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Quantum Theory of Lee-Naughton-Lebed's Angular Effect in Strong Electric Fields

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Abstract: Some time ago, Kobayashi et al. experimentally studied the so-called Lee-Naughton-Lebed's (LNL) angular effect in strong electric fields [K. Kobayashi, M. Saito, E. Omichi, and T. Osada, Phys. Rev. Lett. **96**, 126601 (2006)]. They found that strong electric fields split the LNL conductivity maxima in α-$(ET)_2$-based organic conductor and hypothetically introduced the corresponding equation for conductivity. In this Letter, for the first time we suggest quantum mechanical theory of the LNL angular oscillations in moderately strong electric fields. In particular, we demonstrate that the obtained by us approximate theoretical formula coincides with the hypothetical one and well describes the above mentioned experiments.

Keywords: quantum mechanics; high magnetic fields

It is well known that organic conductors, having quasi-one-dimensional (Q1D) pieces of the Fermi surfaces (FS's), demonstrate unique magnetic properties due to the Bragg reflections of moving electrons from the Brillouin zones boundaries in moderate and strong magnetic fields [1-5]. Among them, are Field-Induced Spin(Charge)-Density-Wave (FIS(C)DW) phase diagrams [3-15], 3D Quantum Hall Effect (3D QHE) [14-16], the so-called Lebed's Magic Angles (LMA) [17-40], the Lee-Naughton-Lebed's (LNL) angular oscillations [41-47], and some others. Note the LMA phenomena [17-40] seem to be very complicated and in most cases possess some non Fermi liquid (FL) properties [27,29,1], whereas the FIS(C)DW, 3D QHE, and LNL phenomena were successfully explained in the framework of the Landau FL approach [1,2]. In particular, the LNL phenomenon was successfully theoretically explained in Refs. [48-54]. Indeed, in Refs. [48-54] there was considered layered Q1D conductor with the electron spectrum,

$$\epsilon_0^{\pm}(\mathbf{p}) = \pm v_F(p_x \mp p_F) + 2t_b \cos(p_y b^*) + 2t_c \cos(p_z c^*), \tag{1}$$

where $v_F p_F \gg t_b \gg t_c$, in an inclined magnetic field,

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

(see Fig.1). Note that in Eq.(1) the upper sign stands for the right piece of the Q1D FS and the lower sign stands for the left one. In the quasi-classical approximation, the following expression for the LNL conductivity was derived by several methods:

$$\sigma_{zz}(H,\theta,\phi) = \sigma_{zz}(0) \sum_{N=-\infty}^{\infty} \frac{J_N^2[\omega_c^*(\theta,\phi)/\omega_b(\theta)]}{1+\tau^2[\omega_c(\theta,\phi) - N\omega_b(\theta)]^2}. \tag{3}$$

Note that in Eq.(3) the so-called electron cyclotron frequencies can be expressed as [54]:

$$\omega_b(\theta) = \frac{ev_F H b^* \cos\theta}{c}, \quad \omega_c(\theta,\phi) = \frac{ev_F H c^* \sin\theta\sin\phi}{c}, \tag{4}$$

$$\omega_c^*(\theta,\phi) = \frac{ev_y^0 H c^* \sin\theta\cos\phi}{c}, \quad v_y^0 = 2t_b b^*. \tag{5}$$

More recently, Kobayashi et al. [55] experimentally studied the LNL phenomenon in rather strong electric fields and found that the strong electric field splits the LNL maxima of conductivity (3). What is also important they suggested a hypothetical theoretical formula which described the above mentioned experimental splitting.

The goal of our paper is to derive the quasi-classical expression for conductivity in moderately strong electric and strong magnetic fields which describes the experimentally observed splitting of the LNL maxima of conductivity [55]. In particular, we show that our equation has a limited area of applicability and is not applicable in very strong electric fields.

First, let us perform the quasi-classical Peierls substitution [56,57] for motion along the conducting chains in Eq.(1),

$$p_x \mp p_F = -i\frac{d}{dx}, \tag{6}$$

in the absence of both magnetic and electric fields:

$$\hat{\epsilon}_0^{\pm}(x, p_y, p_z) = \mp i v_F \frac{d}{dx} + 2t_b \cos(p_y b^*) + 2t_c \cos(p_z c^*). \tag{7}$$

The solution of the corresponding Schrödinger equation is

$$\Psi_0^{\pm}(x, p_y, p_z) = \exp\left(\pm i\frac{\epsilon x}{v_F}\right) \exp\left[\mp i\frac{2t_b x}{v_F}\cos(p_y b^*)\right] \exp\left[\mp i\frac{2t_c x}{v_F}\cos(p_z c^*)\right], \tag{8}$$

where energy ϵ is counted from the Fermi level, $\epsilon_F = p_F v_F$.

Then we introduce the electric field applied along the least conducting **z** axis as a small perturbation to the Hamiltonian (7),

$$\delta\hat{\epsilon}(z) = eEz\,, \tag{9}$$

and perform the one more quasi-classical Peierls substitution [56,57]:

$$\delta\hat{\epsilon}(p_z) = eEz = -ieE\frac{d}{dp_z}. \tag{10}$$

In this case application of the perturbation (10) to the free electron wave function (8) gives

$$\delta\hat{\epsilon}(p_z)\Psi_0^{\pm}(x, p_y, p_z) = \pm\frac{eEx}{v_F}2t_c c^* \sin(p_z c^*)\Psi_0^{\pm}(x, p_y, p_z). \tag{11}$$

It is easy to prove that for not extremely strong electric fields the total Hamiltonian in the electric field can be written as

$$\hat{\epsilon}^{\pm}(x, p_y, p_z) = \mp i v_F \frac{d}{dx} + 2t_b \cos(p_y b^*) + 2t_c \cos\left(p_z c^* \mp \frac{eEc^* x}{v_F}\right). \tag{12}$$

Here, we introduce the magnetic field (2) in the electron Hamiltonian and the electron velocity operator along **z** axis. For the further development, it is convenient to choose vector potential of the magnetic field in the following form:

$$\mathbf{A} = (0, x\cos\theta, -x\sin\theta\sin\phi + y\sin\theta\cos\phi)\;H. \tag{13}$$

To define the corresponding electron wave functions for the case, where $t_b \gg t_c$, as shown in Ref.[51], it is necessary to take into account only two first terms in Hamiltonian (12) and to perform in the second term the following quasi-classical Peierls substitution,

$$p_y \rightarrow p_y - \frac{e}{c}A_y. \tag{14}$$

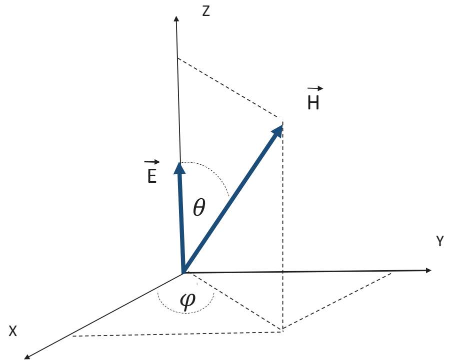

Figure 1. Definition of the azimuthal angle θ and polar angle ϕ for the typical Lee-Naughton-Lebed's experiment, where **z** is the least conducting axis.

In this case wave function in the mixed (x, p_y) representation obeys the following Schrödinger equation [3,51]:

$$\left(\mp i v_F \frac{d}{dx} + 2t_b \cos\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right]\right)\Phi^{\pm}_{\epsilon}(x, p_y) = \epsilon \Phi^{\pm}_{\epsilon}(x, p_y), \tag{15}$$

where the two wave functions (8) and (15) are related by the following equation:

$$\Psi^{\pm}_{\epsilon}(x, p_y) = \exp(\pm i p_F x)\Phi^{\pm}_{\epsilon}(x, p_y). \tag{16}$$

It is important that Eq.(15) can be exactly solved,

$$\Phi^{\pm}_{\epsilon}(x, p_y) = \exp\left(\pm i \frac{\epsilon}{v_F} x\right) \exp\left\{\pm \frac{2it_b}{\omega_b(\theta)}\left(\sin\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right] - \sin[p_y b^*]\right)\right\}. \tag{17}$$

Let us apply the quasi-classical Peierls substitution to energy dependence (12) on momentum component along **z** axis:

$$\hat{\epsilon}^{\pm}_z(x, y, p_z) = 2t_c \cos\left(p_z c^* \mp \frac{eEc^* x}{v_F}\right) \rightarrow 2t_c \cos\left[p_z c^* \mp \frac{eEc^* x}{v_F} + \frac{\omega_c(\theta, \phi)x}{v_F} - \frac{\omega^*_c(\theta, \phi)y}{v^0_y}\right]. \tag{18}$$

Taking into account that in the quasi-classical approximation

$$\hat{v}^{\pm}_z(x, y, p_z) = d[\hat{\epsilon}^{\pm}_z(x, y, p_z)]/dp_z, \quad y = i(d/dp_y), \tag{19}$$

it is possible to write the velocity component operator along **z** axis in the form:

$$\hat{v}^{\pm}_z(x, y, p_z) = -2t_c c^* \sin\left[p_z c^* \mp \frac{eEc^* x}{v_F} + \frac{\omega_c(\theta, \phi)x}{v_F} - i\frac{\omega^*_c(\theta, \phi)(d/dp_y)}{v^0_y}\right]. \tag{20}$$

In Eq.(20) for the further development, we introduce

$$\omega^{\pm}_c(\theta, \phi) = \omega_c(\theta, \phi) \mp eEc^*. \tag{21}$$

It is important that wave functions (17) are eigenfunctions of velocity operator along **z** axis (20),(21) with the following eigenvalues:

$$\hat{v}^{\pm}_z(x, y, p_z)\Phi^{\pm}_{\epsilon}(x, p_y) = -2t_c c^* \sin\left\{p_z c^* + \frac{\omega^{\pm}_c(\theta, \phi)x}{v_F} \pm \frac{\omega^*_c(\theta, \phi)}{\omega_b(\theta)}\right.$$
$$\left. \times \left(\cos\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right] - \cos[p_y b^*]\right)\right\}\Phi^{\pm}_{\epsilon}(x, p_y). \tag{22}$$

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Let us apply the Kubo formula for conductivity [58,51]. We can do this because the electron wave functions (17) and the eigenvalues of velocity operators (22) are known. The total conductivity along **z** axis can be represented as a summation of the following two contributions: one from the right sheet of the FS (1) and another from the left sheet,

$$\sigma_{zz}(H,\theta,\phi) = \sigma^{+}_{zz}(H,\theta,\phi) + \sigma^{-}_{zz}(H,\theta,\phi). \tag{23}$$

By means of the Kubo formalism [58,51] we obtain

$$\sigma^{\pm}_{zz}(H,\theta,\phi) \sim \int_{-\pi}^{\pi} d(p_y b^*) \int_0^{\infty} dx \, \exp\left(-\frac{x}{v_F \tau}\right) \times \cos\left\{\frac{\omega_c^{\pm}(\theta,\phi)x}{v_F} \pm \frac{\omega_c^*(\theta,\phi)}{\omega_b(\theta)}\left(\cos\left[p_y b^* - \frac{\omega_b(\theta)x}{v_F}\right] - \cos[p_y b^*]\right)\right\}, \tag{24}$$

where τ is an electron relaxation time. Complicated double integration in Eq.(24) can be simplified using definitions of the Bessel functions of the N-th order, $J_N(x)$ [59,51],

$$\sigma^{\pm}_{zz}(H,\theta,\phi) = \frac{\sigma_{zz}(0)}{2} \sum_{N=-\infty}^{\infty} \frac{J_N^2[\omega_c^*(\theta,\phi)/\omega_b(\theta)]}{1+\tau^2[\omega_c^{\pm}(\theta,\phi) - N\omega_b(\theta)]^2}, \tag{25}$$

where $\sigma_{zz}(0)$ - conductivity along **z** axis in low electric fields in the absence of the magnetic field. If we make use of the Eq.(23), we finally obtain for the total conductivity in moderately strong electric fields in the presence of the inclined magnetic field (2):

$$\sigma_{zz}(H,\theta,\phi) = \frac{\sigma_{zz}(0)}{2} \sum_{N=-\infty}^{\infty} \left\{\frac{J_N^2[\omega_c^*(\theta,\phi)/\omega_b(\theta)]}{1+\tau^2[\omega_c^{+}(\theta,\phi) - N\omega_b(\theta)]^2} + \frac{J_N^2[\omega_c^*(\theta,\phi)/\omega_b(\theta)]}{1+\tau^2[\omega_c^{-}(\theta,\phi) - N\omega_b(\theta)]^2}\right\}. \tag{26}$$

We stress that Eq.(26) is the main result of our Letter, whereas in Ref.[55] this equation was just guessed. Moreover, we have shown that it is not exact and has to be used for not too high (i.e., moderately high) electric fields. Indeed, let us discuss its applicability. We recall that we have derived Eq.(26) using some approximation: we have suggested that we can use Eq.(12), instead of Eq.(11). It is easy to prove that this can be done under the condition that

$$\frac{eEc^* x_0}{v_F} \ll 1\,, \tag{27}$$

where x_0 is characteristic length where the integral (24) converges. Since, as follows from (24), $x_0 \simeq v_F \tau$ the condition (27) can be written as

$$eEc^* \ll 1/\tau. \tag{28}$$

If we take the lowest experimentally used electric field, $V_0 = Ed = 2$V, $d = 0.2$mm [55], and $\hbar/\tau = $2K [1], we obtain the inequality (28) in the form

$$0.25K \ll 2K, \tag{29}$$

which shows that at lowest voltages analysis [55] is correct, whereas at higher experimental voltages, $V_0 = 20$V [55], Eq.(26) must be used with a great caution, since Eq.(28) gives quantities of the same orders of magnitudes for the left side and for the write one.

Let us briefly discuss one important consequence of Eq.(26) - the splitting of the LNL maxima of conductivity in moderately strong electric field [55]. In the limit of zero electric field at the following typical experimental conditions, where

$$\omega_b(\theta)\tau \gg 1, \quad \omega_c(\theta,\phi)\tau \gg 1, \tag{30}$$

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maxima of conductivity, as follows from Eq.(3), appear at

$$\omega_c(\theta,\phi) = N\omega_b(\theta), \tag{31}$$

where N is an arbitrary integer. Under the experimental condition (30), Eq.(26) splits each maximum into two ones which are defined by the following equations

$$\omega_c(\theta,\phi) = N\omega_b(\theta) \mp \omega_E,\ \omega_E = eEc^*. \tag{32}$$

The effect of splitting was experimentally observed in Ref.[55]. Our analysis of the applicability of Eq.(26), as we discussed above, has shown that Eqs. (32) are valid for lower experimentally used voltages, $V_0 \simeq 2$V, and become controversial at higher ones, $V_0 \simeq 20$V.

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