Interference Commensurate Oscillations in Q1D Conductors

A.G. Lebed\textsuperscript{1,2} and M.J. Naughton\textsuperscript{1}

\textsuperscript{1}Department of Physics, Boston College, Chestnut Hill, MA 02467, USA and
\textsuperscript{2}Landau Institute for Theoretical Physics, 2 Kosygina Street, 117334 Moscow, Russia

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Abstract

We suggest an analytical theory to describe angular magnetic oscillations recently discovered in quasi-one-dimensional conductor (TMTSF)$_2$PF$_6$ [see Phys. Rev. B \textbf{57}, 7423 (1998)] and define the positions of the oscillation minima. The origin of these oscillations is related to interference effects resulting from an interplay of quasi-periodic and periodic ("commensurate") electron trajectories in an inclined magnetic field. We reproduce via calculations existing experimental data and predict some novel effects.
Quasi-one-dimensional (Q1D) organic conductors (TMTSF)$_2$X (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 [4-22,1-3] phases. In the metallic phase [4-22,1-3], the Q1D electron spectra [1-3] of these compounds, 

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

are characterized by two open sheets of Fermi surface (FS). Therefore, traditional magnetic oscillations (related to Landau level 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 phases of (TMTSF)$_2$X materials exhibit a number of unconventional magnetic oscillations related to an open Q1D FS (1). Among them are ”magic angles” (MA) [4-9,1-3], the first angular oscillations with a clear Fermi-liquid (FL) physical meaning - Danner-Kang-Chaikin (DKC) oscillations [10], the ”third angular effect” (TAE) [11-19], and rich angular oscillations recently discovered by Lee and Naughton [12,15,16] in (TMTSF)$_2$PF$_6$ and by Yoshino et al. [17] in (DMET)$_2$I$_3$. We call the latter ”interference commensurate” (IC) oscillations which reflects their physical meaning revealed in this Letter. Note that, despite all these observations of different magnetic oscillations [4-19], a question on the existence or not of FL behavior in Q1D metallic phases of (TMTSF)$_2$X conductors is still controversial [3,9,20-22].

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

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

have given a hint on the FL nature of the IC oscillations. Nevertheless, due to 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] that minima of resistivity $\rho_{zz}(\mathbf{H})$ correspond to some ”commensurate” directions of a magnetic field,

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

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

The goals of our Letter are: 1) to derive an analytical expression for $\rho_{zz}(\mathbf{H})$ and to define the positions of its minima; 2) to reveal a quantum interference nature of the IC oscillations, 3) to compare our results with experiment [15], and 4) 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 $z(c^*)$-axis is non-zero, $\langle v_z(t) \rangle_t \neq 0$ (see Fig.1). Note that an importance of this condition for low-dimensional conductors was pointed out by DKC [10], Osada et al. [24], and by Kartsovnik and Yakovenko et al. [25] in different context.

Below, we consider the most general electron trajectories, characterized by two angles, $\theta$ and $\phi$ [see Eq. (2)]. We show that they correspond to two novel types of angular magnetic oscillations: "commensurate" oscillations and some "generalized DKC" oscillations. In particular, we demonstrate that $\rho_{zz}(H)$ in this case is defined by quantum interference effects related to periodic and quasi-periodic electron motion along the open Q1D FS (1). For small values of $\theta$ [see Eq.(2)], these effects occur between some narrow areas on the Q1D FS (1) [i.e., "effective stripes" (ES) parallel to $p_z^*$-axis ], with their positions being dependent on the magnetic field orientation (see Fig.1c). 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 $\rho_{zz}(H)$ at large enough $\theta$, whereas at smaller $\theta$ ($|\theta| \leq 5^\circ$ in our case) $\rho_{zz}(H)$ minima occur for only even or only odd values of $N$ in Eq. (3), depending on the particular value of $\theta$.

Let us discuss the physical meaning of the IC oscillations by analyzing quasi-classical electron trajectories in an inclined magnetic field (2). As usual, the trajectories are solutions of the equations of motion [23]:

$$\frac{dp}{dt} = \left(\frac{e}{c}\right)[v(p) \times H] , \quad v(p) = \frac{dc(p)}{dp} . \quad (4)$$

For Q1D electron spectrum (1), Eqs.(4) can be rewritten as follows [26]:

$$d(p_yb^*)/dt = \omega_b(\theta) , \quad d(p_zc^*)/dt = \omega_c(\theta, \phi) - \omega^*_c(\theta, \phi) \sin(p_yb^*) , \quad (5)$$

where

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

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

$$p_zc^* = p_0^c c^* + \frac{\omega_c(\theta, \phi)}{\omega_b(\theta)}(p_y - p_0^y) b^* + \frac{\omega^*_c(\theta, \phi)}{\omega_b(\theta)}[\cos(p_yb^*) - \cos(p_0^yb^*)] , \quad (7)$$

with a velocity component along the $z$-axis being

$$v_z(p_y) = -2tc^* \sin \left( p_0^c c^* + \frac{\omega_c(\theta, \phi)}{\omega_b(\theta)}(p_y - p_0^y) b^* + \frac{\omega^*_c(\theta, \phi)}{\omega_b(\theta)}[\cos(p_yb^*) - \cos(p_0^yb^*)] \right) , \quad p_y \sim t. \quad (8)$$
Note that electron trajectories in a reciprocal plane \((p_y, p_z)\) become periodic [27] for "commensurate" directions of a magnetic field (3) (see Figs.1a,b). Therefore, an average velocity over electron path,

\[
<v_z(t)>_t \approx \sin \left[ p_y^b c^* - \frac{\omega_c(\theta, \phi)}{\omega_b(\theta)} p_y^b \cos(p_y^b c^*) \right] J_N \left[ \frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)} \right], \tag{9}
\]

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

\[
J_N \left[ \frac{\omega_c^*(\theta, \phi)}{\omega_b(\theta)} \right] = 0 . \tag{10}
\]

From general metals theory [23,10], it is known that \(<v_z(t)>_t \neq 0\) results in saturating behavior of the conductivity \(\sigma_{zz}(\theta, \phi)\) for high magnetic fields, whereas, at \(<v_z(t)>_t = 0, \sigma_{zz}(\theta, \phi)\) decreases with increasing field. Therefore, there appear maxima in \(\sigma_{zz}(\theta, \phi)\) [i.e., minima in \(\rho_{zz}(\theta, \phi)\)] at "commensurate" angles (3) (see Fig.2) which are a novel type of angular magnetic oscillations. In a similar way, Bessel functions zeros (10) lead to the appearance of maxima in \(\rho_{zz}(H)\) (see Fig.2) 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 \(\rho_{zz}(H)\) at "commensurate" angles (3) which are modulated by oscillatory Bessel functions (10).

Let us discuss electron motion along the \(z\)-axis in real space, \(z(t) = \int_0^t v_z(t') dt'\). Here, contributions to \(z(t)\) from different Brillouin zones [see Eq.(8)] are in-phase for "commensurate" trajectories (3) (see Fig.1c). These interference effects correspond to maxima of conductivity \(\sigma_{zz}(\theta, \phi)\) [i.e., minima of resistivity \(\rho_{zz}(\theta, \phi)\)] (see Fig. 2). For \(\omega_c^*(\theta, \phi)/\omega_b(\theta) \gg 1\) (i.e., for small \(\phi\)), the integral \(z(t) = \int_0^t v_z(t') dt'\) can be evaluated by means of the stationary-phase method and is determined by interference effects between some ES located near the points \(p_y b^* = \arcsin[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)] + 2\pi n\) and \(p_y b^* = \pi - \arcsin[\omega_c^*(\theta, \phi)/\omega_c(\theta, \phi)] + 2\pi n\) on Q1D FS (1) (see Fig.1c), where \(n\) is an integer.

To develop an analytical theory of the IC oscillations and to further demonstrate their quantum interference nature, we make use of the quasi-classical approximation for electron motion [23,28], where a magnetic field is introduced by the Peierls substitution [23,28], \(p \rightarrow \mathbf{P} - (e/c)\mathbf{A}\). We choose a vector-potential of magnetic field (2), in the following form

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

In this case, electron wave functions in a mixed \((p_y, x)\)-representation [28], \(\Psi_{\epsilon}^\pm(p_y, x) = \exp(\pm ip_F x)\psi_{\epsilon}^\pm(p_y, x)\), are solutions of the Schrodinger equations [28],

\[
\left( -i v_F \frac{d}{dx} + 2t_b \cos \left[ p_y b^* - \frac{\omega_b(\theta)x}{v_F} \right] \right) \psi_{\epsilon}^\pm(p_y, x) = \epsilon \psi_{\epsilon}^\pm(p_y, x) , \tag{12}
\]
and can be expressed as

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

Note that the z-component of the quasi-classical velocity operator, \( \hat{v}(p) = d\hat{\epsilon}(p)/dp \) [23], in a gauge (11) is equal to

$$\hat{v}_z(p_z, x, y) = -2t_c c^* \sin \left[p_z c^* - \frac{\omega_c(\theta, \phi) x}{v_F} - \frac{\omega^*_c(\theta, \phi) y}{v_y^0}\right], \quad y = i \frac{d}{p_y}. \quad (14)$$

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

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

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

$$\sigma_{zz}(H, \theta, \phi) \sim \int_0^{2\pi} d(p_y b^*) \int_0^\infty dx \exp\left(-\frac{x}{v_F \tau}\right) \times \cos\left(-\frac{\omega_c(\theta, \phi) x}{v_F} + \frac{\omega^*_c(\theta, \phi)}{\omega_b(\theta)} \left[\cos \left(p_y b^* - \frac{\omega_b(\theta) x}{v_F}\right) - \cos[|p_y b^*|]\right]\right), \quad (16)$$

where \( \tau \) is an electron relaxation time. Double integral (16) can be rewritten in a simple form:

$$\sigma_{zz}(H, \theta, \phi) = \sigma_{zz}(0) \sum_{N=-\infty}^{+\infty} \frac{J^2_N[\omega^*_c(\theta, \phi)/\omega_b(\theta)]}{1 + \tau^2[\omega_c(\theta, \phi) - N\omega_b(\theta)]^2}, \quad (17)$$

where for a Q1D conductor (1):

$$\rho_{zz}(H, \theta, \phi) \simeq 1/\sigma_{zz}(H, \theta, \phi). \quad (18)$$

To summarize, Eqs.(17) and (18) provide analytical expressions for 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 Eqs.(17),(18), predicts no angular oscillations [29] 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. We also stress that the integration of the quasi-periodic function in Eq.(16) corresponds to interference effects in matrix elements of velocity operator (15) and, thus, directly demonstrates the interference nature of the IC oscillations. Indeed, two different periods in Eq.(16) become commensurate at 
\[ \omega_c(\theta, \phi) = N \omega_b(\theta, \phi) \] [i.e., for "commensurate" trajectories (3)] and, therefore, the integral (16) is increased due to these interference effects.

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),(17):
\[ J_N(2t_b c^*/v_F \tan \theta) \approx \cos(2t_b c^*/v_F \tan \theta - \pi/4 - \pi N/2). \]
Therefore, depending on the value of parameter \( 2t_b c^*/v_F \tan \theta \), the Bessel functions of even orders are bigger than those of odd orders or vice versa. At \( \omega_c \tau, \omega_b \tau \approx 1 \), this results in the appearance of minima of \( \rho_{zz}(\phi, \theta) \) in Eqs.(17),(18) only for all even or only for all odd values of the integer \( N \). We call this phenomenon "even-odd" angular resonance (see Fig.2b). It is important that Eq.(17) demonstrates also another kind of angular oscillations (i.e., "extended DKC" oscillations) related to zeros of the Bessel functions (10). By analyzing Eqs.(16)-(18), it is possible to show that \( \rho_{zz}(H, \theta, \phi) \) is characterized by an unusual linear behavior for "non-commensurate" directions of a magnetic field and small \( \theta \ll 2t_b b^*/v_F \),
\[ \rho_{zz}(H, \theta, \phi) \sim |H|, \] whereas, for commensurate directions (3), \( \rho_{zz}(H, \theta, \phi) \) saturates with increasing magnetic field. The latter effect is different from the linear magnetoresistance predicted in Ref. [14].

In Fig.2, we compare the experimental data [15] with Eqs. (17),(18) using the same values of parameters, \( t_a/t_b = 8.5 \) and \( \omega_c(\theta = 0, \phi = \pi/2, H = 1 \ T) \tau = 15 \), for all three theoretical curves. These curves not only demonstrate qualitative but quantitative agreement between theory (17),(18) and experiment [15], in a broad region of magnetic field orientations, \( \phi \leq 20^\circ \) [26]. Note that, for \( \theta = 3^\circ \), \( \rho_{zz}(H, \theta, \phi) \) minima appear both theoretically and experimentally only for odd integers \( N \) in Eq.(3) [see Fig.(2)] which is an agreement with the "odd" angular resonance effect discussed above. The agreement is far 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. We have initiated more detailed experiments to try to confirm other effects predicted in the Letter such as "even" angular resonance, "generalized DKC" oscillations (10), and linear magnetoresistance (19).

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 points" (EP) in \( (p_y, x) \)-space:
\[ \omega_b(\theta) z_n/v_F = \arcsin[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)] + 2\pi n, \ z = x - v_F p_y b^*/\omega_b(\theta), \quad (20) \]
\[
\omega_b(\theta) z_n/v_F = \pi - \arcsin\left[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)\right] + 2\pi n, \quad z = x - v_F p_y b^*/\omega_b(\theta),
\] (21)

where \(n\) is an integer. In quantum mechanical language, these EP (20),(21) correspond to ES on the Q1D FS (1) discussed above. The contributions to (16) from the EP (20),(21) are characterized by non-zero phase shifts with their values being dependent on magnetic field orientation (2). Note that these phase shifts are integer values of \(2\pi\) for different \(n\) in Eqs.(20),(21) only at \(\omega_c(\theta, \phi) = N\omega_b(\theta, \phi)\). Therefore, at small angles \(\theta\), the IC oscillations (3),(10) can be interpreted in terms of interference effects between these two infinite series of electron waves (20),(21). It is easy to show that, in our picture, different integers \(n\) in Eqs.(20),(21) correspond to different Brillouin zones for a quasi-classical electron motion picture in the extended Brillouin zone.

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FIG. 1: For a "commensurate" electron trajectory (a) shown in the extended Brillouin zone \((p_y, p_z)\) for \(N = 1\) and \(\omega_c^*(\theta, \phi)/\omega_b(\theta) = 15\) [see Eqs. (3),(7)], the velocity component \(v_z(t)\) (b) is a periodic function of \(t \sim p_y\) with an average value \(<v_z(t)>\) being given by Eq.(9). Electron transport along z-axis, \(z(t)\), (c) is a step-like function of \(t \sim p_y\) and is defined by the interference effects between "effective stripes" (ES) located near the following two series of points in the extended Brillouin zone:

\[
p_y = \arcsin[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)] + 2\pi n \quad \text{and} \quad p_y = \pi - \arcsin[\omega_c(\theta, \phi)/\omega_c^*(\theta, \phi)] + 2\pi n,
\]

where \(n\) is an integer. As it follows from Fig.1c, the ES are "in phase" in the extended Brillouin zone \((p_y, p_z)\) for the "commensurate" electron orbits given by Eq.(3).
FIG. 2: IC oscillations of resistivity $\rho_{zz}(\theta, \phi)$ calculated for (a) $\theta = 0^\circ$, (b) $\theta = 3^\circ$, and (c) $\theta = 9^\circ$ by means of Eqs. (17),(18) (solid lines) are compared with the experimental data [15] (dotted lines). Note that at $\theta = 9^\circ$ $\rho_{zz}$ minima occur at all integers $N$ in Eq.(3), whereas at $\theta = 3^\circ$ they correspond only to odd integers $N$ in Eq.(3).