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Lebed resonance in quasi-one-dimensional organic conductors

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We consider a strongly anisotropic three-dimensional conductor in a magnetic field perpendicular to the most conducting direction. We show that the magnetoresistance exhibits a series of resonancelike dips when the magnetic field takes particular angles in the b-c plane where periodic motion in the b and the c direction becomes commensurate. The model is consistent with the initial idea of Lebed and describes recent experiments in $(TMTSF)_2ClO_4$ (where TMTSF is tetramethyltetraselenafulvalene) quite well.

In a remarkable paper Lebed[1] proposed geometrical resonance in the electronic motion in a quasi-one-dimensional conductor in a magnetic field perpendicular to the most conducting direction (say, the a direction) and tilted from the c axis when the electron motion in the b and c direction becomes commensurate. In particular, Lebed predicted that this resonance would induce instability of the normal metallic state. In spite of an extensive search, no such instability has been established experimentally.[2,3] On the other hand, it has been discovered that the magnetoresistance of relaxed $(TMTSF)_2ClO_4$ (di-tetramethyltetraselenafulvalene perchlorate) exhibits a series of dips at these commensurate points.[4,5] In order to account for this anomaly in the resistance, Lebed and Bak[6] proposed a model with resonance scattering of electrons at commensurate points; the electron scattering is enhanced at the commensurate points due to resonance in the electron motion. Unfortunately, however, this model gives peaks rather than dips in the magnetoresistance contrary to the experiments. This behavior can be understood more clearly as follows. In the vicinity of the spin-density-wave transition, the fluctuation of the order parameter gives rise to the extra scattering.[7] Now, this term is very sensitive to the magnetic field since the transverse coherence lengths ξ_b and ξ_c associated with the fluctuation depend sensitively on the magnetic field.[8] In particular, ξ_c decreases sharply at the commensurate points resulting in sharp peaks in the magnetoresistance. Therefore, we can exclude the fluctuation effect which is essentially multiple scattering effect as well as the scattering effect from the source of dips in magnetoresistance.

In this Rapid Communication, we show that there exist a simple geometrical effect which has been overlooked so far. We shall consider the free electron in the tight-binding model, since the electron-electron interaction as well as the presence of field-induced spin-density wave (FISDW) is irrelevant to the present question. Then we analyze the electron motion in a magnetic field in the b-c plane with an angle θ from the c axis within semiclassical approximation. Then we calculate $\sigma_{zz}(H,\theta)$, the electric conductivity in the c direction within single relaxation-time approximation,[9] which exhibits as series of peaks associated with the commensurate resonance. Other conductivity tensors can be analyzed in a similar way but the effect of the resonance is most clear in $\sigma_{zz}(H,\theta)$. We shall also discuss briefly the effect of the FISDW transition on $\sigma_{zz}(H,\theta)$.

First, let us consider the quasiparticle energy

$$E(\mathbf{p}) = -2t_a\cos(ap_1) - 2t_b\cos[b(p_2+eBx\cos\theta)] - 2t_c\cos[c(p_3-eBx\sin\theta)] - \mu\,, \tag{1}$$

where μ is the chemical potential and a magnetic field B is applied in the b-c plane with an angle θ from the c axis. In the following, we assume

$$t_b/t_a,\ t_c/t_b \ll 1\,, \tag{2}$$

as usually the case with Bechgaard salts [i.e., $(TMTSF)_2$ salts]. Then the equation of motion for the electron is given by

$$\frac{dp_1}{dt} = eB\{2t_b b\cos\theta\sin[b(p_2+eB\cos\theta x)] - 2t_c c\sin\theta\sin[c(p_3-eB\sin\theta x)]\} \tag{3}$$

and

$$\frac{dx}{dt} = 2t_a a\sin(ap_1)\,. \tag{4}$$

In the limit $t_c=0$ and for small t_b/t_a, this set of equations are integrated after linearizing Eq. (4) in $p_1 \mp p_F$ in the vicinity of $p_1 = \pm p_F$ as

$$\left(\frac{dx}{dt}\right)^2 = v^2 - 4t_b av\cos[b(p_2+eB\cos\theta x)] \tag{5}$$

or

$$x \simeq v\left[1+\frac{3}{2}\left(\frac{t_b}{t_a}\right)^2\right]^{-1}\left[t-\sqrt{2}\left(\frac{t_b}{t_a}\right)\omega_b^{-1}\sin(\omega_b' t)\right] \tag{6}$$

where

$$\omega_b = vebB\cos\theta,\quad \omega_b' = \omega_b\left[1+\frac{3}{2}\left(\frac{t_b}{t_a}\right)^2\right]^{-1}, \tag{7}$$

v is the Fermi velocity, and ω_b is the cyclotron frequency associated with electron motion along the b axis. Here, we neglected the higher-order terms in $(t_b/t_a)^2$ for simplicity except for the modification of the frequency. A more complete solution of Eq. (5) may be obtained in terms of the elliptic integral, but Eq. (6) suffices for our present purpose.

The electric current along the c axis is given by

$$j_z = 2et_c c \sin[c(p_3 - eB\sin\theta x)] . \tag{8}$$

Substituting Eq. (6) into Eq. (8), we obtain

$$j_z \cong 2et_c c \sin\left[cp_3 - \omega_c' t + \sqrt{2}\frac{t_b}{t_a}\left(\frac{\omega_c}{\omega_b}\right)\sin(\omega_b' t)\right]$$

$$= 2et_c c\left[\sin(cp_3 - \omega_c' t)\left(J_0(z) + 2\sum_{k=1}^{\infty} J_{2k}(z)\cos(2k\omega_b' t)\right) + 2\cos(cp_3 - \omega_c' t)\sum_{k=0}^{\infty} J_{2k+1}(z)\sin[2(k+1)\omega_b' t]\right] \tag{9}$$

where

$$\omega_c = vecB\sin\theta, \quad \omega_c' = \omega_c\left[1 + \frac{3}{2}\left(\frac{t_b}{t_a}\right)^2\right]^{-1}, \quad z = \sqrt{2}\frac{t_b}{t_a}\left(\frac{c}{b}\tan\theta\right), \tag{10}$$

and $J_k(z)$ is the Bessel function.

Since the electron motion in the x direction contains an oscillatory term with period $2\pi/\omega_b'$ [see Eq. (6)], this gives rise to a series of resonances in j_z.

Finally, the electric conductivity parallel to the c axis is given within the single relaxation-time approximation[10,11] as

$$\sigma_{zz}(B,\theta) = \sigma_{zz}^0\left\{J_0^2(z)[1 + (\tau\omega_c')^2]^{-1} + \sum_{k=0}^{\infty} J_k^2(z)\{[1 + (\tau(\omega_c' - k\omega_b'))^2]^{-1} + [1 + (\tau(\omega_c' + k\omega_b'))^2]^{-1}\}\right\} \tag{11}$$

where τ is the relaxation time. The exact value of weight factor in the limit $t_b/t_a \ll 1$ is obtained[12] as $(\sqrt{2}t_b/t_a)^{2k} \times C^2(k)$ which replaces $J_k^2(z)$ in Eq. (11) where $C(k) = \Gamma(k+\frac{1}{2})/\Gamma(k+1)\Gamma(\frac{1}{2})$. This coefficient is read off directly from the time average of j_z.

The electric conductivity exhibits a series of resonance-like peaks when θ takes

$$\frac{c}{b}\tan\theta = k , \tag{12}$$

with k an integer. The strength of this resonance is controlled by

$$(\sqrt{2}t_b/t_a)^{2k}C^2(k) \simeq (\pi k)^{-1}(\sqrt{2}t_b/t_a)^{2k}$$

for $t_b/t_a \ll 1$. Therefore, the strength of the resonance decreases rapidly with increasing k. A similar analysis of σ_{xx} indicates that it also exhibits similar resonances but only in the terms higher orders in $(t_c/t_a)^2$, and these resonances are much weaker. This is readily seen since j_x is given as[13]

$$j_x \simeq e\{v - 2a\cot(ap_F)[t_b\cos(b(p_2 - eB\cos\theta_x)) + t_c\cos(c(p_3 - eB\sin\theta x))]\} .$$

Therefore, we believe that the commensurate resonance observed in the magnetoresistance in the chain direction originated from σ_{zz}, where the effect of resonance is most clearly seen. Within the present approximation, we have no fractional terms. However, such resonances appear in the conductivity tensor when we include the higher-order terms in $(t_c/t_a)^2$. But, in $(TMTSF)_2ClO_4$ such terms are extremely small [note $(t_c/t_a)^2 \sim 10^{-5}$] and it is rather unlikely we see any fractional resonance in $(TMTSF)_2ClO_4$ in accordance with Naughton *et al.*[5]

So far, we have neglected the effect of the electron-electron interaction. In the presence of the interaction, the system undergoes the FISDW transition. The principal effect of the FISDW transition in the present context is opening of the quasiparticle energy gap and decrease in the quasiparticle density. The magnetoconductivity along the c axis is still given by Eq. (11). But σ_{zz}^0 has to be replaced with $\sigma_{zz}^0[1 - f_c(B,\theta)]$, and $f_c(B,\theta)$ is the condensate density,[13]

$$f_c(B,\theta) = (2\Delta)^2\int_\Delta^\infty dE(E^2-\Delta^2)^{-1/2}(\omega_b^2 + 4\Delta^2 - 4E^2)^{-1} \times\tanh(\tfrac{1}{2}\beta E) . \tag{13}$$

In summary, we have shown that the commensurability in the orbital motions along the b and c axes in a tilted magnetic field gives rise to a series of resonancelike structures in the magnetoconductivity along the c axis. The position of the resonance is independent of the field strength and controlled by the purely geometrical factor [Eq. (12)]. In a higher magnetic field and at low temperature, the resonances become much sharper. Further, in $(TMTSF)_2ClO_4$, we expect resonances only at integral value of k's. These are fully consistent with recent observation of dips in the magnetoresistance in the commensurability points.[4,5] Also, this phenomenon should be quite general and be observable in most of the quasi-one-dimensional systems, where the Fermi surfaces consist of a pair of warped sheet in the transverse directions.

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