Interference Commensurate Oscillations in Quasi-One-Dimensional Conductors

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We suggest an analytical theory to describe angular magnetoresistance oscillations recently discovered in the quasi-one-dimensional conductor $(TMTSF)_2PF_6$ [see Phys. Rev. B **57**, 7423 (1998)] and define the positions of the oscillation minima. The origin of these oscillations is related to interference effects resulting from Bragg reflections which occur as electrons move along quasiperiodic and periodic ("commensurate") electron trajectories in the extended Brillouin zone. We reproduce via calculations existing experimental data and predict some novel effects.

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Quasi-one-dimensional (Q1D) organic conductors $(TMTSF)_2X$ ($X = PF_6$, ClO_4, etc.) demonstrate a variety of unique properties in a magnetic field in their superconducting [1–3], field-induced spin-density wave [1–3], and metallic [1–22] phases, including evidence for non-Fermi-liquid (nFL) behavior [3,9,20–22]. In the metallic phase [1–22], the Q1D electron spectra [1–3] of these compounds,

$$\epsilon^{\pm}(\mathbf{p}) = \pm v_F(p_x \mp p_F) + 2t_b \cos(p_y b^*) + 2t_c \cos(p_z c^*),$$
$$v_F p_F \gg t_b \gg t_c, \tag{1}$$

are characterized by two open sheets of Fermi surface (FS). Therefore, traditional magnetic oscillations (related to Landau quantization) [23] cannot exist in these materials. [Here + (−) stands for the right (left) sheet of the Fermi surface, v_F and p_F are the Fermi velocity and Fermi momentum, respectively; t_b and t_c are the overlapping integrals between electron wave functions; $\hbar \equiv 1$].

Surprisingly, the metallic phase of the $(TMTSF)_2X$ materials exhibits a number of unconventional magnetic oscillations related to an open Q1D FS (1). Among them are "magic angles" (MA) [1–9], the first angular oscillations with a clear Fermi-liquid (FL) physical meaning—Danner-Kang-Chaikin (DKC) oscillations [10], the "third angular effect" [11–19], and rich angular oscillations recently discovered by Lee and Naughton [12,15,16] in $(TMTSF)_2PF_6$ and Yoshino *et al.* [17] in $(DMET)_2I_3$. We call the latter "interference commensurate" (IC) oscillations which reflects their physical meaning revealed in this Letter.

Pioneering numerical solutions [15,16,18,19] of the Boltzmann kinetic equation for Q1D metal (1) in the extended Brillouin zone in an inclined magnetic field,

$$\mathbf{H} = H(\cos\theta \cos\phi, -\cos\theta \sin\phi, \sin\theta), \tag{2}$$

have given a hint on the FL nature of the IC oscillations. Nevertheless, due to the very complex behavior of these oscillations, their physical meaning has not been revealed and their properties have not been described in detail. In particular, a hypothesis [15,19] that minima in resistivity $\rho_{zz}(\mathbf{H})$ correspond to some "commensurate" directions of a magnetic field,

$$\sin\phi = N\left(\frac{b^*}{c^*}\right)\tan\theta \tag{3}$$

(where N is an integer) has not been theoretically proven.

The goals of our Letter are (i) to derive an analytical expression for $\rho_{zz}(\mathbf{H})$ and to define the positions of its minima; (ii) to reveal the interference nature of the IC oscillations; (iii) to compare our results with experiment [15]; and (iv) to predict some novel qualitative effects. In particular, we demonstrate that the origin of the IC oscillations is related to special commensurate electron trajectories in a magnetic field (different from the MA trajectories [4]), where an average electron velocity along the $\mathbf{z}(\mathbf{c}^*)$ axis is nonzero, $\langle v_z(t)\rangle_t \neq 0$. Note that an importance of this condition for low-dimensional conductors was pointed out by DKC [10], Osada *et al.* [24], and Kartsovnik and Yakovenko *et al.* [25] in different contexts.

Below, we consider the most general electron trajectories, characterized by two angles, θ and ϕ [see Eq. (2)]. We show that they correspond to two novel types of angular magnetic oscillations: some commensurate oscillations and "generalized DKC" oscillations [26]. In particular, we demonstrate that $\rho_{zz}(\mathbf{H})$ in this case is defined by quasiclassical interference effects related to periodic and quasiperiodic electron trajectories along the open Q1D FS (1) in the extended Brillouin zone [27]. For small values of θ [see Eq. (2)], these effects occur between some narrow areas on the Q1D FS (1) (i.e., "effective stripes" parallel to the $\mathbf{p}_z$ axis), with their positions being dependent on magnetic field orientation. These unique features demonstrate an unusual physical meaning of the IC oscillations. We also show that the commensurate directions of a magnetic field (3) indeed correspond to minima in $\rho_{zz}(\mathbf{H})$ at large enough θ, whereas at smaller θ ($|\theta| \leq 5°$ in our case), $\rho_{zz}(\mathbf{H})$ minima occur for only even or only odd values of N in Eq. (3), depending on the particular value of θ [see Fig. 1(b)].

Let us discuss the physical meaning of the IC oscillations by analyzing electron trajectories in an inclined

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magnetic field (2), where trajectories are solutions of the equations of motion [23]:

$$d\mathbf{p}/dt = (e/c)[\mathbf{v}(\mathbf{p}) \times \mathbf{H}], \qquad \mathbf{v}(\mathbf{p}) = d\epsilon(\mathbf{p})/d\mathbf{p}. \quad (4)$$

For Q1D electron spectrum (1), Eqs. (4) can be rewritten as follows:

$$d(p_y b^*)/dt = \omega_b(\theta),$$
$$d(p_z c^*)/dt = \omega_c(\theta, \phi) - \omega_c^*(\theta, \phi)\sin(p_y b^*), \quad (5)$$

where

$$\omega_b(\theta) = ev_F H b^* \sin\theta/c,$$
$$\omega_c(\theta, \phi) = ev_F H c^* \cos\theta \sin\phi/c,$$
$$\omega_c^*(\theta, \phi) = (v_y^0/v_F)(ev_F H c^*/c)\cos\theta\cos\phi, \quad (6)$$
$$v_y^0 = 2t_b b^*.$$

From Eqs. (5), one defines electron trajectories in a reciprocal plane (p_y, p_z):

$$p_z c^* = p_z^0 c^* + \frac{\omega_c(\theta, \phi)}{\omega_b(\theta)}(p_y - p_y^0)b^* + \frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)}[\cos(p_y b^*) - \cos(p_y^0 b^*)], \quad (7)$$

with a velocity component along the $\mathbf{z}$ axis being

$$v_z(p_y) = -2t_c c^* \sin\left(p_z^0 c^* + \frac{\omega_c(\theta, \phi)}{\omega_b(\theta)}(p_y - p_y^0)b^* + \frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)}[\cos(p_y b^*) - \cos(p_y^0 b^*)]\right),$$
$$p_y \sim t. \quad (8)$$

Note that electron trajectories in a reciprocal plane (p_y, p_z) become periodic for commensurate directions of a magnetic field (3). Thus, an average velocity over electron path [28],

$$\langle v_z(t)\rangle_t \sim \sin\left[p_z^0 c^* - \frac{\omega_c(\theta, \phi)}{\omega_b(\theta)}p_y^0 b^* - \frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)}\cos(p_y^0 b^*)\right] \times J_N\left[\frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)}\right] \quad (9)$$

(which is zero for all "noncommensurate" trajectories), for commensurate orbits (3) and (7), becomes zero only at zero values of the N-order Bessel functions:

$$J_N\left[\frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)}\right] \equiv J_N\left[\frac{2t_b c^* \cos\phi}{v_F \tan\theta}\right] = 0. \quad (10)$$

Therefore, there appear maxima in $\sigma_{zz}(\theta, \phi)$ [i.e., minima in $\rho_{zz}(\theta, \phi)$] at commensurate angles (3) [see Figs. 1(b) and 1(c)] which are a novel type of angular magnetic oscillation. In a similar way, Bessel function zeros (10) lead to the appearance of maxima in $\rho_{zz}(\mathbf{H})$ which are a generalization of the DKC oscillations corresponding to $N = 0$ in Eq. (10). In other words, the IC oscillations are characterized by minima in $\rho_{zz}(\mathbf{H})$ at commensurate angles (3) which are modulated by oscillatory Bessel functions (10).

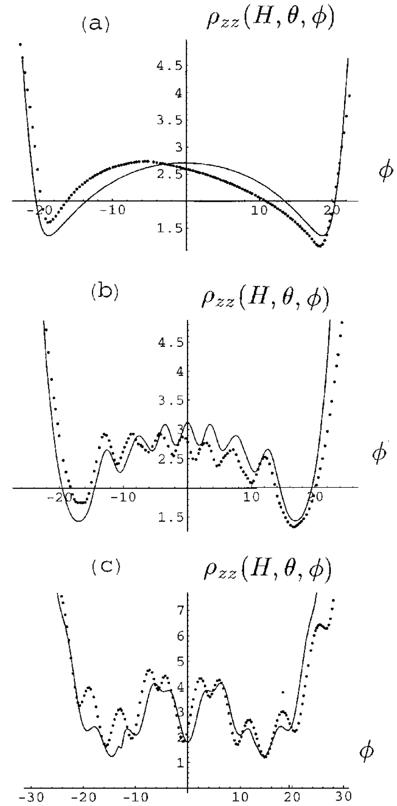

FIG. 1. IC oscillations of resistivity $\rho_{zz}(\theta, \phi)$ calculated for (a) $\theta = 0°$, (b) $\theta = 3°$, and (c) $\theta = 9°$ by means of Eq. (17) (solid lines) are compared with the experimental data [15] (dotted lines). Note that at $\theta = 9°$ ρ_{zz} minima occur at all integers N in Eq. (3), whereas at $\theta = 3°$ they correspond only to odd integers N in Eq. (3).

To develop an analytical theory of the IC oscillations and to further demonstrate their quantum interference nature, we make use of the Peierls substitution method [23], $\mathbf{p} \to \mathbf{P} - (e/c)\mathbf{A}$, for electron motion in the extended Brillouin zone [29]. We choose a vector potential of magnetic field (2), in the following form:

$$\mathbf{A} = (0, x\sin\theta, x\cos\theta\sin\phi + y\cos\theta\cos\phi)H. \quad (11)$$

In this case, electron wave functions in a mixed (p_y, x) representation [29], $\Psi_\epsilon^\pm(p_y, x) = \exp(\pm i p_F x)\psi_\epsilon^\pm(p_y, x)$, are solutions of the Schrödinger equations,

$$\left(\mp i v_F \frac{d}{dx} + 2t_b \cos\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right]\right)\psi_\epsilon^\pm(p_y, x) = \epsilon\psi_\epsilon^\pm(p_y, x), \quad (12)$$

and can be expressed as

$$\psi_{\epsilon}^{\pm}(p_y, x) = \exp\left(\pm i\frac{\epsilon}{v_F}x\right)\exp\left[\pm\frac{2it_b}{\omega_b(\theta)}\left(\sin\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right] - \sin[p_y b^*]\right)\right]. \quad (13)$$

Note that the **z** component of the quasiclassical velocity operator, $\hat{\mathbf{v}}(\mathbf{p}) = d\hat{\epsilon}(\mathbf{p})/d\mathbf{p}$ [23], in gauge (11) is equal to

$$\hat{v}_z(p_z, x, y) = -2t_c c^* \sin\left[p_z c^* - \frac{\omega_c(\theta,\phi)x}{v_F} - \frac{\omega_c^*(\theta,\phi)y}{2t_b b^*}\right], \quad y = i\frac{d}{p_y}. \quad (14)$$

It is possible to show that wave functions (13) are eigenfunctions of velocity operator (14) with their eigenvalues and expectation values being

$$\hat{v}_z(p_z, x, p_y)\psi_{\epsilon}^{\pm}(p_y, x) = -2t_c c^* \sin\left[p_z c^* - \frac{\omega_c(\theta,\phi)x}{v_F} \pm \frac{\omega_c^*(\theta,\phi)}{\omega_b(\theta)}\left(\cos\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right] - \cos[p_y b^*]\right)\right]\psi_{\epsilon}^{\pm}(p_y, x), \quad (15)$$

$$\langle v_z(p_y, p_z)\rangle \sim \lim_{N\to\infty}\frac{1}{2N}\int_{-\pi v_F/\omega_b(\theta)}^{+\pi v_F/\omega_b(\theta)} dx \sum_{n=-N}^{N}\sin\left[p_z c^* - \frac{\omega_c(\theta,\phi)x}{v_F} - 2\pi n\frac{\omega_c(\theta,\phi)}{\omega_b(\theta)} \pm \frac{\omega_c^*(\theta,\phi)}{\omega_b(\theta)}\left(\cos\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right] - \cos[p_y b^*]\right)\right]. \quad (16)$$

Since wave functions (13) and their matrix elements (15) and (16) are known, $\sigma_{zz}(H,\theta,\phi)$ can be evaluated by means of the Kubo formalism. After straightforward but rather complicated calculations, we obtain

$$\frac{\sigma_{zz}(H,\theta,\phi)}{\sigma_{zz}(0)} = \sum_{N=-\infty}^{+\infty}\left(\frac{J_N^2[\omega_c^*(\theta,\phi)/\omega_b(\theta)]}{1+\tau^2[\omega_c(\theta,\phi) - N\omega_b(\theta)]^2}\right), \qquad \rho_{zz}(H,\theta,\phi) \simeq \frac{1}{\sigma_{zz}(H,\theta,\phi)}, \quad (17)$$

where τ is an electron relaxation time.

To summarize, Eq. (17) provides analytical expressions for the experimentally measured resistivity $\rho_{zz}(H,\theta,\phi)$ [15,16]. As is seen from Eq. (17), $\sigma_{zz}(H,\theta,\phi)$ possesses maxima [i.e., $\rho_{zz}(H,\theta,\phi)$ possesses minima] at $\omega_c(\theta,\phi) = N\omega_b(\theta)$ if $\omega_c(\theta,\phi)$, $\omega_b(\theta) \geq 1/\tau$. This coincides with the "commensurability" condition (3). It is important to note that this theory, based on Eq. (17), predicts no angular oscillations [30] at MA directions of a magnetic field [4] (i.e., at $\phi = \pi/2$) since $\omega_c^* = 0$ in Eq. (17). Therefore, the previous interpretation [15–19] of the IC oscillations as a simple combination of the MA effects and the DKC oscillations is too oversimplified.

The interference nature of the IC oscillations is directly seen from Eq. (16). Indeed, the expectation values of the velocity operator (15) are defined by a summation of an infinite number of electron waves with their relative phases, $2\pi n[\omega_c(\theta,\phi)/\omega_b(\theta)]$, being dependent on the orientation of the magnetic field (2). From a physical point of view, these interference effects are due to multiple Bragg reflections of electron waves from Brillouin zone boundaries which occur as electrons move along open orbits in the extended Brillouin zone.

Let us consider Eq. (17) at small enough angles, $\phi \ll \pi/2$ and $\theta \ll 2t_b c^*/v_F$. In this case, one can make use of an asymptotic expression for the Bessel functions in Eqs. (10) and (17): $J_N(2t_b c^*/v_F \tan\theta) \simeq \cos(2t_b c^*/v_F \tan\theta - \pi/4 - \pi N/2)$. Therefore, depending on the value of parameter $2t_b c^*/v_F \tan\theta$, the Bessel functions of even order are larger than those of odd order or vice versa. At $\omega_c\tau$, $\omega_b\tau \simeq 1$, this results in the appearance of minima of $\rho_{zz}(\phi,\theta)$ in Eq. (17) for strictly even or strictly odd values of the integer N. We call this phenomenon "even-odd" angular resonance (see Fig. 1(b)). It is important that Eq. (17) demonstrates also another kind of angular oscillation (i.e., "extended DKC" oscillations [26]) related to zeros of the Bessel functions (10). By analyzing Eq. (17), it is possible to show that $\rho_{zz}(H,\theta,\phi)$ is characterized by an unusual linear behavior for "noncommensurate" directions of a magnetic field and small $\theta \ll 2t_b b^*/v_F$,

$$\rho_{zz}(H,\theta,\phi) \sim |H|, \quad (18)$$

whereas, for commensurate directions (3), $\rho_{zz}(H,\theta,\phi)$ saturates with increasing magnetic field.

In Fig. 1, we compare the experimental data [15] with Eq. (17) using the same values of parameters, $t_a/t_b = 8.5$ and $\omega_b(\theta = 0, \phi = \pi/2, H = 7T)\tau = 15$, for all three theoretical curves. These curves not only demonstrate qualitative but quantitative agreement between theory (17) and experiment [15], in a broad region of magnetic field orientations, $\phi \leq 20°$. Note that, for $\theta = 3°$, $\rho_{zz}(H,\theta,\phi)$ minima appear both theoretically and experimentally only for odd integers N in Eq. (3) [see Fig. 1(b)] which is in agreement with the "odd" angular resonance effect discussed above. The agreement is markedly better than what has been achieved with numerical solutions of the kinetic equation [15–19], which do not account in full for the interference nature of the IC oscillations, particularly at small angles θ. We have initiated more detailed experiments [32] to try to confirm other effects predicted in this Letter such as "even" angular resonance, generalized DKC oscillations (10), and linear magnetoresistance (18).

Let us discuss peculiarities of the interference effects at small angles $\theta \ll 2t_b b^*/v_F$ in a clean limit where $\omega_c(\theta, \phi)\tau, \omega_b(\theta)\tau \to \infty$. In this case, the integral (16) can be evaluated by means of the stationary-phase method and is determined by the close proximity of the following two series of "effective stripes" (ES) in (p_y, p_z, x) space:

$$\omega_b(\theta)z_n/v_F = \arcsin[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)] + 2\pi n, \quad z = x - v_F p_y b^*/\omega_b(\theta), \tag{19}$$

$$\omega_b(\theta)z_n/v_F = \pi - \arcsin[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)] + 2\pi n, \quad z = x - v_F p_y b^*/\omega_b(\theta), \tag{20}$$

where n is an integer. The contributions to (16) from the ES (19) and (20) are characterized by nonzero phase shifts with their values being dependent on magnetic field orientation (2). Note that these phase shifts are integer values of 2π for different n in Eqs. (19) and (20) only at $\omega_c(\theta, \phi) = N\omega_b(\theta, \phi)$. Therefore, at small angles θ, the IC oscillations (3) and (10) can be interpreted in terms of interference effects between these two infinite series of electron waves (19) and (20).

Finally, we suggest an experimental study of the IC oscillations as a test of FL versus nFL behavior in low-dimensional $(TMTSF)_2X$ and $(ET)_2X$ conductors. Indeed, a comparison of our theory with experiment [15] shows the validity of a FL description in $(TMTSF)_2PF_6$ under 8.3 kbar pressure [15], whereas it is claimed to be broken in the same compound at higher pressures [3,9,20–22], where DKC and IC oscillations are not observed [20].

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