Magic angle effects of the one-dimensional axis conductivity in quasi-one dimensional conductors

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In quasi-one-dimensional conductors, the conductivity in both one-dimensional axis and interchain direction shows peaks when magnetic field is tilted at the magic angles in the plane perpendicular to the conducting chain. Although there are several theoretical studies to explain the magic angle effect, no satisfactory explanation, especially for the one-dimensional conductivity, has been obtained. We present a new theory of the magic angle effect in the one-dimensional conductivity by taking account of the momentum-dependence of the Fermi velocity, which should be large in the systems close to a spin density wave instability. The magic angle effect is explained in the semiclassical equations of motion, but neither the large corrugation of the Fermi surface due to long-range hoppings nor hot spots, where the relaxation time is small, on the Fermi surface are required.

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Quasi-one-dimensional organic conductors show a lot of interesting phenomena, such as unconventional superconductivity, spin density wave (SDW), field-induced spin density wave, quantum Hall effect, etc.\textsuperscript{1} By studying the interaction of electrons with impurities as well as interaction between electrons Lebed and Bak\textsuperscript{2} have predicted that the resistance, $R_{xx}$, has peaks at the magic angles $\theta = \tan^{-1}\left(\frac{\sqrt{3}}{3}\right)$, where $p$ and $q$ are mutually prime integers and $b$ and $c$ are lattice constants, when the magnetic field is rotated in the plane perpendicular to the most conducting axis. Experimentally, dips, instead of peaks, of the magnetoresistance, unphysically large values of the heights of peaks are proportional to $\sigma_{zz}$, and constant relaxation time $\tau$ are observed by the metallic and non-metals at the magic angles and at other directions of the magnetic field are observed by the metallic and non-metallic states at the magic angles. Osada et al.\textsuperscript{15} have shown that the conductivity in the $z$ axis $\sigma_{zz}$ shows peaks at the magic angles. In quasi-one-dimensional conductors the energy dispersion is described as $\epsilon_{k} = -2t_{c}\cos k_{x} - 2t_{b}\cos k_{y} - 2t_{c}\cos k_{z} - \mu$. Here we take the simple cubic lattice with lattice constant $a$, $b$, and $c$ for simplicity. Since $t_{a} \gg t_{b} \gg t_{c}$, the Fermi surface is two nearly parallel sheets at $k_{x} \approx \pm k_{F}$ and $k_{F} = \frac{\pi}{a}$ for the quarter-filled band. Osada et al.\textsuperscript{15} used the linearized dispersion in the $k_{x}$ direction as

$$\epsilon_{k}(k) = \pm \hbar v_{F}(|k_{x}| - k_{F}) - \sum_{m,n} t_{mn} \cos(mbk_{y}+nck_{z}),$$

and constant relaxation time $\tau$. They have shown that peaks appear in $\sigma_{yy}$ and $\sigma_{zz}$ at the magic angles and the heights of peaks are proportional to $t_{pq}^{2}$. In order to explain the experimental results of the perpendicular magnetoresistance, unphysically large values of $t_{pq}$ are required. This model also fails to explain the magnitude of the recently observed giant Nernst effect\textsuperscript{30} at the magic angles. Maki\textsuperscript{21} has used the similar approximation of the linearized dispersion and constant $\tau$, but took account of the $k_{y}$ dependence of $v_{x}$ in perturbation in $\frac{k_{y}}{\hbar}$. Recently, Lebed et al.\textsuperscript{26,27} have emphasized the importance of the $k_{y}$ dependence of $v_{x}$, or the density of states on the Fermi surface. They show that there occurs the
1D to 2D dimensional crossover when the magnetic field is at magic angles. In these approximation resonance-like peaks in $\sigma_{xx}$ at the magic angle with $q = 1$ is obtained, but its height is proportional to $(\frac{B}{c})^{2\theta}$ and very small in the case of $t_b \ll t_c, \Sigma_1$.

The more serious discrepancy between the semiclassical theories of MAE and experiments is encountered in the one-dimensional conductivity $\sigma_{xx}$. In the model of Osada et al. $\Sigma_2$, $\sigma_{xx}$ does not depend on the direction of the magnetic field. Maki $\Sigma_2$ has pointed out that $\sigma_{xx}$ shows peaks at magic angles, if the $k_y$ and $k_z$ dependence of $v_x$ is taken into account. It is, however, very weak, i.e., it is of the order of $(\frac{B}{t_c})^2$. Meanwhile, Chaikin $\Sigma_2$ has shown that the angular-dependence of $\sigma_{xx}$ can be explained, if there are hot spots on the Fermi surface, where $\tau$ is small.

In this letter we show that the peaks in one-dimensional conductivity $\sigma_{xx}$ at the magic angles are dramatically enhanced, when $v_x$ depends strongly on $k_y$ and $k_z$ on the Fermi surface, even when long-range hopping terms and hot spots are absent. In quasi-one dimensional organic conductors, electrons correlate strongly and the one-dimensional conductivity $\sigma_{xx}$ is small. When $k_y$ and $k_z$ dependence of $v_x$ is small.

\begin{equation}
\sigma_{ij} = \frac{2e^2}{V} \sum_k \left( -\frac{df}{dk} \right) v_i(k(0)) \int_0^\infty v_j(k(t)) e^{\frac{t^2}{\tau}} dt \tag{2}
\end{equation}

where $i$ and $j$ are $x$, $y$ or $z$, and $v_i(k(t))$ is the velocity on the Fermi surface in the semiclassical picture

\begin{equation}
v(k(t)) = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k(t)}. \tag{3}
\end{equation}

The velocity $v(k(t))$ depends on time via the time dependence of the wave vector $k(t)$ as

\begin{equation}
\hbar \frac{dk(t)}{dt} = -e v(k(t)) \times B \tag{4}
\end{equation}

where we take the magnetic field $B$ in the $y - z$ plane, $B_x = 0$, $B_y = B \sin \theta$, and $B_z = B \cos \theta$.

When $\theta = \tan^{-1}(\frac{2\pi}{\pi})$, $k$ started from some point $k(0)$ moves in the commensurate trail on the Fermi surface before coming back to $k(0)$, while it travels all the Fermi surface when $\frac{2\pi}{\tau} \tan \theta$ is an irrational number. This is the main idea of the Chaikin’s hot spots and other semiclassical theories of MAE. In order to simplify the calculation, we assume $v_x = v_0$ except for in the rectangular region of $2\pi \delta \times 2\pi \delta w$, where $v_x = \alpha v_0$ ($\alpha \neq 1$), as shown in Fig. $1$ and $a = b = c = 1$. In the quasi-one dimensional system the density of states on the Fermi surface can be expressed as a function of energy $\epsilon$, $k_y$ and $k_z$ as

\begin{equation}
N(\epsilon, k_y, k_z) = \frac{1}{[\hbar v_x(\epsilon, k_y, k_z)]} \tag{5}
\end{equation}

At low temperature we can replace $\frac{\partial E}{\partial k}$ by $\delta(\epsilon - \epsilon F(k_y, k_z))$ in Eq. (2) and we obtain

\begin{equation}
\sigma_{xx} = \frac{2e^2}{\hbar V} \sum_{k_y, k_z} \int_0^\infty v_x(k(t)) e^{\frac{t^2}{\tau}} dt, \tag{6}
\end{equation}

where summation on $k_y$ and $k_z$ should be done on the right sheet of the Fermi surface ($v_x(k(0)) > 0$). A factor of 2 comes from the contribution of the left sheet of the Fermi surface. Although $\sigma_{zz}$ is given by the correlation of $v_z(k(0))$ and $v_z(k(t))$ in Eq. (2), $\sigma_{xx}$ in quasi-one dimensional system is simply given by the momentum-space average of the time average (weighted by $\exp(\frac{t^2}{\tau})$) of $v_x(k(t))$. We consider the case of $eB\tau \gg 1$. Then integration over $t$ can be approximated by $\tau$ times the time average of $v_x(k(t))$ over the trajectory of $k(t)$. It might

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**Fig. 1:** (a) Simple model that $v_x$ is $\alpha v_0$ in the small rectangular region and $v_0$ in the other region in the Brillouin zone. (b) Extended Brillouin zone for $\tan \theta = \frac{\pi}{\pi} = \frac{2}{3}$. The gray region should be translated to the first Brillouin zone.
be thought that $\sigma_{xx}$ does not depend on the direction of the magnetic field, but it does, since the time-average is performed on the trajectory, which depends on the angle of the magnetic field. Since the speed of $k(t)$ in the momentum space is proportional to $v_x(k(t))$ when $|v_x| \gg v_y, |v_z|$, as seen from Eq. (3), time average of $v_x(k(t))$ can be calculated as follows.

First, we consider the commensurate case, $\tan \theta = \frac{p}{q}$, where $p$ and $q$ are mutually prime integers. Brillouin zone is extended $q$ times $p$ as shown in Fig. 1(b). In the black region (area $S_1 = (2\pi)^2 w^2 \delta^2$), $v_x = \alpha v_0$. The gray and black regions in Fig. 1(b) is defined as the set of $\mathbf{k}(0)$ that goes into the black region at some $t$. The area of the gray region is

$$S_0 = (2\pi)^2 p (1 + \frac{w}{\tan \theta}) \delta - S_1$$

$$= (2\pi)^2 (p + qw - \delta w) \delta. \quad (7)$$

We define $s_0 = \frac{S_0}{(2\pi)^2} = (p + qw - \delta w) \delta$ and $s_1 = \frac{S_1}{(2\pi)^2} = w \delta^2$. The gray region in Fig. 1(b) should be translated in the first Brillouin zone. Therefore, if $(p + qw) \delta > 1$, all the first Brillouin zone becomes black or gray region, i.e., every $\mathbf{k}(0)$ goes into $S_1$. If $(p + qw) \delta < 1$, however, we can divide the first Brillouin zone into two regions, the first region $(S_1 + S_0)$, and the second region $(2\pi)^2 - (S_1 + S_1)$. If $\mathbf{k}(0)$ is in the first region, $v_x(\mathbf{k}(t))$ changes the value as $\mathbf{k}(t)$ travels on the commensurate trajectory on the Fermi surface, while $v_x(\mathbf{k}(t))$ is time-independent constant $v_0$ for the $\mathbf{k}(0)$ in the second region. Now, we calculate the momentum-space average and time average of $v_x$, when the magnetic field is at the magic angle $\theta = \tan^{-1} \frac{p}{q}$ and $(p + qw) \delta < 1$. If $\mathbf{k}(0)$ is in $S_1$ or $S_0$, the duration when $\mathbf{k}(t)$ is in the region $S_1$ is approximately proportional to $\frac{s_0}{v_0}$, while that in $S_0$ is approximately proportional to $\frac{s_1}{v_0}$. Thus the time average of $v_x(\mathbf{k}(t))$ when $\mathbf{k}(0)$ is in $S_1 + S_0$ is given by

$$\langle v_x \rangle^{(S_1 + S_0)} \approx \alpha v_0 \frac{s_0}{s_1 + s_0} + v_0 \frac{s_1}{s_1 + s_0}$$

$$= v_0 \frac{s_1 + s_0}{s_1 + s_0} \quad (8)$$

After the summation over $\mathbf{k}(0)$ in the Brillouin zone, we get the time and momentum-space average of $v_x$ for the magic angle (commensurate orbit) as

$$\langle v_x \rangle^C = v_0 (1 - s_1 - s_0) + \langle v_x \rangle^{(S_1 + S_0)} (s_1 + s_0)$$

$$= v_0 \left(1 + \frac{s_1 (s_1 + s_0) (1 - \frac{1}{\alpha})}{\alpha + s_0}\right) \quad (9)$$

Next, the time and momentum-space average of $v_x$ is calculated for the case that $\tan \theta$ is irrational number or $(p + qw) \delta > 1$. In this case, $\mathbf{k}(t)$ goes into the region $S_1$ at some $t$ regardless of the initial point $\mathbf{k}(0)$, i.e. the trajectory is incommensurate. The average of $v_x$ is calculated as

$$\langle v_x \rangle^{IC} = \alpha v_0 \frac{s_1}{s_1 + \frac{1 - s_1}{\alpha} + v_0 \frac{1 - s_1}{s_1 + \frac{1 - s_1}{\alpha}}}$$

$$= v_0 \frac{1}{1 - s_1 (1 - \frac{1}{\alpha})} \quad (10)$$

From the above result we get the normalized peak heights of conductivity at the magic angles as

$$\frac{\sigma_{xx} - \sigma_{xx}^{IC}}{\sigma_{xx}^{IC}} = \frac{\langle v_x \rangle^C - \langle v_x \rangle^{IC}}{\langle v_x \rangle^{IC}}$$

$$= \frac{(1 - \alpha)\alpha^2 w^3}{\alpha (p + qw) + w (1 - \alpha) \delta}, \quad (11)$$

where the condition $(p + qw) \delta < 1$ should be satisfied.

In both cases of small velocity ($\alpha < 1$) and large velocity ($\alpha > 0$) in region $S_1$, we get $\sigma_{xx} \geq \sigma_{xx}^{IC}$. The peak
heights becomes large ($\propto 1/\alpha$) as $\alpha$ approaches to 0. In Figs. 2 and 3 we plot \((\sigma_{xx} - \sigma_{xx}^{IC})/\sigma_{xx}^{IC}\) for several parameters of $\alpha$, $\delta$ and $\omega$. If $s_1$ is small, there are a lot of peaks at magic angles, $\tan^{-1}1 = 45^\circ$, $\tan^{-1}2 \approx 63.4^\circ$, $\tan^{-1}3 \approx 26.6^\circ$, $\tan^{-1}4 \approx 18.4^\circ$, etc. as seen in Fig. 2 but the heights of peaks are small. On the other hand, the number of peaks is small but their heights are large for larger $s_1$ (Fig. 3).

In conclusion we show that peaks in $\sigma_{xx}$ at magic angles are large, when $v_x$ depends on $k_y$ and $k_z$ on the Fermi surface of the quasi-one dimensional conductors. In the simple model that $v_x = v_{0y}$ is constant except for in the rectangular region on the Fermi surface, where $v_x$ is another constant value $v_x = \alpha\omega$, we get the approximate form of $\sigma_{xx}$ by using the simple calculation of taking the momentum-space average on the Fermi surface and the time average on the trajectory of $k(t)$. MAE is the consequence of the fact that $k(t)$ stays shorter time in the region where $|v_x(k_y, k_z)|$ is large, and in the region of small $|v_x(k_y, k_z)|$, $k(t)$ stays longer time. In this Letter, only $\sigma_{xx}$ as a function of the tilting angle of the magnetic field is studied. The similar mechanism works also for $\sigma_{zz}$ and the peak heights of $\sigma_{zz}$ at the magic angles will be much more enhanced by considering the strong $k_y$ and $k_z$ dependence of $v_x$ as done in this paper than that studied by Maki.[21] and Lebed et al.[24, 27] in the perturbation theory in $\frac{\omega}{E}.$ If we take account of the momentum-dependent relaxation time and more realistic momentum dependence of the velocity $v_x(k_y, k_z)$, experimentally observed peaks of $\sigma_{xx}$ and $\sigma_{zz}$ at magic angles will be explained better. Although MAE of $\sigma_{xx}$ can be explained within the semiclassical theory, the strong momentum-dependence of the Fermi velocity, which may be caused by interactions between electrons, plays a crucial role to understand the magnitudes of the peak heights. This feature is in contrast to the other angle dependence of the conductivity in quasi-one and quasi-two dimensional conductors[17, 20] and usual quantum oscillations such as Shubnikov-de Haas oscillations, where the shape of the Fermi surface is important.

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