# Cr pi-phase shift

Wednesday, October 25, 2023 10:02 AM

Outline:

Introduction { Properties of Cr
SdH observations.

Semiclassical Boltzmann theory of magnetotransport { Physical meaning of the solution (Pippard)
Application to circular & open orbits (Ziman)

Solution for coupled orbits. { Introduce magnetic breakdown junction.
Geometric series — Dyson

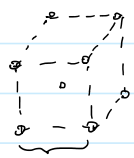
Application to the model { Qualitative behavior of 4 cases: $(P=0,1)\otimes(E\parallel\hat{x},\hat{y})$
Introduce quantum interference.
$\pi$-phase shift

Conclusion — can be found in other incommensurate density wave systems.

## Introduction

Cr properties:

bcc



n.n. bond length: $a_0 = \frac{\sqrt{3}}{2}\times 2.97 \simeq 0.866\times 2.97 \cong 2.57\,\text{Å}$

$a \equiv 2.97\,\text{Å}$ — conventional u.c.

1BZ corresponding to the primitive cell

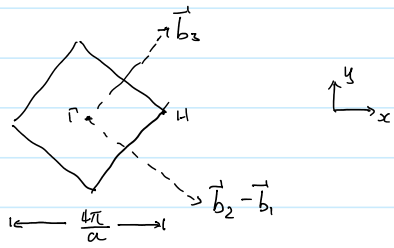
$$\left.\begin{aligned}\vec{a}_1 &= \tfrac{1}{2}(\hat{x}+\hat{y}+\hat{z})a\\ \vec{a}_2 &= \tfrac{1}{2}(\hat{x}-\hat{y}+\hat{z})a\\ \vec{a}_3 &= \tfrac{1}{2}(\hat{x}+\hat{y}-\hat{z})a\end{aligned}\right\} \Rightarrow \left\{\begin{aligned}V &= \frac{a^3}{2}\\ \vec{b}_1 &= \frac{2\pi}{a}(\hat{y}+\hat{z})\\ \vec{b}_2 &= \frac{2\pi}{a}(\hat{z}+\hat{x})\\ \vec{b}_3 &= \frac{2\pi}{a}(\hat{x}+\hat{y}).\end{aligned}\right\} \Rightarrow$$

periodicity in reciprocal space along $\hat{x}$ is:

$$\boxed{\vec{b}_2+\vec{b}_3-\vec{b}_1 = \frac{4\pi}{a}\hat{x}.}$$

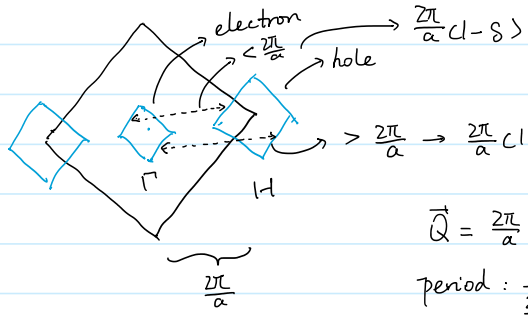
Other shorter periods in the xy plane: $\boxed{\begin{aligned}\vec{b}_3 &= \frac{2\pi}{a}(\hat{x}+\hat{y})\\ \vec{b}_2-\vec{b}_1 &= \frac{2\pi}{a}(\hat{x}-\hat{y}).\end{aligned}}$

$\therefore$




Incommensurate SDW below $T_N = 311\,K$

Fermi surface:




$\delta \simeq 0.05 \pm 0.005.$

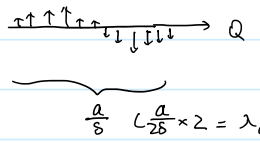
$$\vec{Q} = \frac{2\pi}{a}(1 \pm \delta)\hat{x}$$

period: $\dfrac{2\pi}{\frac{2\pi}{a}\delta} = \dfrac{a}{\delta} \simeq 20a$

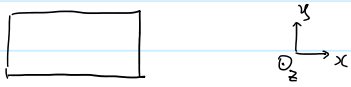
Exp wavelength: $\frac{a}{\delta} = 6.0\,\text{nm}$ at $T < 10\,K \Rightarrow \delta = \frac{2.97}{60} \simeq 0.0495$

spin direction: $(1 - 0.952 = 0.048$ in paper$)$

$$\begin{cases} \hat{S} \parallel \hat{Q} & T < T_{SF} = 123\,K \\ \hat{S} \perp \hat{Q} & T > T_{SF}. \end{cases}$$

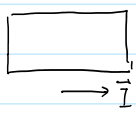



Experiment: $(T = 1.65\,K)$

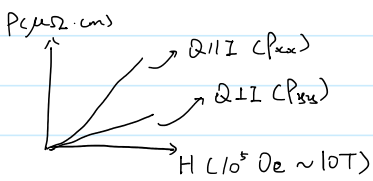



$\vec{H} \parallel \hat{z}$, $\vec{Q} \parallel \hat{x}$

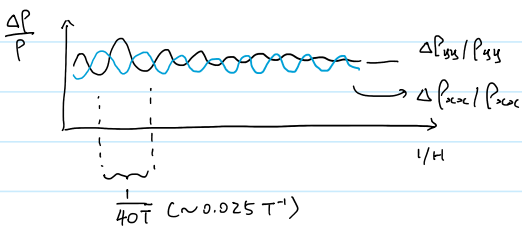
$\to \vec{Q}, \vec{I} \Rightarrow \rho_{xx}$



$\uparrow \vec{Q} \Rightarrow \rho_{xy}$ (due to 4-fold rotation symmetry)




$(Q \perp I$ — near linear, $Q \parallel I$ — quadratic$)$




but SdH oscillation should not depend on current direction.

Naive picture: (2D LL).

$\frac{1}{2m}(-i\hbar\nabla + |e|\vec{A})^2\psi = \varepsilon\psi \Rightarrow \varepsilon = \hbar\omega_c(n + \frac{1}{2})$ $\quad \omega_c = \frac{eB}{m^*}$

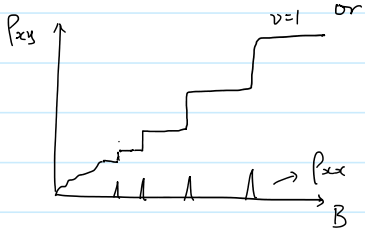
number of electrons in each LL: $N_B = \frac{A}{2\pi l_B^2} = \frac{A}{2\pi}\frac{eB}{\hbar}$

$\therefore$ If the system has $N_0$ electrons, there will be a gap at the Fermi energy whenever $N_0 = n \times N_B = n\frac{A}{2\pi}\frac{eB}{\hbar} \Rightarrow B_n = \frac{1}{n}\frac{2\pi\hbar N_0}{eA}$

or $\Delta B_n = \frac{1}{n(n-1)}\frac{2\pi\hbar N_0}{eA}$

$\rho_{xy} \uparrow$ $\quad \nu = 1$

energy whenever $\Delta\varepsilon_0 = \hbar\omega = \frac{\hbar eB}{m^*}$ if $2\pi\hbar$ , $\varepsilon_n = n$ $eA$




or $\Delta B_n = \frac{1}{n(n-1)} \frac{2\pi\hbar N_0}{eA}$

$$\sigma_{xy} = \nu \frac{e^2}{h} \Rightarrow \rho_{xy} = \frac{h}{\nu e^2}$$

$\therefore \rho_{xx}$ should oscillate with $\frac{1}{B}$ with the period $\Delta(\frac{1}{B}) = \frac{eA}{2\pi\hbar N_0} = \frac{e}{\hbar n_e}$

This is when there is a gap at the FS $\Rightarrow$ all longitudinal $\sigma_{ii}$ (in 3D) should have a minimum, all $\rho_{ii}$ should have a maximum.

$\Rightarrow$ <u>why can $\rho_{xx}(\frac{1}{H})$ and $\rho_{xy}(\frac{1}{H})$ have opposite phases ??</u>

## Semiclassical Boltzmann theory of magnetotransport.

Two ingredients: ① equations of motion, ② Boltzmann equation.

① : $\begin{cases} \dot{\vec{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}} \\ \dot{\vec{k}} = -\frac{e}{\hbar}(\vec{E} + \dot{\vec{r}} \times \vec{B}) \end{cases}$ ($\dot{\vec{r}}$ can have more corrections if TRS is broken: $\frac{1}{\hbar}\frac{\partial \varepsilon_{Zeeman}}{\partial \vec{k}} - \dot{\vec{k}} \times \vec{\Omega}$, $\varepsilon_{Zeeman} = -(\vec{m}_{orb} + \vec{m}_{spin}) \cdot \vec{B}$)

② $\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec{r}} \cdot \dot{\vec{r}} + \frac{\partial f}{\partial \vec{k}} \cdot \dot{\vec{k}} = -\frac{f - f_0}{\tau}$

For Cr SDW — TR + translation is a symmetry, I is a symmetry.

$\Rightarrow$ The correction terms for $\dot{\vec{r}}$ can be ignored.

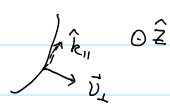
② $\xrightarrow[\text{state}]{\text{steady, uniform}}$ $\left.\begin{array}{l} \frac{\partial f}{\partial \vec{k}} \cdot \dot{\vec{k}} = -\frac{g}{\tau} \quad (g \equiv f - f_0) \\ \dot{\vec{k}} = -\frac{e}{\hbar}(\vec{E} + \dot{\vec{r}} \times \vec{B}) \end{array}\right\} \Rightarrow \underbrace{\frac{\partial f}{\partial \vec{k}} \cdot (-\frac{e}{\hbar})\vec{E}}_{-\frac{e}{\hbar}\frac{\partial f_0}{\partial \vec{k}} \cdot \vec{E}} + \underbrace{\frac{\partial f}{\partial \vec{k}} \cdot (-\frac{e}{\hbar})(\dot{\vec{r}} \times \vec{B})}_{-\frac{e}{\hbar}\frac{\partial g}{\partial \vec{k}} \cdot (\dot{\vec{r}} \times \vec{B})} = -\frac{g}{\tau}$ *

(linear response) (since $\frac{\partial f_0}{\partial \vec{k}} \cdot (\dot{\vec{r}} \times \vec{B}) = 0$)

without loss of generality, assume $\vec{B} = B\hat{z}$.

Then $-\frac{e}{\hbar}\frac{\partial g}{\partial \vec{k}} \cdot (\vec{v} \times \vec{B}) = \frac{eB}{\hbar}(\hat{z} \times \vec{v}) \cdot \frac{\partial g}{\partial \vec{k}}$

$= \frac{eB}{\hbar} v_\perp \underbrace{\hat{k}_{\parallel} \cdot \nabla_k}_{\equiv \frac{\partial}{\partial s}} g$




change the coordinate system: $\hat{k}_x, \hat{k}_y, \hat{k}_z \to \hat{k}_\perp, \hat{k}_\parallel, \hat{k}_z \to \begin{cases} dk_\perp = \frac{d\varepsilon(k_z)}{v_\perp} \\ dk_\parallel \equiv ds \\ dk_z = dk_z. \end{cases}$

$* \Rightarrow \left.\begin{array}{l} \frac{eB}{\hbar} v_\perp \frac{\partial g}{\partial s} + \frac{g}{\tau} = \frac{\partial f_0}{\partial \vec{k}} \cdot \frac{e}{\hbar}\vec{E} \\ \frac{eB}{\hbar} \equiv \ell^2 \end{array}\right\} \Rightarrow \frac{\partial g}{\partial s} + \frac{\ell^2}{v_\perp \tau} g = \frac{e\ell^2}{\hbar v_\perp}\frac{\partial f}{\partial \vec{k}} \cdot \vec{E} \sim \frac{dy}{dx} + ay = b.$

$\frac{dy}{dx} + ay = b$ can be solved by turning the l.h.s. into a single derivative.

Note $\frac{d}{dx}\exp[\int_{-\infty}^{x} a(x')dx'] = a(x)\exp[\int_{-\infty}^{x} a(x')dx']$

$\frac{dy}{dx} + ay = b$ can be solved by turning the l.h.s. into a single derivative.

Note $\frac{d}{dx}\exp\left[\int_{-\infty}^{x} a(x')dx'\right] = a(x)\exp\left[\int_{-\infty}^{x} a(x')dx'\right]$

Then $\underbrace{\frac{dy}{dx} e^{\int_{-\infty}^{x} a(x')dx'} + a e^{+\int_{-\infty}^{x} a(x')dx'} y}_{\frac{d}{dx}\left[y e^{\int_{-\infty}^{x} a(x')dx'}\right]} = b e^{\int_{-\infty}^{x} a(x')dx'} \Rightarrow y e^{\int_{-\infty}^{x} a(x')dx'} = y(-\infty) + \int_{-\infty}^{x} b(x') e^{\int_{-\infty}^{x'} a(x'')dx''} dx'$

if $y(-\infty) = 0$

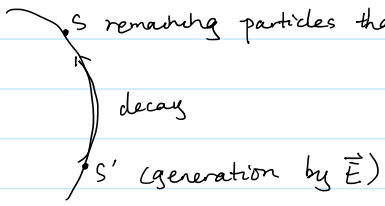
$$\Rightarrow \boxed{y(x) = \int_{-\infty}^{x} b(x') e^{-\int_{x'}^{x} a(x'')dx''} dx'}$$

*

$$\Rightarrow \boxed{g(s) = \int_{-\infty}^{s} \underbrace{\frac{\ell^2}{v_\perp}\left(\frac{e}{\hbar}\frac{\partial f}{\partial \vec{k}}\cdot\vec{E}\right)\Big|_{s'}}_{\equiv F_1(s')} e^{-\int_{s'}^{s} \underbrace{\frac{\ell^2}{v_\perp \tau}\Big|_{s''}}_{\equiv F_2(s'')} ds''} ds'} \quad ③.$$

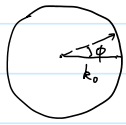
Physical meaning: $F_1(s') \propto$ particles excited by $\vec{E}$ at position $s'$

$F_2(s') \propto$ decay along the path from $s'$ to $s$.

$\Rightarrow$ 


<u>Examples:</u>

1. circular orbits.




$ds = k_0 d\phi$

$\vec{E} = E\hat{x}$

$v_\perp = \text{const}$

$\frac{\partial f}{\partial \vec{k}}\cdot\vec{E} = \frac{\partial f}{\partial \varepsilon}\hbar v_\perp E\cos\phi$

$\Rightarrow F_1(s') = \frac{\partial f}{\partial \varepsilon}\ell^2 eE\cos\phi'$

$F_2(s'') = \frac{\ell^2}{v_\perp \tau} = \text{const}$

$$\Rightarrow g(s) = g(\phi) = \int_{-\infty}^{\phi} k_0 d\phi' \left(\frac{\partial f}{\partial \varepsilon}\ell^2 eE\right)\cos\phi' e^{-(\phi-\phi')\frac{k_0\ell^2}{v_\perp\tau}}$$

$$\omega_c = \frac{2\pi}{T} = \frac{2\pi}{\int_0^T dt} = \frac{2\pi}{\int_0^{2\pi}\frac{dt}{d\phi}d\phi} = \frac{2\pi}{\int_0^{2\pi}\frac{d\phi}{\frac{\dot{s}}{k_0}}} = \frac{2\pi}{\int_0^{2\pi}\frac{k_0 d\phi}{\frac{eB}{\hbar}v_\perp}} = \frac{eBv_\perp}{\hbar k_0} = \frac{v_\perp}{\ell^2 k_0}$$

$$\therefore \omega_c\tau = \frac{v_\perp\tau}{\ell^2 k_0} \Rightarrow \frac{k_0\ell^2}{v_\perp\tau} = \frac{1}{\omega_c\tau}$$

$$\Rightarrow g(s) = \int_{-\infty}^{\phi}\left(\frac{\partial f}{\partial \varepsilon}k_0\ell^2 eE\right)\cos\phi' d\phi' e^{-\frac{\phi-\phi'}{\omega_c\tau}}$$

$$\propto \int_0^{\infty}\cos(\phi-\phi') e^{-\frac{\phi'}{\omega_c\tau}} d\phi' = \sum_{n=0}^{\infty} e^{-\frac{2\pi n}{\omega_c\tau}}\int_0^{2\pi}\cos(\phi-\phi') e^{-\frac{\phi'}{\omega_c\tau}} d\phi'$$

$$= \frac{1}{1-e^{-\frac{2\pi}{\omega_c\tau}}}\int_0^{2\pi}\cos(\phi-\phi') e^{-\frac{\phi'}{\omega_c\tau}} d\phi' \simeq \frac{\omega_c\tau}{2\pi}\int_0^{2\pi}\cos(\phi-\phi')\sum_{n=0}^{\infty}\frac{(-\phi')^n}{n!}(\omega_c\tau)^{-n} d\phi'$$

0th order: $\int_0^{2\pi}\cos(\phi-\phi') = 0.$

1st order: $\sigma_{yx} \propto \ell^2 \propto \frac{1}{B}$, $\sigma_{xx} = 0.$

2nd order: $\sigma_{xx} \propto \frac{1}{B^2}$

1st order : $\sigma_{yx} \propto \ell^2 \propto \frac{1}{B}$, $\sigma_{xx} = 0$.

2nd order : $\sigma_{xx} \propto \frac{1}{B^2}$

2. open orbits. $(\parallel \hat{x})$



$$\vec{v}_\perp = v_\perp \hat{y},$$

$$\frac{\partial f}{\partial \vec{k}} \cdot \vec{E} = \frac{\partial f}{\partial \varepsilon} \hbar v_\perp \hat{y} \cdot \vec{E} = \begin{cases} 0 & \vec{E} \parallel \hat{x} \\ \frac{\partial f}{\partial \varepsilon} \hbar v_\perp E & \vec{E} \parallel \hat{y}. \end{cases}$$

$\therefore$ open orbit can contribute to $\sigma_{\alpha\beta}$ if $\beta$ is perpendicular to the orbit.

consider $\sigma_{yy}$ :

$$g(s) = \int_{-\infty}^{s} \left( \frac{\partial f}{\partial \varepsilon} \hbar v_\perp E \frac{e\ell^2}{v_\perp \hbar} \right) e^{-\frac{(s-s')\ell^2}{v_\perp \tau}} ds' = \frac{\partial f}{\partial \varepsilon} eE \ell^2 \int_0^\infty e^{-\frac{s'\ell^2}{v_\perp \tau}} ds'$$

$$= \frac{\partial f}{\partial \varepsilon} eE \ell^2 \frac{v_\perp \tau}{\ell^2} \sim O(B^0)$$

$\therefore \sigma_{yy} \sim$ const.

$$\therefore \rho = \begin{pmatrix} \frac{A_{xx}}{B^2} & -\frac{A_H}{B} \\ \frac{A_H}{B} & A_{yy} \end{pmatrix}^{-1} = \frac{B^2}{A_{xx}A_{yy} + A_H^2} \begin{pmatrix} A_{yy} & \frac{A_H}{B} \\ -\frac{A_H}{B} & \frac{A_{xx}}{B^2} \end{pmatrix}$$

$\Rightarrow \rho_{xx} \sim B^2$ (non-saturating) $(I \parallel Q)$

$\rho_{yy} \sim$ const (saturating) $(I \perp Q)$

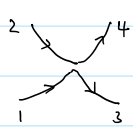
Keys : closed orbit : $\sigma_{xx} \sim (\omega_c \tau)^{-2}$

open orbit : $(\parallel \hat{x})$. $\begin{cases} \sigma_{yy} \sim \text{const} \times \tau \\ \sigma_{xx} \sim 0. \end{cases}$

<u>Solution for coupled orbits.</u>

when orbits cross, a gap is usually opened due to degenerate perturbation.

$\Downarrow$




Under a finite B, since $\dot{\vec{k}} = -\frac{e}{\hbar} \dot{\vec{r}} \times \vec{B}$, particles have two possible choices : continue along the original orbit (no gap) — P

or switch to the other orbit (finite gap). — $1-P = Q$

$P \sim \exp(-\frac{H_0}{H})$ $H_0 = H_0(\varepsilon_F, p_z)$ — Blount.

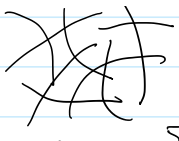
$$\boxed{\begin{pmatrix} N_3 \\ N_4 \end{pmatrix} = \begin{pmatrix} Q & P \\ P & Q \end{pmatrix} \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}}$$

$\Rightarrow$ $H \gg H_0$ — $P = 1$ (complete breakdown)

$H \to 0$ — $P = 0$ (no breakdown).

Now consider an infinitely complex network of coupled orbits.

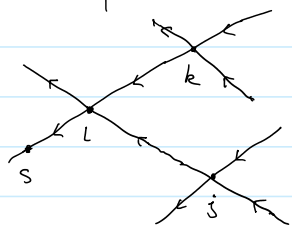
— how to get a $g(s)$ ?



— how to get a $g(s)$ ?

Ansatz : $g(s) = \sum_{path} P_{path}\, g(s_{path})$ $\quad P_{path}$ — probability of taking a particular path.

To perform the path summation, focus first on a MB junction in the network.




$j, k, l$ — label all MB junctions in the network.

Goal : $g(s)$.

First $g(s)$ in terms of $g(s_0)$ and $s-s_0$.

$$g(s) = \int_{-\infty}^{s} F_1(s')\exp\left[-\int_{s'}^{s} F_2(s'')ds''\right] ds'$$

$$= \int_{-\infty}^{s_0} F_1(s')\exp\left[-\int_{s'}^{s_0} F_2(s'')ds'' - \int_{s_0}^{s} F_2(s'')ds''\right] ds' + \int_{s_0}^{s} F_1(s')e^{-\int_{s'}^{s} F_2(s'')ds''} ds'$$

$$= e^{-\int_{s_0}^{s} F_2(s'')ds'}\, g(s_0) + \int_{s_0}^{s} F_1(s')e^{-\int_{s'}^{s} F_2(s'')ds''} ds'$$

$$\equiv \boxed{c(s,s_0)\, g(s_0) + v(s,s_0)}$$

Now, $g(s) = v(s, s_{l0}) + c(s, s_{l0})\, g(s_{l0})$

$$\left.\begin{aligned} g(s_{l0}) &= P_{k_1\to l_0}\, g(s_{k1}) + P_{j_1\to l_0}\, g(s_{j1}) \\ g(s_{k1}) &= v(s_{k1}, s_{k0}) + c(s_{k1}, s_{k0})\, g(s_{k0}) \\ g(s_{j1}) &= v(s_{j1}, s_{j0}) + c(s_{j1}, s_{j0})\, g(s_{j0}) \end{aligned}\right\}$$

$$\Rightarrow \underbrace{\begin{pmatrix} g(s_{j0}) \end{pmatrix}}_{\equiv I} = \begin{pmatrix} P_{k_1\to j_0} \end{pmatrix} \begin{pmatrix} g(s_{k1}) \end{pmatrix}$$

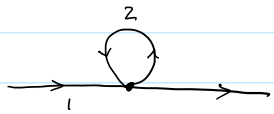
$$= \underbrace{\begin{pmatrix} P_{k_1\to j_0} \end{pmatrix}}_{\equiv M} \left[ \underbrace{\begin{pmatrix} v(s_{k1}, s_{k0}) \end{pmatrix}}_{\equiv V} + \underbrace{\begin{pmatrix} \ddots & & \\ & c(s_{k1}, s_{k0}) & \\ & & \ddots \end{pmatrix}}_{\equiv C} \underbrace{\begin{pmatrix} g(s_{k0}) \end{pmatrix}}_{= I} \right]$$

$$\Rightarrow I = M\cdot V + M\cdot C\cdot I \Rightarrow \boxed{I = (\mathbb{I} - M\cdot C)^{-1}\cdot M\cdot V}$$

After solving $I$ or $g(s_{j0})$, we finally have

$$\boxed{g(s) = c(s, s_{j0})\, g(s_{j0}) + v(s, s_{j0}).} \quad **$$

## Application to a minimal model:




$P=0$ : 1 & 2 are decoupled

$P=1$ : 1 & 2 form a single orbit.

1 – open, $\parallel \hat{x}$

2 – closed,

One can calculate $\sigma_{\alpha\beta}$ exactly using **, but let us consider four special cases below.

$$\begin{cases} \vec{E} \parallel \hat{x} \begin{cases} P=0 & ① \\ P=1 & ② \end{cases} \\ \vec{E} \parallel \hat{y} \begin{cases} P=0 & ③ \\ P=1 & ④ \end{cases} \end{cases}$$

① $(\vec{E} \parallel \hat{x},\ P=0)$

orbit 1 has no contribution to $g(s)$ $(\vec{v}_\perp \cdot \vec{E} = 0)$ $\Rightarrow$ $\boxed{\sigma_{xx} \sim (\omega_{c_2}\tau)^{-2}}$

$P=0 \Rightarrow$ decoupled.

② $(\vec{E} \parallel \hat{x},\ P=1)$

orbit 1 can contribute through $e^{-\int_{s'}^{s} F_2(s'')ds''}$

particles effectively have to travel longer distances in order to finish a cycle $\Rightarrow$ more effective decay, or smaller $(\omega_{c_2}\tau)$.

$\Rightarrow$ $\boxed{\sigma_{xx} \sim (\omega_{c_2}\tau)^{-2} \text{ increases}}$

③ $(\vec{E} \parallel \hat{y},\ P=0)$

orbit 1 is dominant $\Rightarrow$ $\sigma_{yy} \sim \text{const.} \times \tau$

④ $(\vec{E} \parallel \hat{y},\ P=1)$

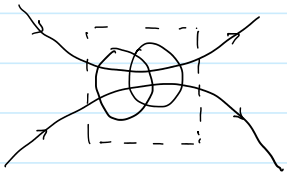
orbit 2 makes 1 effectively longer — more decay due to $e^{-\int_{s'}^{s} F_2(s'')ds''}$

$\Rightarrow$ $\boxed{\sigma_{yy} \sim \text{const} \times \tau \text{ decreases.}}$

①, ②, ③, ④ $\Rightarrow$ $\begin{cases} \sigma_{xx} \text{ increases w/ } P \\ \sigma_{yy} \text{ decreases w/ } P. \end{cases}$

Oscillation ? $P = P_0 + P_1 \cos\left(\frac{H_0}{H} + \phi_0\right)$

Why? The "MB junction" is not a single junction but a small coherent network, e.g.



the classical tunneling probability can be calculated by solving a QM scattering problem.

classical orbits + QM effective MB junctions = semiclassical theory of (low frequency) SdH in coupled orbits

Recap:

① Incommensurate DW — intricate network of
- semiclassical closed orbits.
- semiclassical open orbits $\parallel \vec{Q}$
- effective, coherent junctions of small remant FS pieces.

②. coupling to open orbit will increase the $\sigma$ due to closed orbits $(L\omega_c\tau) \downarrow$ )
closed decrease open ( $\tau$ $\downarrow$ )

③ "$\pi$ phase shift" — no drama.