0.4.

The negative Hall constant in some region of the magnetic field<sup>38,39</sup> has been explained by the  $t_3$  and  $t_4$  terms.<sup>15</sup> When  $V=0$ , the terms with  $t_3/t_b=0.02$  and  $t_4/t_b=0.002$  make



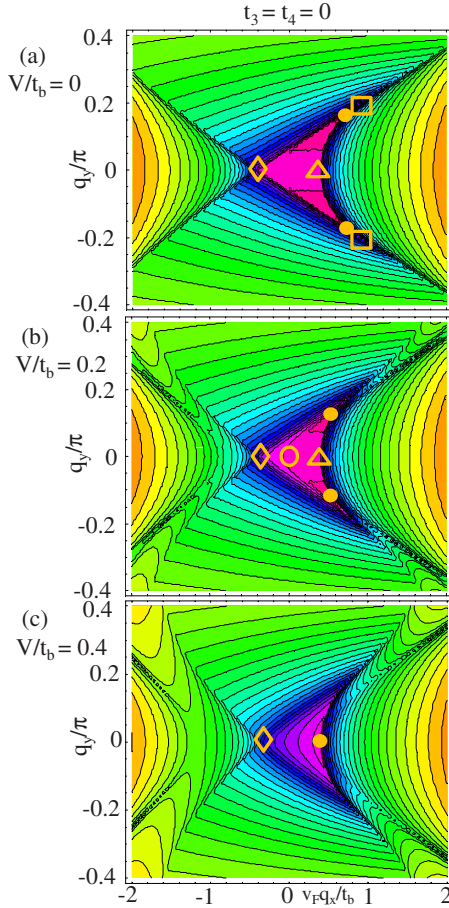


FIG. 20. (Color online) The contour plot of  $\chi_0(\mathbf{Q}_0+\mathbf{q})$ . The filled circles show the location of the maximum (best nesting vector). The diamonds, the open circles, the triangles, and the squares are  $\mathbf{q}_1$ ,  $\mathbf{q}_2$ ,  $\mathbf{q}_3$ , and  $\mathbf{q}_4$ , respectively. We take  $t'_b/t_b=0.1$  and  $t_3=t_4=0$ .

the absolute maximum of  $\chi_0(\mathbf{Q})$  in the zero magnetic field to be at  $\mathbf{q}_1$  (best nesting vector), while the best nesting vector is located near  $\mathbf{q}_4$  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  $\mathbf{q}_2$  (see the lower figures in Fig. 18 and the middle figure in Fig. 21). As far as  $V<2t'_b-2t_4$ , the negative Hall constant is possible since  $q_{2x}<0$ . If  $V>2t'_b-2t_4$ , however, the best nesting vector  $\mathbf{q}_2$  has the positive  $x$  component as seen in the lower figures in Figs. 18 and 19. Therefore, the negative Hall constant is difficult to be stabilized when  $V>2t'_b-2t_4$ . Recently, the authors<sup>33</sup> 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  $0.03 \leq V/t_b \leq 0.2$  ( $0.3 \leq V/t'_b \leq 2$ ) 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. 33). 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 for  $V/t'_b \geq 0.3$  is understood by the effect of  $V$  that will make  $\chi_0(\mathbf{Q}_0+\mathbf{q})$  at  $\mathbf{q} \approx \mathbf{q}_4$  smaller. Experimentally, a negative Hall effect is observed when the system is cooled slowly (less

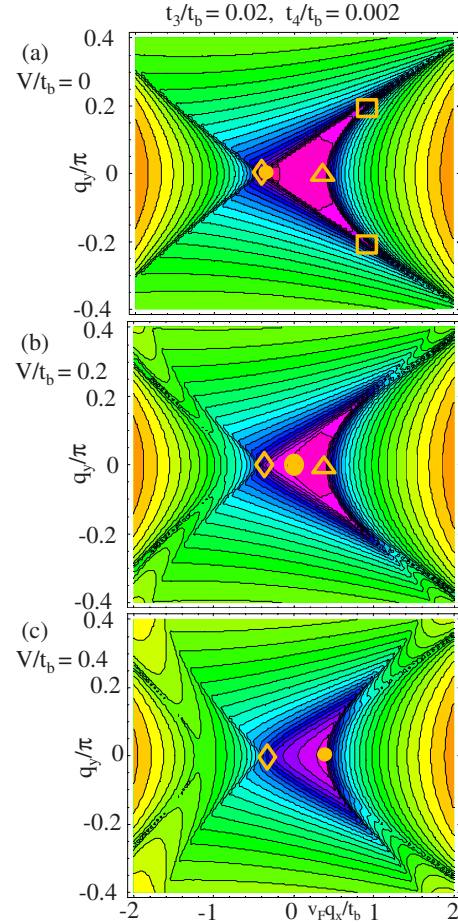


FIG. 21. (Color online) The same as Fig. 20 with  $t'_b/t_b=0.1$ ,  $t_3/t_b=0.02$ , and  $t_4/t_b=0.002$ .

than 0.03 K/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 0.000 09 K/s) (Ref. 38). It is expected that the magnitude of the periodic potential  $V$  becomes larger at the slower cooling rate. Therefore, we can conclude from the existence of the negative Hall effect in  $(\text{TMTSF})_2\text{ClO}_4$  that  $V<2t'_b-2t_4$ . The value of  $V$  estimated from the magnetic-field-angle dependence of the conductivity<sup>34-36</sup> is close to the border of this condition.

## VI. SUMMARY AND DISCUSSIONS

We have studied the nesting vector and  $\chi_0(\mathbf{Q})$  in the quasi-one-dimensional systems having the imperfectly nested Fermi surface (the imperfectness is measured by  $t'_b$ ). We have obtained the plateaulike maximum of  $\chi_0(\mathbf{Q})$  when  $\mathbf{Q}$  is in the *sweptback* region with the apexes  $\mathbf{q}_1$  and  $\mathbf{q}_4$ . The absolute maximum of  $\chi_0(\mathbf{Q})$  is obtained near but not at  $\mathbf{Q}=\mathbf{Q}_0+\mathbf{q}_4$  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  $(\text{TMTSF})_2\text{ClO}_4$ ], the sweptback region (with apexes  $\mathbf{q}_2$  and  $\mathbf{q}_4$ ) becomes smaller as  $V$  increases and shrinks to  $\mathbf{q}_3$  when  $V=4t'_b$ . The best nesting vector moves to  $\mathbf{Q} \approx \mathbf{Q}_0+\mathbf{q}_3$ . The absolute maximum of  $\chi_0(\mathbf{Q})$  is located at  $\mathbf{Q}=\mathbf{Q}_0+\mathbf{q}_3$  when  $V>4t'_b$ . The negative Hall coefficient observed in the field-

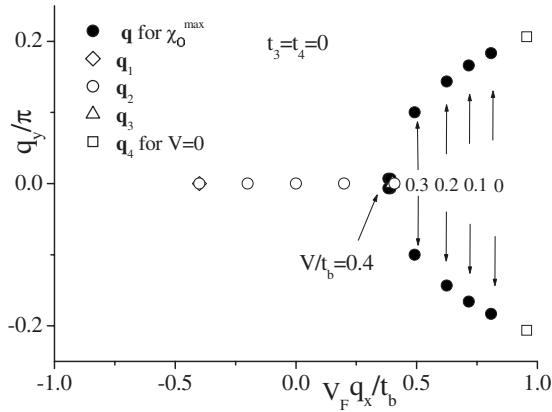


FIG. 22. Open diamond, open triangle, and open squares are  $\mathbf{q}_1$ ,  $\mathbf{q}_3$ , and  $\mathbf{q}_4$  for  $V=0$ , respectively. Open circles and closed circles are  $\mathbf{q}_2$  and the locations of the maximum of  $\chi_0(\mathbf{Q})$  (best nesting vector), respectively, for  $V/t_b=0, 0.1, 0.2, 0.3$ , and  $0.4$ . We take  $t'_b/t_b=0.1$  and  $t_3=t_4=0$ .

induced spin-density wave states in some region of the magnetic field is shown to be possible only when  $V < 2t'_b - 2t_4$ , in which case the vectors  $\mathbf{q}$ 's giving the plateaulike maximum of  $\chi_0(\mathbf{Q}_0 + \mathbf{q})$  (*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  $(\text{TMTSF})_2\text{ClO}_4$ , where the sign reversal of the Hall effect has been observed.

Recently, a lot of interest is attracted by the quasi-one-dimensional conductor  $(\text{Per})_2M(\text{mnt})_2$  (where  $\text{Per}=\text{perylene}$ ,

$\text{mnt}=\text{maleonitriledithiolate}$ , and  $M=\text{Au}$  and  $\text{Pt}$ ) (Refs. 42–46). The charge-density wave (CDW) state is realized in  $(\text{Per})_2M(\text{mnt})_2$  and the successive transitions of the field-induced CDW has been observed in high magnetic field<sup>42</sup> in contrast to the field-induced SDW in  $(\text{TMTSF})_2\text{ClO}_4$ . This material has a similar band structure as  $(\text{TMTSF})_2\text{ClO}_4$ , but the origin of the pairs of the quasi-one-dimensional Fermi surface in  $(\text{Per})_2M(\text{mnt})_2$  is different from that in  $(\text{TMTSF})_2\text{ClO}_4$ . The origin of the four pairs of the quasi-one-dimensional Fermi surface in  $(\text{Per})_2M(\text{mnt})_2$  is the existence of four perylene molecules in the unit cell in the perpendicular plane to the conduction axis,<sup>46</sup> while the origin of the two pairs of the quasi-one-dimensional Fermi surface in  $(\text{TMTSF})_2\text{ClO}_4$  is the periodic potential caused by the anion ordering. It will be interesting to study the similarity and the difference between the two materials, since the spin susceptibility  $\chi_0(\mathbf{Q})$  and the charge susceptibility  $\chi_c(\mathbf{Q})$  for the noninteracting system have the same  $\mathbf{Q}$  dependence caused by the nesting properties of the Fermi surface, except for the effects of the Zeeman splitting of the Fermi surface, which play an important role only for CDW.

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