Pis'ma v ZhETF, vol. 119, iss. 8, pp. 622 – 623

Theory of Lee–Naughton–Lebed's oscillations in moderately strong electric fields in layered quasi-one-dimensional conductors

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Submitted 4 March 2024
Resubmitted 23 March 2024
Accepted 28 March 2024

DOI: 10.31857/S123456782408010X, EDN: XKYXBQ

Metallic phases of layered quasi-one-dimensional (Q1D) organic materials are very unusual and demonstrate two original types of angular magnetic oscillations: the so-called Lebed's magic angles (LMA) [1] and the Lee–Naughton–Lebed's (LNL) oscillations [1–8]. As to the LMA effects, they still contain lots of unexplained features, whereas the LNL oscillations are well explained by present moment [6, 9–15]. More recently Kobayashi et al. in the pioneering work [16] have considered effects of moderately strong electric fields on the LNL phenomenon and, in particular, have experimentally shown that the strong electric field splits the LNL maxima of conductivity. The goal of our paper is to show that the hypothetical formula of [16] can be obtained by using some moderately high electric field approximation for quasi-classical extension of the Boltzmann kinetic equation.

Let us consider the following Q1D Fermi surface in a layered conductor in a tight-binding model:

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

Under the condition of the LNL experiment the Q1D conductor is placed in the inclined magnetic field,

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

whereas the constant electric field is applied perpendicular to the conducting layers,

$$\mathbf{E} = E\ (0, 0, 1). \tag{3}$$

In the so-called τ-approximation, the Boltzmann kinetic equation can be written as [10]:

$$\left\{e\mathbf{E} + \left(\frac{e}{c}\right)[\mathbf{v}(\mathbf{p}) \times \mathbf{H}]\right\}\frac{dn(\mathbf{p})}{d\mathbf{p}} = -\frac{n(\mathbf{p}) - n_0(\mathbf{p})}{\tau}. \tag{4}$$

Using the standard approach, we can now represent the quasi-classical Boltzmann kinetic equation (4) in the following form:

$$e\mathbf{E}\mathbf{v}(\mathbf{p})\left[\frac{dn_0(\epsilon)}{d\epsilon} - \frac{d^2n_0(\epsilon)}{d\epsilon^2}\Psi(\mathbf{p})\right] - \left\{e\mathbf{E} + \left(\frac{e}{c}\right)[\mathbf{v}(\mathbf{p}) \times \mathbf{H}]\right\}\frac{dn_0(\epsilon)}{d\epsilon}\frac{d\Psi(\mathbf{p})}{d\mathbf{p}} = \frac{dn_0(\epsilon)}{d\epsilon}\frac{\Psi(\mathbf{p})}{\tau}. \tag{5}$$

Note that the Boltzmann kinetic equation is usually studied in metals in small electric fields, whereas the magnetic fields can be strong. Therefore, there is usually considered a variant of the equation, which is linear with respect to the electric field. Since $\Psi(\mathbf{p})$ and $d\Psi(\mathbf{p})/d\mathbf{p}$ are both proportional to electric field, the following two terms

$$-e\mathbf{E}\mathbf{v}(\mathbf{p})\frac{d^2n_0(\epsilon)}{d\epsilon^2}\Psi(\mathbf{p}) - e\mathbf{E}\frac{dn_0(\epsilon)}{d\epsilon}\frac{d\Psi(\mathbf{p})}{d\mathbf{p}} \tag{6}$$

are usually omitted in the Boltzmann equation (5) (see, for example, [9, 10]). In this article, for the first time we theoretically consider the case of moderately strong electric fields, where we disregard the first term but keep the second one of the above mentioned two terms (6). It is easy to see that we can disregard the first term in Eq. (6), if it much less than the right side of Eq. (5):

$$\left|e\mathbf{E}\mathbf{v}(\mathbf{p})\frac{d^2n_0(\epsilon)}{d\epsilon^2}\Psi(\mathbf{p})\right| \ll \left|\frac{dn_0(\epsilon)}{d\epsilon}\frac{\Psi(\mathbf{p})}{\tau}\right|. \tag{7}$$

Since

$$|\mathbf{v}(\mathbf{p})| = |-2t_\perp d_\perp \sin(p_z d_\perp)| \sim t_\perp d_\perp \tag{8}$$

and

$$\left|\frac{d^2n_0(\epsilon)}{d\epsilon^2}\right| \sim \frac{1}{T}\left|\frac{dn_0(\epsilon)}{d\epsilon}\right|, \tag{9}$$

Equation (7) can be rewritten as

$$eE(t_\perp d_\perp)\tau \ll T. \tag{10}$$

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The physical meaning of Eqs. (7)–(10) is now clear. Electric field has to be small enough in order not to change electron energy on the scale of the temperature. As a result of disregarding the above discussed term in Eq. (5), instead of Eq. (5), we obtain

$$e\mathbf{E}\mathbf{v}(\mathbf{p})-\left\{e\mathbf{E}+\left(\frac{e}{c}\right)[\mathbf{v}(\mathbf{p})\times\mathbf{H}]\right\}\frac{d\Psi(\mathbf{p})}{d\mathbf{p}}=\frac{\Psi(\mathbf{p})}{\tau}. \quad (11)$$

It is important that Eq. (11) is different from the weak electric field approximation equations considered in [9, 10] and, thus, we call the former equation the quasiclassical kinetic equation for moderately strong electric fields.

Straightforward calculations [10] result in the following expression for the total conductivity:

$$\sigma_{zz}(\theta,\phi,E,H)=\frac{\sigma_{zz}(0)}{2}\sum_{n=-\infty}^{+\infty}J_n^2\left[\frac{\omega_c^*(\theta,\phi)}{\omega_b(\theta)}\right]\times\left\{\frac{1}{1+[\omega_c(\theta,\phi)+\omega_E-n\omega_b(\theta)]^2\tau^2}+\frac{1}{1+[\omega_c(\theta,\phi)-\omega_E-n\omega_b(\theta)]^2\tau^2}\right\}. \quad (12)$$

Note that Eq. (12) describes splitting of the LNL maxima of conductivity for the LNL oscillations (see Fig. 2 of [16]). Indeed, in pure layered Q1D metals it has two maxima at

$$\omega_c(\theta,\phi)=n\omega_b(\theta)\pm\omega_E \quad (13)$$

or

$$\tan(\theta^{\pm})\sin(\phi)=n\left(\frac{b^*}{d_\perp}\right)\pm\frac{Ec}{v_F H\cos(\theta)}, \quad (14)$$

where n is an integer. We note that, using Eq. (14) and experimental data on splitting the LNL maxima, the authors of work [16] evaluated the Fermi velocity v_F (1) in compound α-(BEDT-TTF)$_2$KHg(SCN)$_4$, corresponding to open sheets of the Fermi surface, $v_F \simeq \simeq 10^7$cm/s. We suggest to use the above described effect to determine Fermi velocities in other Q1D conductors, where heating of a sample under experiment allows to observe such splitting and where inequality (10) is fulfilled.

To summarize we stress that the derived above in moderately high electric fields (i.e., when inequality (10) is fulfilled). Eq. (12) was guessed in [16] as a strict equation, which is not correct. Although Eq. (12) coincides with Eq. (4) from [16], we have to check if inequality (10) is true under the experimental conditions of [16]. Indeed, the experimental conditions were the following: voltage $V = 2-20$ V, thickness of the sample $d = 0.1$ mm, temperature $T = 1.8$ K [16]. If we take into account the following band structure parameters of α-(BEDT-TTF)$_2$KHg(SCN)$_4$ organic material [16]: $d_\perp = 20$ Å [1] and $t_\perp \simeq 30\,\mu$eV [1], then at $V = 2$ V, Eq. (10) can be written as

$$eE(t_\perp d_\perp)\tau \simeq 0.14\text{ K} \ll T = 1.8\text{ K}, \quad (15)$$

whereas at $V = 20$ V both sides of Eq. (10) become of the same order. So, although the overall comparison of the experimental results [16] with the theoretical Eq. (12) can be justified at small voltages, at high voltages this has to be done with some caution.

The author is thankful to N. N. Bagmet (Lebed) for useful discussions.

Funding. This work was supported by ongoing University of Arizona funding. No additional grants to carry out or direct this particular research were obtained.

Conflict of interests. The author of this work declares that he has no conflicts of interest.

This is an excerpt of the article "Theory of Lee–Naughton–Lebed's oscillations in moderately strong electric fields in layered quasi-one-dimensional conductors". Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364024600915

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