The angular dependence of the quantum oscillations of the magnetoresistance in strongly anisotropic quasi-two-dimensional layered conductors

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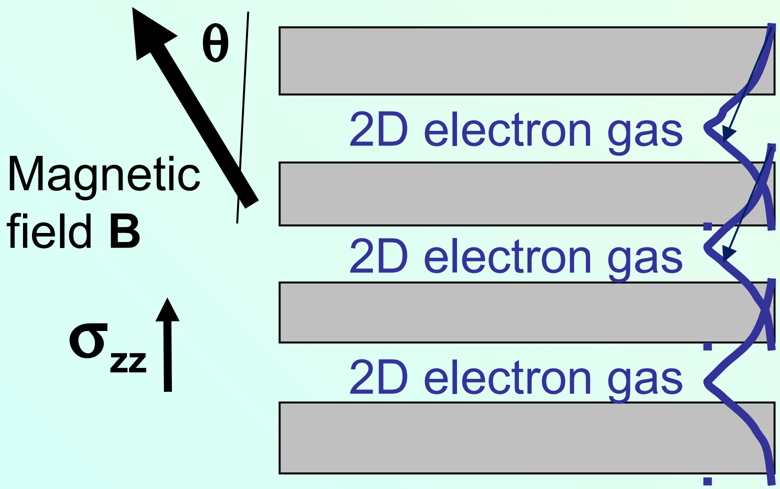
Main question to be studied:

How the angular oscillations of magnetoresistance (MR) interfere with (or influence on) the magnetic quantum oscillations (MQO) of interlayer MR.

Layered quasi-2D metals

(Examples: heterostructures, organic metals, all high-Tc superconductors)



Electron wave functions overlap leads to the finite interlayer transfer integral t_z

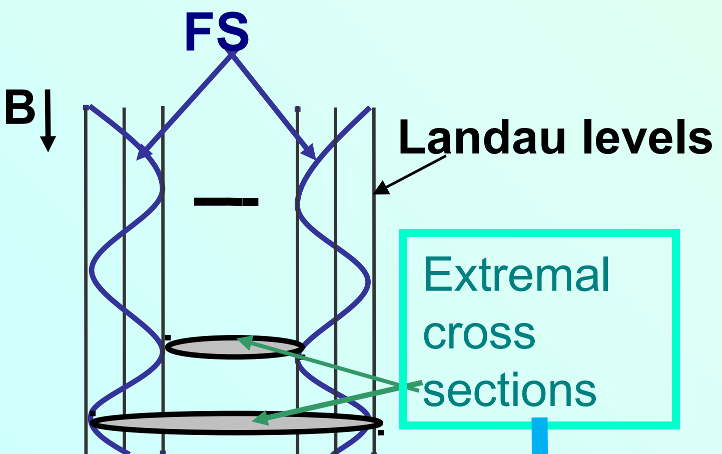
Electron dispersion in the tight-binding approximation is highly anisotropic:

$$\varepsilon(p)=\varepsilon_{||}(p_{||})+2t_z \cos(p_z d/\hbar),$$

$$t_z << E_F$$

(coherent-tunneling, conserving $p_{||}$)

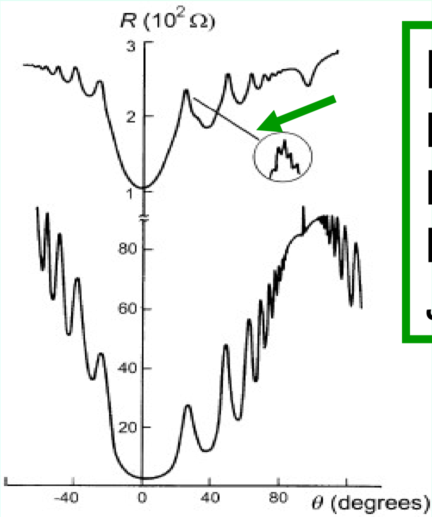
$$\varepsilon_{||}(p_{||})=p^2_{||}/2m_{||}$$



Fermi surface in layered Q2D metals is a warped cylinder. The size of warping $W=4t_z \sim \hbar\omega_c$

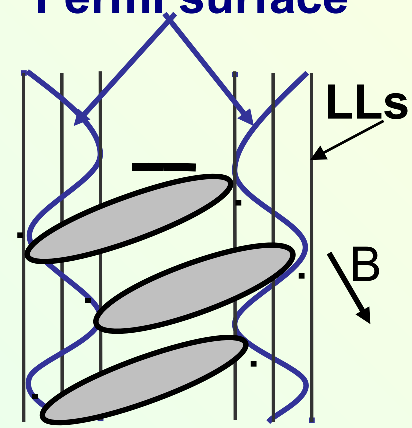
Two close frequencies => beats of MQO

Angle-dependent magnetoresistance oscillations (AMRO) in quasi-2D metals.



First observation:
M.V. Kartsovnik, P. A. Kononovich, V. N. Laukhin, I. F. Schegolev, *JETP Lett.* ***48***, *541 (1988).*

First theory:
K.J. Yamaji, Phys. Soc. Jpn. **58, 1520, (1989).**



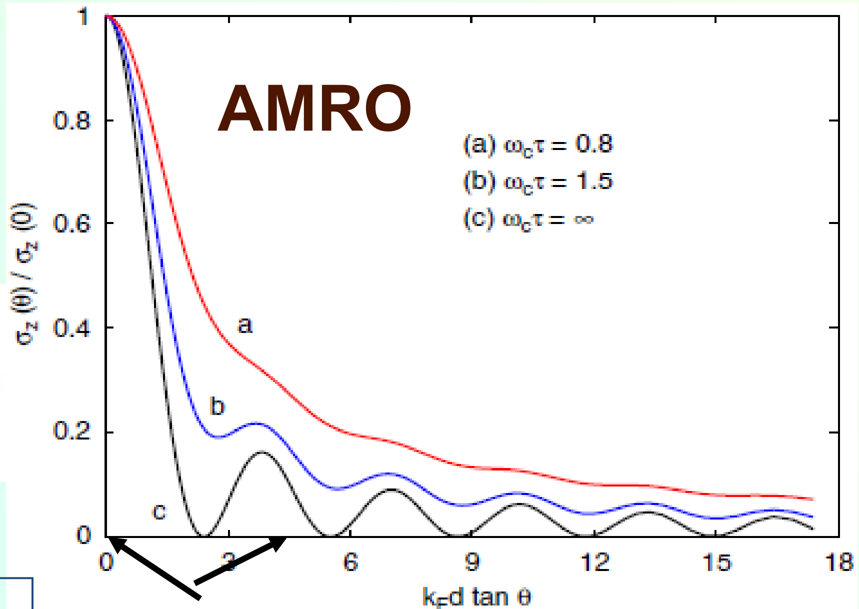
$$\sigma_{zz}^{3D} = e^2 \tau \sum_{FS} v_z^2, \; v_z = \partial \varepsilon / \partial p_z$$

For axially symmetric dispersion and in the first order in t_z the Shockley tube integral gives:
[R. Yagi et al., J. Phys. Soc. Jap. **59**, 3069 (1990)]

$$\frac{\sigma_z(\boldsymbol{B})}{\sigma_z(0)} = J_0^2(k_F d \tan\theta) + 2\sum_{j=1}^{\infty} \frac{J_j^2(k_F d \tan\theta)}{1 + (j\omega_c \tau)^2}.$$

gives AMRO

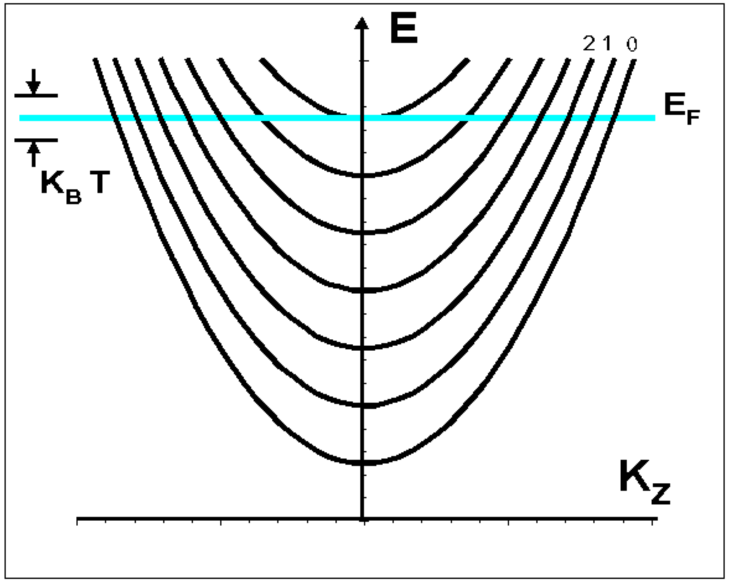
gives damping of AMRO by disorder



Yamaji angles

Origin of magnetic quantum oscillations in metals

For parabolic electron dispersion in zero magnetic field
$\varepsilon(p)= p_x^2/2m_x + p_y^2/2m_y + p_z^2/2m_z$, **in magnetic field directed along z-axis the dispersion relation is**
$\varepsilon(n,p_z)=\hbar\omega_c(n+1/2)+p_z^2/2m_z$,
where $\omega_c=eB/mc$ **(Landau level quantization).**



As the magnetic field increases the Landau levels periodically cross Fermi level.

This results in magnetic quantum oscillations (MQO) of thermodynamic (DoS, magnetization) and transport electronic properties of metals.

In 3D the DoS oscillations are weak, because the integration over p_z smears them out.

In 2D the DoS oscillations can be strong and sharp, leading to the sharp and non-sinusoidal MQO.

Lifshitz-Kosevich formula for MQO

Quantum oscillations of magnetization (de Haas – van Alphen effect)

$$M \propto eF\sqrt{H/A''}\sum_{p=1}^{\infty} p^{-3/2}\sin\left[2\pi p\left(\frac{F}{H}-\frac{1}{2}\right)\pm\frac{\pi}{4}\right]R_T(p)R_D(p)R_S(p),$$

only difference between 3D and 2D ? [D. Shoenberg]

where the dHvA fundamental frequency $F = chA_{extr}/(2\pi)\,e,$

The temperature damping factor $R_T(p) = \pi\kappa p/\sinh(\pi\kappa p),$

$\kappa \equiv 2\pi\, k_B T/h\omega_C\,,\ \omega_C = eH/m^*c\,.$

The scattering (Dingle) damping factor $R_D(p) = \exp\left(\frac{-\pi p}{\tau\omega_C}\right) = \exp\left(\frac{-2\pi^2 T_D p}{\omega_C}\right),$

$\tau = h/(2\pi)^2 k_B T_D$ **is the mean free scattering time.**

The spin factor $R_s(p) = \cos\left(\frac{\pi p g m^*}{2m_0}\right).$

General motivation

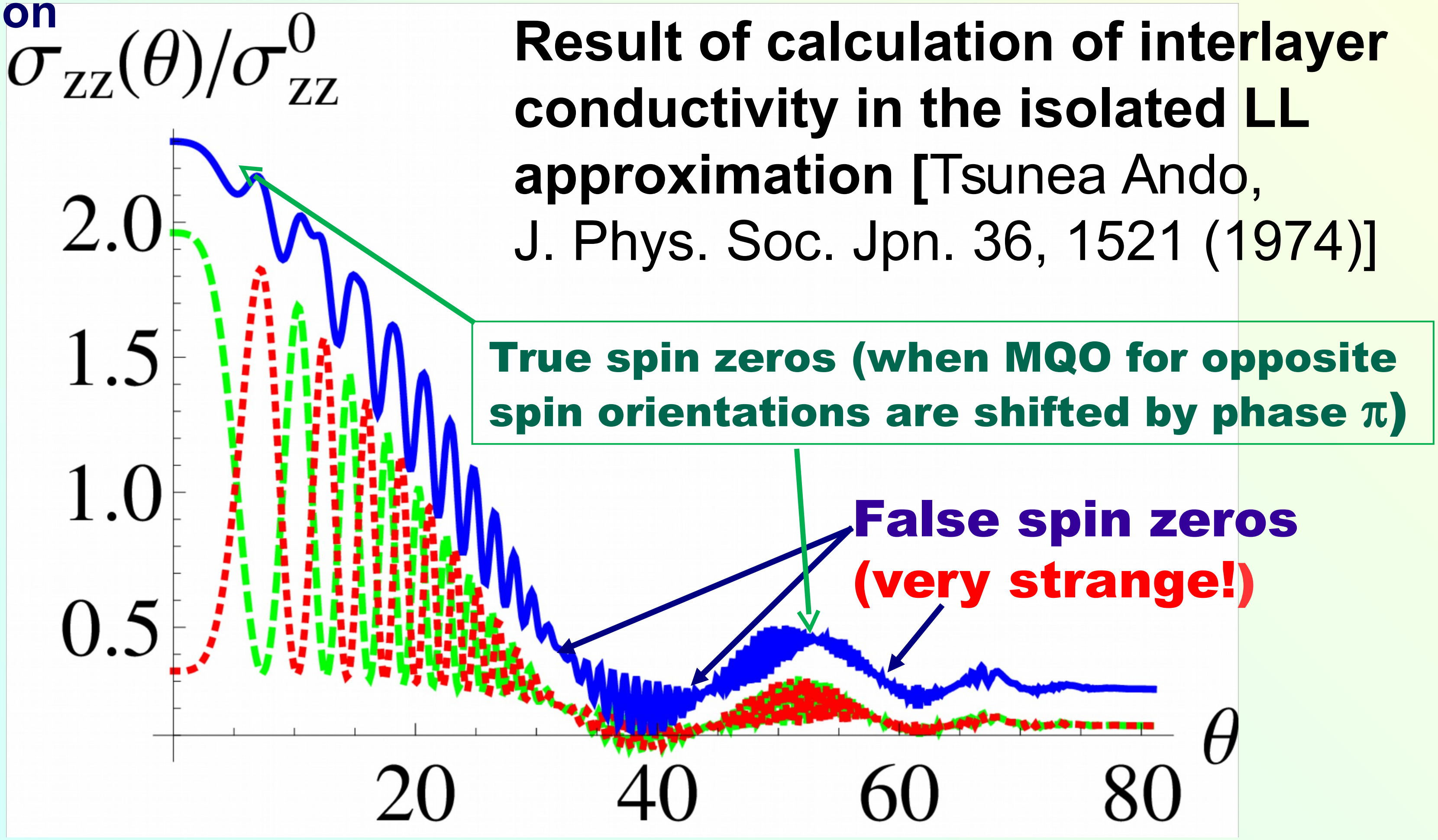
Layered compounds are very common: high-Tc cuprates, pnictides, organic metals, intercalated graphites, heterostructures, etc.
Magnetoresistance (MQO and AMRO) is used to measure the quasi-particle dispersion, Fermi surface, effective mass, mean scattering time.
It is an important complementary tool to ARPES.

Aim:

Our task is to investigate the interplay between angular and magnetic quantum oscillations (MQO), i.e. to calculate the MQO of magnetoresistance taking into account angular oscillations and find out if the false spin zeros are possible.

Motivation

Result of calculation of interlayer conductivity in the isolated LL approximation [Tsunea Ando, J. Phys. Soc. Jpn. 36, 1521 (1974)]



The calculated angular dependence of the interlayer conductivity for spin-up component (dashed green line), spin-down component (dotted red line), and the their sum (solid blue line) for the g-factor g=2 for Gaussian LL shape.

Expected false spin-zeroes at angle θ ≈ 32˚, 44˚, 58˚, …

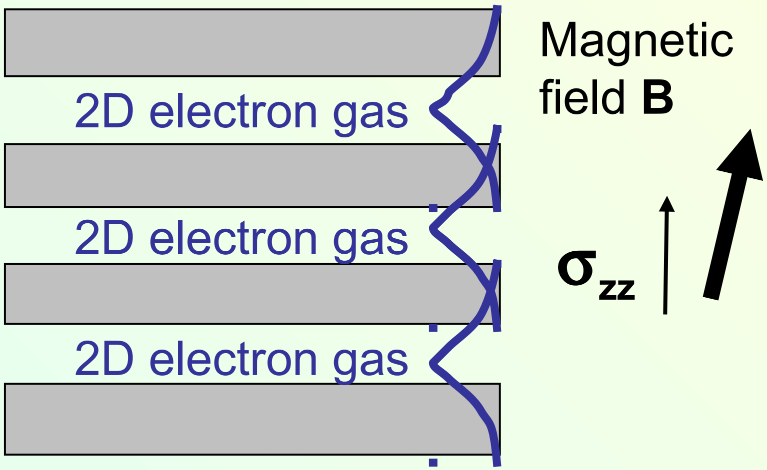
Incorrect, as will be shown later!

The two-layer tunneling model

The Hamiltonian contains 3 terms:

$$\hat{H} = \hat{H}_0 + \hat{H}_t + \hat{H}_I$$

1 2 3



1. The 2D free electron Hamiltonian in magnetic field summed over all layers:

$$\hat{H}_0 = \sum_{m,j} \varepsilon_{2D}(m)\, c^{+}_{m,j} c_{m,j},$$

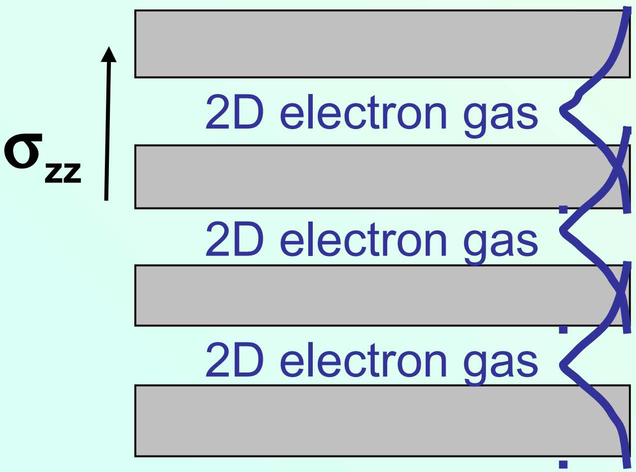
2. The coherent electron tunneling between any two adjacent layers:

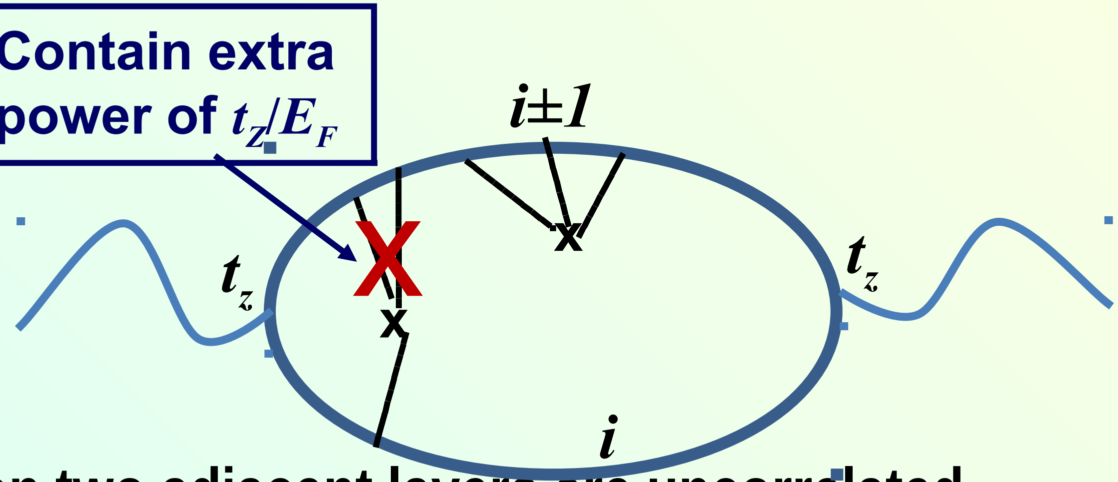
$$\hat{H}_t = 2t_z \sum_j \int dxdy [\Psi_j^{\dagger}(x,y)\Psi_{j-1}(x,y) + \Psi_{j-1}^{\dagger}(x,y)\Psi_j(x,y)],$$

3. The short-range impurity potential: $\hat{H}_I = \sum_i V_i(r)$ where $V_i(r) = U\delta^3(r - r_i)$

$\Gamma_0 \gtrsim \hbar\omega_c >> t_z$ **[A.D. Grigoriev, P.D. Grigoriev, Физ. низких темп. 40(4), 472 (2014)]**

Impurity averaging





The impurity distributions on two adjacent layers are uncorrelated, and the vertex corrections are small by the parameter t_Z/E_F=>

$$\sigma_{zz}=\frac{4e^2t_z^2d}{L_xL_y}\int d^2rd^2r'\int\frac{d\varepsilon}{2\pi}\left[-n_F'(\varepsilon)\right]\langle \mathrm{Im}\,G(r,r',j,\varepsilon)\rangle\langle \mathrm{Im}\,G(r',r,j+1,\varepsilon)\rangle.$$

Vertex corrections can be ignored

The calculation of interlayer conductivity reduces to 2D electron Green's function

Calculation of the angular dependence of MR

[started in P. Moses and R. H. McKenzie, Phys. Rev. B 60, 7998 (1999).]
P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011), P. D. Grigoriev, T. I. Mogilyuk Phys. Rev. B 90, 115138 (2014)

The impurity averaging on adjacent layers can be done independently:

$$\sigma_{zz}=\frac{e^2 t_z^2 d}{L_x L_y}\int d^2 r d^2 r' \int \frac{d\varepsilon}{2\pi}\langle A(r,r',j,\varepsilon)\rangle\langle A(r',r,j+1,\varepsilon)\rangle\left[-n'_F(\varepsilon)\right],$$

where the spectral function $A(r,r',j,\varepsilon)=i\left[G_A(r,r',j,\varepsilon)-G_R(r,r',j,\varepsilon)\right].$

In tilted magnetic field $B=(B_x,0,B_z)=(B\sin\theta,0,B\cos\theta)$
the vector potential is $A=(0,xB_z-zB_x,0)$ **, the electron wave functions on adjacent layers acquire the coordinate-dependent phase difference** $\Lambda(r)=-yB_x d=-yBd\sin\theta,$ **and the Green's functions acquire the phase** $G_R(r,r',j+1,\varepsilon)=G_R(r,r',j,\varepsilon)\exp\{ie[\Lambda(r)-\Lambda(r')]\},$

The expression for conductivity has the form:

$$\sigma_{zz}=\frac{2e^2 t_z^2 d}{\hbar}\int\int\frac{d\varepsilon}{2\pi}d^2 r\left[-n'_F(\varepsilon)\right]\left[G^2(r,\varepsilon)\cos\left(\frac{eByd}{h/2\pi}\sin\theta\right)-\mathrm{Re}\left[G_R^2(r,\varepsilon)\exp\left(\frac{ieByd}{h/2\pi}\sin\theta\right)\right]\right].$$

$G_R G_A$

New term! $G_R G_R$

Angular dependence of harmonic amplitudes for arbitrary LL shapes

(P. D. Grigoriev, T. I. Mogilyuk, Phys. Rev. B 90, 115138 (2014))

The angular dependence of interlayer conductivity is given by a double sum over Landau levels:

$$\frac{\sigma_{zz}/\sigma_{zz}^0}{\Gamma_0\hbar\omega_c} = \frac{2}{\pi}\sum_{n,p\in Z} Z(n,p)\mathrm{Im}G(\varepsilon,n)\mathrm{Im}G(\varepsilon,n+p),$$

$$Z(n,p) = \exp\left(-\frac{(ql_H)^2}{2}\right)\left(\frac{(ql_H)^2}{2}\right)^p \left(L_n^p\left[\frac{(ql_H)^2}{2}\right]\right)^2 \left(\frac{n!}{(n+p)!}\right)$$

where $q = eBd\sin\theta/\hbar c$ **and the Laguerre polynomials**

$$L_n^\alpha(z) \approx \frac{\Gamma(\alpha+n+1)}{n!}\left(\left(n+\frac{\alpha+1}{2}\right)z\right)^{-\frac{\alpha}{2}} \exp\left(\frac{z}{2}\right) J_\alpha\left(2\sqrt{\left(n+\frac{\alpha+1}{2}\right)z}\right)$$

Angular dependence of harmonic amplitudes with AMRO for Lorentzian LL shapes

For Lorentzian LL shape:

$$\frac{\sigma_{zz}^{L}}{\sigma_{zz}^{0}} = \frac{\Gamma_0}{\Gamma} \sum_{k=-\infty}^{\infty} (-1)^k \exp\left(\frac{2\pi i k \epsilon_F}{\hbar\omega_c}\right) R_D(k)\, R_T(k)$$

$$\times R_S(k) \left\{ \left[J_0(\kappa)\right]^2 \left(1 + \frac{\pi |k|}{\omega_c \tau}\right) + \sum_{p=1}^{\infty} \frac{2\left[J_p(\kappa)\right]^2}{1 + (p\omega_c\tau)^2} \right\},$$

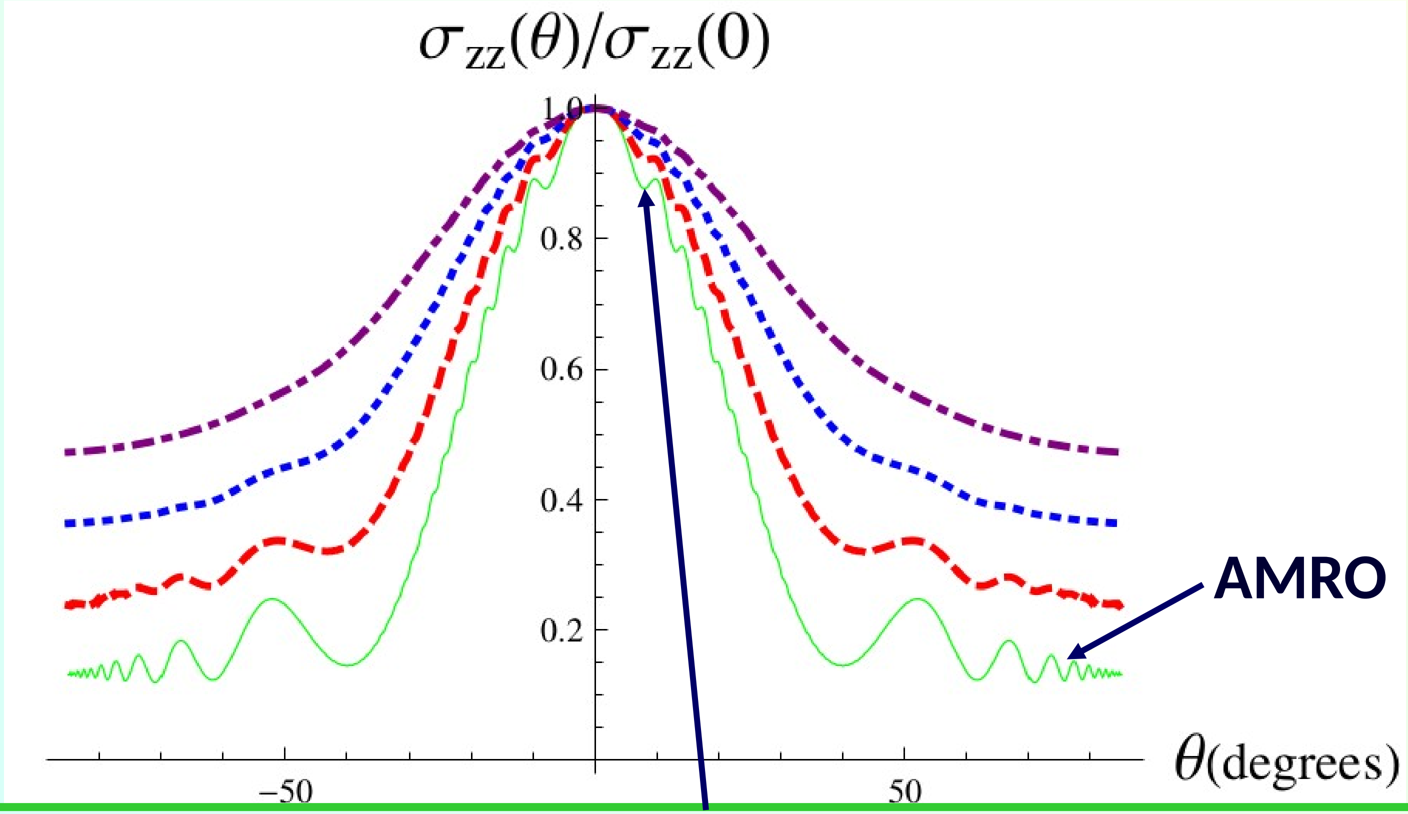
$$\kappa \equiv k_F d \tan\theta$$

$$! \; \tau = \tau_0 \left(\Gamma_0 / \Gamma\right) \propto 1/\sqrt{B \cos\,\theta}$$

For Gaussian LL shape the p≠0 terms are exponentially small at $\omega_c\tau \gg 1$, **which leads to a strong enhancement of AMRO amplitudes.**

Angular dependence of MQO amplitudes is given not only by the spin-zero factor

$$R_S(k) = \cos\left(\frac{\pi k \; m^*}{m_e \cos\theta}\right)$$



Weak magnetic quantum oscillations in the presence of AMRO

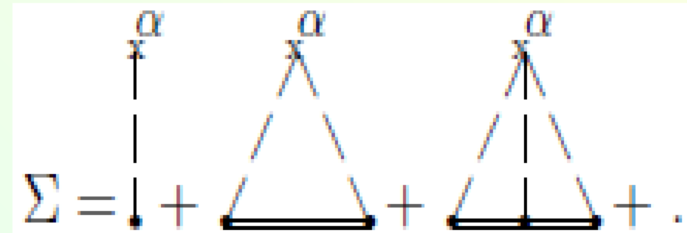
The angular dependence of normalized interlayer conductivity for Lorentzian LL With four different values $\omega_c \tau_0 = 10$ (thin solid green curve), 10/3 (dashed red curve), 5/3 (dotted blue curve), and 1 (dash-dotted purple curve). The other parameters $k_F d = 3, \mu = 605\,K,\ T = 3\,K,\ B_0 \approx 11.6\,T,$ which for cyclotron mass $m = m_e$ and for $\theta = 0$ corresponds to $\hbar\omega_c = 10\,K$

Isolated LL: approxi-mation

The 2D electron Green's function with disorder in B_z

The point-like impurities are included in the "non-crossing" approximation, which gives:

$$G(r_1, r_2, \varepsilon) = \sum_{n, k_y, k'_y} \Psi^{0*}_{n, k_y}(r_2)\, \Psi^{0}_{n, k'_y}(r_1)\, G(\varepsilon, n),$$



where, if Landau levels do not overlap,

Tsunea Ando, J. Phys. Soc. Jpn. 36, 1521 (1974)

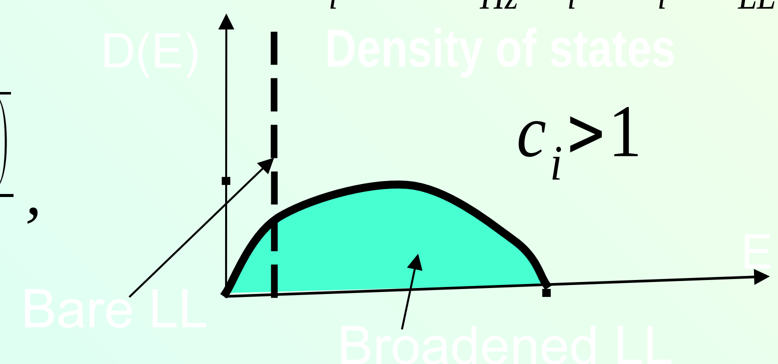
$$G_R(E, n) = \frac{E + E_g(1 - c_i) \pm \sqrt{(E - E_1)(E - E_2)}}{2 E E_g},$$

$$E_1 = E_g\left(\sqrt{c_i} - 1\right)^2, \quad E_2 = E_g\left(\sqrt{c_i} + 1\right)^2,$$

where $E_g = V_0 / 2\pi l_{Hz}^2 \propto B,$
$c_i = 2\pi l_{Hz}^2 N_i = N_i / N_{LL}.$

The density of states on each LL has a dome-like shape:

$$D(E) = -\frac{\operatorname{Im} G_R(E)}{\pi} = \frac{\sqrt{(E - E_1)(E_2 - E)}}{2\pi |E| E_g},$$



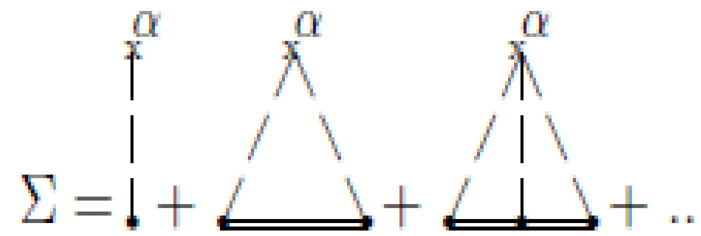
LL width

$$c_i = 2\pi l_{Hz}^2 N_i = N_i / N_{LL}.$$

In this approximation we obtain false spin zeros! (very strange)

The 2D electron Green's function with disorder in B_z

The point-like impurities are included in the "non-crossing" approximation, which gives:



$$G(r_1, r_2, \varepsilon) = \sum_{n,\, k_y,\, k'_y} \Psi^{0*}_{n,\, k_y}(r_2)\, \Psi^{0}_{n,\, k'_y}(r_1)\, G(\varepsilon, n),$$

where $G(\varepsilon, n) = \dfrac{1}{\varepsilon - \hbar\omega_c(n + 1/2) - \Sigma(\varepsilon)}, \quad \Sigma(\varepsilon) = \dfrac{n_i U}{1 - U G(\varepsilon)},$

At $\Gamma_0 \sim \hbar\omega_c$ one cannot consider each LL separately, =>

$$G(\varepsilon) = \sum_{n, k_y, k_z} G(\varepsilon, n) = \frac{g_{LL}}{d} \sum_n G(\varepsilon, n) = -\frac{\pi g_{LL}}{\hbar\omega_c d} \tan\left[\pi \frac{\varepsilon - \Sigma(\varepsilon)}{\hbar\omega_c}\right]$$

The system of equations in SCBA (self-consistent Born approximation) becomes

$$\frac{\gamma}{\gamma_0} = \frac{\sinh(\gamma)}{\cosh(\gamma) + \cos(\alpha)}, \qquad \alpha - \frac{2\pi\varepsilon}{\hbar\omega_c} = \frac{\gamma_0 \sin(\alpha)}{\cosh(\gamma) + \cos(\alpha)}$$

where $\alpha \equiv 2\pi(\varepsilon - \mathrm{Re}\Sigma(\varepsilon))/\hbar\omega_c, \;\; \gamma \equiv 2\pi|\mathrm{Im}\Sigma(\varepsilon)|/\hbar\omega_c$

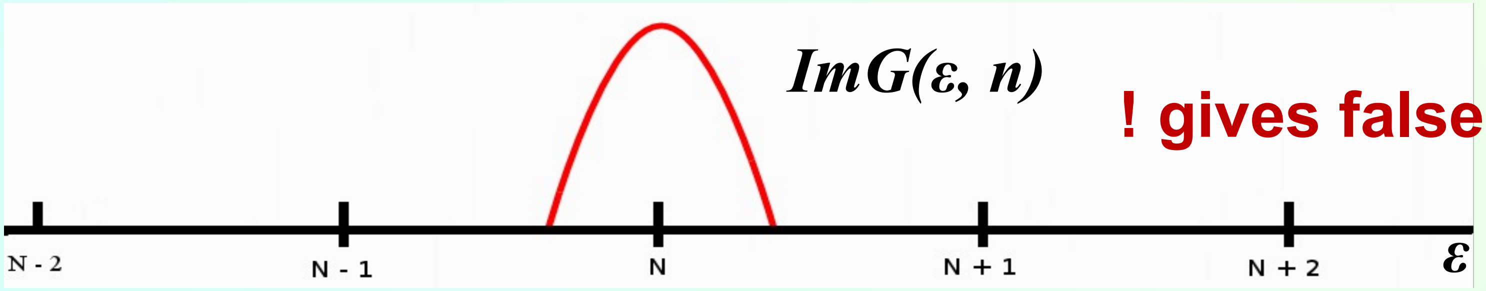
In SCBA with many LLs the false spin zeros are absent

Green's functions of one Landau level $G(\varepsilon, n)$

Contribution to the total Green's function from each Landau level

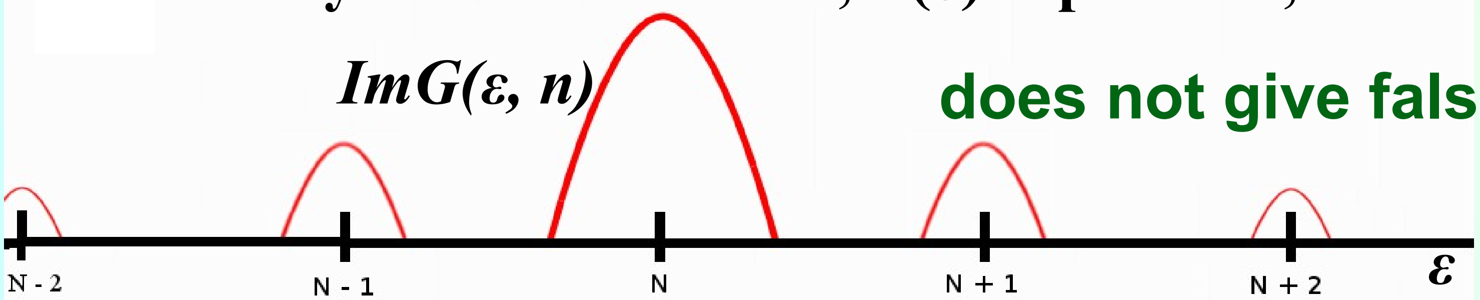
$$G\left(\varepsilon,n\right)=\frac{1}{\varepsilon-\hbar\omega_{c}\left(n+1/2\right)-\Sigma\left(\varepsilon\right)},$$

Approximation of isolated LLs: Im Σ(ε)≠0 only near the n-th LL [Tsunea Ando, J. Phys. Soc. Jpn. 36, 1521 (1974)]



! gives false spin-zeros

When many LLs are included, Σ(ε) is periodic, which gives



does not give false spin-zeros

The total Green's function

$$G\left(\varepsilon\right)\ =\ \sum_{n,k_y,k_z}G\left(\varepsilon,n\right)=\frac{g_{LL}}{d}\sum_{n}G\left(\varepsilon,n\right)$$

Angular dependence of harmonic amplitudes with AMRO for general LL shapes

$$\frac{\sigma_{zz}}{\sigma_{zz}^{0}} = \int d\varepsilon \frac{\Gamma_0}{2\Gamma(\epsilon)} \sum_{s=\pm 1} \left[-n_F'(\varepsilon)\right] \sum_{p=-\infty}^{\infty} A_p \left[J_p(\kappa)\right]^2$$

$$A_0 \equiv \sum_{n\in Z} \frac{(2/\pi)\hbar\omega_c\Gamma^3}{\left[\left(\epsilon^* - \hbar\omega_c\left(n+\frac{1}{2}\right)\right)^2 + \Gamma^2\right]^2} = \frac{\sinh(\gamma)}{(\cos(\alpha)+\cosh(\gamma))} - \gamma\frac{1+\cos(\alpha)\cosh(\gamma)}{(\cos(\alpha)+\cosh(\gamma))^2}$$

$$A_p \equiv \sum_{n\in Z} \frac{(2/\pi)\hbar\omega_c\Gamma^3}{\left[\left(\epsilon^* - \hbar\omega_c(n+1/2)\right)^2 + \Gamma^2\right]} \frac{1}{\left[\left(\epsilon^* - \hbar\omega_c(n+p+1/2)\right)^2 + \Gamma^2\right]} = \frac{\sinh(\gamma)}{(\cos(\alpha)+\cosh(\gamma))\left[1+(p\pi/\gamma)^2\right]}$$

$$\alpha \equiv 2\pi\left(\varepsilon - \mathrm{Re}\Sigma(\varepsilon)\right)/\hbar\omega_c, \;\; \gamma \equiv 2\pi\left|\mathrm{Im}\Sigma(\varepsilon)\right|/\hbar\omega_c$$

Results B: formula for large $\gamma \equiv 2\pi \left|\mathrm{Im}\Sigma(\varepsilon)\right| / \hbar\omega_c$

(weak magnetic field or/and high tilt angle & dirty sample)

For $\gamma_0 >> 1$ amplitude of oscillations is exponentially suppressed.

One can find the following values of extremal values of quantum oscillations of interlayer conductivity:

$$\frac{<\sigma_{zz}(\mu)>}{\sigma_{zz}^0} \approx \int_{\hbar\omega_c n_F}^{\hbar\omega_c(n_F+1)} \frac{\sigma_{zz}(\mu)}{\sigma_{zz}^0}\frac{d\mu}{\hbar\omega_c} \approx 2\gamma_0 \exp(-\gamma_0)|J_{\gamma_0 i/\pi}(\kappa)|^2 \approx \begin{cases} \gamma_0/(\pi\kappa), & 1 \ll \gamma_0 \ll \kappa, \\ 1 \ll \gamma_0, & \kappa \sim 1. \end{cases}$$

if $\kappa\pi^2 >> \gamma_0^2 >> 1$ (high-tilted angle) **:**

$$\frac{\sigma_{zz}^{min}(\kappa)}{\sigma_{zz}^0} \approx \frac{\gamma_0}{\pi\kappa}\left(1-\left(2+4\cos^2\left(\kappa-\frac{\pi}{4}\right)\right)\exp(-\gamma_0)\right),$$

$$\frac{\sigma_{zz}^{max}(\kappa)}{\sigma_{zz}^0} \approx \frac{\gamma_0}{\pi\kappa}\left(1+\left(2+4\cos^2\left(\kappa-\frac{\pi}{4}\right)\right)\exp(-\gamma_0)\right).$$

$\kappa \equiv k_F d \tan\theta$

if $\kappa\pi << \gamma_0$ **:**

$$\frac{\sigma_{zz}^{min}(\kappa)}{\sigma_{zz}^0} \approx 1-\frac{\kappa^2\pi^2}{2\gamma_0^2} - 2\exp(-\gamma_0)\left(J_0^2(\kappa)\gamma_0+\frac{\kappa^2\pi^2}{\gamma_0^2}\right),$$

$$\frac{\sigma_{zz}^{max}(\kappa)}{\sigma_{zz}^0} \approx 1-\frac{\kappa^2\pi^2}{2\gamma_0^2} + 2\exp(-\gamma_0)\left(J_0^2(\kappa)\gamma_0+\frac{\kappa^2\pi^2}{\gamma_0^2}\right).$$

Results C: formula for small $\gamma \equiv 2\pi \left|\mathrm{Im}\Sigma(\varepsilon)\right| / \hbar\omega_c$

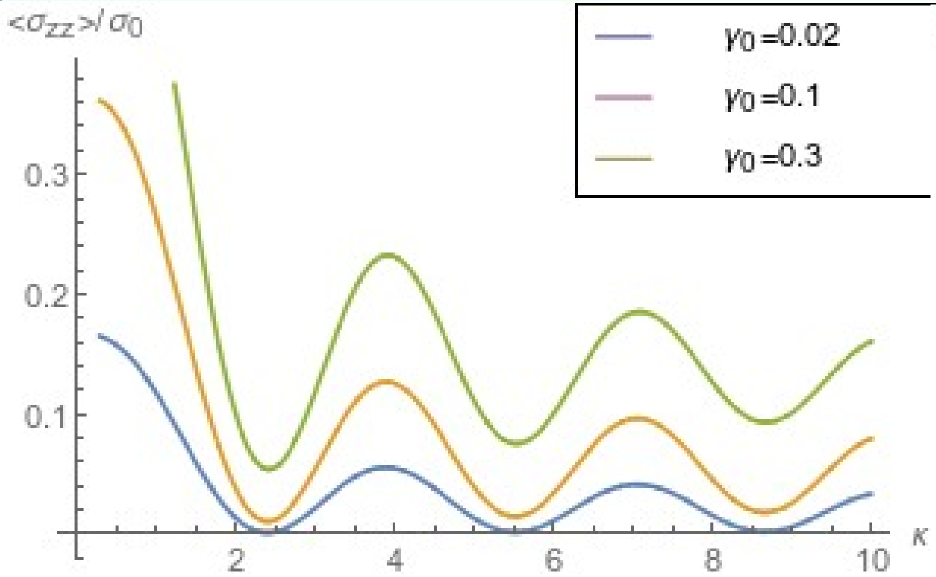
(strong magnetic field or/and clean sample)

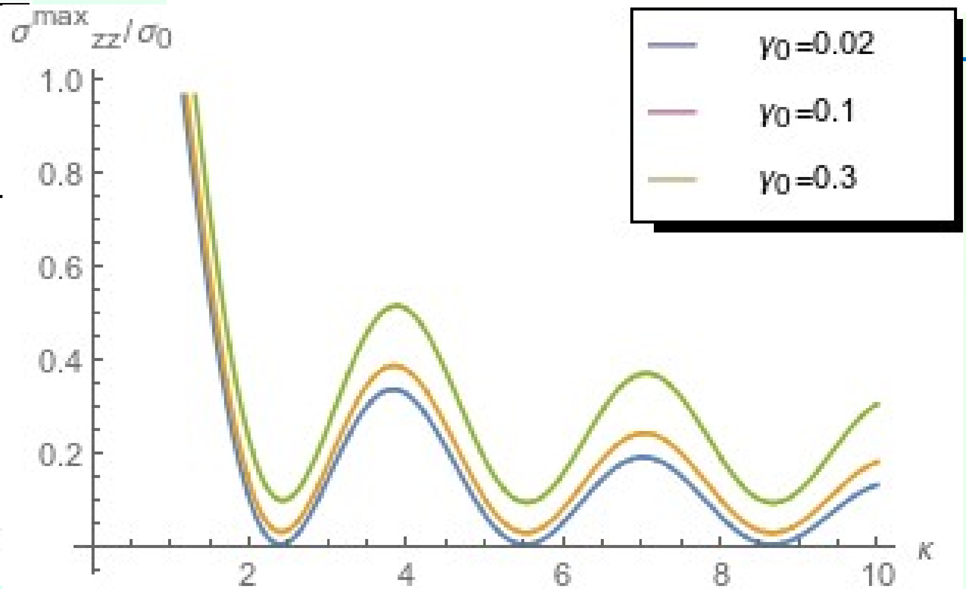
For γ_0 << 1 / 2 amplitude of oscillations is strongly angular dependent. $\kappa \equiv k_F d \tan\theta$

One can find the following values of extremal values of quantum oscillations of interlayer conductivity at γ_0 << κ ($k_F d = 1$):

$$\frac{\sigma_{zz}^{min}(\kappa)}{\sigma_{zz}^{0}} = 0 \qquad \frac{\sigma_{zz}^{max}(\kappa)}{\sigma_{zz}^{0}} \approx 2J_0^2(\kappa) + \frac{\gamma_0}{2}\left(Y_0^2(\kappa) - \frac{8}{\pi^2} J_0(\kappa) \frac{\partial^2 J_\nu(\kappa)}{\partial \nu^2}|_{\nu=0}\right)$$

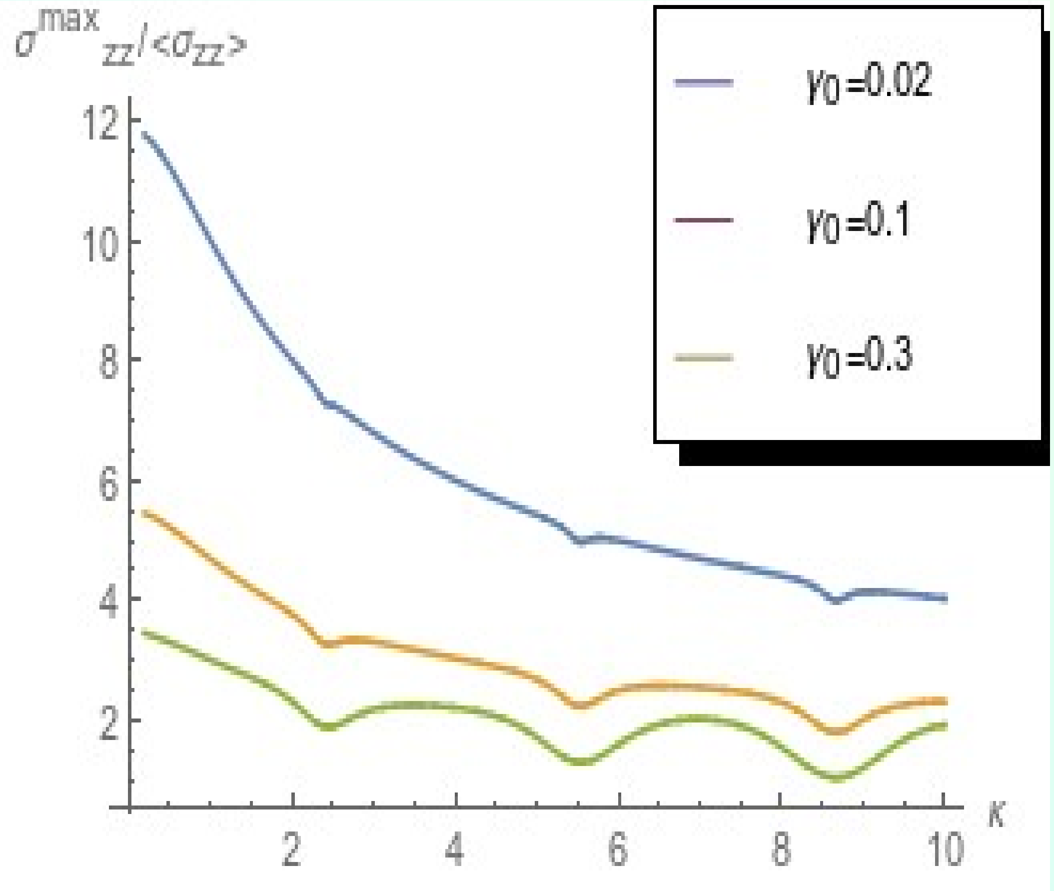
$$\frac{<\sigma_{zz}(\mu)>}{\sigma_{zz}^{0}} \approx \frac{8J_0^2(\kappa)}{3\pi}(2\gamma_0)^{\frac{1}{2}} + \frac{(2\gamma_0)^{\frac{3}{2}}}{3\pi}\left(Y_0^2(\kappa) - \frac{5}{3}J_0^2(\kappa) - \frac{8}{\pi^2} J_0(\kappa) \frac{\partial^2 J_\nu(\kappa)}{\partial \nu^2}|_{\nu=0}\right)$$





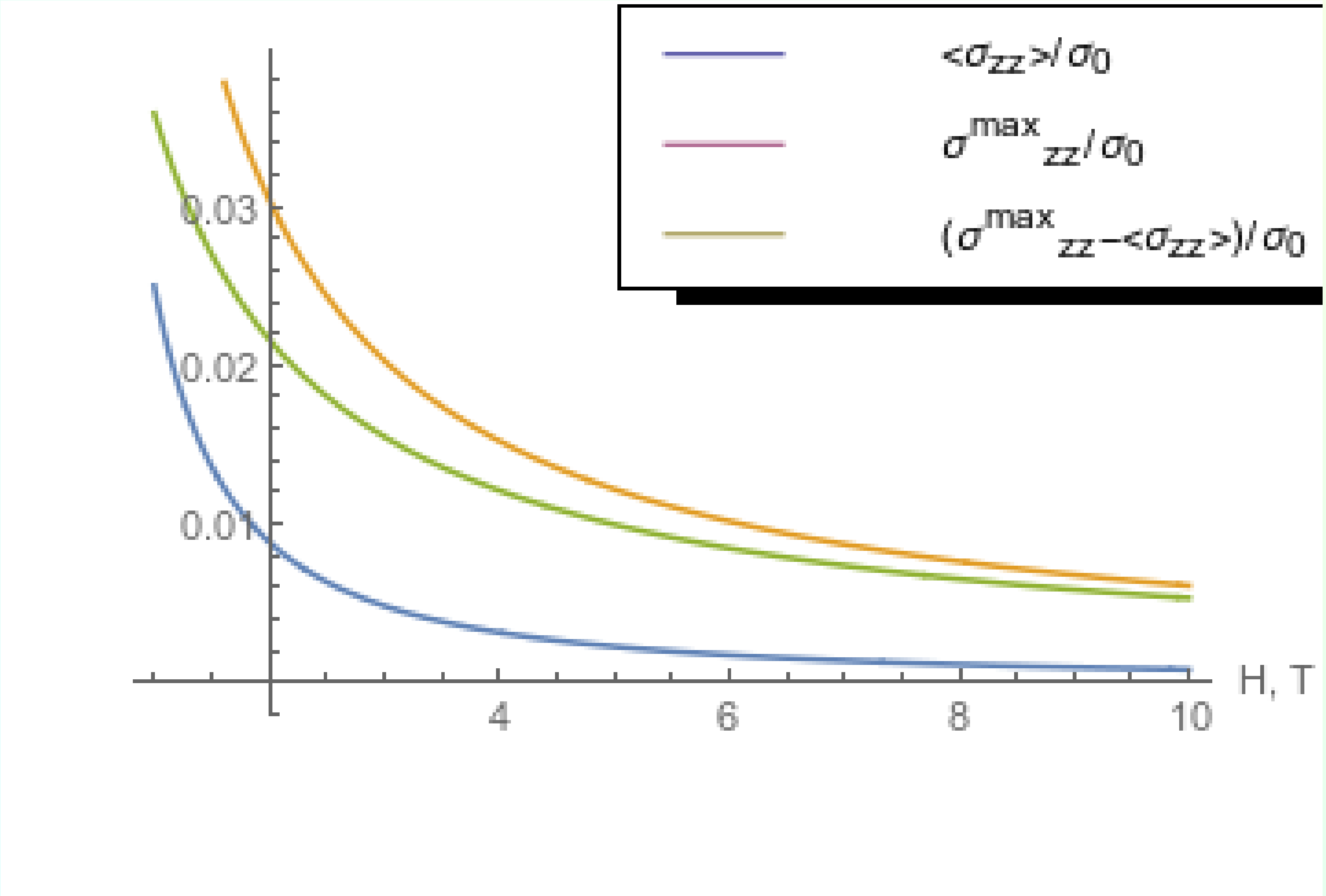
Results C: formula for small $\gamma \equiv 2\pi \left| \mathrm{Im}\Sigma\left(\varepsilon\right)\right| / \hbar\omega_c$ (strong magnetic field or/and clean sample)

Ratio of oscillating to monotonic part of interlayer conductivity for various magnetic field

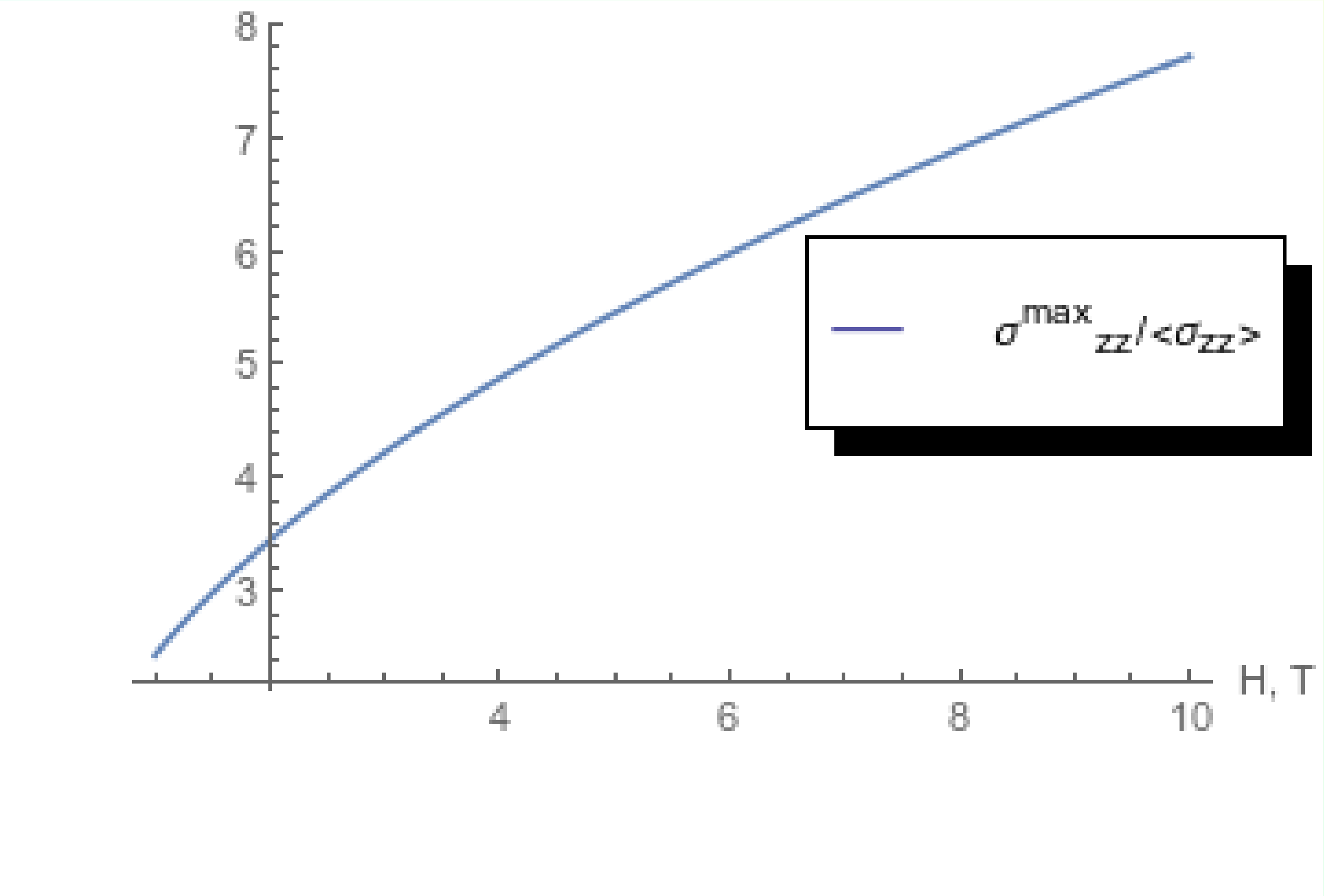


At the Yamaji angles the ratio of the oscillating to monotonic part of interlayer conductivity has dips, which become stronger for smaller magnetic field (larger γ_0).

Oscillating and monotonic part of MR at first Yamaji angle



Relative amplitude of oscillations of MR at first Yamaji angle



Conclusions

1. The interplay of angular and quantum oscillations of MR in quasi-2D metals is investigated. The amplitude MQO of σ_{zz} is weakly affected by the angular MR oscillations.

2. The false spin zeros (minima of the amplitude of MQO at some tilt angles of B) may appear in the approximation of isolated LL [T. Ando (1974)], but when many LLs are included the false spin zeros are absent.

3. The amplitude of MQO as a function of the tilt angle θ of magnetic field is calculated taking into account the interplay between magnetic and angular MR oscillations. Maxima and minima of conductivity oscillations are found analytically.

4. The behavior of monotonic and oscillating part of MR in the vicinity of Yamaji angles is analyzed.