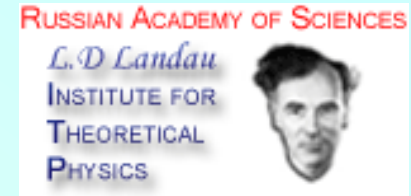


Interlayer magnetoresistance in strongly anisotropic quasi-2D layered metals

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Plan of the talk:

1. Calculation of longitudinal interlayer MR in SCBA starting from the strongly-anisotropic quasi-2D electron dispersion. Its comparison with the two-layer tunneling approach.

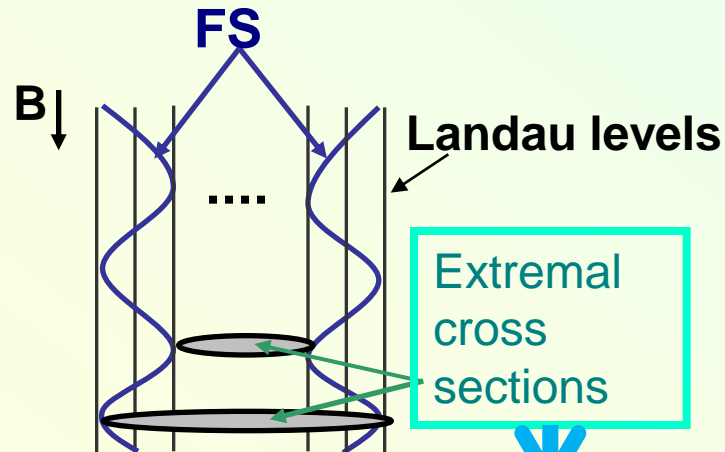
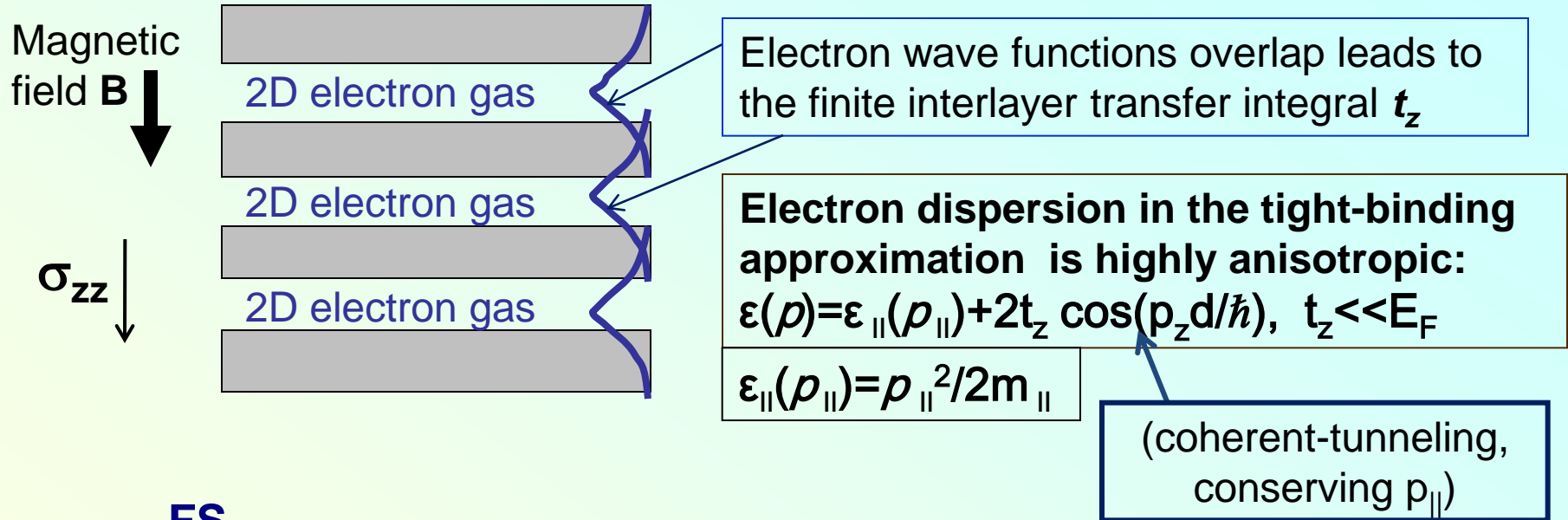
Crossover from linear to square-root longitudinal MR at $t_z \sim \sqrt{\omega_c \Gamma_0}$.

[P. D. Grigoriev, arXiv:1212.6926, submitted to PRB]

2. Angular dependence of monotonic and oscillating parts of interlayer MR for various LL shapes (with T.I. Mogilyuk).

Layered quasi-2D metals

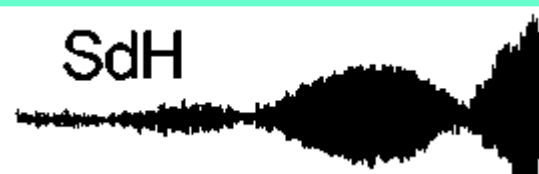
(Examples: heterostructures, organic metals, all high-T_c superconductors)



Two close frequencies => beats of MQO

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

SdH



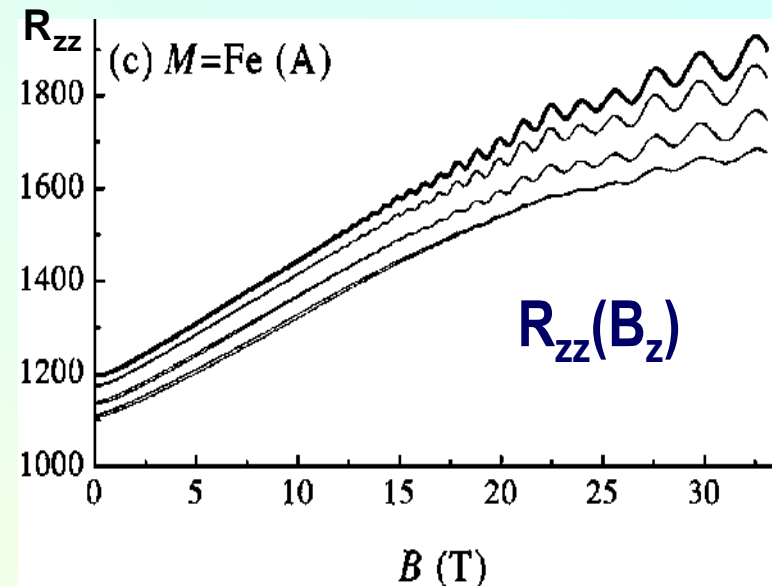
Motivation and urgency

Layered compounds are very common: high- T_c 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.

Experimentally observed dimensional crossover: 3D \rightarrow quasi-2D \rightarrow 2D shows many new qualitative features:

- (1) monotonic growth of $R_{zz}(B_z)$,
- (2) different damping of MQO,
- (3) different angular dependence of MR



$\beta'' - (BEDT - TTF)_4[(H_3O)Fe(C_2O_4)_3]C_5H_5N$

ARPES (Angle resolved photoemission spectroscopy)

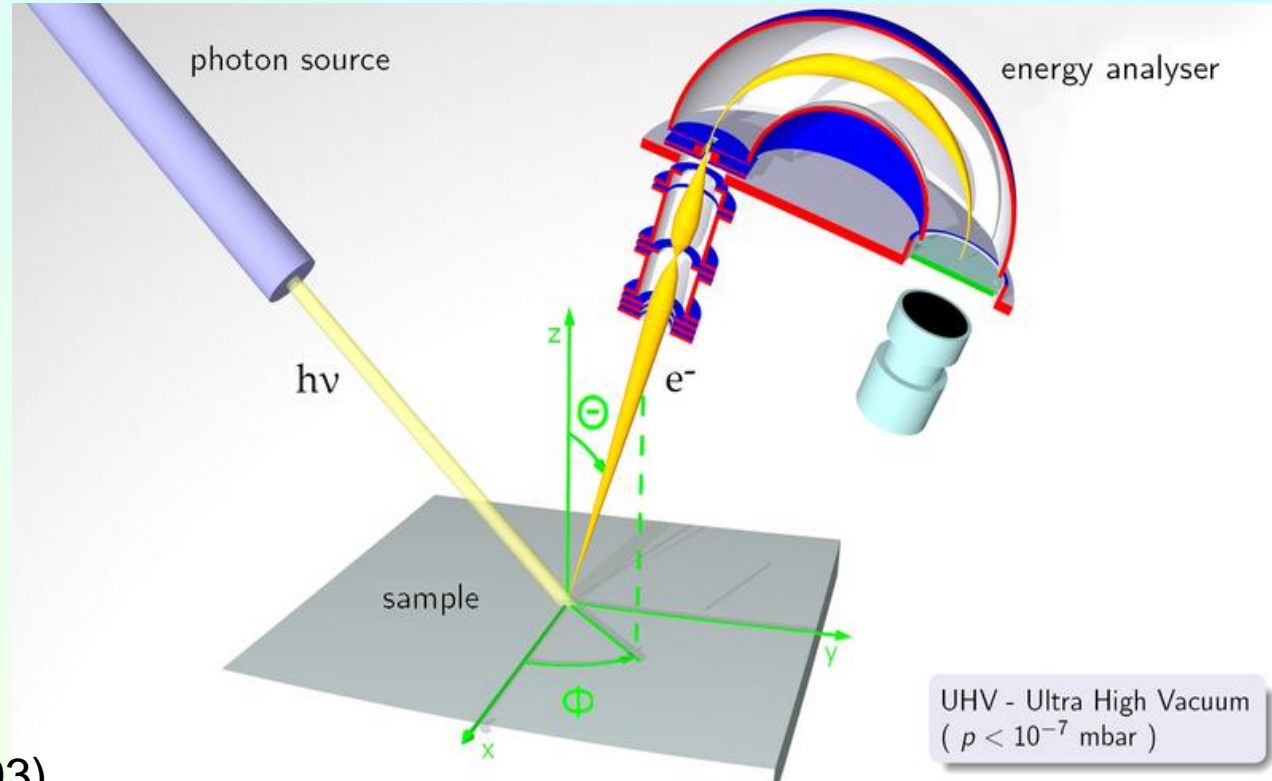
Main idea:

$$E = \hbar\omega - E_k - \phi$$

E_k = kinetic energy of the outgoing electron — can be measured.

$\hbar\omega$ = incoming photon energy - known from experiment, ϕ = known electron work function.

Angle resolution of photoemitted electrons gives their momentum.



Rev.Mod.Phys. 75, 473 (2003)

The photocurrent intensity is proportional to a one-particle spectral function multiplied by the Fermi function:

$$I(\mathbf{k}, \omega) = A(\mathbf{k}, \omega) f(\omega)$$

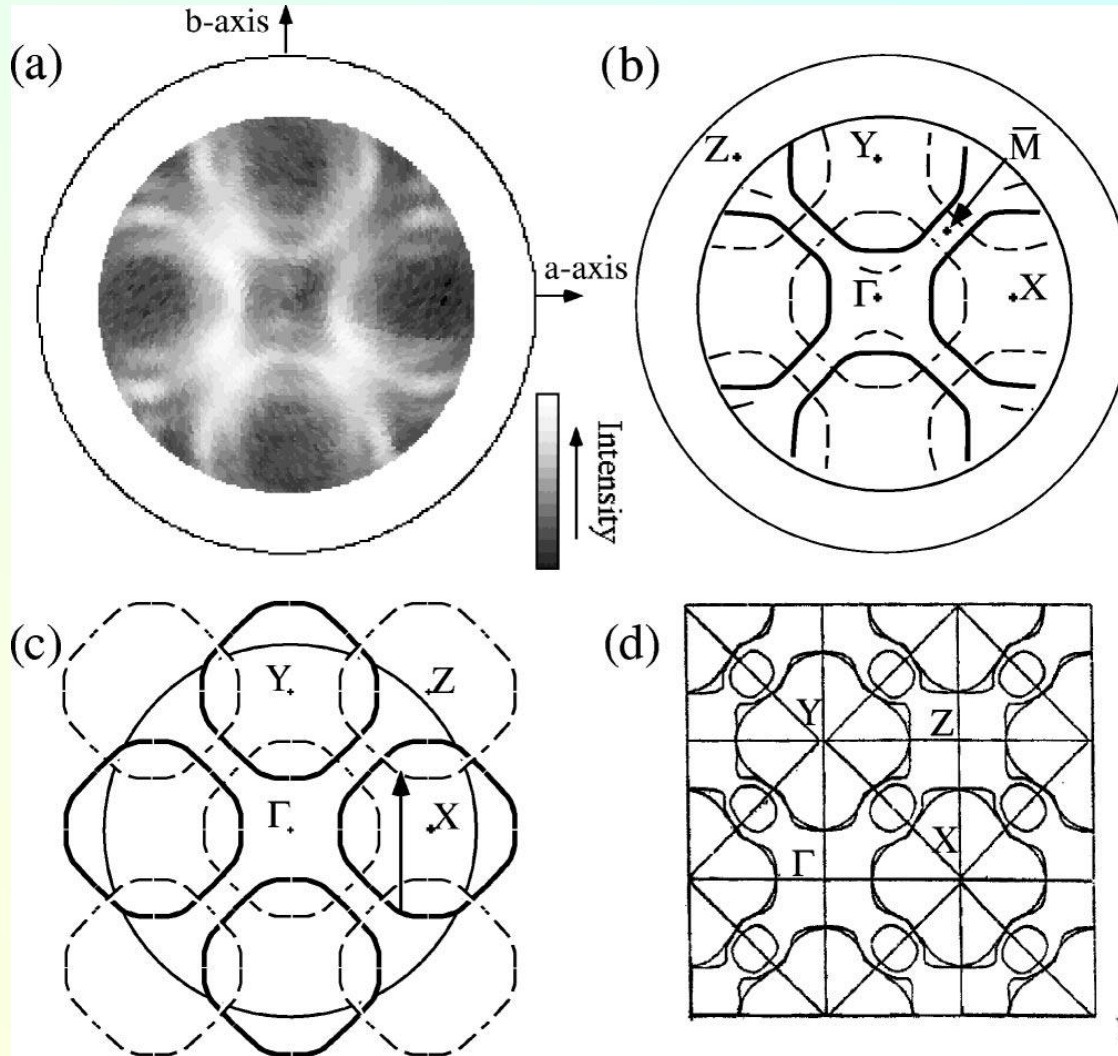
$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(\mathbf{k}) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$

Therefore can find out information about $E(\mathbf{k})$

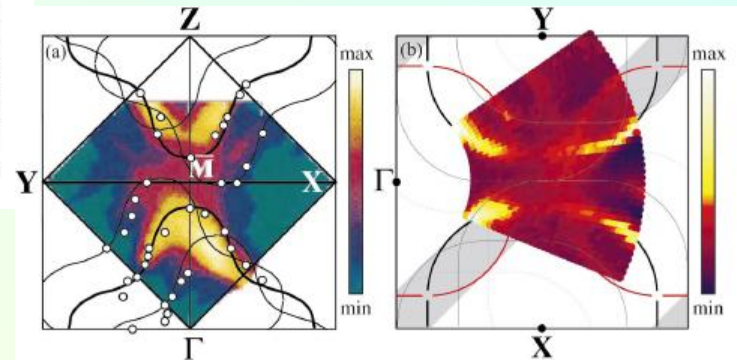
Drawback 1: Only surface electrons participate!

Motivation

ARPES data and Fermi-surface shape



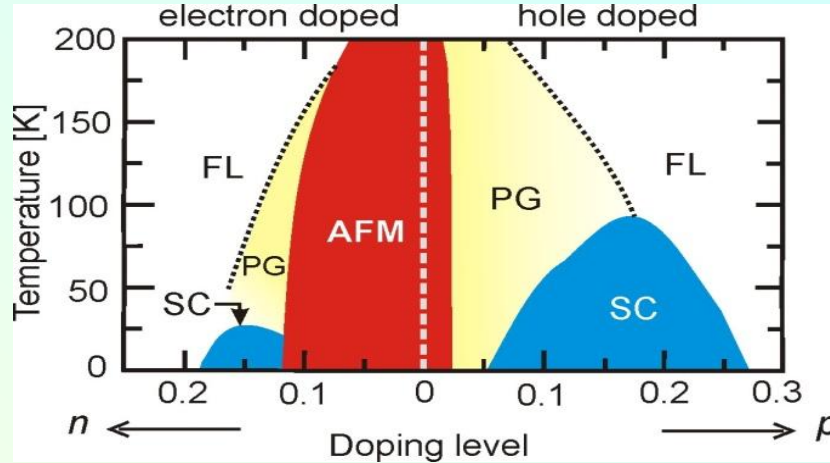
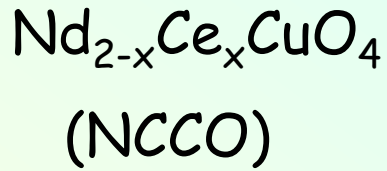
The Fermi surface of near optimally doped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (a) integrated intensity map (10-meV window centered at E_F) for Bi2212 at 300 K obtained with 21.2-eV photons (HeI line); (b),(c) superposition of the main Fermi surface (thick lines) and of its (p,p) translation (thin dashed lines) due to backfolded shadow bands; (d) Fermi surface calculated by Massidda *et al.* (1988).



Drawback 2: Ambiguous interpretation.

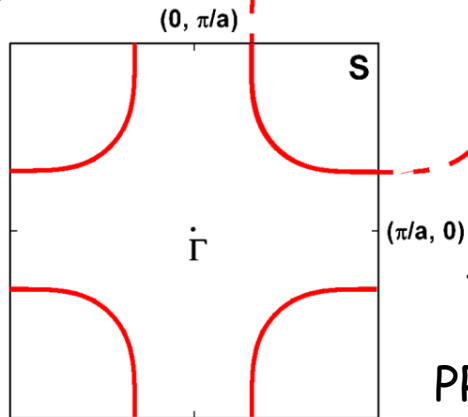
Phase diagram of high- T_c cuprate SC.

High T_c and quantum phase transition



Theory predicts shift of the QPT point in SC phase? How strong is this shift?

Original FS:

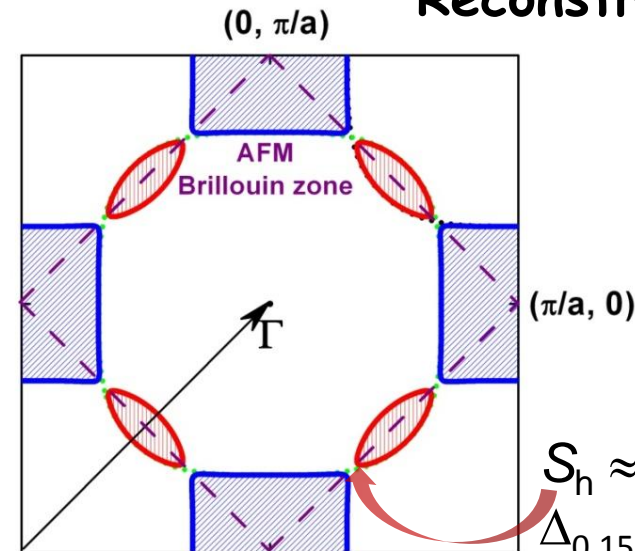


$$n = 0.17$$

$$S_h = 41.5\% \text{ of } S_{BZ}$$

T. Helm et al.,
PRL 103, 157002
(2009)

Reconstructed FS:



$$n = 0.15 \text{ and } 0.16$$

$$S_h \approx 1.1\% \text{ of } S_{BZ};$$

$$\Delta_{0.15} \approx 64 \text{ meV};$$

$$\Delta_{0.16} \approx 36 \text{ meV}$$

Angular dependence of background magnetoresistance

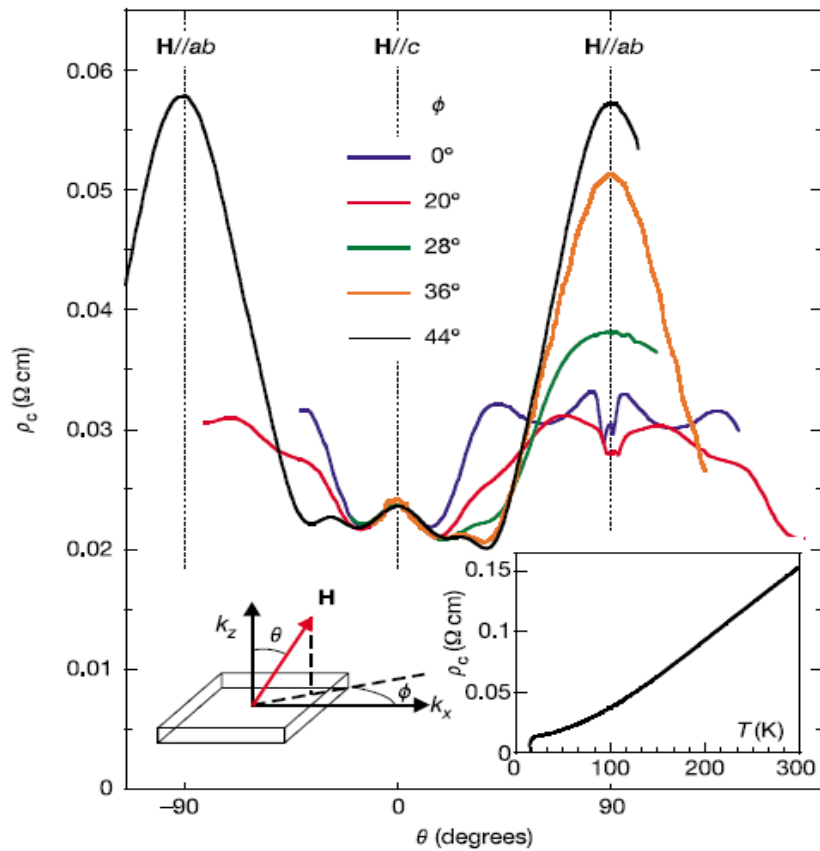
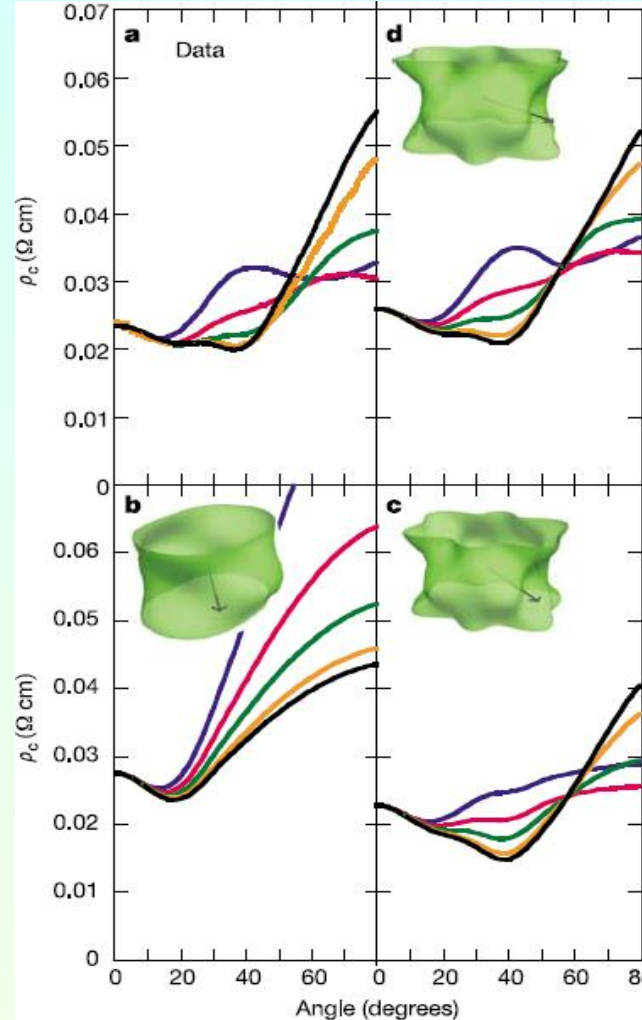


Figure 1 Polar AMRO sweeps in an overdoped Ti2201 single crystal ($T_c \approx 20$ K). The data were taken at $T = 4.2$ K and $H = 45$ T. The different azimuthal orientations ($\pm 4^\circ$) of each polar sweep are stated relative to the Cu–O–Cu bond direction. The key features of the data are as follows: (1) a sharp dip in ρ_\perp at $\theta = 90^\circ$ for low values of ϕ , which we attribute to the onset of superconductivity at angles where $H_{c2}(\phi, \theta)$ is maximal, (2) a broad peak around $\mathbf{H}||ab$ ($\theta = 90^\circ$) that is maximal for $\phi \approx 45^\circ$, consistent with previous azimuthal AMRO studies in overdoped Ti2201 (ref. 16), (3) a small peak at $\mathbf{H}||c$ ($\theta = 0^\circ$), and (4) a second peak in the range $25^\circ < \theta < 45^\circ$ whose position and intensity vary strongly with ϕ . These last two features are the most critical for our analysis. Similar



Reconstruction of the FS in $Ti_2Ba_2CuO_{6+d}$ from polar AMRO data.

N. E. Hussey et al., "A coherent 3D Fermi surface in a high- T_c superconductor", Nature 425, 814 (2003)

Magnetoresistance studies of organic metals

There are very many papers on the study of electronic properties of organic metals using magnetoresistance measurements.

Some books:

1. J. Wosnitzer, *Fermi Surfaces of Low-Dimensional Organic Metals and Superconductors* (Springer-Verlag, Berlin, 1996).
2. T. Ishiguro, K. Yamaji, and G. Saito, *Organic Superconductors*, 2nd ed. (Springer-Verlag, Berlin, 1998).
3. A.G. Lebed (ed.), *The Physics of Organic Superconductors and Conductors*, (Springer Series in Materials Science, 2009).

Some review papers:

1. D. Jérôme and H.J. Schulz, *Adv. Phys.* 31, 299 (1982).
2. J. Singleton, *Rep. Prog. Phys.* 63, 1111 (2000).
3. M.V. Kartsovnik, *High Magnetic Fields: A Tool for Studying Electronic Properties of Layered Organic Metals*, *Chem. Rev.* 104, 5737 (2004).
4. M.V. Kartsovnik, V.G. Peschansky, *Galvanomagnetic Phenomena in Layered Organic Conductors*, *FNT* 31, 249 (2005) [LTP 31, 185].

Introduction.

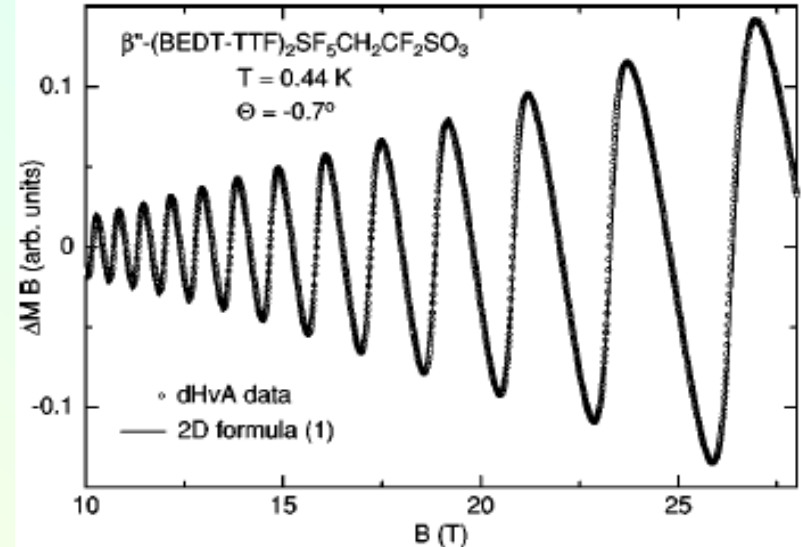
MQO of all thermodynamic quantities can be easily calculated from the DoS

The thermodynamic potential is given by the integral of DoS:

$$\Omega(\mu, B, T) = -T \int_0^{\infty} \rho(E, B) \ln \left[1 + \exp \left(\frac{\mu - E}{T} \right) \right] dE$$

Magnetization is given by the derivative

$$\tilde{M}(B) = - \frac{\partial \tilde{\Omega}}{\partial B}$$



But the transport quantities cannot be calculated so simply!

Theory of magnetoresistance is not as simple

While the thermodynamic potential is a linear functional of the DoS, conductivity has nonlinear dependence on DoS.

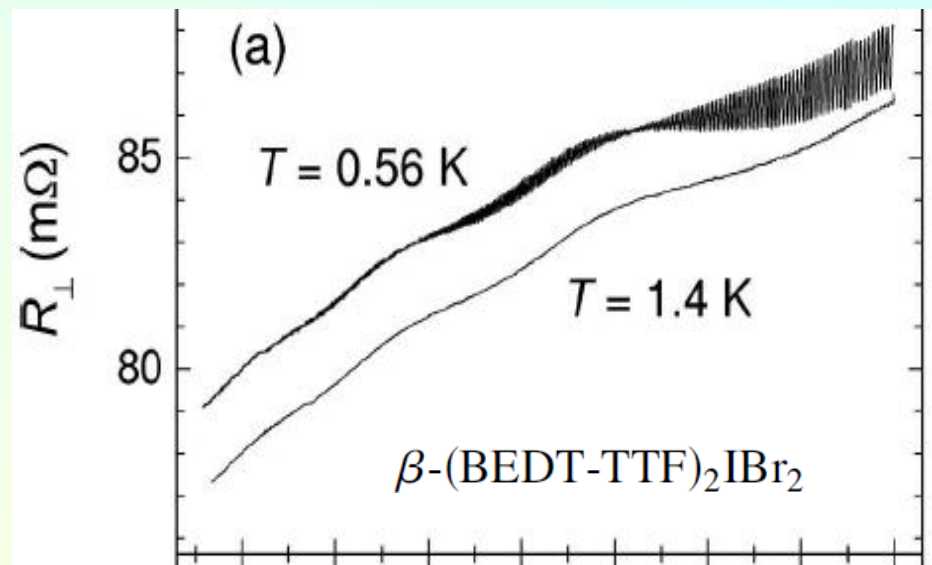
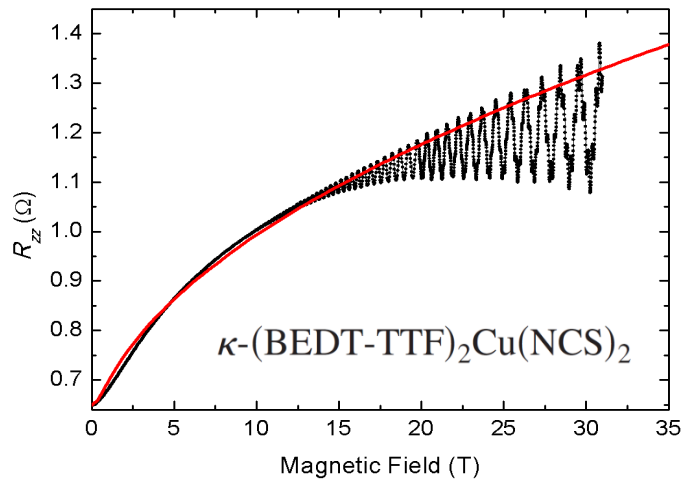
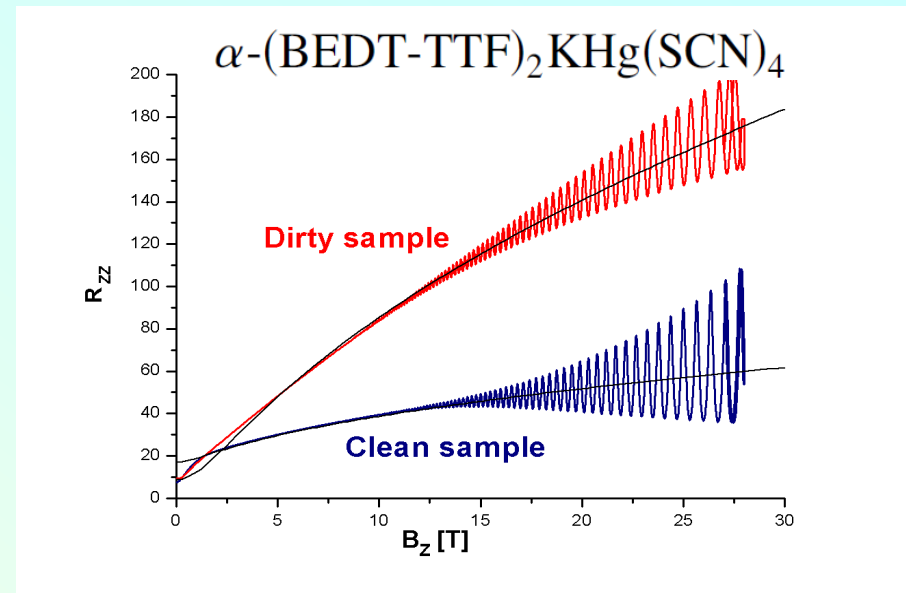
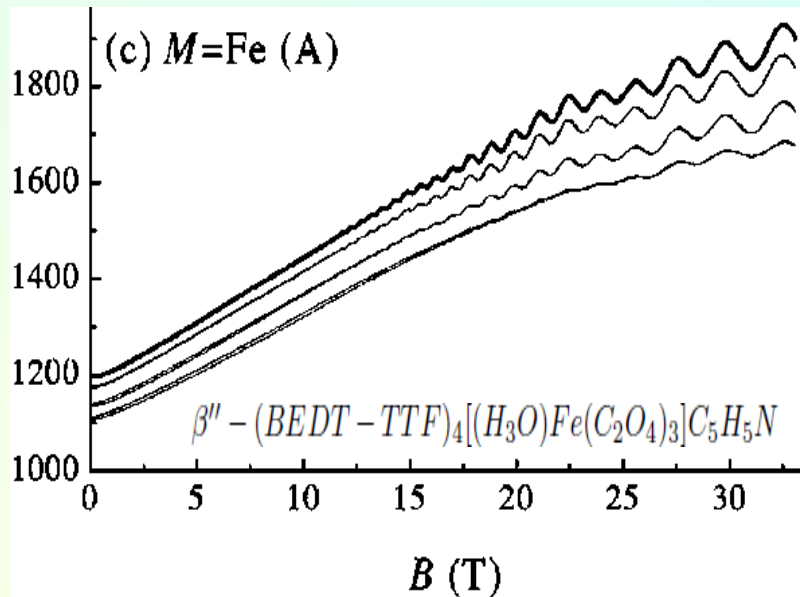
Usually one separates monotonic (background) classical MR and MQO:

$$\sigma(B) = \sigma_{cl}(B) + \tilde{\sigma}(B).$$

In quasi-2D metals the oscillations (MQO) are strong, **and such separation in the theory is incorrect** even if MQO are smeared by T or long-range disorder.

Accurate calculation of longitudinal MR in the presence of MQO explains the monotonic growth of MR even in the one-particle approximation (electrons + B + disorder).

Monotonic longitudinal MR remains unexplained



Results 1Recent theoretical predictions for interlayer MR $R_{zz}(B)$

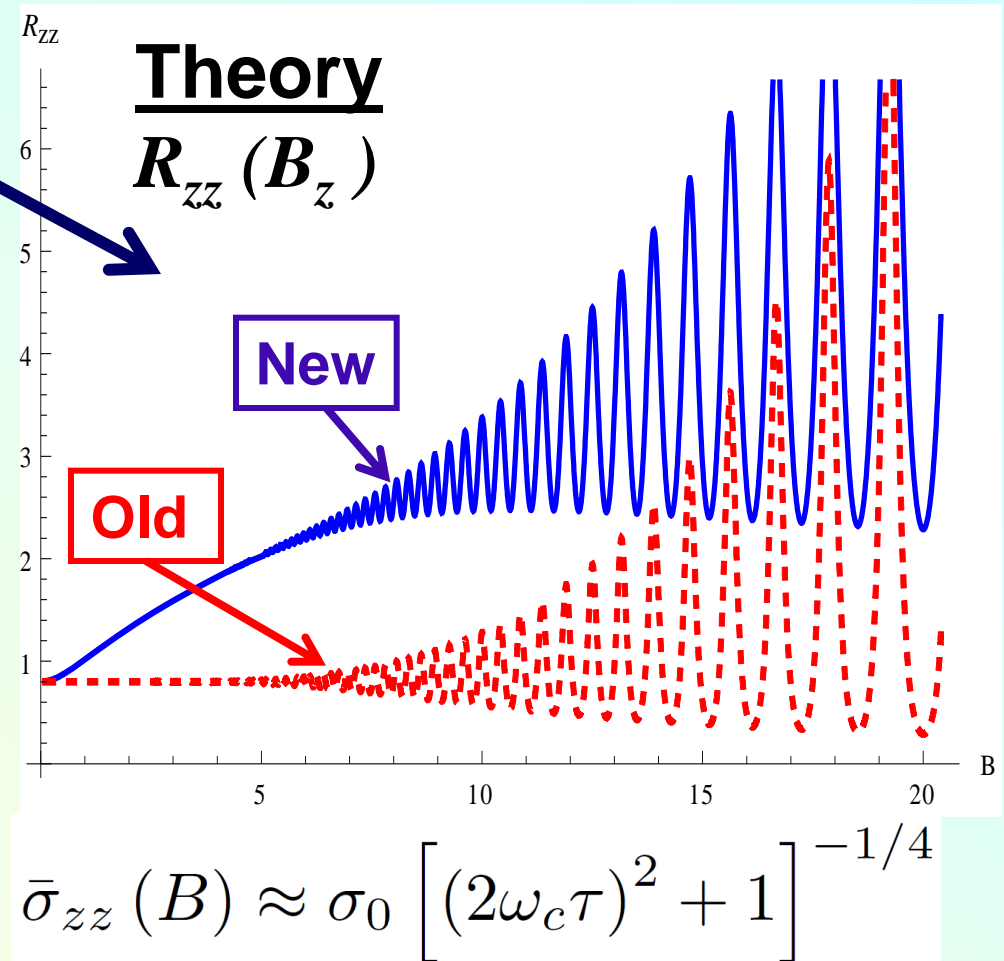
[1] P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011).

[2] P. D. Grigoriev, JETP Lett. 94, 48 (2011) [arXiv:1104.5122].

1. Longitudinal interlayer magnetoresistance (MR) grows with B_z at $\omega_c \tau > 1$: $R_{zz} \sim B_z^{1/2}$. It grows even if MQO are damped by T or by long-range disorder.

2. B_z -dependence of MQO amplitude changes. The Dingle low $R_D = \exp(-B_0/B_z)$ is not valid (as in 2D case)

3. Angular dependence of MR changes: both the monotonic part and the amplitude of AMRO.



The coefficient 2 slightly depends on the LL shape

The model of weakly coherent regime

P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011); JETP Lett. 94, 48 (2011).

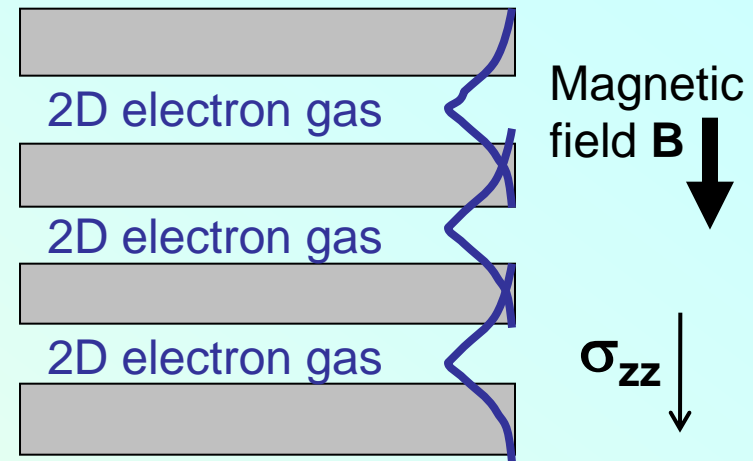
The Hamiltonian contains 3 terms:

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

1 3 2

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

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



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

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

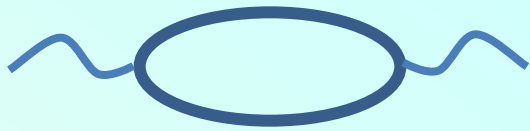
2. The short-range impurity potential:

$$\hat{H}_I = \sum_i V_i(r) \quad \text{where} \quad V_i(r) = U \delta^3(r - r_i)$$

Calculation of conductivity in q2D metals (standard theory, generalization to $\hbar\omega_c \sim 4\pi t_z$)

Electron dispersion in the tight-binding approximation is highly anisotropic: $\epsilon(\rho) = \epsilon_{||}(\rho_{||}) + 2t_z \cos(p_z d/\hbar)$, $t_z \ll E_F$

Conductivity (the linear response to external electric field) is calculated from the Kubo formula:



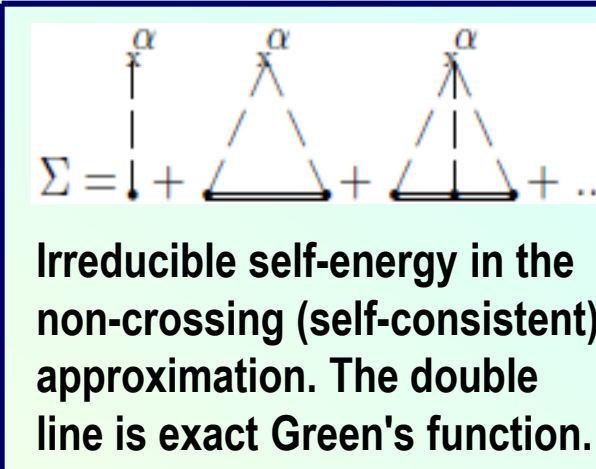
$$\sigma_{ZZ} = \frac{e^2}{V} \sum_m v_z^2(m) \int \frac{d\epsilon}{2\pi} [2 \text{Im} G_R(m, \epsilon)]^2 [-n'_F(\epsilon)],$$

where $m=(n, k_y, k_z)$, the electron velocity $v_z(\epsilon, n) = \partial\epsilon / \partial k_z$, is determined by the 3D electron dispersion,

$G_R(m, \epsilon)$ - retarded electron Green's function,

$$n'_F(\epsilon) = -1 / \{4T \cosh^2[(\epsilon - \mu) / 2T]\}$$

- derivative of the Fermi distribution function.



Previous theoretical results on Shubnikov - de Haas effect in quasi-2D metals

Equations for the Green's function in self-consistent Born approximation in quasi-2D metals are complicated:

$$\Sigma^R(m, \epsilon) = \left\langle \sum_i U^2 G(r_i, r_i, E) \right\rangle = C_i U^2 \int d^3 r G(r, r, E), \quad \text{where}$$

$$G(E) = \frac{-N_{LL}}{\hbar\omega_c} \left\{ A(E) + i\pi \left[1 + 2 \sum_{k=1}^{\infty} (-1)^k J_0 \left(\frac{4\pi kt}{\hbar\omega_c} \right) \exp \left(2\pi i k \frac{E - \Sigma(E)}{\hbar\omega_c} \right) \right] \right\}$$

Conductivity was calculated before only in the simple Born approximation

Quasi-2D case, $\hbar\omega_c \ll 4\pi t_z$

[P.D. Grigoriev, cond-mat/0204270 (April 2002);
PRB 67, 144401 (2003) (Submitted April 2002)]

Use expansion in the small parameter

$$J_0(4\pi t_z / \hbar\omega_c) \exp(-2\pi |\text{Im}\Sigma^R(\epsilon)| / \hbar\omega_c) \ll 1$$

Almost 2D case, $\hbar\omega_c \gg t_z$

[T. Champel and V.P. Mineev, PRB 66,
195111 (2002) (Submitted June 2002)]

Introduce very large electron reservoir
to damp MQO of the electron DoS.

Electron Green's function in SCBA in q2D metals

Hamiltonian contains q2D free electrons + short-range impurity scattering:

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \hat{H}_0 = \sum \epsilon_{3D}(m) c_m^\dagger c_m, m \equiv \{n, k_y, k_z\}, \hat{H}_I = \sum_i V_i(r)$$

we use 3D (or Q2D) electron dispersion in tight-binding approximation:

$$\epsilon_{3D}(\mathbf{k}) \approx \epsilon_{2D} - 2t_z \cos(k_z d), \quad \epsilon_{2D} = \epsilon_{2D}(n) = \hbar\omega_c (n + \gamma)$$

This gives the system of equations:

$$\Sigma(\epsilon) \approx n_i U + n_i U^2 G(\epsilon), \quad G(\epsilon) = \sum_n \frac{g_{LL}/d}{\sqrt{(\epsilon - \epsilon_{2D}(n) - \Sigma(\epsilon))^2 - 4t_z^2}}$$

If $4t_z < \hbar\omega_c$, one can consider each LL separately and equation on Σ simplifies to 4-order algebraic equation:

$$\Sigma_*^2 \left[(\Delta\epsilon - \Sigma_*)^2 - 4t_z^2 \right] = (\Gamma_0 \hbar\omega_c)^2$$

where $\Sigma_* \equiv \Sigma(\epsilon) - n_i U$

and $\Delta\epsilon = \epsilon - \epsilon_{2D}(n_F) - n_i U$

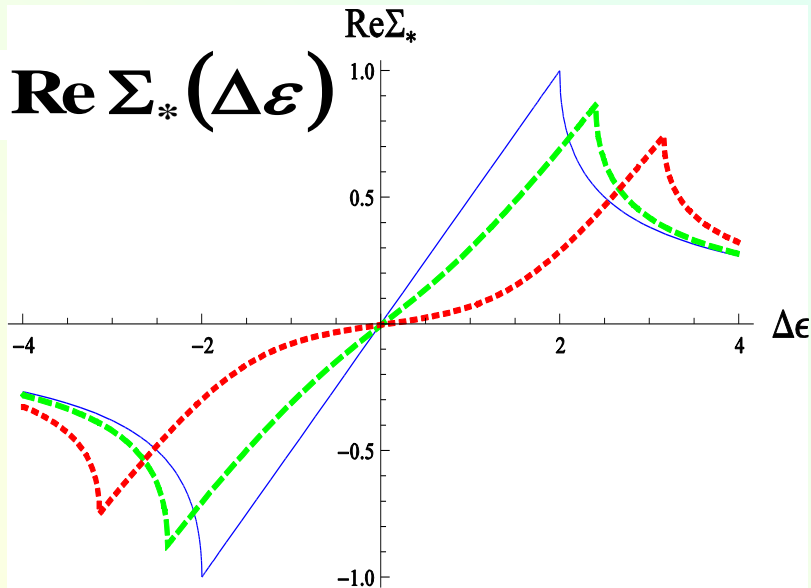
Two limits depending on $t_z / \sqrt{\omega_c \Gamma_0}$

Electron self energy in SCBA in q2D metals

Equation on electron self-energy

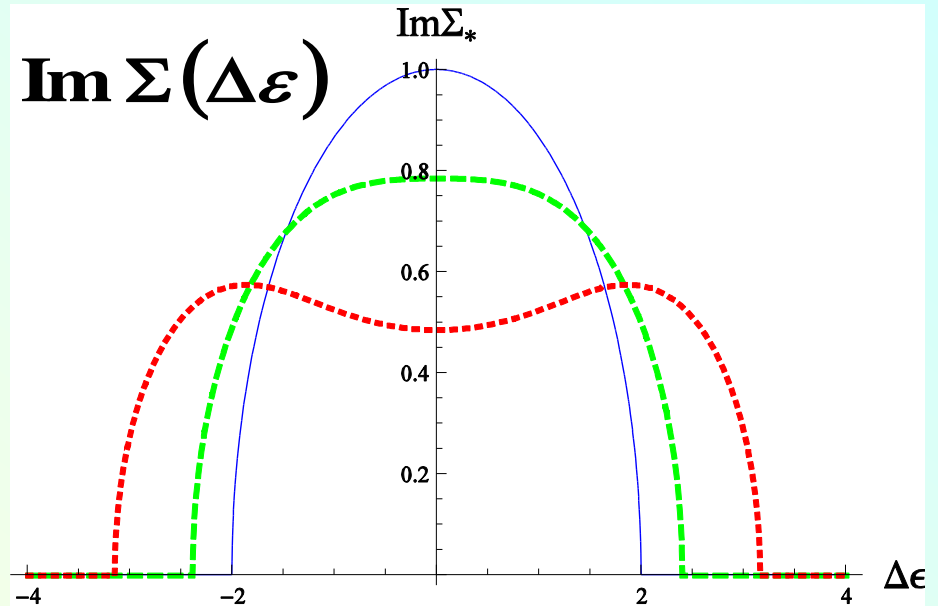
$$\Sigma_*^2 \left[(\Delta\varepsilon - \Sigma_*)^2 - 4t_z^2 \right] = (\Gamma_0 \hbar \omega_c)^2$$

gives the following solution for 3 values of $t_z / \sqrt{\omega_c \Gamma_0} = \mathbf{0, 0.5, 1.0}$



$$\text{Re } \Sigma_*(\Delta\varepsilon = 0) = 0$$

$$\text{Re } \Sigma_*(\Delta\varepsilon \rightarrow \infty) \rightarrow 0$$



$\text{Im } \Sigma_*(\Delta\varepsilon) \neq 0$ only in finite interval around each Landau level

Interlayer conductivity

From Kubo formula for 3D metals with anisotropic dispersion

$$\sigma_{zz} = \int d\varepsilon [-n'_F(\varepsilon)] \sigma_{zz}(\varepsilon), \quad \text{where } -n'_F(\varepsilon) = 1/\{4T \cosh^2[(\varepsilon - \mu)/2T]\},$$

independence of background MR on T

$$\sigma_{zz}(\varepsilon) = \frac{e^2 \hbar}{2\pi} \sum_m v_z^2(k_z) [2\text{Im}G_R(m, \varepsilon)]^2 \quad m \equiv \{n, k_y, k_z\}$$

$$\epsilon_{3D}(\mathbf{k}) \approx \epsilon_{2D} - 2t_z \cos(k_z d)$$

Substituting

$$\text{Im}G_R(m, \varepsilon) = \frac{\text{Im}\Sigma^R(\varepsilon)}{[\varepsilon - \epsilon(m) - \text{Re}\Sigma^R(\varepsilon)]^2 + [\text{Im}\Sigma_n^R(\varepsilon)]^2}$$

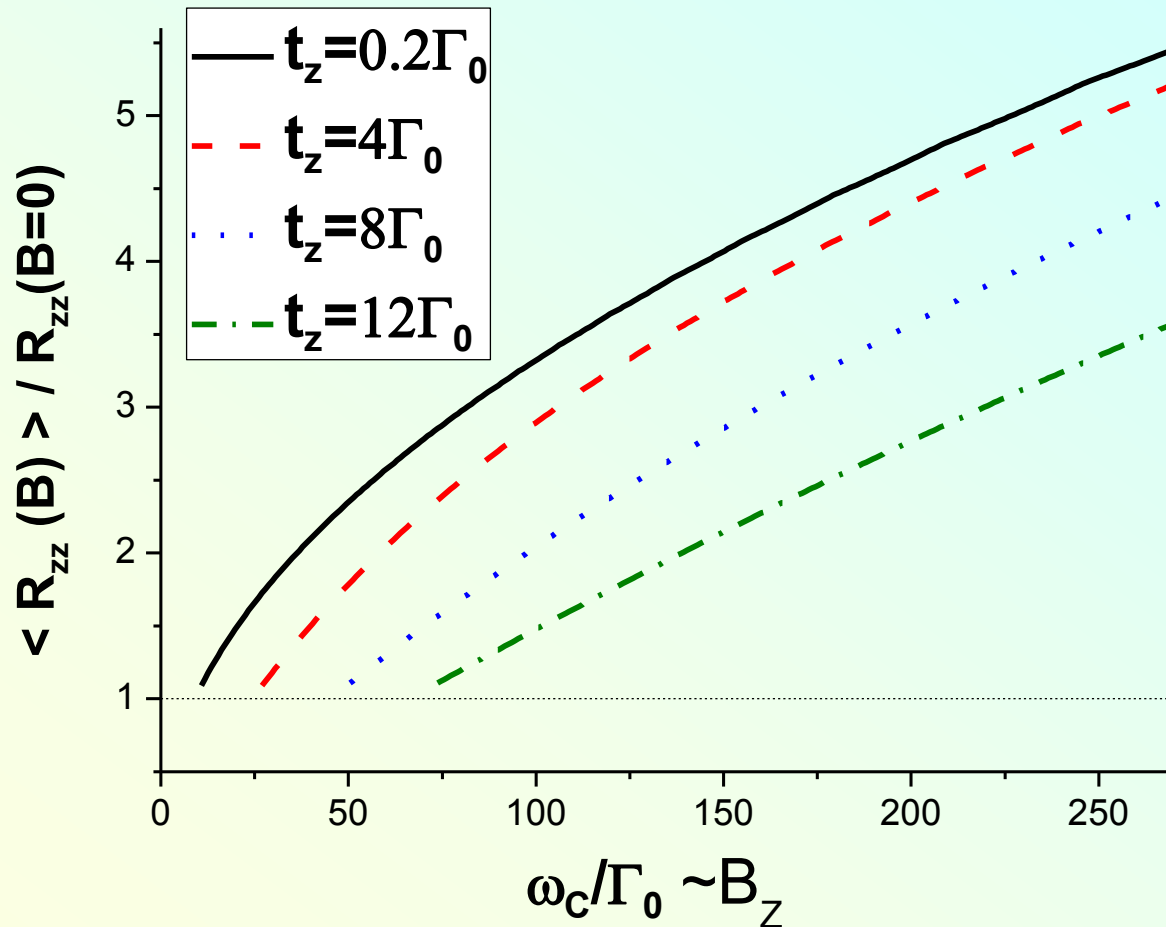
and integrating over k_z we obtain:

$$\sigma_{zz}(\varepsilon) \equiv \frac{\sigma_0 \hbar \omega_c \Gamma_0}{2\pi t_z^2 |\text{Im}\Sigma^R(\varepsilon)|} \text{Re} \frac{4t_z^2 - (\Delta\varepsilon)^2 + i \Delta\varepsilon |\text{Im}\Sigma^R(\varepsilon)|}{\sqrt{4t_z^2 - (\Delta\varepsilon - i |\text{Im}\Sigma^R(\varepsilon)|)^2}},$$

The electron self-energy is given equation in SCBA

$$\Sigma_*^2 \left[(\Delta\varepsilon - \Sigma_*)^2 - 4t_z^2 \right] = (\Gamma_0 \hbar \omega_c)^2$$

Result 2. $R_{zz}(B_z)$ at finite interlayer transfer integral t_z



Linear MR for
 $\omega_c < (2t_z)^2 / \Gamma_0$

Square-root MR
 $R_{zz} \propto \sqrt{B_z}$
 at higher field B_z
 or at smaller t_z

Calculation is
 valid at $\omega_c > 4t_z$

Therefore linear MR
 is obtained only at

$$\omega_c \gg \Gamma_0$$

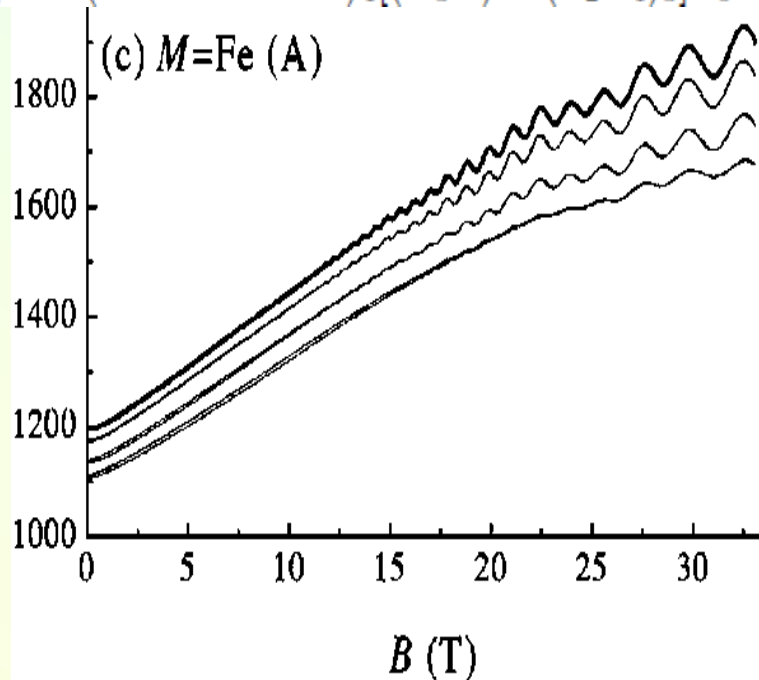
! Crossover from square-root to linear field dependence
 (observed in many high- T_c superconducting materials)

Result 2

Comparison with experiments on interlayer longitudinal MR at finite t_z

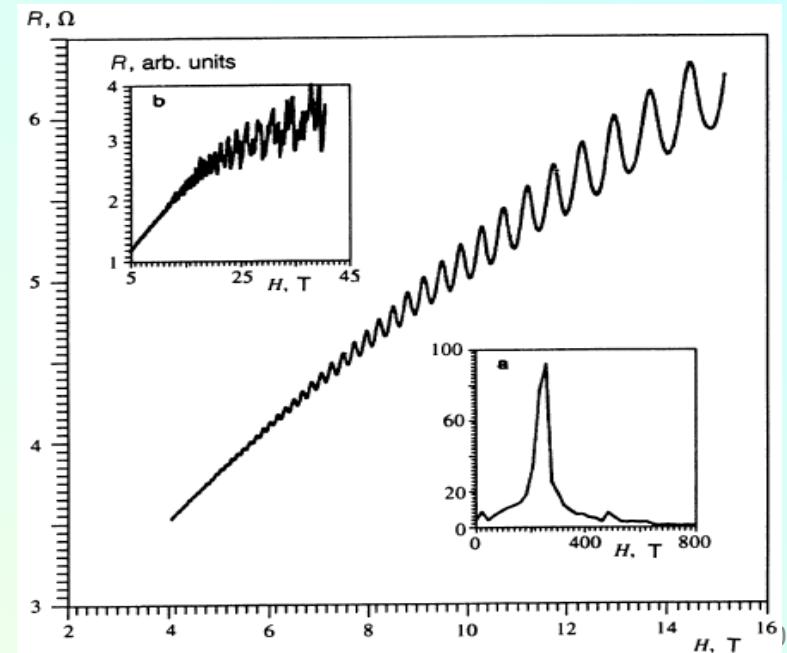
A.I. Coldea et al., PRB 69, 085112 (2004)

$\beta'' - (BEDT - TTF)_4[(H_3O)Fe(C_2O_4)_3]C_5H_5N$



R.B. Lyubovskii, S.I. Pesotskii et al.,

JETP 80, 946 (1995) $ET_8[Hg_4Cl_{12}(C_6H_5Cl)_2]$



theoretical prediction: crossover from linear to square-root field dependence of MR at $t_z \sim \sqrt{\omega_c \Gamma_0}$

Result 1

Experiments on longitudinal interlayer MR $R_{zz}(B)$ (magnetic field dependence: background resistance)

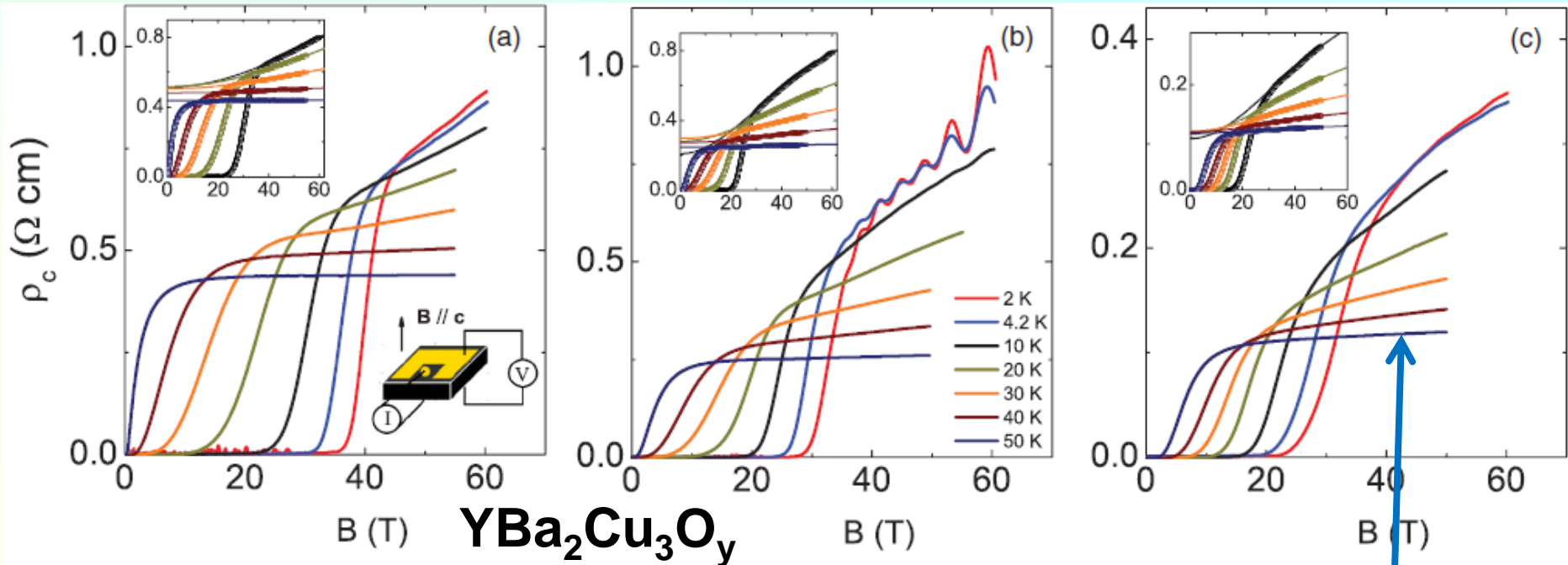
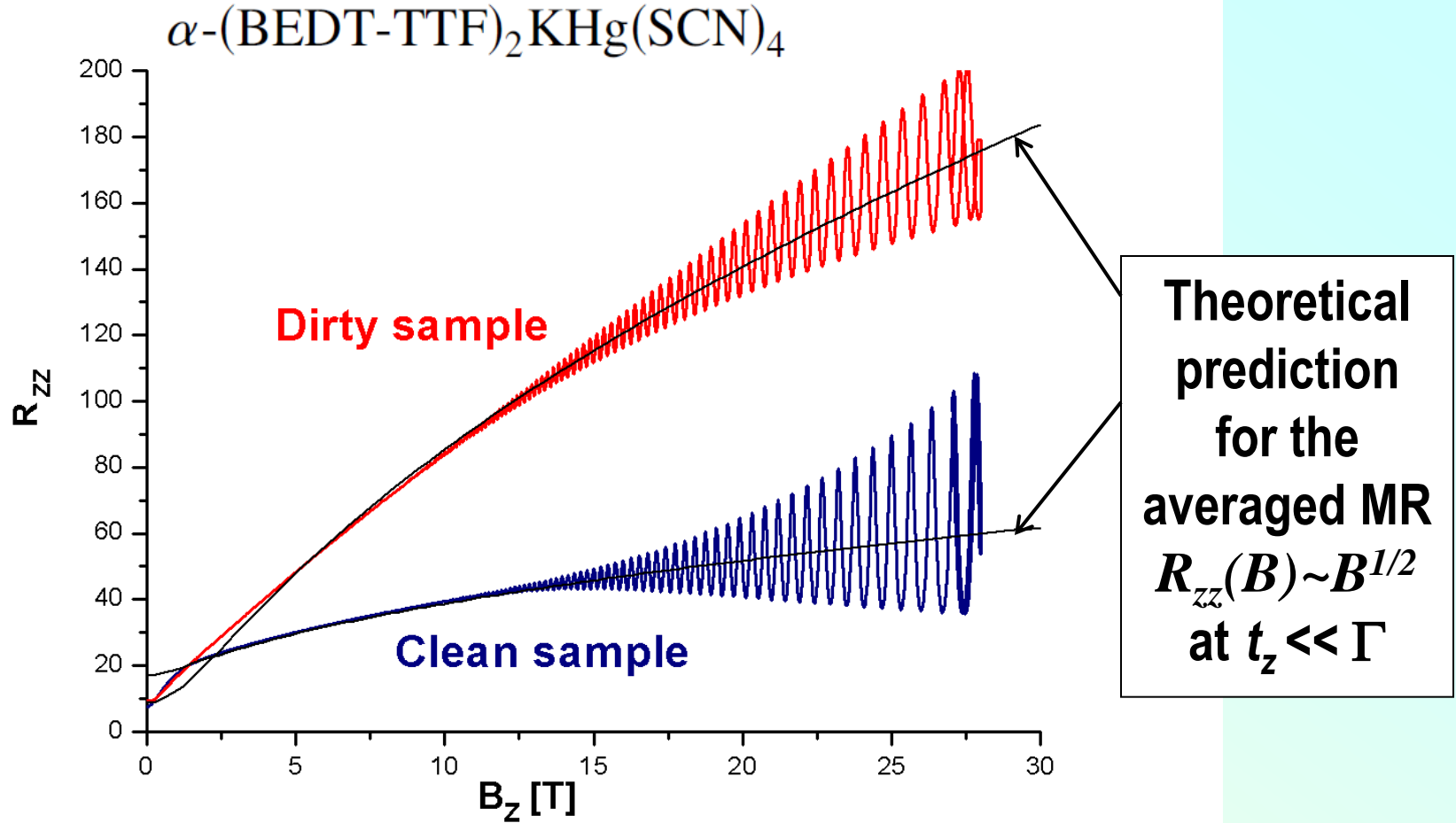


FIG. 1. (Color online) Electrical resistivity ρ_c of $\text{YBa}_2\text{Cu}_3\text{O}_y$ for a current I and a magnetic field B along the c axis ($I \parallel B \parallel c$). Three underdoped samples were measured at different temperatures below T_c (as indicated) in pulsed magnetic fields up to 60 T. The doping level of each sample is (a) $p = 0.097$, (b) $p = 0.109$, and (c) $p = 0.120$. Insets: Same data between 10 and 50 K with a fit of each isotherm (thin solid lines) using a two-band model above the superconducting transition (see Sec. V).

B. Vignolle et al.,
PRB 85, 224524 (2012)

linear MR transforms
to $B^{1/2}$ at lower T ?

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background and MQO)



P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, PRB 86, 165125 (2012)

Agreement is excellent, especially in clean sample!

Interlayer conductivity in the maxima

When chemical potential is in the center of LL, $\Delta\varepsilon = 0$

Then equation on SE simplifies $\Sigma_*^2 \left[(\Delta\varepsilon - \Sigma_*)^2 - 4t_z^2 \right] = (\Gamma_0 \hbar \omega_c)^2$

$$\text{Re } \Sigma(\mathbf{0}) = \mathbf{0}$$

$$|\text{Im} \Sigma_*| = \sqrt{\sqrt{4t_z^4 + (\Gamma_0 \hbar \omega_c)^2} - 2t_z^2}$$

and the interlayer conductivity

$$\sigma_{zz}(\varepsilon) \equiv \frac{\sigma_0 \hbar \omega_c \Gamma_0}{2\pi t_z^2 |\text{Im} \Sigma^R(\varepsilon)|} \text{Re} \frac{4t_z^2 - (\Delta\varepsilon)^2 + i \Delta\varepsilon |\text{Im} \Sigma^R(\varepsilon)|}{\sqrt{4t_z^2 - (\Delta\varepsilon - i |\text{Im} \Sigma^R(\varepsilon)|)^2}},$$

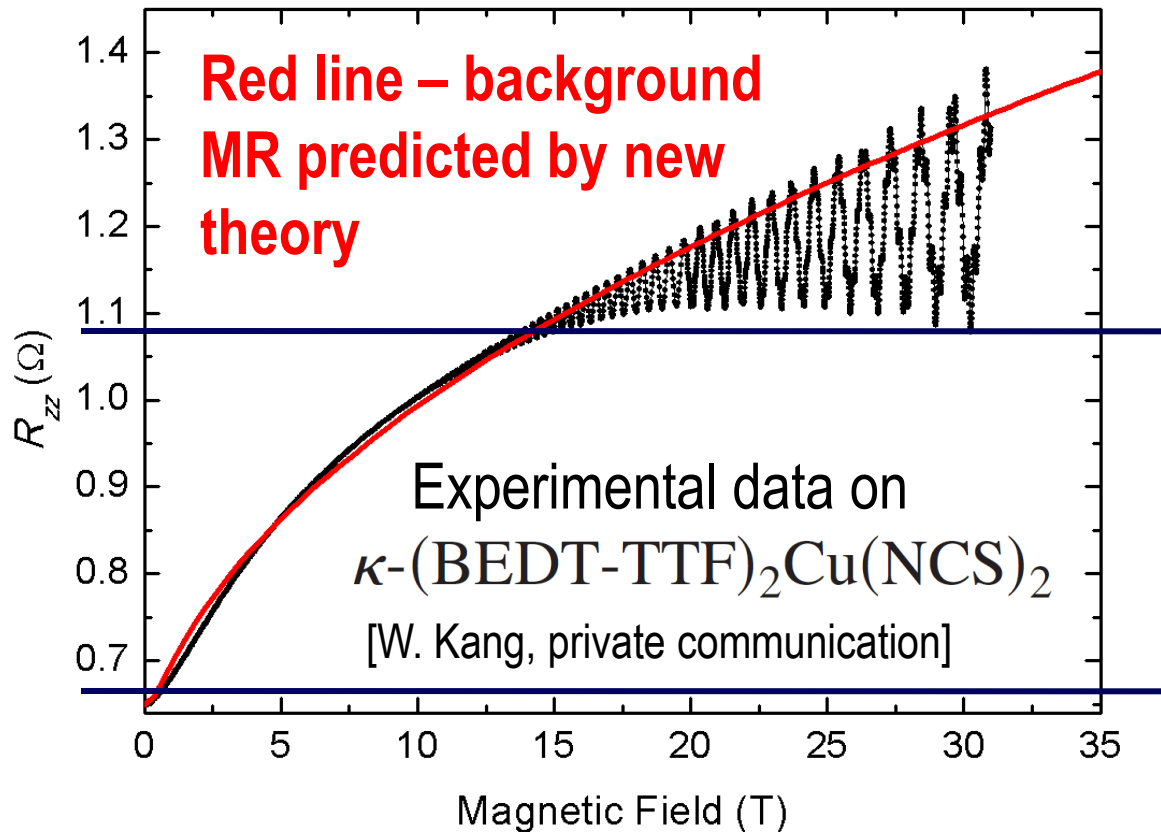
at $\Delta\varepsilon=0$ in SCBA
simplifies to

$$\sigma_{zz}(0) \approx 2\sigma_0/\pi \quad \text{for any } t_z/\sqrt{\omega_c \Gamma_0} !$$

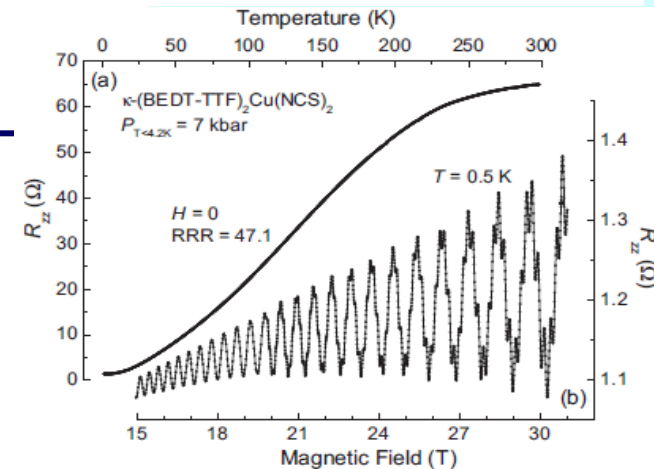
$$\text{but } 4t_z < \hbar \omega_c$$

Result

MR $R_{zz}(B)$ in the minima of MQO (magnetic field dependence: background and MQO)



The temperature dependence of conductivity is metallic-type:



[W. Kang et al., PRB
80, 155102 (2009)]

$$R_{\min}(B \rightarrow \infty) / R_{\min}(B = 0) \approx 1.08 / 0.67 = 1.6 \approx \pi / 2!$$

Again a very good agreement of theory with experiment!

2. $R_{zz}(B_z)$ at finite interlayer transfer integral t_z (qualitative arguments)

Contribution to σ_{zz} from one LL at : $\omega_c / \Gamma_0 = 40 \gg 1$

$\sigma_{zz}(\epsilon)/\sigma_0$

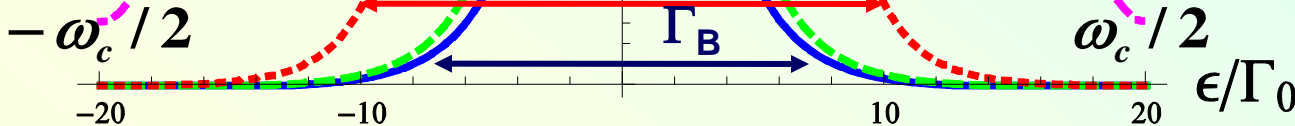
even at $t_z=0$
the LL width

$$\Gamma_B = \sqrt{\omega_c \Gamma_0} \gg \Gamma_0$$

4 values of t_z : $t_z / \Gamma_0 = 0.1, 2, 5, 10$

**! Crossover from
square-root to linear
field dependence
at $2t_z \sim \Gamma_B$**

$$\sigma_{zz}(0) \approx 2\sigma_0/\pi.$$



$$\bar{\sigma}_{zz} = \int_{-\hbar\omega_c/2}^{\hbar\omega_c/2} \frac{d\epsilon}{\hbar\omega_c} \sigma_{zz}(\epsilon) \approx \sigma_0 (t_z / \hbar\omega_c) \propto 1/B_z.$$

Conclusions (Part 1)

The standard 3D theory of magnetoresistance (MR) (derived in the Born or even τ -approximations) is not applicable to strongly anisotropic layered compounds.

The reduction of dimensionality + magnetic field increase the effect of impurities, lead to strong longitudinal MR, change the Dingle plot and angular dependence of MR.

In the limit $t_z < \sqrt{\omega_c \Gamma_0} \ll \omega_c$ longitudinal MR $R_{zz} \propto \sqrt{B_z}$

In the limit $\sqrt{\omega_c \Gamma_0} \leq 4t_z < \omega_c$ longitudinal MR $R_{zz} \propto B_z$
 and $\sigma_{zz} \propto t_z^3$ contrary to usual $\sigma_{zz} \propto t_z^2$

This dependence is not damped by temperature (if impurity scattering is stronger than phonon scattering of conducting electrons)

General conclusion: in quasi-2d to calculate MR one must consider MQO even if they are damped by T.

Technical conclusion on MR calculation $R_{zz}(B)$ in strong magnetic field

1. The approach starting from the 3D strongly-anisotropic dispersion is valid even at $t_z < \Gamma_0$, but the Born approximation is not valid. In the second order in t_z both approaches sum the same set of diagrams.

2. The two-layer approach violates at $t_z > \Gamma_B = (\omega_c \Gamma_0)^{1/2}$

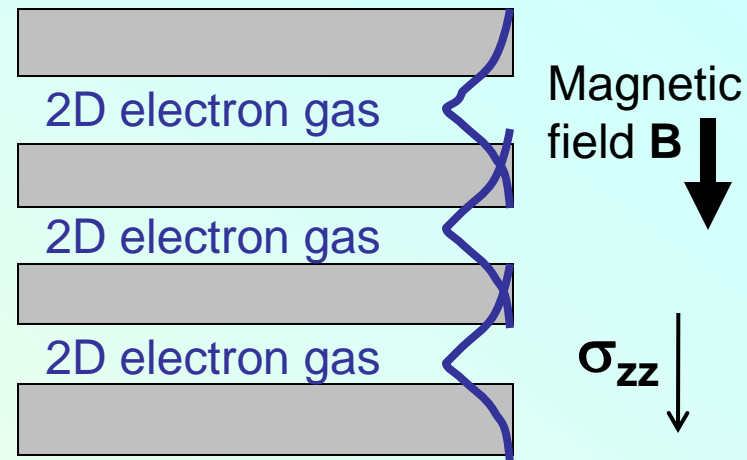
The Hamiltonian contains 3 terms:

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

1
3
2

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

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



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

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

2. The short-range impurity potential:

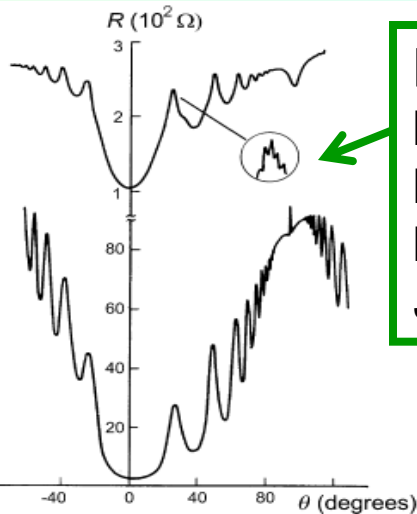
$$\hat{H}_I = \sum_i V_i(r) \quad \text{where} \quad V_i(r) = U \delta^3(r - r_i)$$

Part 2: Angular dependence of MR in strongly anisotropic layered metals

Started in P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011)

Continued in P.D. Grigoriev, T.I. Mogilyuk, to be published

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



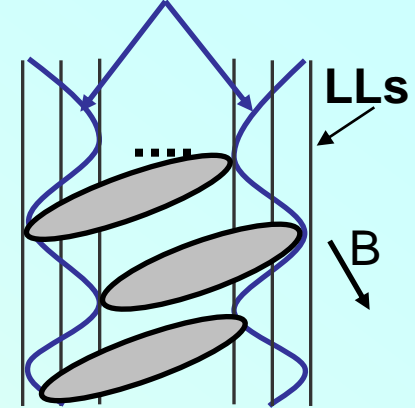
First observation:

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).

Fermi surface



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

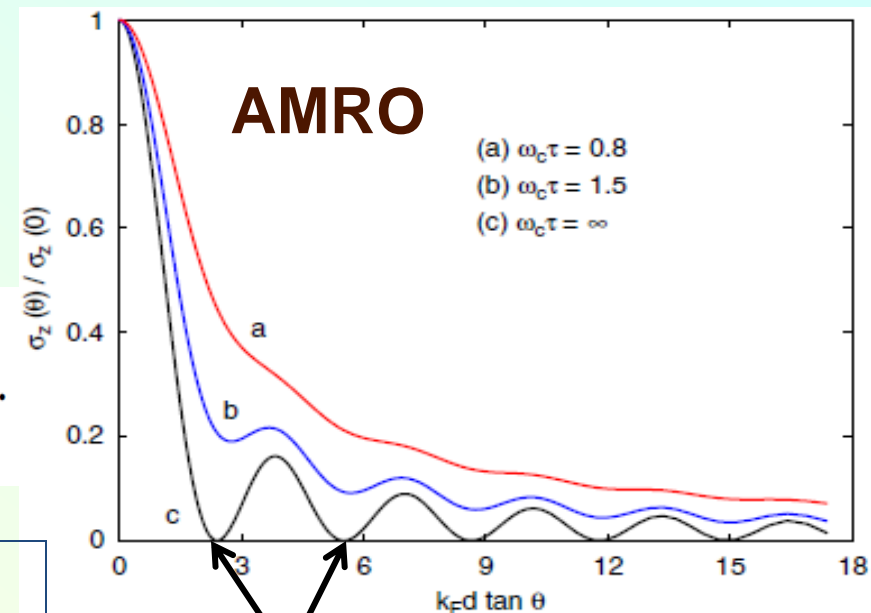
For axially symmetric dispersion and in the first order in t_z the Shockley tube integral gives:

[R. Yagi et al., *J. Phys. Soc. Jap.* **59**, 3069 (1990)]

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

gives AMRO

gives damping of AMRO by disorder



Yamaji angles

The two-layer tunneling model

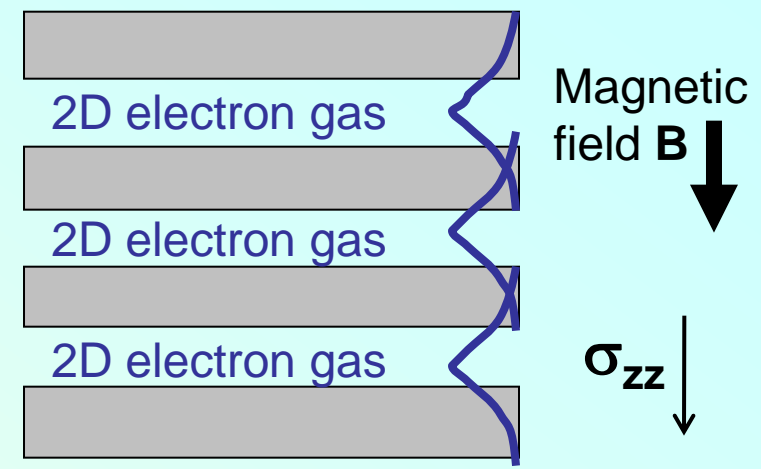
The Hamiltonian contains 3 terms:

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

1 3 2

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

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



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

2. The short-range impurity potential:

$$\hat{H}_I = \sum_i V_i(r) \quad \text{where} \quad V_i(r) = U \delta^3(r - r_i)$$

Calculation of the angular dependence of MR

[started in P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011)].

The impurity averaging on adjacent layers can be done independently:

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

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

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:

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

New term! $G_R G_R$ $G_R G_A$

Result 2011 Angular dependence of magnetoresistance in the weakly incoherent regime [PRB 2011]

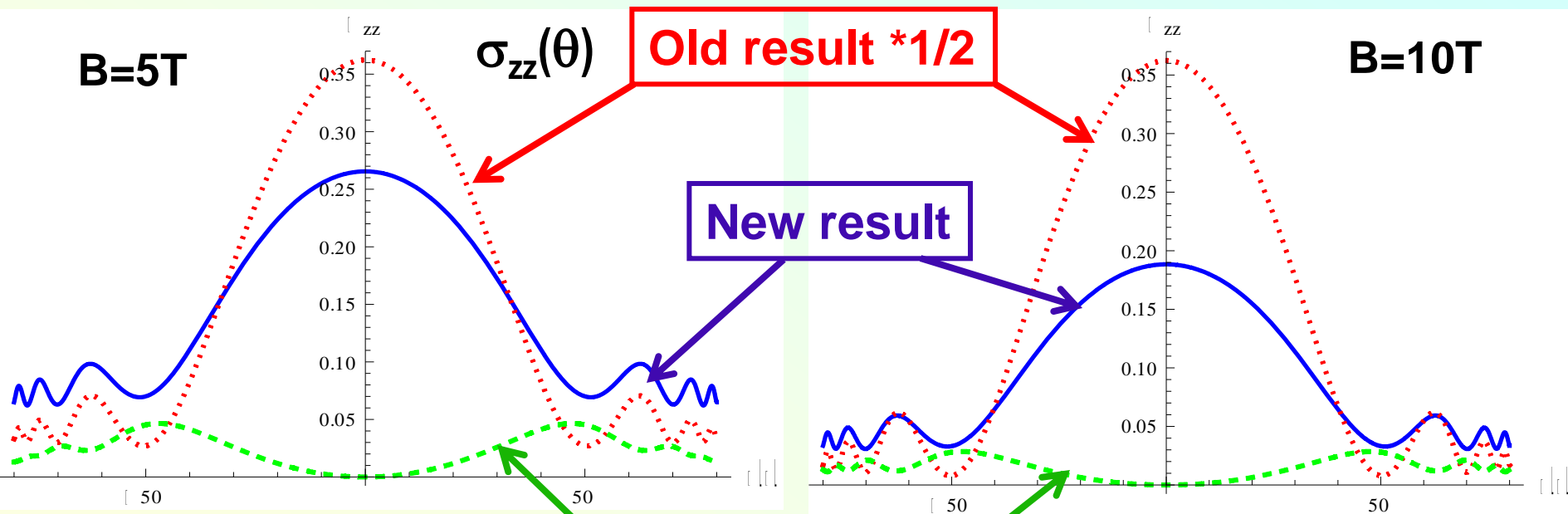
Result for Lorentzian LL shape is very approximate:
It modifies for $\omega\tau > 1$.

$$\sigma_{zz} = \sigma_0(B_Z) \left\{ [J_0(\kappa)]^2 + 2 \sum_{\nu=1}^{\infty} \frac{[J_{\nu}(\kappa)]^2}{1 + (\nu\omega_c\tau_B)} \right\},$$

where $\kappa \equiv k_F d \tan\theta$, but τ depends on B_Z : $\tau_B = \tau_0 (\Gamma_0 / \Gamma_B) \propto 1 / \sqrt{B \cos\theta}$

and the prefactor acquires the angular dependence:

$$\sigma_0(B_Z) \propto 1 / \sqrt{B_Z} = 1 / \sqrt{B \cos\theta}.$$



The difference comes from the high harmonic contributions and from the prefactor

Angular dependence of harmonic amplitudes for arbitrary LL shapes

(P.D. Grigoriev, T.I. Mogilyuk)

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

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

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

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 for Lorentzian and Gaussian LL shapes

(P.D. Grigoriev, T.I. Mogilyuk)

For Lorentzian LL shape:

$$\frac{\sigma_{zz}^L}{\sigma_{zz}^0} = \frac{\Gamma_0}{\Gamma} \sum_{k=-\infty}^{\infty} (-1)^k \exp\left(\frac{2\pi i k \epsilon_F}{\hbar \omega_c}\right) R_D(k) R_T(k) \times R_S(k) \left\{ [J_0(\kappa)]^2 \left(1 + \frac{\pi k}{\omega_c \tau}\right) + \sum_{p=1}^{\infty} \frac{2 [J_p(\kappa)]^2}{1 + (p \omega_c \tau)^2} \right\},$$

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

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

For Gaussian LL shape the $p \neq 0$ 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 $R_S(k) = \cos\left(\frac{\pi k m^*}{m_e \cos \theta}\right)$

Spin current is considerable in strong field!

Conclusions

Part 1: The standard 3D theory of magnetoresistance (MR) (derived in the Born or even τ - approximation) is not applicable to strongly anisotropic layered compounds. The reduction of dimensionality + magnetic field increase the effect of impurities, lead to strong longitudinal MR, change the Dingle plot and angular dependence of MR.

In the limit $t_z < \sqrt{\omega_c \Gamma_0} \ll \omega_c$ longitudinal MR $R_{zz} \propto \sqrt{B_z}$
 This dependence is not damped by temperature

In the limit $\sqrt{\omega_c \Gamma_0} \leq 4t_z < \omega_c$ longitudinal MR $R_{zz} \propto B_z$
 and $\sigma_{zz} \propto t_z^3$ contrary to usual $\sigma_{zz} \propto t_z^2$

Part 2: Angular dependence of MR depends on LL shape. For Gaussian LL shape AMRO are much stronger. Angular dependence of MQO harmonics is calculated. Spin current

Thank you for your attention !.

But no AMRO is predicted in these models,
which contradicts the experiments on $R_{zz}(\theta)$

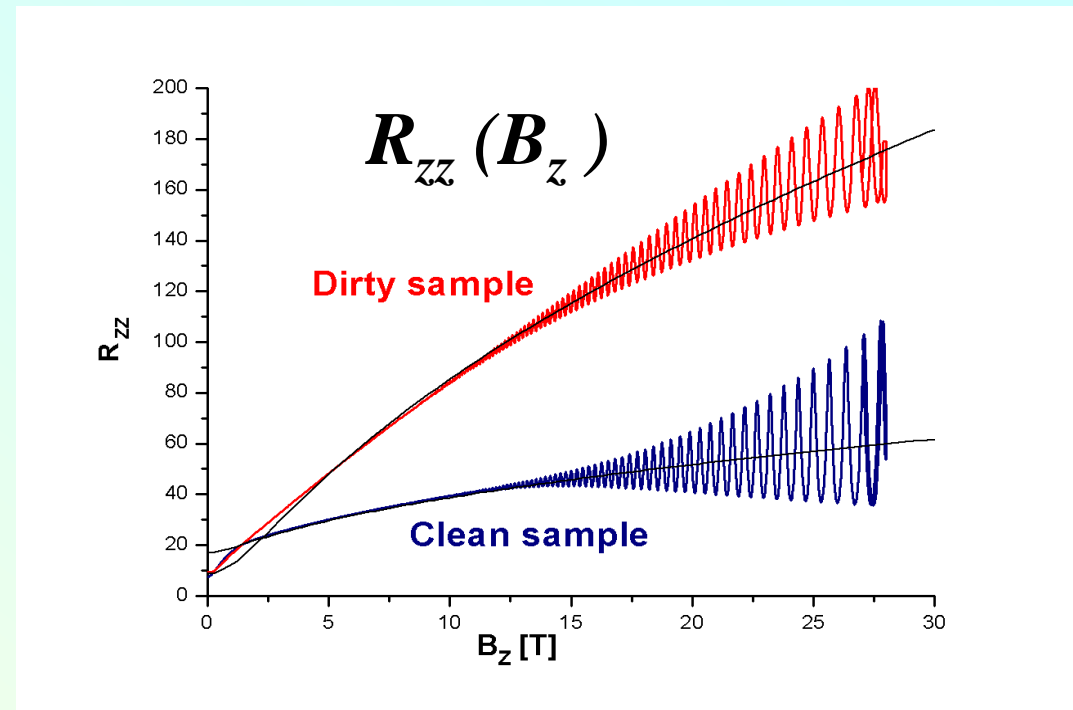
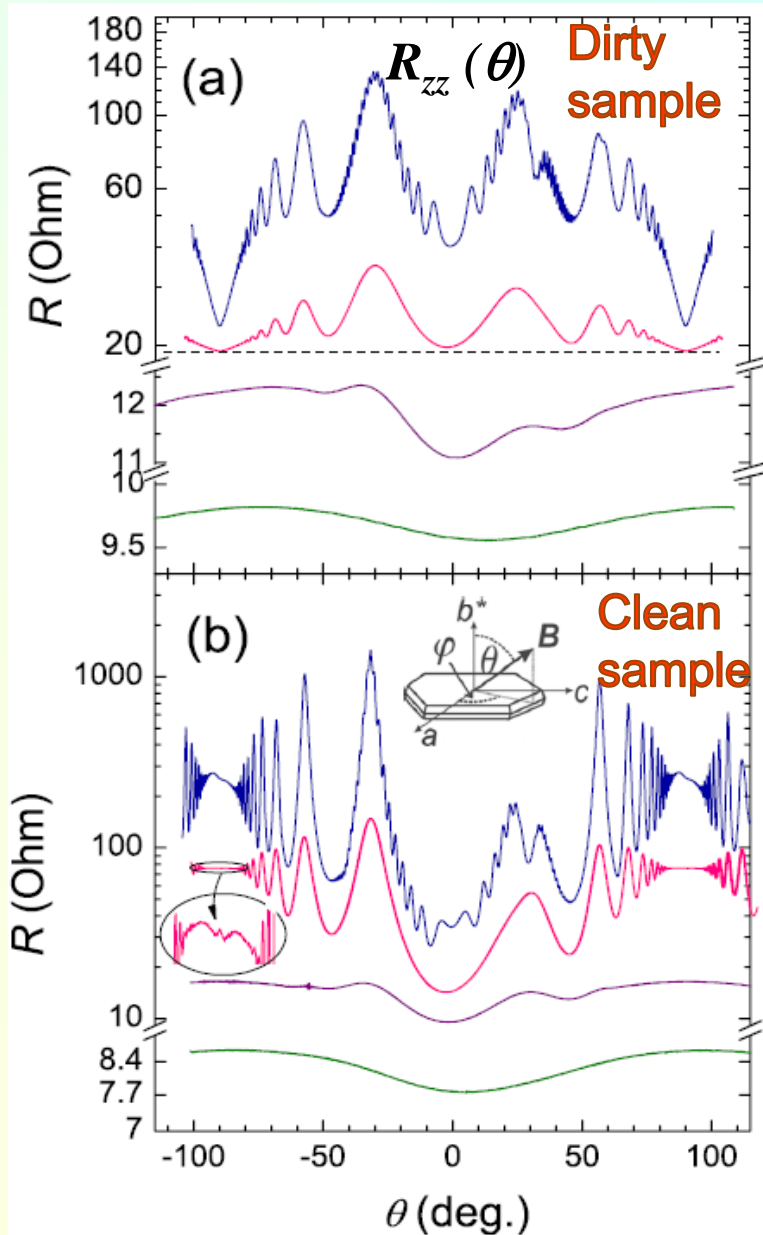


FIG. 1. (Color online) (a) Angle-dependent interlayer magnetoresistance of a relatively dirty sample, 1, of α -(BEDT-TTF) $_2$ KHg(SCN) $_4$ in the high-pressure metallic state recorded at $T=1.4$ K at magnetic fields (bottom to top): 0.12, 0.5, 3, and 15 T; $\varphi \approx 20^\circ$. (b) Same for a very clean sample, 2. The upper inset illustrates the definition of angles θ and φ ; the lower inset: enlarged fragment of the 3 T curve showing a small “coherence peak.” [PRB 79, 165120 (2009).]

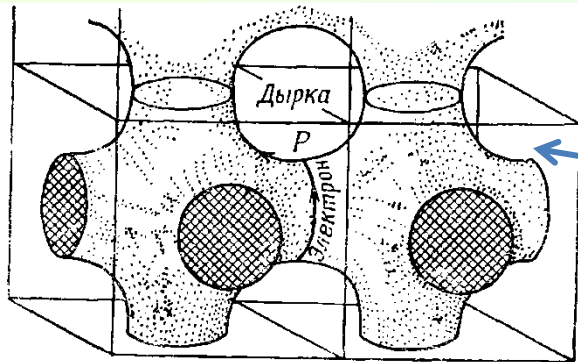
Appendices

Background magnetoresistance in 3D metals (strong field)

In strong magnetic field B ($\omega_c \tau \gg 1$) magnetoresistance (MR) depends on the shape and topology of Fermi surface (FS),
but $B//J$ produces no MR. Only $B \perp J$ gives MR.

For closed trajectories
the conductivity tensor

$$\sigma = \begin{pmatrix} \frac{A_{xx}}{H^2} & -\frac{A_{yx}}{H} & -\frac{A_{zx}}{H} \\ \frac{A_{yx}}{H} & \frac{A_{yy}}{H^2} & -\frac{A_{zy}}{H} \\ \frac{A_{zx}}{H} & \frac{A_{zy}}{H} & A_{zz} \end{pmatrix}$$

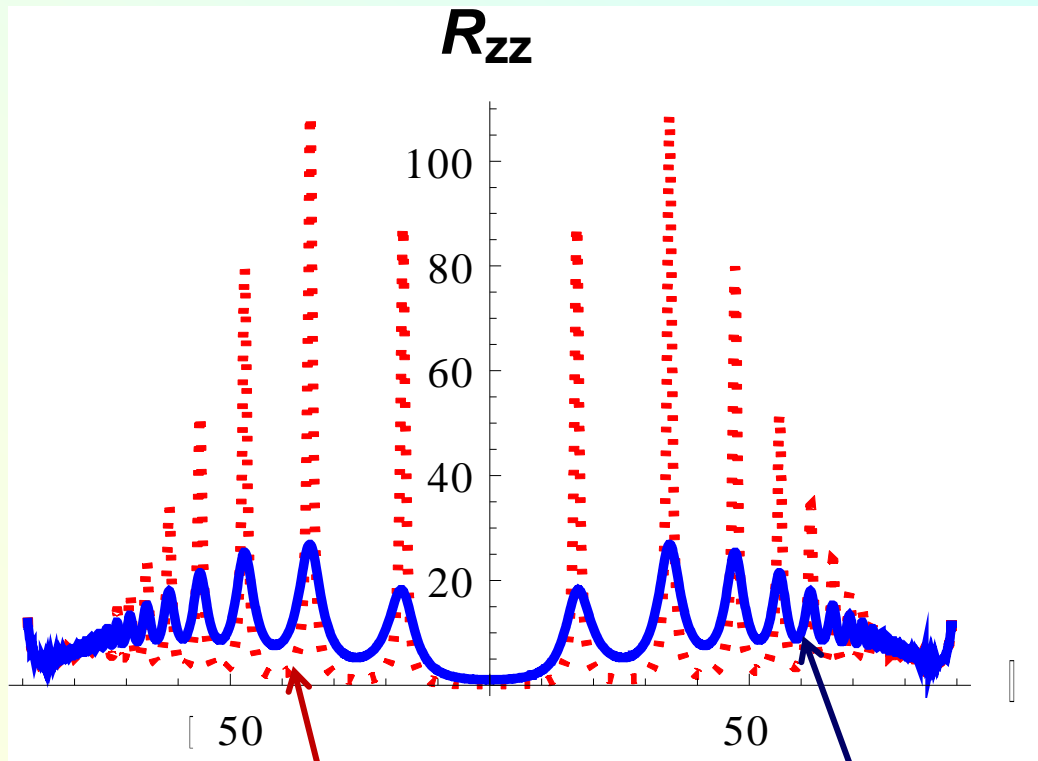


FS, containing
open and closed
trajectories

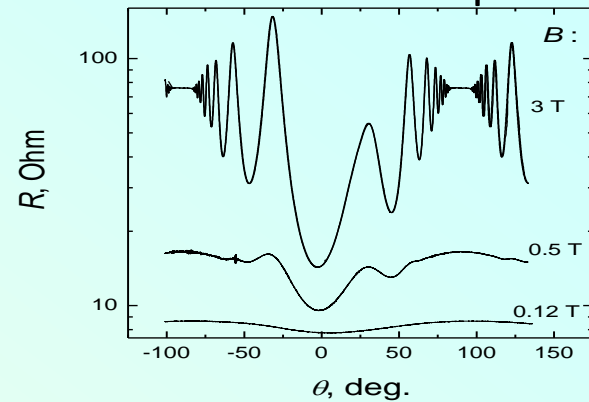
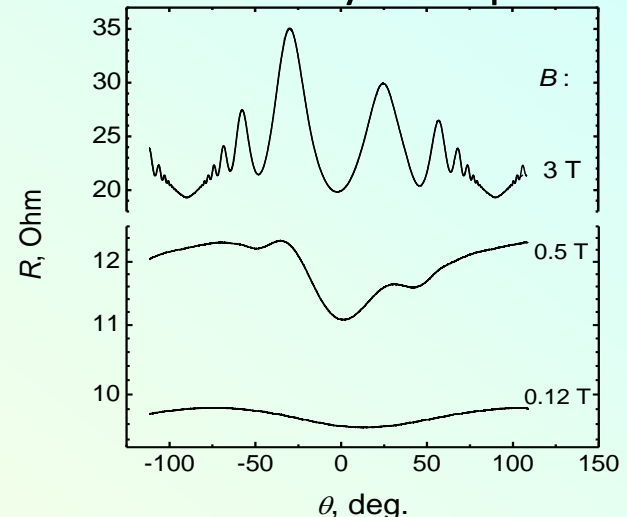
$$\sigma = \begin{pmatrix} B_{xx} & -\frac{A_{yx}}{H} & -B_{zx} \\ \frac{A_{yx}}{H} & \frac{A_{yy}}{H^2} & -\frac{A_{zy}}{H} \\ B_{zx} & \frac{A_{zy}}{H} & A_{zz} \end{pmatrix}$$

For open trajectories (open
orbit along x-axis)
the conductivity tensor is

A.A. Abrikosov, *Fundamentals of the theory of metals*, North-Holland, 1988.

Result 3.**Comparison with experiment on angular oscillations of magnetoresistance (AMRO)****Theory (qualitative view):****Old result****new result**

**P. Moses and R.H. McKenzie,
Phys. Rev. B 60, 7998 (1999).**

**Experiment:
“Clean” sample****“Dirty” sample**

**M. Kartsovnik et al.,
PRB 79, 165120 (2009)**

Result 2

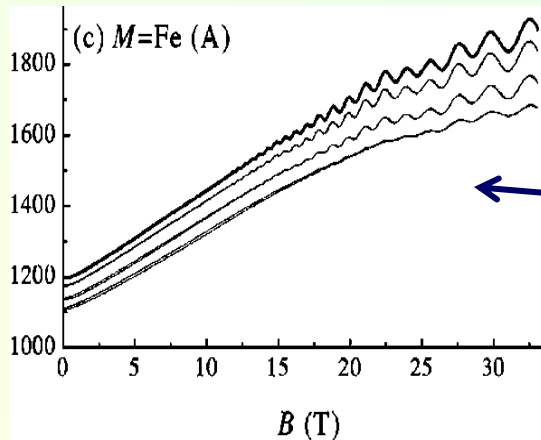
Generalization of the theory of interlayer longitudinal MR for finite t_z

Aim: extend applicability + explain experiments

Previous two-layer approach gives square-root $R_{zz}(B_z)$ and is applicable at $t_z \ll \Gamma_0 \ll h\omega_c$

New approach is applicable at $\Gamma_0 \sim t_z < h\omega_c/4$

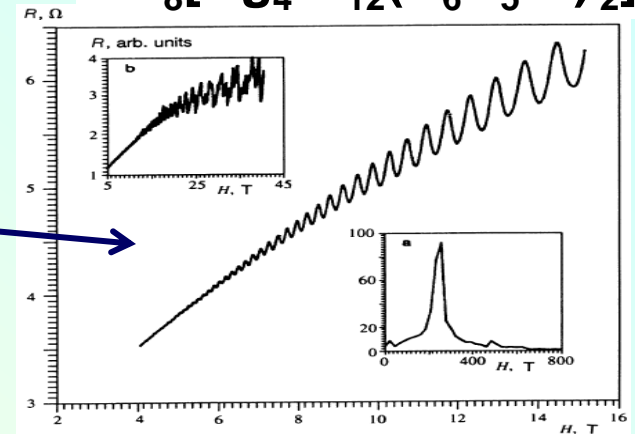
$\beta'' - (BEDT - TTF)_4[(H_3O)Fe(C_2O_4)_3]C_5H_5N$



A.I. Coldea et al., PRB 69, 085112 (2004)

Longitudinal interlayer MR experiment $R_{zz}(B_z)$

$ET_8[Hg_4Cl_{12}(C_6H_5Cl)_2]$

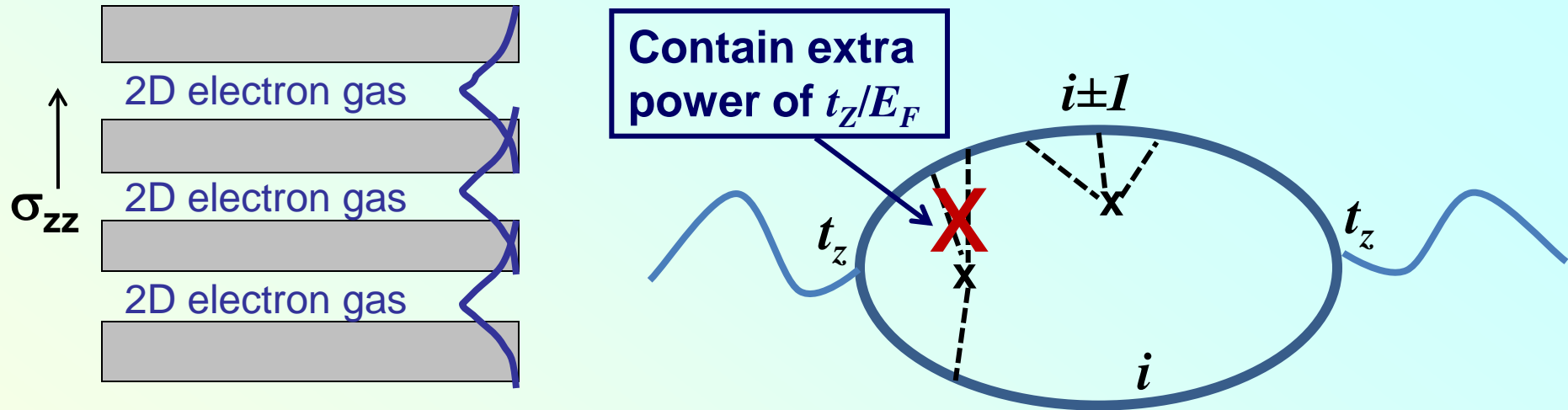


R.B. Lyubovskii, S.I. Pesotskii et al., JETP 80, 946 (1995)

40

New result: crossover from linear to square-root field dependence of MR at $2t_z \approx \sqrt{\omega_c \Gamma_0} \ll \omega_c$.

Impurity averaging



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

$$\sigma_{zz} = \frac{4e^2 t_z^2 d}{L_x L_y} \int d^2 r d^2 r' \int \frac{d\varepsilon}{2\pi} [-n'_F(\varepsilon)] \langle \text{Im} G(r, r', j, \varepsilon) \rangle \langle \text{Im} G(r', r, j+1, \varepsilon) \rangle,$$

Vertex corrections can be ignored

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

Shubnikov – de Haas oscillations in 3D metals

MQO of conductivity in 3D metals mainly come from the oscillations of electron mean free time $\tau \sim 1/\rho(E_F)$. The DoS $\rho(E_F)$ oscillates because of Landau level quantization.

$$\sigma_{zz}^{3D} = e^2 \tau \sum_{FS} v_z^2,$$

where in the Born approximation the scattering rate is given by golden Fermi rule:

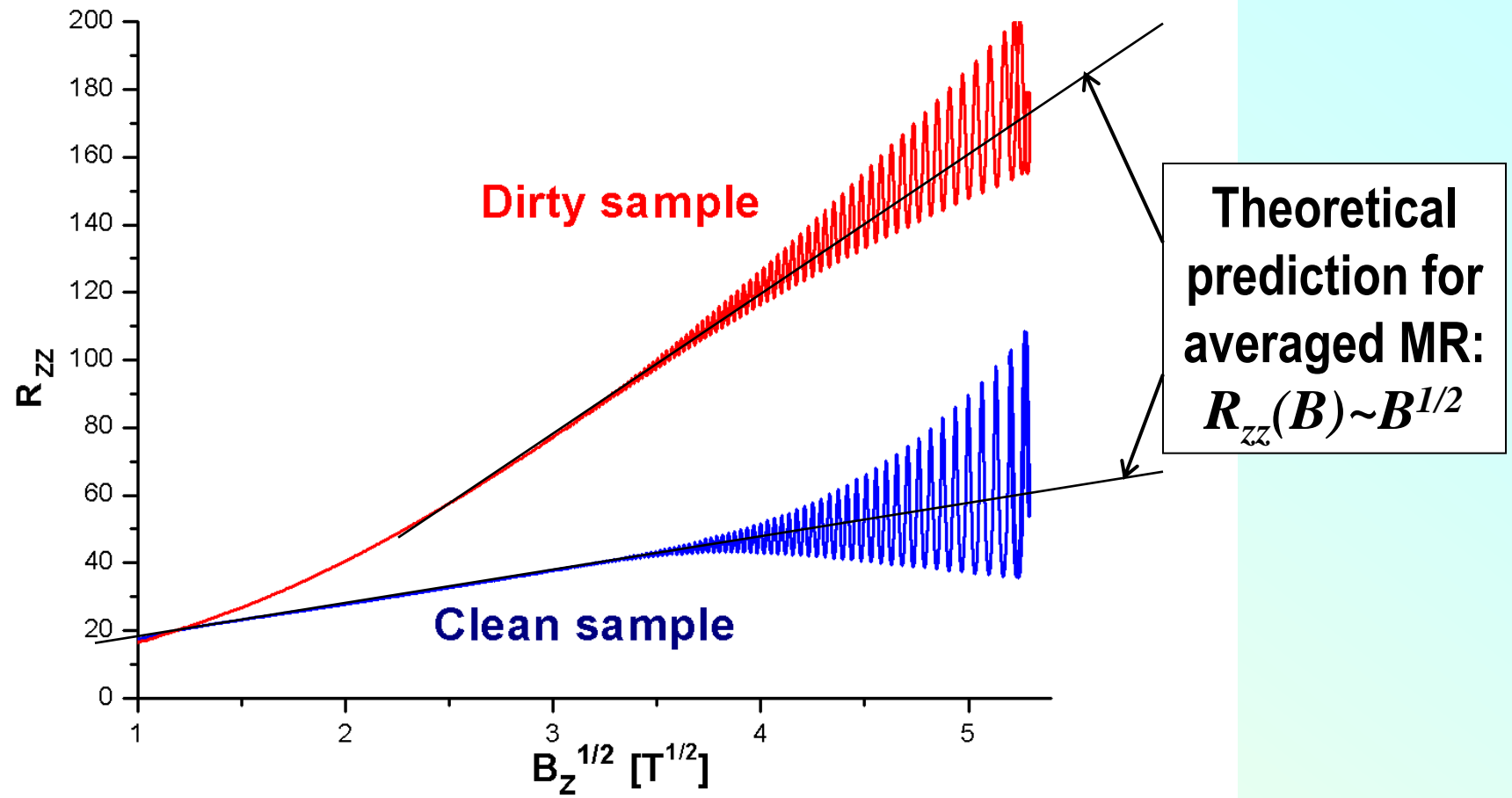
$$1/\tau = \frac{2\pi}{\hbar} n_i |v|^2 \int dp_z \sum_n \delta(\epsilon(n, p_z) - \mu) \frac{eH/c}{(2\pi\hbar)^2}. \quad \leftarrow \text{DoS}$$

So, in 3D conductivity is inversely proportional to the DoS, because oscillations of scattering rate $1/\tau$ dominate oscillations of mean square electron velocity averaged over FS.

In 2D maxima of conductivity coincide with DoS maxima, because between the LLs there is no electron states to conduct => the phase of Shubnikov-de Haas oscillations in 2D and 3D differs by π => 2D and 3D cases are not described by the same formula!

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background and MQO)

α -(BEDT-TTF)₂KHg(SCN)₄



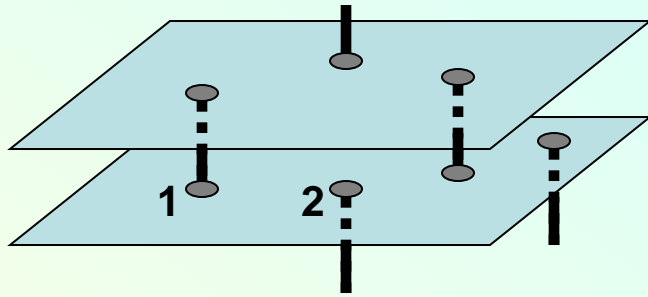
Theoretical prediction for averaged MR:
 $R_{zz}(B) \sim B^{1/2}$

P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, PRB 86, 165125 (2012);

Agreement is excellent, especially in clean sample!

The model of incoherent conductivity channel

[Phys. Rev. B 79, 165120 (2009)]



The resistance through each hopping center contains two in-series elements:

$$R_{\perp} = R_{hc} + R_{\parallel}.$$

The hopping-center resistance R_{hc} is almost independent of magnetic field and has nonmetallic temperature dependence.

The in-plane resistance R_{\parallel} depends on the magnetic field \perp to the conducting layers, and has the metallic temperature dependence. It can be calculated in the limit when the concentration of hopping centers $n_i = 1/l_i^3$ is much less than the concentration of normal impurities $n_{\tau} = 1/l_{\tau}^3$. Then the resistance R_{\parallel} is determined by the in-plane conductivity:

$$R_{\parallel} = \ln(l_i/l_{\tau}) / \pi \sigma_{\parallel} d.$$

The total incoherent part of conductivity:

σ_{\parallel} depends on magnetic field \perp layers and has metallic T-dependence.

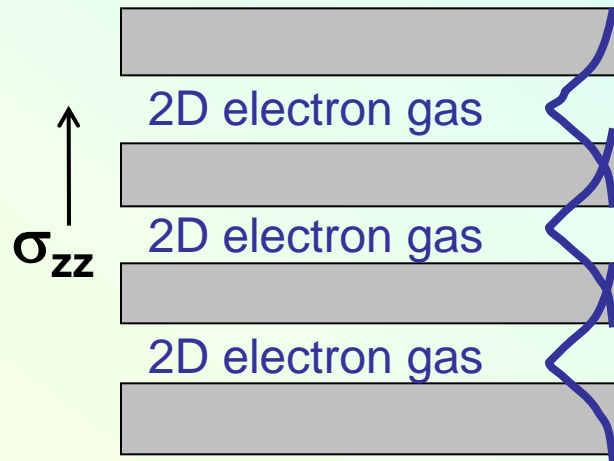
$$\sigma_i = \frac{\pi \sigma_{\parallel} n_i d^3}{\pi d \sigma_{\parallel} R_{hc} + \ln(l_i/l_{\tau})}.$$

**Another experimental indication
of the 3D \rightarrow quasi-2D crossover when
LL separation becomes greater than t_z**

**Landau level shape and harmonic damping
of MQO can answer if electron dynamics is
2D or 3D in particular compounds**

**P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher,
Phys. Rev. B 86, 165125 (2012)**

Calculation of interlayer conductivity in the weakly incoherent regime [PRB 83, 245129 (2011)]

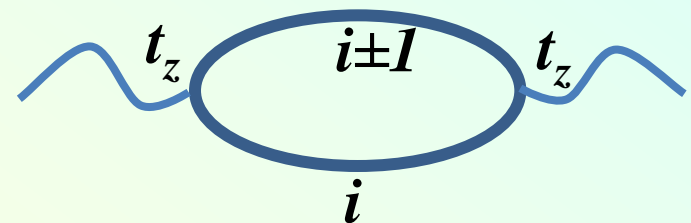


The interlayer transfer integral $t_z \ll \Gamma_0$ is the smallest parameter. We take it into account in the lowest order (after the magnetic field and impurity potential are included as accurately as possible). Interlayer conductivity is calculated as the tunneling between two adjacent layers using the Kubo formula:

$$\sigma_{zz} = \frac{e^2 t_z^2 d}{L_x L_y} \left\langle \int d^2 r d^2 r' \int \frac{d\varepsilon}{2\pi} 4 \text{Im} G_R(r, r', j, \varepsilon) \text{Im} G_R(r', r, j+1, \varepsilon) [-n'_F(\varepsilon)] \right\rangle,$$

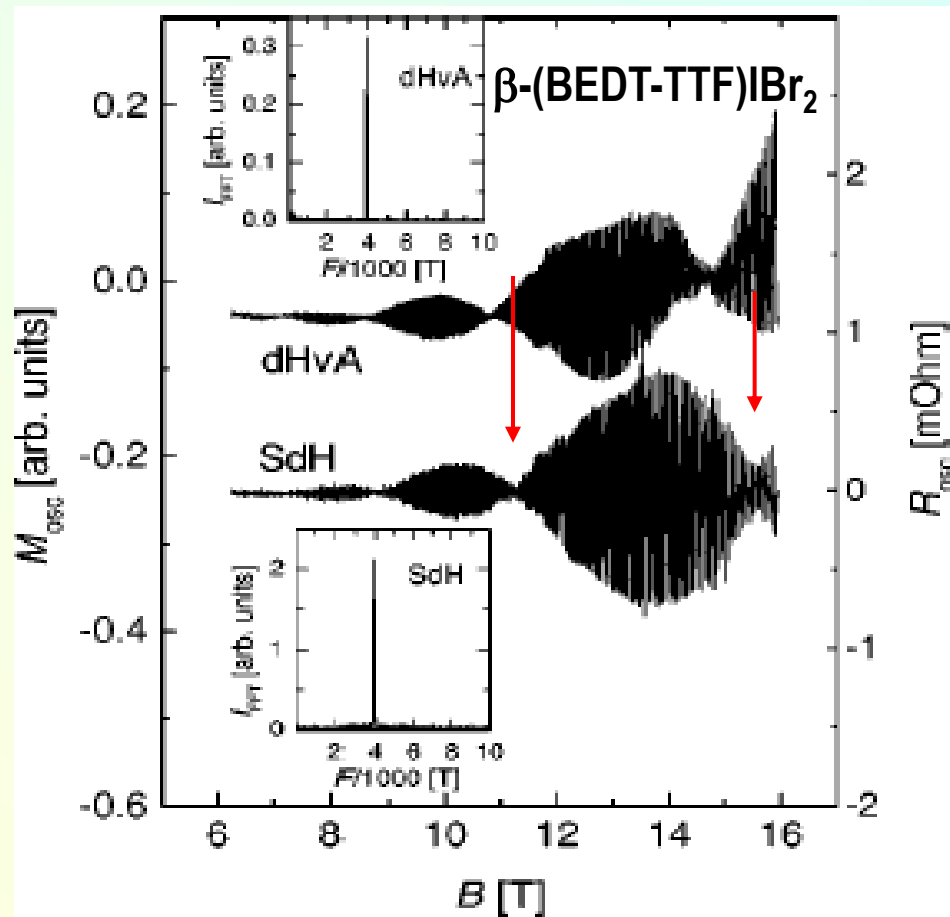
where the Green's function $G_R(r, r', j, \varepsilon)$ includes magnetic field and impurity scattering.

Conductivity (the linear response to external electric field) is again calculated from the Kubo formula:

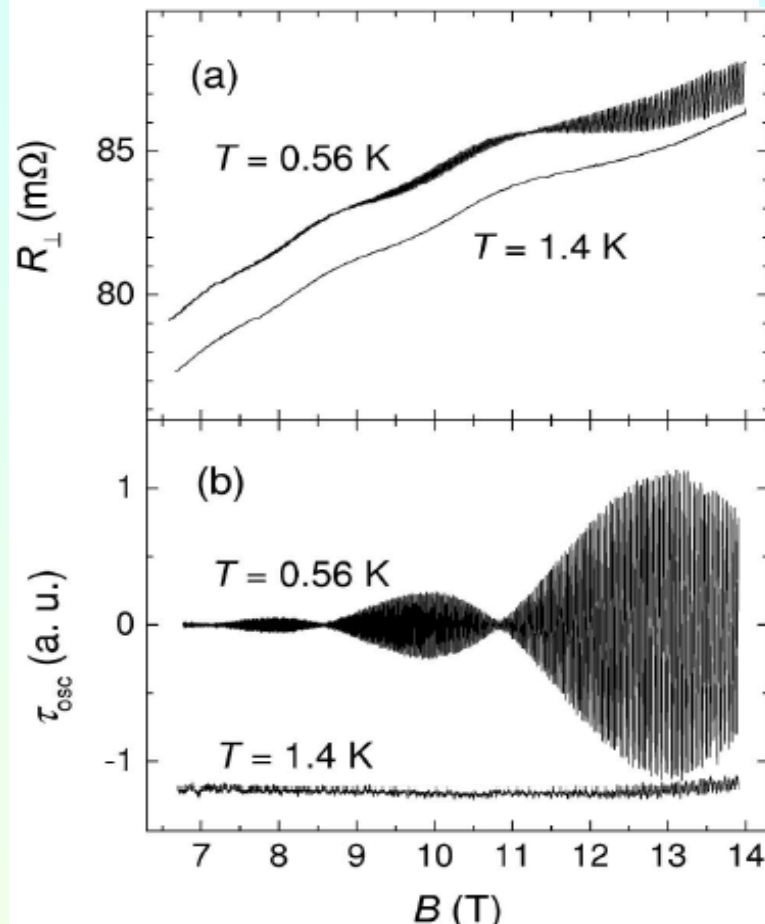


New features of MQO of conductivity in Q2D appear already in the first order in $\hbar\omega_c/4\pi t_z \ll 1$

Phase shift of beats



Slow oscillations of MR



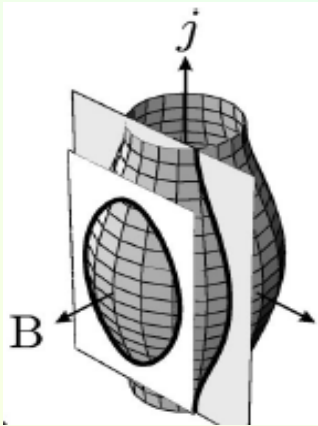
P.D. Grigoriev et al., Phys. Rev. B 65, 60403(R) (2002). Phys. Rev. Lett. 89, 126802 (2002);
Rigorous calculation is performed in P.D. Grigoriev, PRB 67, 144401 (2003).

Introduction

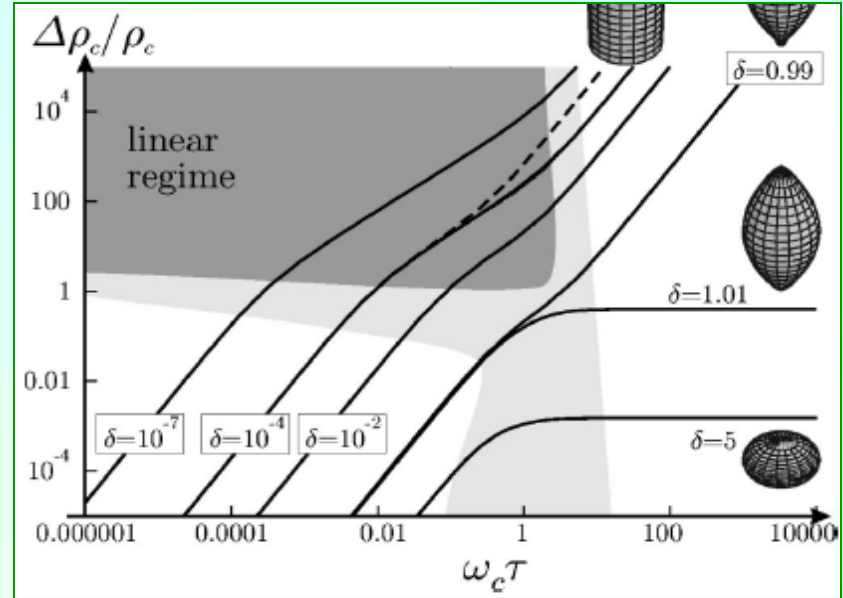
When $B \perp J$, strong MR $R_{zz}(B_x)$ is not surprising

Only longitudinal magnetoresistance is strange

The transverse magnetoresistance $R_{zz}(B_x)$ can be quadratic, linear,

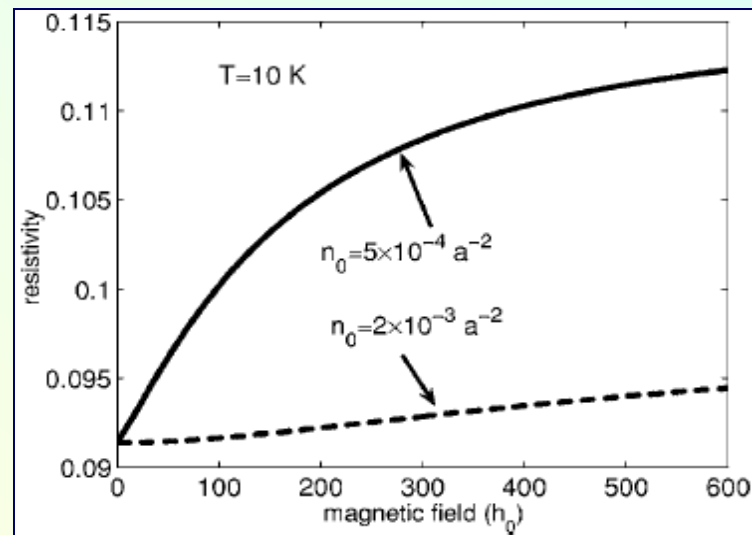


[A.F. Ho, A.J. Schofield, arXiv:cond-mat/0211675; A.J. Schofield and J.R. Cooper, Phys. Rev. B 62, 10779 (2000); ..]



or even $R_{xx}(B_z) \sim B_z^{1/2}$
as in graphen

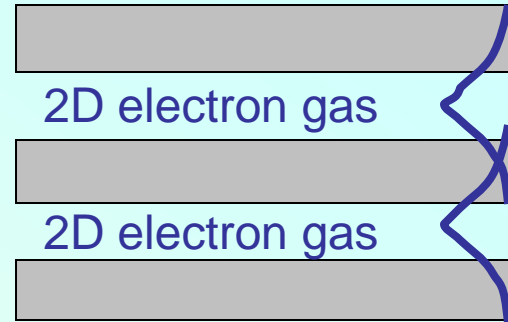
[L.A. Falkovsky, Phys. Rev. B 75, 033409 (2007)]



Previous theoretical results on Shubnikov - de Haas effect in quasi-2D metals (3)

V. M. Gvozdkov, PRB 76, 235125 (2007)

Title: Incoherence, metal-to-insulator transition, and magnetic quantum oscillations of interlayer resistance in an organic conductor

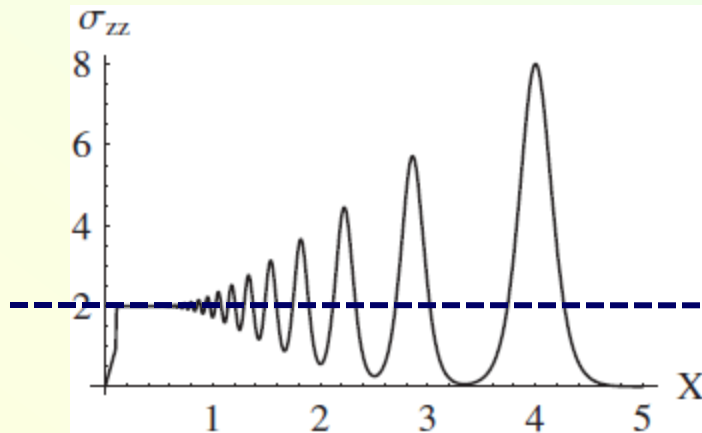


Variable-range hopping model for interlayer electron transport

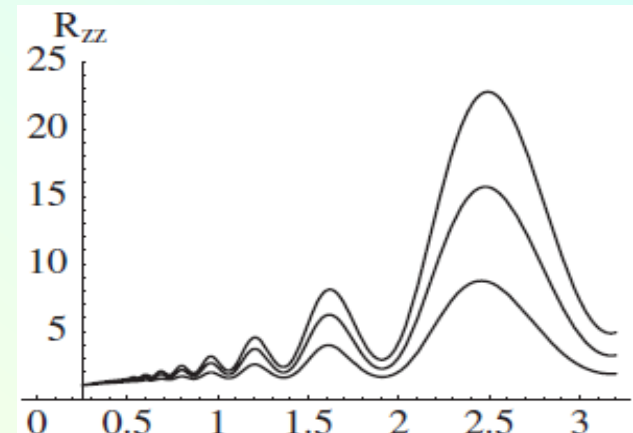
$$\sigma_{\tau}(T_0/T) = \sigma_{\tau}(0) \exp(-\sqrt{T_0/T}).$$

To explain the particular experiment he also assumed

$$\sqrt{\frac{T_0}{T}} \propto \sqrt{\frac{|B - B_0|^{\gamma}}{T}} = \left(\frac{|B - B_0|}{T^{1/\gamma}} \right)^{\gamma/2}$$



But in fact no VRH in Q2D componds



Do any new features in the theory of angular and field dependence of MR appear as we go from 3D to quasi-2D limit?

Generally accepted opinion [P. Moses and R. H. McKenzie, PRB 60, 7998 (1999)] that during coherent-weakly incoherent crossover ($t_z < \Gamma_0$) no changes.

This conclusion is incorrect.

It is based on oversimplified model for the interaction with impurities: Born approximation + neglect of MQO => constant electron self energy)

They have used the following 2D electron Green's function $G_R(n, \varepsilon) = \frac{1}{\varepsilon - \varepsilon_{2D}(n, k_y) - i\Gamma_0}$, disorder wrong

In PRB 83, 245129 (2011) I have shown, that

In strong magnetic field, when $\Gamma_0 < \hbar\omega_c \sim t_z$, MQO produce monotonic (background) MR, leading to strong longitudinal MR for $B \perp$ layers. **This changes the angular dependence of MR and reduces AMRO amplitude.**

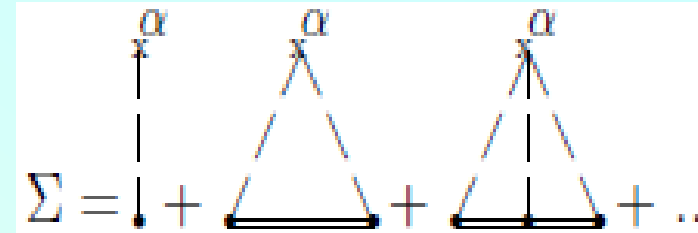
The 2D electron Green's function with disorder in B_z

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

$$G(r_1, r_2, \varepsilon) = \sum_{n, k_y} \Psi_{n, k_y}^{0*}(r_2) \Psi_{n, k_y}^0(r_1) G(\varepsilon, n),$$

where

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

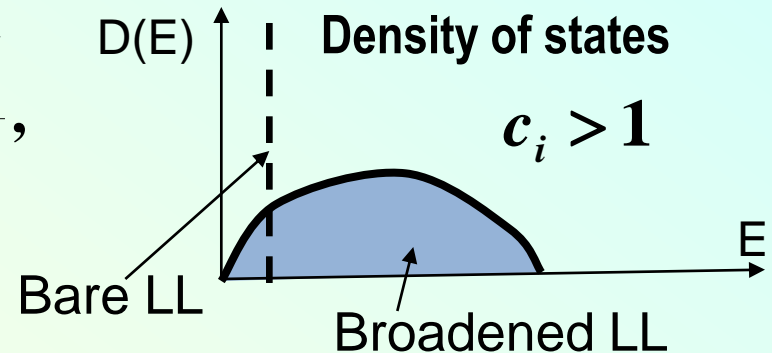


Tsunea Ando, J. Phys. Soc. Jpn. 36, 1521 (1974)

$$E_1 = E_g(\sqrt{c_i} - 1)^2, \quad E_2 = E_g(\sqrt{c_i} + 1)^2, \quad E_g = V_0 / 2\pi l_{\text{Hz}}^2 \propto B, \quad c_i = 2\pi l_{\text{Hz}}^2 N_i = N_i / N_{LL}.$$

The density of states on each Landau level has the dome-like shape:

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



Landau level width

$$\Gamma_B \equiv (E_2 - E_1) / 2 = 2E_g \sqrt{c_i} \propto \sqrt{B}.$$

In strong magnetic field the effective electron level width is much larger than without field:

$$\frac{\Gamma_B}{\Gamma_0} = \sqrt{\frac{4\omega_c}{\pi \Gamma_0}} \gg 1$$

Four-site approximation

Tsunea Ando, J. Phys. Soc. Japan 37, 622 (1974)].

Diagrams with intersections of impurity lines:

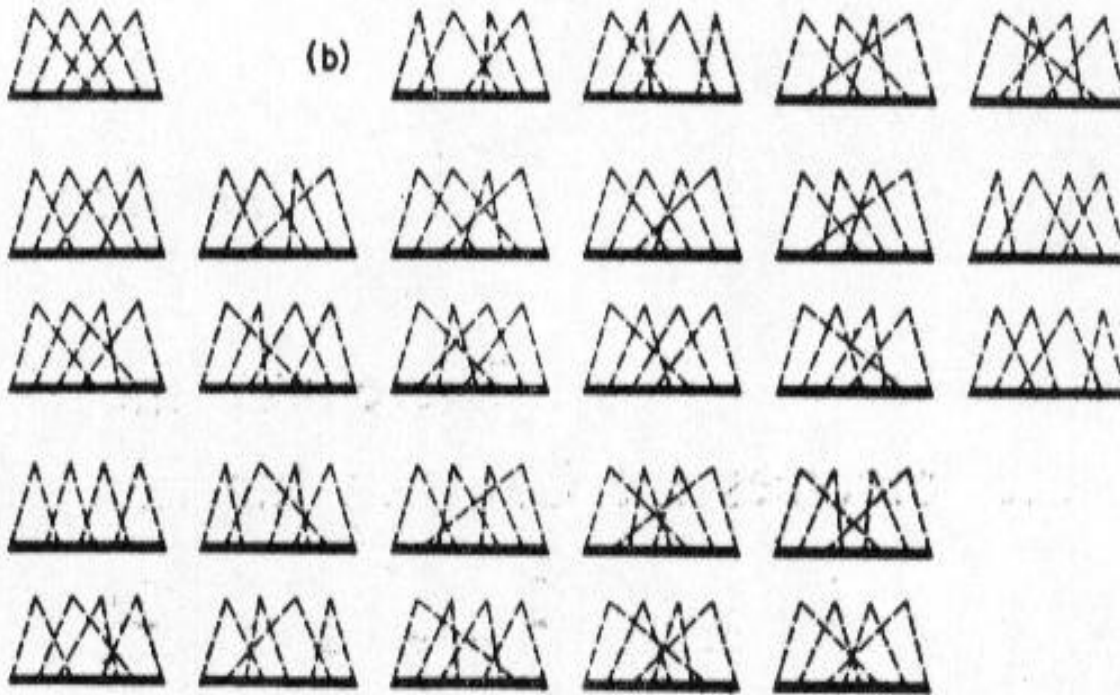


Fig. 9. The self-energies in the 4SA.

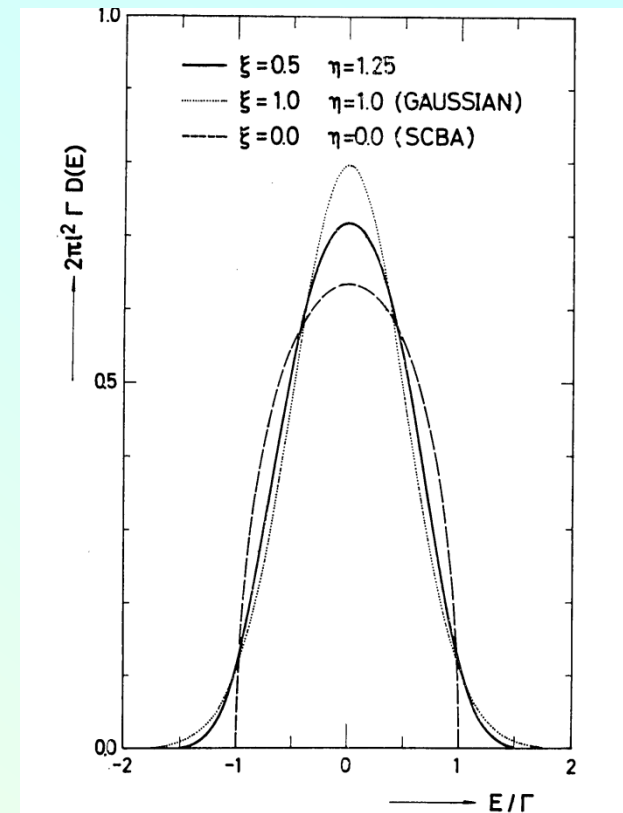
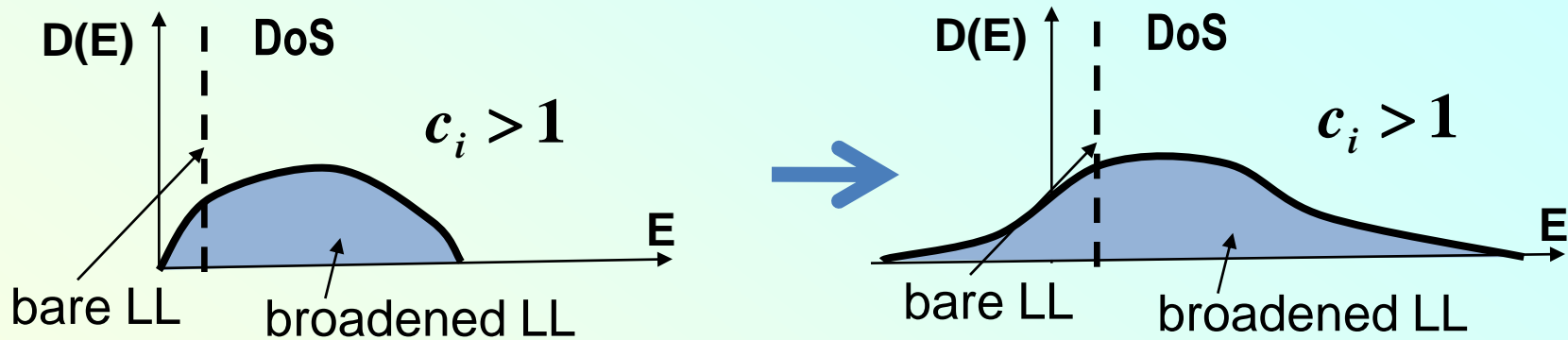


Fig. 7. The density of states of the ground Landau level. The solid line is the present result, the broken line is that in the SCBA, and the dotted line is the Gaussian density of states. The present result is something like an average of the Gaussian density of states and that in the SCBA.

The shape of LLs is not as important as their width!

The inclusion of diagrams with intersection of impurity lines in 2D electron layer with disorder only gives the tails of the DoS dome. The width of this dome remains unchanged and $\sim B_Z^{1/2}$:



The conductivity is not sensitive to the shape of LLs, but strongly depends on their width.

Therefore, we can take the DoS:

$$D(E) \approx \frac{\Gamma_B / \pi}{E^2 + \Gamma_B^2}.$$

where $\Gamma_B \approx \Gamma_0 \left[\left(4\omega_c / \pi \Gamma_0 \right)^2 + 1 \right]^{1/4}$

and Γ_0 is the electron level width without magnetic field

The corresponding Green's function is

$$G_R(n, \varepsilon) = \frac{1}{\varepsilon - \varepsilon_{2D}(n, k_y) - i\Gamma_B},$$

which gives $\bar{\sigma}_{zz} = \sigma_0 \sqrt{\pi \Gamma_0 / 4\omega_c} \approx 0.89 \sigma_0 \sqrt{\Gamma_0 / \omega_c} = 0.63 \sigma_0 / \sqrt{\omega_c \tau_0} \propto 1 / \sqrt{B_Z}$.

Result 1a**Monotonic part of conductivity for $B \parallel z$**

The averaging over impurities on two adjacent layers is not correlated.

For $B = B_z$ we get

$$\sigma_{zz} = \frac{\sigma_0 \Gamma_0 \hbar \omega_c}{\pi} \int d\varepsilon [-n'_F(\varepsilon)] \sum_n |\text{Im} G_R(\varepsilon, n)|^2.$$

In weak magnetic field this gives

$$\sigma_{zz}(B) = \sigma_0 \Gamma_0 / |\text{Im} \Sigma(\mu, B)|$$

Substituting Green's functions in the various approximations gives the monotonic part of interlayer conductivity [P.D.Grigoriev, JETP Lett. 94, 47 (2011)]

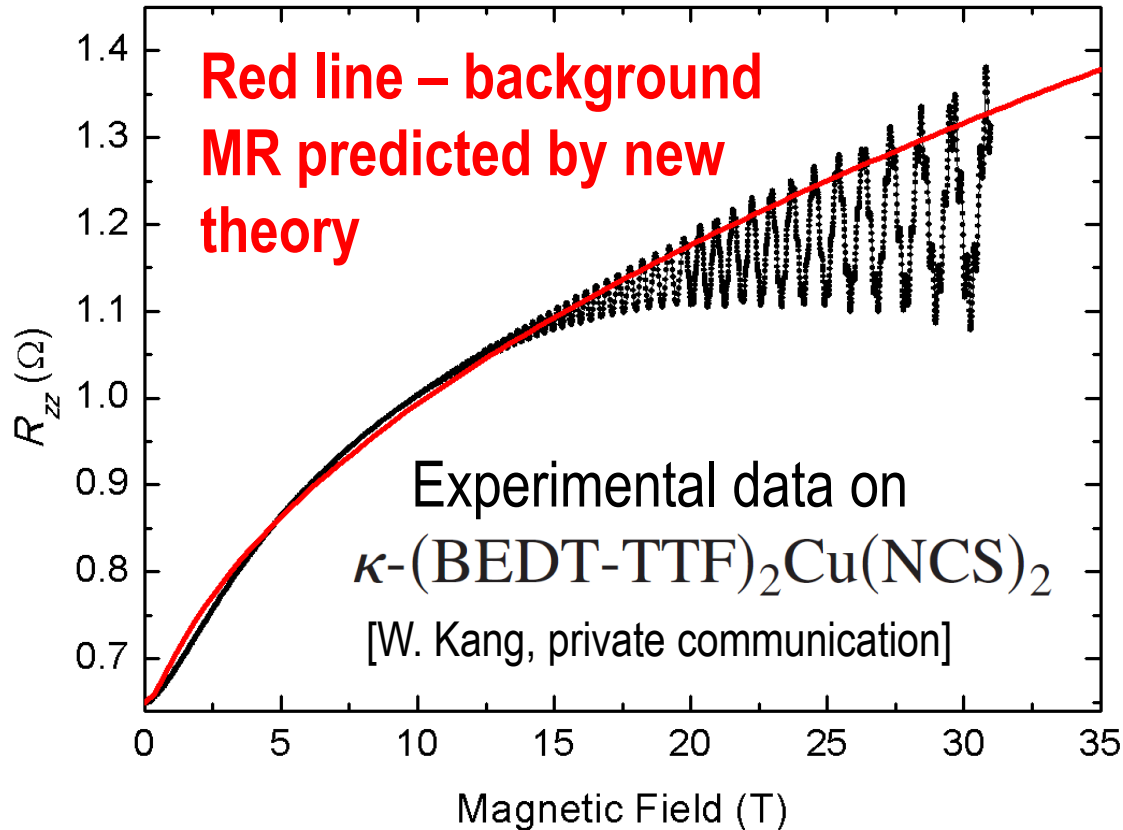
$$\bar{\sigma}_{zz} = \int_{E_1}^{E_2} \sigma_{zz}(E) dE / \hbar \omega_c = \frac{2\sigma_0 \Gamma_0}{\pi E_g} \left[\frac{1 + c_i}{2} \ln \left(\frac{\sqrt{c_i} + 1}{\sqrt{c_i} - 1} \right) - \sqrt{c_i} \right].$$

where $c_i = 2\pi l_{Hz}^2 N_i = N_i / N_{LL}$ and $\Gamma_0 = \pi c_i E_g^2 / \omega_c$.

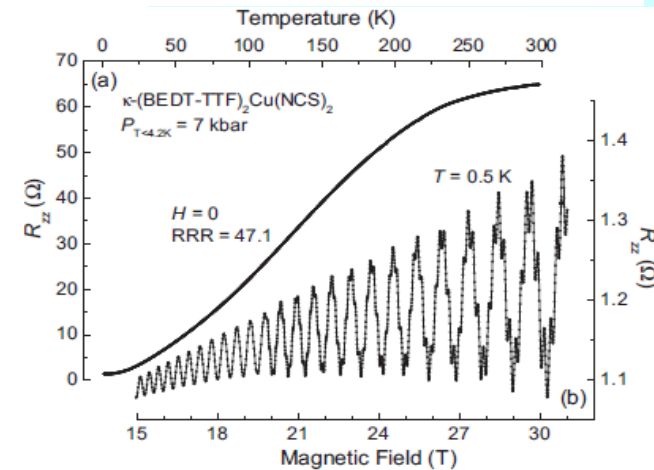
When $c_i \gg 1$, this simplifies to $\bar{\sigma}_{zz} \approx \frac{2\sigma_0 \Gamma_0}{\pi E_g \sqrt{c_i}} = \sigma_0 \sqrt{\frac{4\Gamma_0}{\pi \hbar \omega_c}} \approx \sigma_0 \sqrt{\frac{\Gamma_0}{\omega_c}} 1.13 \propto \sqrt{\frac{1}{B_z}}$

In the SC Born approximation $\bar{\sigma}_{zz} = \sigma_0 \sqrt{\frac{\Gamma_0}{\omega_c}} \frac{8}{3\sqrt{\pi}} \approx \sigma_0 \sqrt{\frac{\Gamma_0}{\omega_c}} 1.5 \approx \frac{\sigma_0 1.06}{\sqrt{\omega_c \tau_0}}$.

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background and MQO)



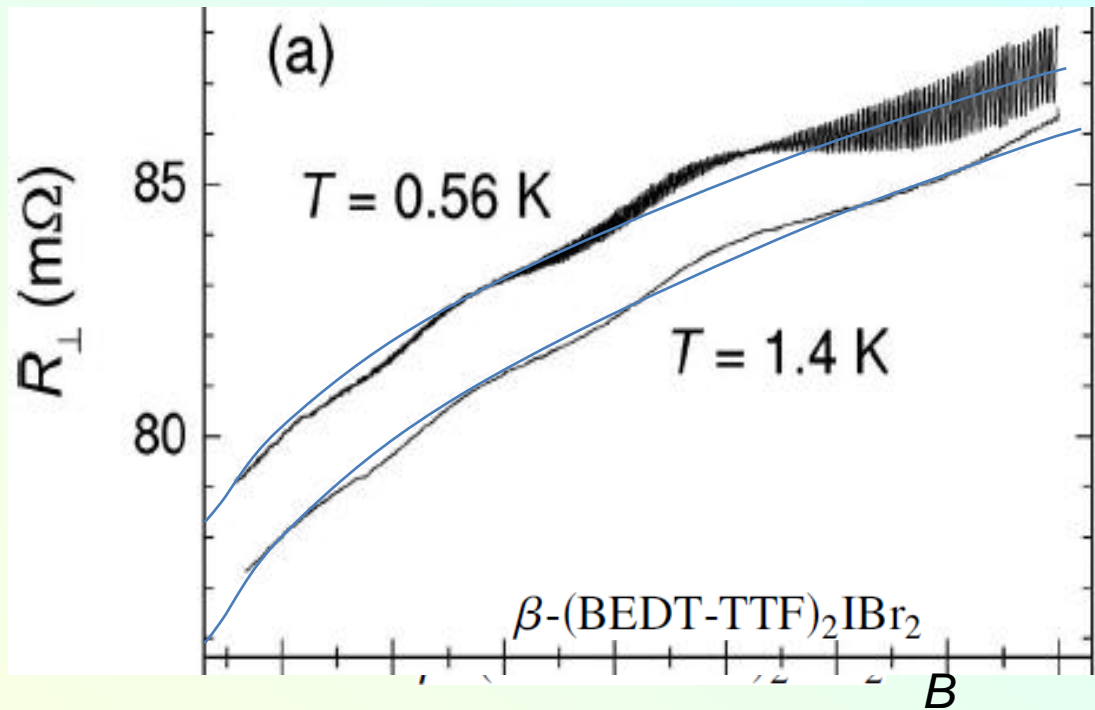
The temperature dependence of conductivity is metallic-type:



[W. Kang et al., PRB **80**, 155102 (2009)]

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background and MQO)

MR growth appears also at large $t_z \sim \Gamma$, as in β -(BEDT-TTF)₂IBr₂



PRL 89, 126802 (2002);

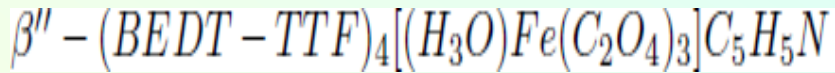
Plans for future:
study MR at $t_z \sim \Gamma$

! Beautiful effect: Both slow oscillations and background MR originate from MQO but survive at much higher T

Result 1

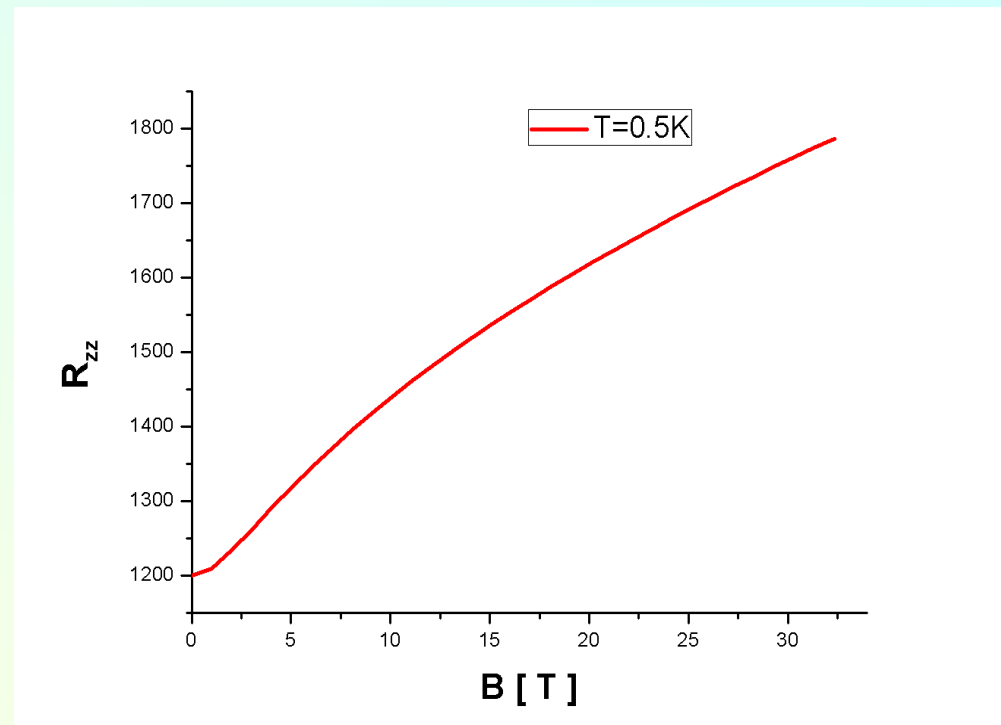
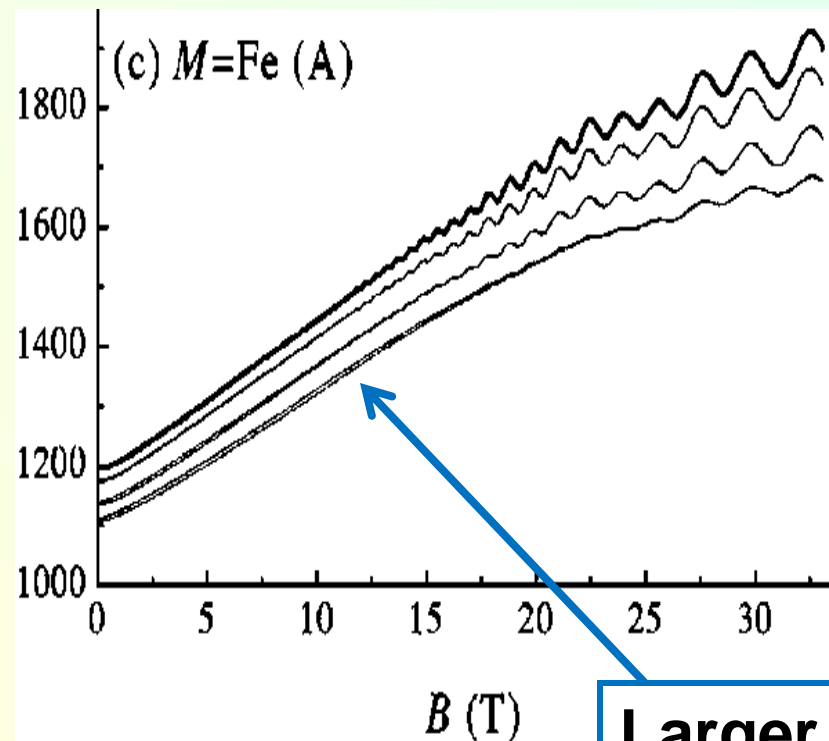
Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background and MQO)

measured field dependence of
magnetoresistance in



A.I. Coldea et al., PRB **69**, 085112 (2004)

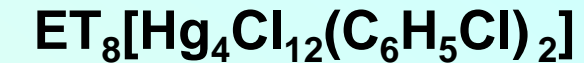
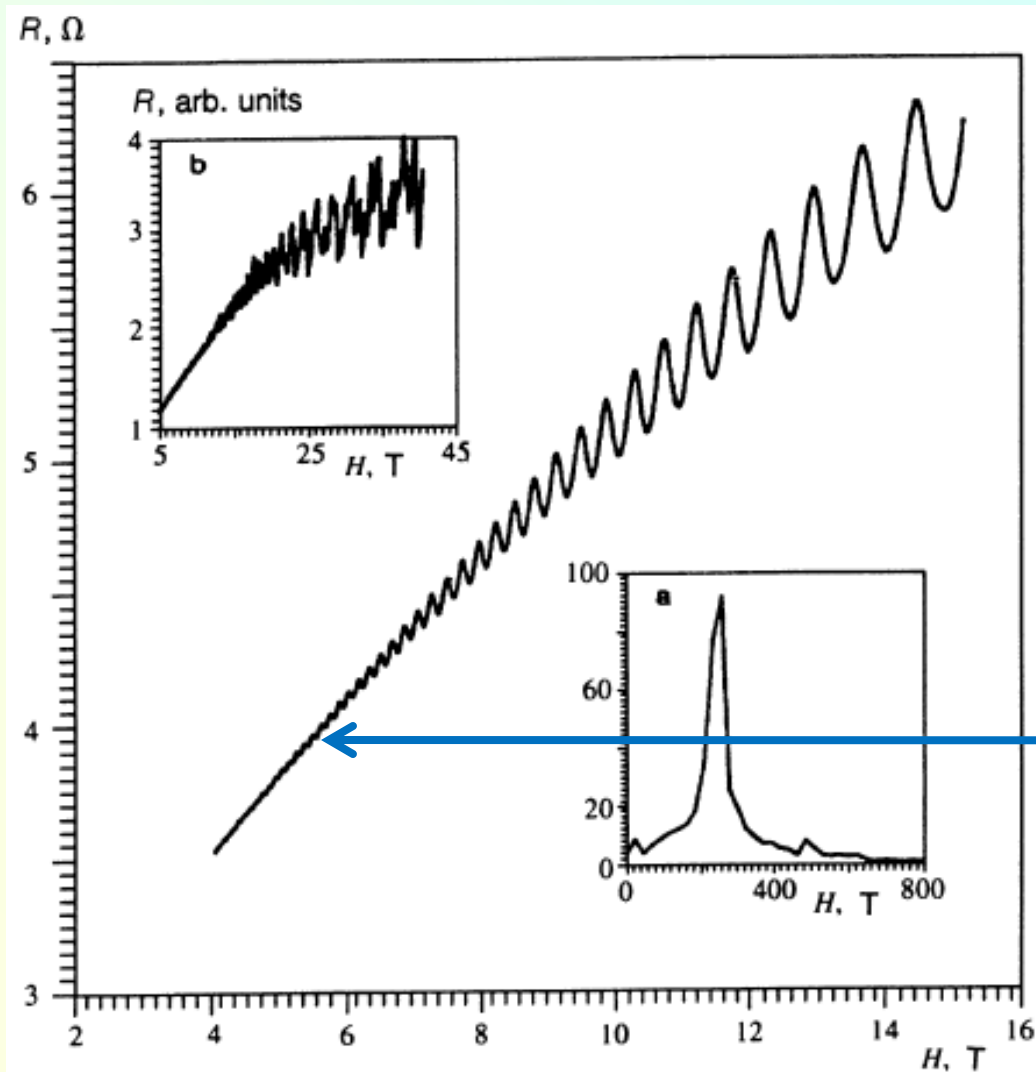
predicted field dependence
of non-oscillating part of
magnetoresistance



Larger $t_z \Rightarrow$ longer range of linear MR

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background and MQO)

Longitudinal MR crossover from linear to square-root at $t_z \sim \omega_c$

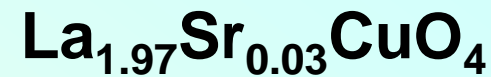
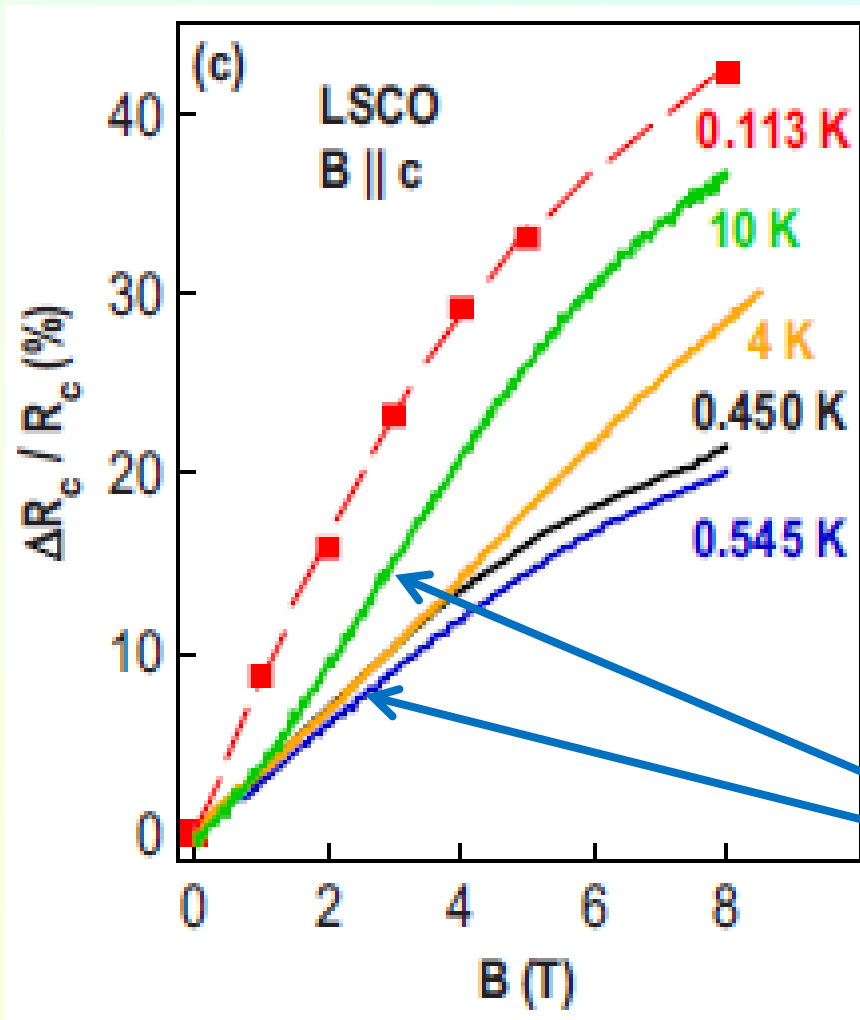


R.B. Lyubovskii, S.I. Pesotskii et al., JETP **80** (5), 946 (1995)

long range
of linear MR

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$ (magnetic field dependence: background resistance)

MR growth crossover from linear to square-root at $t_z \sim \omega_c$



I. Raičević, D. Popović et al.,
PRB 81, 235104 (2010)

linear MR transforms
to $B^{1/2}$ at higher field

Interlayer magnetoresistance in Fe-based high- T_c superconductors

Usually attributed to the field-induced spin-density wave (FISDW) state with partially gapped FS, but it is not correct because FISDW with $T_c > 100\text{K}$ require much stronger magnetic field

But it agrees with the proposed theory of longitudinal MR in quasi-2D metals

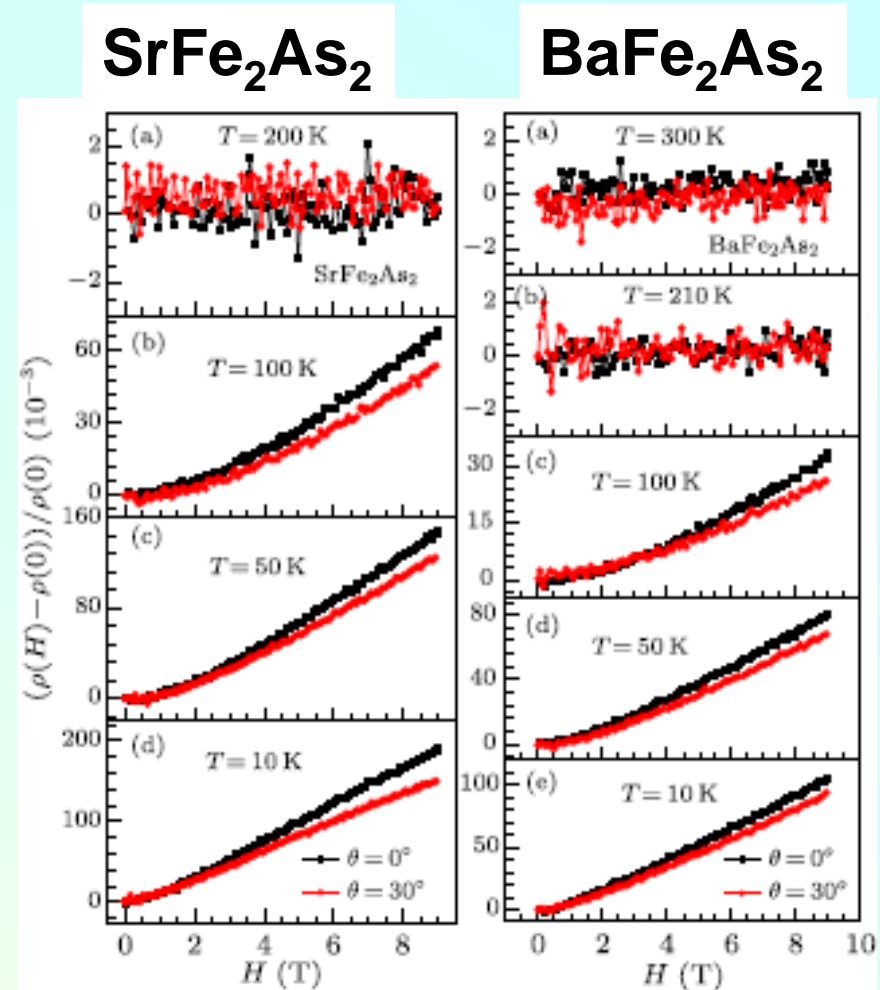


Fig. 2. Magnetoresistivity of SrFe_2As_2 (left): (a) $T = 200\text{ K}$, (b) $T = 100\text{ K}$, (c) $T = 50\text{ K}$, and (d) $T = 10\text{ K}$, and BaFe_2As_2 (right): (a) $T = 300\text{ K}$, (b) $T = 210\text{ K}$, (c) $T = 100\text{ K}$, (d) $T = 50\text{ K}$, and (e) $T = 10\text{ K}$ for the fields in the azimuths of $\theta = 0^\circ$ and 30° with respect to the c axis.

Chin. Phys. Lett. 26(10) 107401 (2009);
Chen G F, Li Z et al 2008 Phys. Rev. B 78 224512

**Two-layer theory, predicting
the square-root MR $R_{zz}(B_z)$,
is applicable at $t_z \ll \Gamma_0 \ll h\omega_c$**

What happens at larger t_z , or at smaller B_z ?

Damping of MQO for various LL shapes in 2D

The Dingle factor depends on the LL DoS $D(E)$ as

$$R_D(k) = \frac{\Gamma}{\pi} \int_{-\infty}^{\infty} \exp\left(\frac{2\pi i k E}{\hbar\omega_c}\right) |D(E)|^2 dE$$

Possible damping laws for MQO harmonics:

For Lorentzian LL shape and Γ independent of B one obtains standard Dingle factor: $R_{DL}(k) = \exp(-const \cdot k/B_z)$

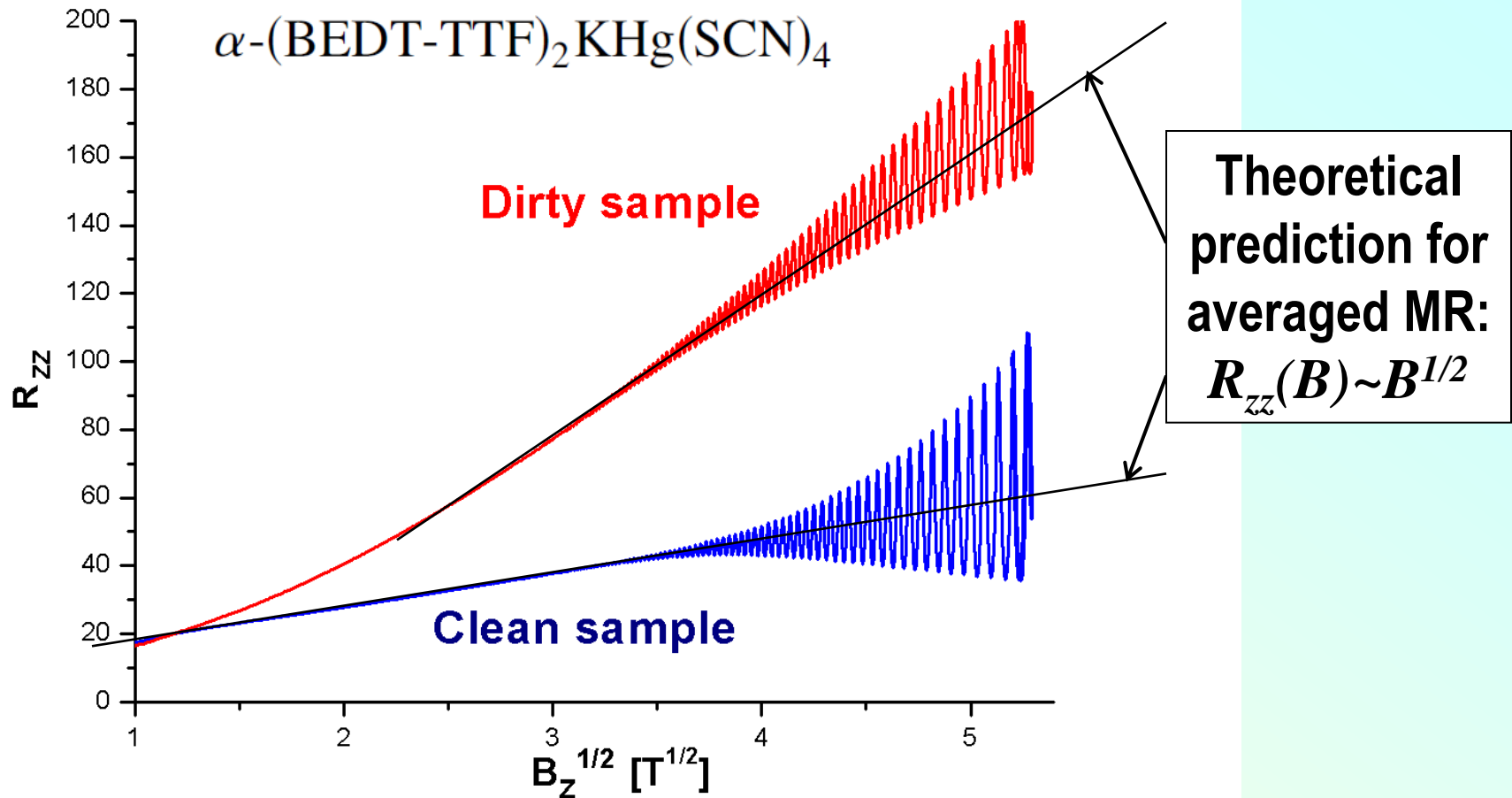
For Lorentzian LL shape and $\Gamma \sim B^{1/2}$ (as for short-range disorder in 2D): $R_{DL}^*(k) = \exp(-const \cdot k/\sqrt{B_z})$

For Gaussian LL shape and Γ independent of B (long-range disorder in 2D): $R_{DG}(k) = \sqrt{\pi/2} \exp[-const \cdot k^2/B_z^2]$

For Gaussian LL shape and $\Gamma \sim B^{1/2}$ (short-range disorder in 2D):

$$R_{DG}^*(k) = \sqrt{\pi/2} \exp[-const \cdot k^2/B_z]$$

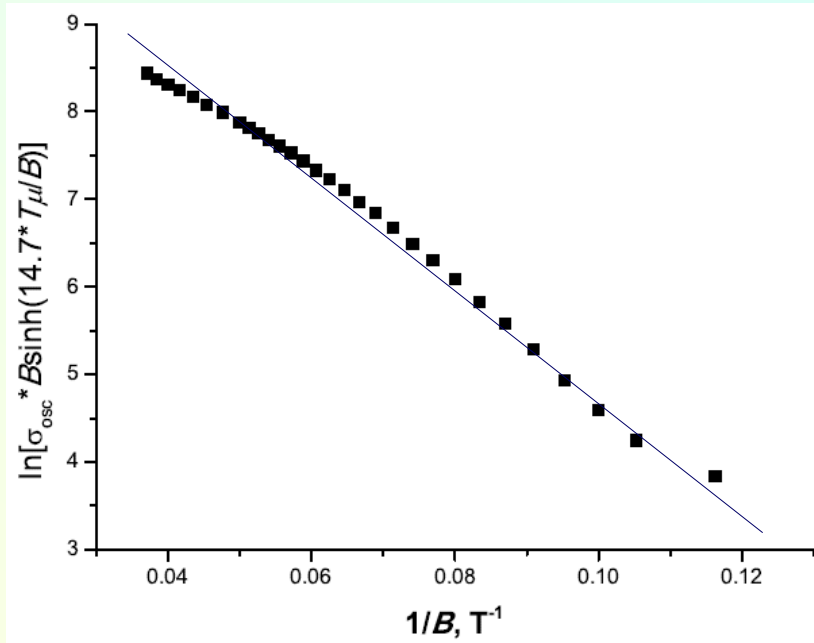
We take the same compound where there was excellent agreement on field-dependence of interlayer MR $R_{zz}(B)$



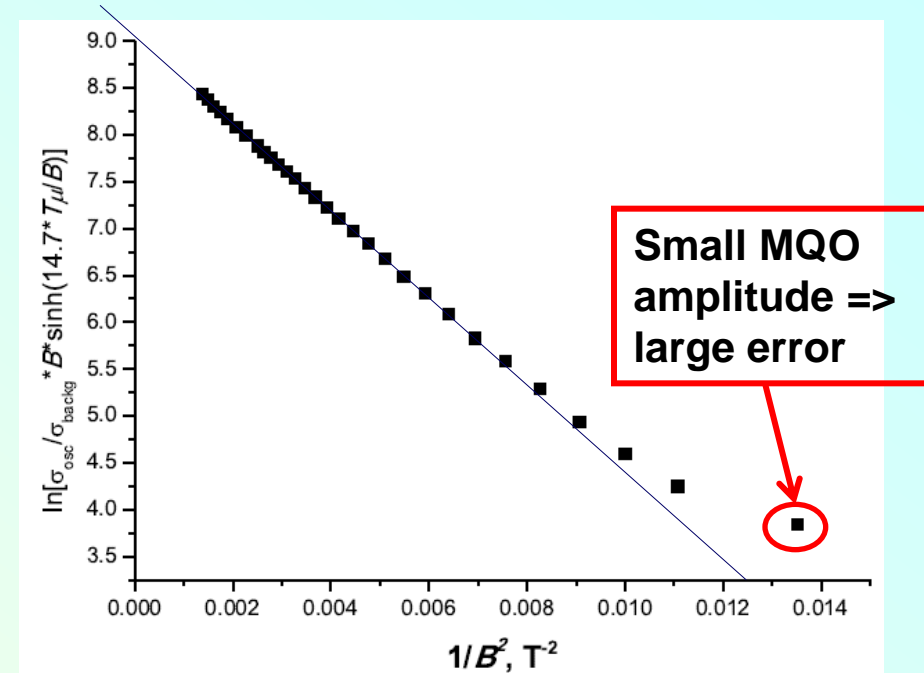
P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, PRB 86, 165125 (2012)

Result 2

Field-dependence of MQO amplitude in layered organic metal α -(BEDT-TTF)₂KHg(SCN)₄



The Dingle plot, i.e. the logarithm of the amplitude of the first harmonic of MQO divided by the temperature damping factor R_T , plotted as function of the inverse magnetic field $1/B$.

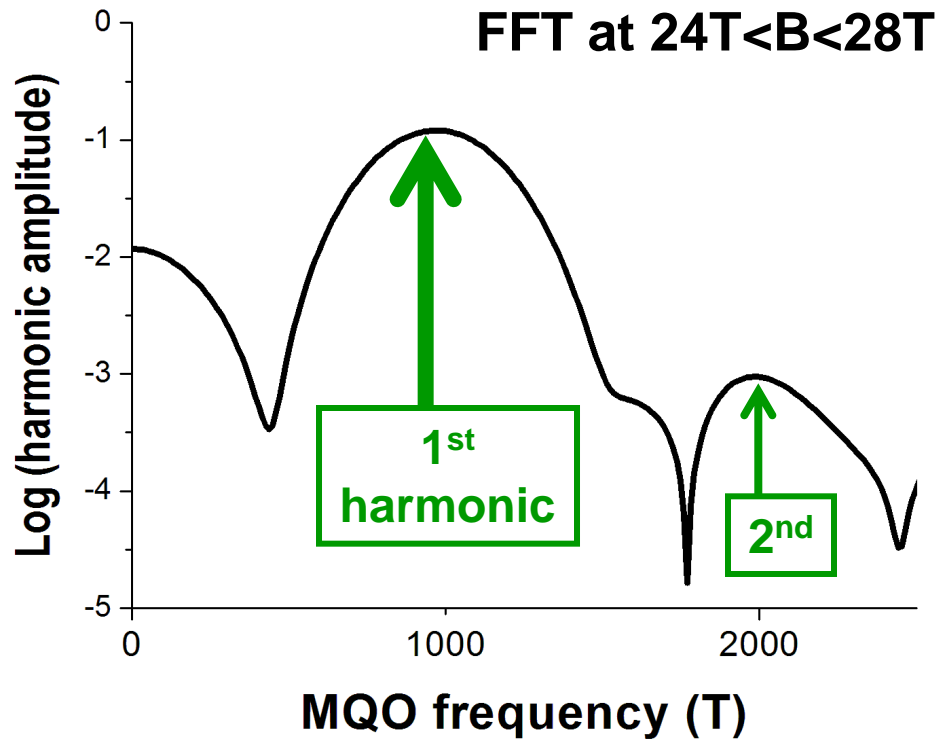


The modified Dingle plot: the logarithmic plot of the amplitude of the first harmonic of MQO divided by the temperature damping factor R_T as function of the inverse magnetic field squared $1/B^2$.

This corresponds to
Gaussian LL shape =>

$$R_{DG}(k) = \sqrt{\pi/2} \exp \left[-const \cdot k^2 / B_z^2 \right]$$

Damping of higher harmonics of MQO in α -(BEDT-TTF)₂KHg(SCN)₄



Calculation shows, that observed harmonic damping obeys that for Gaussian LL shape and Γ independent of B (long-range disorder in 2D)
[P.D. Grigoriev, M.V. Kartsovnik, W. Biberacher, arXiv:1205.0041]:

$$R_{DG}(k) = \sqrt{\pi/2} \exp \left[-const \cdot k^2 / B_z^2 \right]$$

This is in strong contrast to 3D Dingle law but agrees with 2D DoS !

P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, PRB 86, 165125 (2012)

Conclusions from comparison with experiment

1. In strongly anisotropic layered metals the standard 3D theory of MR is not valid. The new **quasi-2D weakly coherent** regime show up by appearance of strong longitudinal interlayer MR, originating from MQO but surviving at much higher temperature.
2. The electron dynamics in this regime is indeed closer to 2D than to 3D, as derived also from analysis of MQO, Dingle plot, harmonic damping and LL shape.
3. The main qualitative features of the proposed theory of MR in new weakly coherent regime (growth of MR, damping of MQO) agree with experiment.

The field-induced dimensional crossover of MR is proposed

Further work

Above analysis is only the first step in the theory of MR in layered metals

There is still much work to do:

second
part of
the talk

- ▼ 1. New accurate calculation of the angular dependence of MR
- ▼ 2. Change of angular dependence of harmonic amplitudes of MQO
- ▼ 3. The crossover 2D --> quasi-2D --> 3D ($t_z \sim \Gamma_0$)
- ▼ 4. Very high field, when the growth of $R_{zz}(B)$ is faster than $\sim B^{1/2}$.
- 5. The crossover weak --> strong magnetic field ($\omega_c \sim \Gamma_0$).
- 6. Influence of chemical potential oscillations and electron reservoir.
- 7. Quasi-1D anisotropic metals.

Probably, due to Coulomb anomaly in compounds with low electron density

▼ - currently studied by P.G. and (hopefully) solved in the simplest model

Conclusions

The standard 3D theory of magnetoresistance (MR) is not applicable to strongly anisotropic layered compounds.

In one-electron approach the reduction of dimensionality + magnetic field increase the effect of impurities, leading to strong longitudinal MR and changes in the Dingle plot and angular dependence of MR.

The e-e interaction may additionally suppress interlayer conductivity, leading to the magnetic-field dependent Coulomb blockade => strong magnetoresistance.

Thank you for attention!

Recent theoretical predictions for interlayer MR $R_{zz}(B)$

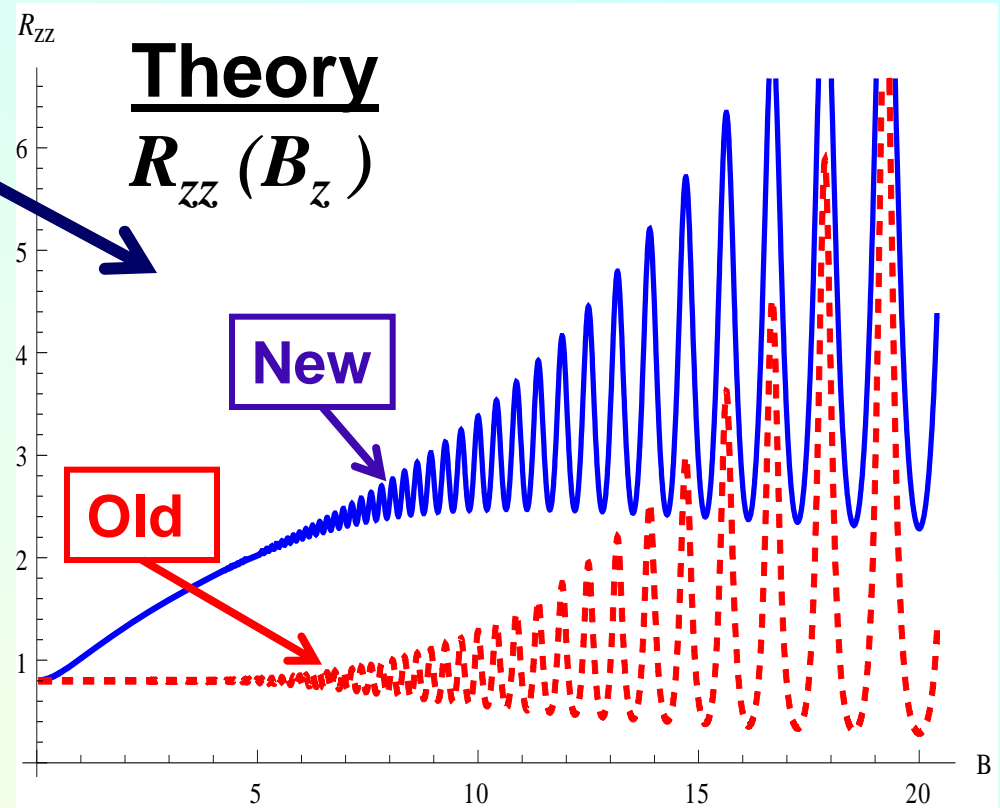
[1] P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011).

[2] P. D. Grigoriev, JETP Lett. 94, 48 (2011) [arXiv:1104.5122].

1. Longitudinal interlayer magnetoresistance (MR) grows with B_z at $\omega_c \tau > 1$: $R_{zz} \sim B_z^{1/2}$. It grows even if MQO are damped by T or by long-range disorder.

2. B_z -dependence of MQO amplitude changes. The Dingle low $R_D = \exp(-B_0/B_z)$ is not valid (as in 2D case)

3. Angular dependence of MR changes: both the monotonic part and the amplitude of AMRO.



$$\bar{\sigma}_{zz}(B) \approx \sigma_0 \left[(2\omega_c \tau)^2 + 1 \right]^{-1/4}$$

The coefficient 2 slightly depends on the LL shape

Applicability of Kubo formula

If electronic states in the layers are localized, the discrete electron energy spectrum with level separation $\delta \sim \hbar^2/m\xi^2$ may violate the Kubo formula when $\delta > \sim T, \hbar/\tau, t_z$.

Localization length of 2D electrons in magnetic field [Bodo Huckestein, RMP 67, 357 (1995)]

$$\xi \sim R_c \exp(\pi^2 g_0^2)$$

where the

Larmor radius

$$R_c = \hbar k_F c / eB = k_F l_H^2 = (2N_{LL} + 1) / k_F,$$

and dimensionless
conductivity

$$g_0 = (h/e^2) \sigma_{xx} \approx (2N_{LL} + 1) / \pi$$

Hence the localization length $\xi \sim R_c \exp\{(2N_{LL} + 1)^2\}$

where N_{LL} is the number of filled Landau levels; usually $N_{LL} \gg 1$.

In organic metals for highest available fields $N_{LL} > 10$ (usually $N_{LL} \sim 100$)

No electron localization at $N_{LL} \gg 1$ and Kubo formula works!

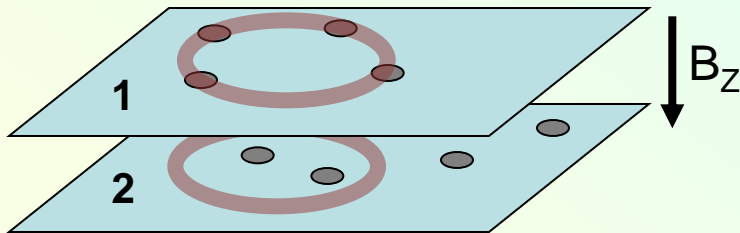
Because $T, \hbar/\tau, t_z \gg [\omega_c / (2N_{LL} + 1)] \exp[-(2N_{LL} + 1)^2]$!

Physical reason for the increase of interlayer resistivity in high magnetic field

Rough explanation: low dimensionality + strong magnetic field enhance the effective interaction with impurities and the mean scattering rate $1/\tau$
=> increase of resistivity according to

$$\sigma_{zz} \approx e^2 \tau \left\langle v_z^2 \right\rangle_{FS} \rho(E_F)$$

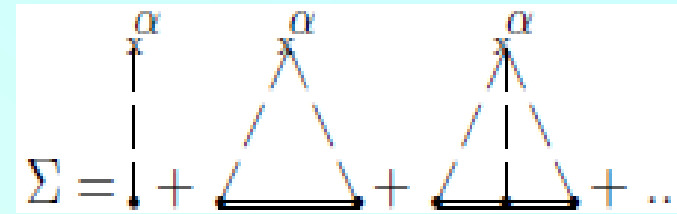
Another explanation:



The impurity distributions on adjacent layers are different. When an electron tunnels between two layers, its in-plane wave function does not change, but the energy shift due to impurities differs by the LL width $\Gamma_W \approx (\Gamma_0 \omega_C)^{1/2} \sim B_Z^{1/2}$

Why $\Gamma_W \sim B_Z^{1/2}$? Because the area where $\Psi_e \neq 0$, approximately, $S \sim 1/B_Z$, and the number of effectively interacting with the electron impurities $c_i \approx SN_i \sim 1/B_Z$ fluctuates as $c_i^{1/2} \sim B_Z^{-1/2}$, => the average shift of electron energy due to impurities $W = SN_i V_0$ fluctuates as $W/c_i^{1/2} \sim (SN_i)^{1/2} V_0 \sim B_Z^{1/2}$.

To calculate the in-plane Green's function one can use the non-crossing approximation with short-range impurity scattering.



Just Born approximation gives qualitatively wrong result (no B_z dependence of R_{zz}).
Self-consistent Born approximation is much better and only gives a wrong factor ~ 1 .

Why the non-crossing approximation is applicable?

Why only the short-range impurities are included?

In 2D in magnetic field the center of electron Larmor orbit drifts along the equipotential lines of long-range disorder (hills and valleys). This gives QHE, mobility edges, etc.

In quasi-2D metals the long-time 2D electron dynamics is cut-off by the new time scale of interlayer electron hopping \hbar/t_z , therefore the QHE has not been observed in layered quasi-2D compounds

Motivation

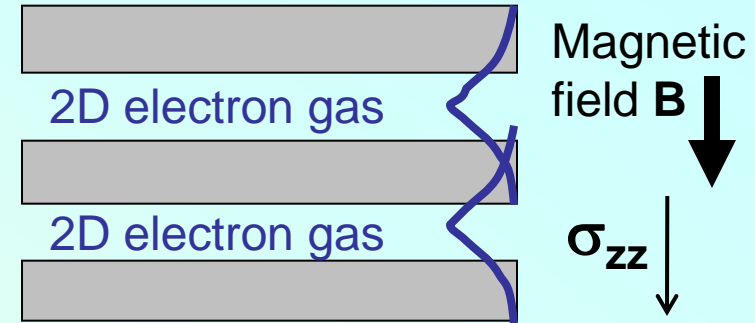
Is inelastic scattering time necessary for this calculation?

As we restrict to only two layers, without coherent tunneling to next layer, do we need the condition $\tau_\phi < \tau_h$?

The Hamiltonian of the model contains 3 terms:

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

1
3
2



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

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

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

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

2. The short-range impurity potential:

$$\hat{H}_I = \sum_i V_i(r) \quad \text{where} \quad V_i(r) = U \delta^3(r - r_i)$$

AMRO do not require 3D Fermi surface, but only a coherent (momentum conserving) interlayer tunneling

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

with 2D free electrons in magnetic field summed over all layers:

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

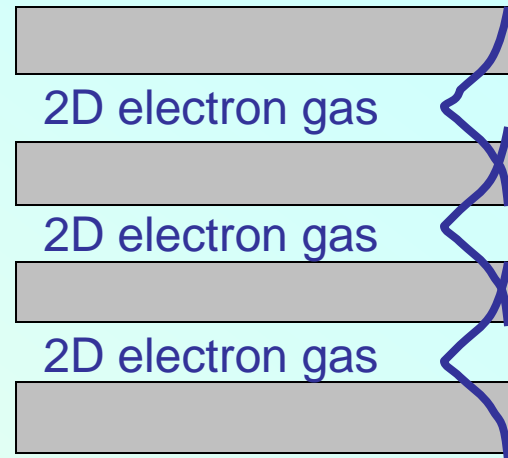
and the coherent electron tunneling between any two adjacent layers:

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

gives AMRO due to the overlap of electron wave functions, because they shift in tilted magnetic field for different layers j :

$$\Psi_{n,k_y,j}(x, y) = \Psi_n(x - l_{Hz}^2 [k_y + jd/l_{Hx}^2]) e^{ik_y y}$$

where magnetic length $l_{H\alpha} = \sqrt{\hbar c / e H_\alpha}$



[Y. Kurihara,
J. Phys. Soc. Jpn.
61, 975 (1992)]

Landau level broadening in 2D case depends on the range of impurities

For a white-noise or Gaussian correlator of the impurity potential $U(\mathbf{r})$:

$$Q(\mathbf{r}) \equiv \langle U(\mathbf{0}) U(\mathbf{r}) \rangle \propto \exp(-r^2/2d^2)$$

one obtains dome-like (“non-crossing” approx.) and **Gaussian** LL shape (in better approx.):

$$D(\varepsilon) = \frac{\exp(-\varepsilon^2/2\Gamma_N^2)}{2\pi l_H^2 \sqrt{2\pi}\Gamma_N}$$

with the LL width:

$$\begin{aligned} \Gamma_N^2 &= \int Q_{\mathbf{k}} \exp\left(-\frac{k^2 l_H^2}{2}\right) \left[L_N\left(\frac{k^2 l_H^2}{2}\right) \right]^2 \frac{d^2 k}{(2\pi)^2} \\ &= \int Q(\mathbf{r}) \exp\left(-\frac{r^2}{2l_H^2}\right) \left[L_N\left(\frac{r^2}{2l_H^2}\right) \right]^2 \frac{d^2 r}{2\pi l_H^2}, \end{aligned}$$

and L_N is a Laguerre polynomial

For a long-range impurity potential, when $d \ll l_H$, the LL width Γ is independent of B (but may depend on LL number N), while for short-range disorder in strong field $\omega_c \tau \gg 1$ the LL width $\Gamma \propto \sqrt{B}$ as in the “non-crossing” approximation.

Landau level shape in 2D

The LL shape in 2D depends on theoretical model

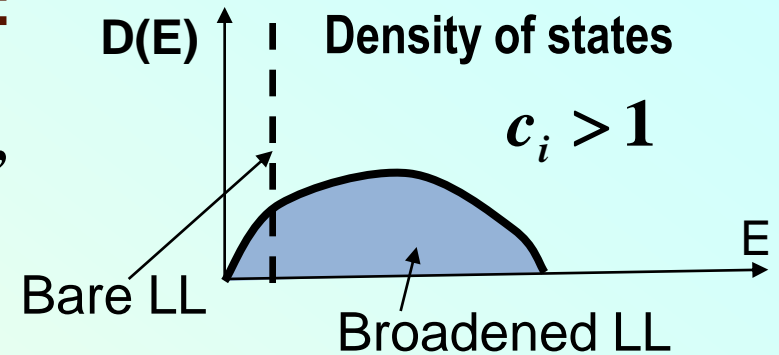
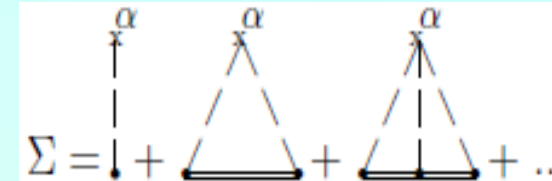
For point-like impurities in the “non-crossing” approximation gives **dome-like LL** shape

[Tsuneo Ando, J. Phys. Soc. Jpn. 36, 1521 (1974)]:

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

Landau level width

$$\Gamma_B \equiv (E_2 - E_1)/2 = 2E_g \sqrt{c_i} \propto \sqrt{B}.$$



For a white-noise or Gaussian correlator of the impurity potential $U(\mathbf{r})$:

$$Q(\mathbf{r}) \equiv \langle U(\mathbf{0}) U(\mathbf{r}) \rangle \propto \exp(-r^2/2d^2)$$

one obtains **Gaussian** shape of the Landau levels [see review in

I.V. Kukushkin, S.V. Meshkov and V.B. Timifeev, Sov.Phys. Usp. 31, 511 (1988).]

Any case, in 2D the LL shape is not Lorentzian !

Why result of [E. Brezin, D.I. Gross, C. Itzykson. Nucl. Phys. B 235, 24 (1984)] is applicable only for lowest LL

The lowest Landau level is spanned by the orthogonal set of functions [3]

$$u_{0,m}(r) = (2^{m+1}\pi m!)^{-1/2} \kappa^{m+1} (x + iy)^m \exp\left(-\frac{1}{4}\kappa^2(x^2 + y^2)\right), \quad (m = 0, 1, \dots), \quad (6a)$$

$$\kappa^2 \equiv \frac{eB}{\hbar}. \quad (6b)$$

Introducing the complex variable $z = x + iy$, one can thus express the condition that a state $\varphi(\mathbf{r})$ belongs to the $n = 0$ subspace (i.e. is an arbitrary square-integrable linear combination of the $u_{0,m}$) as the condition

$$\varphi(x, y) = e^{-\frac{1}{4}\kappa^2|z|^2} u(z), \quad (7)$$

in which $u(z)$ is an holomorphic function [4], namely

$$\frac{\partial}{\partial z^*} u(z) = 0, \quad (8)$$

Summary (part I)

A dimensional crossover and the new regime of electron transport in layered metals is proposed, when the interlayer tunneling time is longer than the cyclotron period. In this regime the effect of impurities is much stronger than in standard 3D theory. This qualitatively changes the angular and field dependence of magnetoresistance:

- 1. The background interlayer MR grows $\sim B^{1/2}$ with increasing field $B \parallel \sigma$.**
- 2. The Dingle temperature grows $\sim B^{1/2}$ + contains the terms from long-range disorder. This leads to the stronger damping of MQO.**
- 3. The angular dependence of MR changes: additional $(\cos\theta)^{-1/2}$ factor appears and the AMRO are weaker.**

The predictions of new theory nicely agree with experiment

Publications:

[1] P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011).

[2] P. D. Grigoriev, JETP Lett. 94, 48 (2011) [arXiv:1104.5122].

[3] P.D. Grigoriev, Low Temp. Phys./Fiz. Nizk. Temp. 37, 738 (2011).

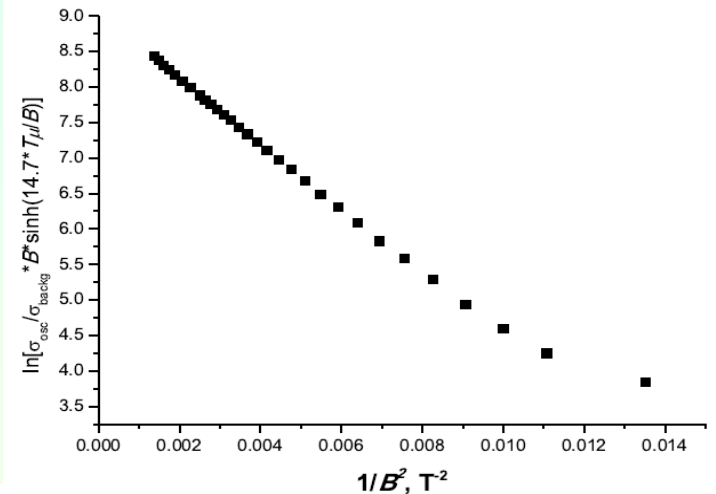
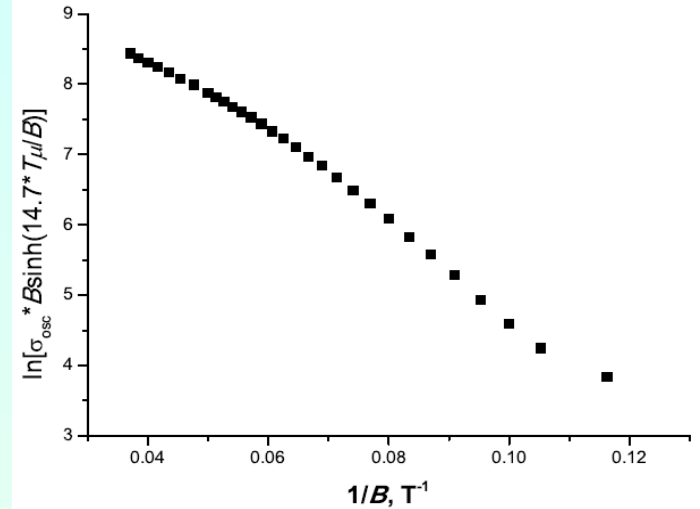
[4] P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, PRB 86, 165125 (2012)

Details of the analysis of harmonic damping

For the Lorentzian LL shape with field-independent $\Gamma \approx 11K$ one obtains from Eq. (9) at $B_a = 22T$ the Dingle factors $R_{DL}(1) \approx 0.017$ and $R_{DL}(2) \approx 0.00028$. The predicted harmonic amplitudes for the Lorentzian LL shape are $A_{1t} = R_{DL}(1) R_T(1) R_{s1} \approx 0.017 * 0.64 * 0.852 = 0.0093$ and $A_{2t} = R_{DL}(2) R_T(2) R_{s2} \approx 0.00028 * 0.22 * 0.453 = 0.000028$, which by orders of magnitude differs from the experimental values $A_{1ex} \approx 0.3$ and $A_{2ex} \approx 0.002$. The smaller value $\Gamma \approx 7K$ obtained for Gaussian LL shape gives the Dingle factors $R_{DL}(1) \approx 0.074$ and $R_{DL}(2) \approx 0.0055$, and the harmonic amplitude $A_{1t} = R_{DL}(1) R_T(1) R_{s1} \approx 0.074 * 0.64 * 0.852 = 0.04$ and $A_{2t} = R_{DL}(2) R_T(2) R_{s2} \approx 0.0055 * 0.22 * 0.453 = 0.0005$, which still very strongly differs from the experimental data. Thus the observed harmonic damping cannot be explained by the traditional 3D Dingle factor, corresponding to the Lorentzian LL shape.

For the Gaussian LL shape with field-independent $\Gamma \approx 7K$ one obtains from Eq. (12) at $B_a = 22T$ the Dingle factors $R_{DG}(1) \approx 0.45$ and $R_{DG}(2) \approx 0.02$. Then the calculated harmonic amplitudes for the Gaussian LL shape are $A_{1t} = R_{DG}(1) R_T(1) R_{s1} \approx 0.45 * 0.64 * 0.852 = 0.25$ and $A_{2t} = R_{DG}(2) R_T(2) R_{s2} \approx 0.02 * 0.22 * 0.453 = 0.002$, which nicely agrees the experimental values $A_{1ex} \approx 0.3$ and $A_{2ex} \approx 0.002$. This analysis gives additional

$$R_{DL}(k) = \exp(-2\pi k\Gamma/\hbar\omega_c)$$



$$R_{DG}(k) = \sqrt{\pi/2} \exp\left[-(\pi k\Gamma/\hbar\omega_c)^2 / 2\right]$$

Green's function (coherent limit)

If the energy levels ε_m and wave functions Ψ_m of quantum states m are known, the Green's function writes down as

$$G_R^0(r_1, r_2, \varepsilon) = \sum_m \frac{\Psi_m^{0*}(r_2) \Psi_m^0(r_1)}{\varepsilon - \varepsilon_m - i0}$$

One cannot find exactly the electron energy levels and Green's functions of macroscopic system with impurity scattering.

Therefore, one applies the perturbation theory, with averaging over disorder. Then, in the Born approximation, impurity scattering leads to the energy-dependent imaginary part of electron self energy.

Green's function in quasi-2D metals (coherent limit)

$$G_R^0(r_1, r_2, j, \varepsilon) = \sum_{n, k_y, k_z} \frac{\Psi_{n, k_y, j}^{0*}(x_2, y_2) \Psi_{n, k_y, j}^0(x_1, y_1) e^{ik_z(z_1 - z_2)}}{\varepsilon - \varepsilon_{2D}(n, k_y) + 2t_z \cos(k_z d) - i\Gamma(\varepsilon, B)}$$

impurity effect

where Ψ^0 – are the wave functions of 2D electrons in magnetic field, and the level broadening Γ oscillates as function of energy ε and magnetic field around the field-independent value $\Gamma_0 \approx \hbar/2\tau$, being proportional to the density of states.

Incorrect in the weakly incoherent limit

Applicability of Kubo formula

If electronic states in the layers are localized, the discrete electron energy spectrum with level separation $\delta \sim \hbar^2/m\xi^2$ may violate the Kubo formula when $\delta > \sim T, \hbar/\tau, t_z$.

Localization length of 2D electrons in magnetic field [Bodo Huckestein, RMP 67, 357 (1995)]

$$\xi \sim R_c \exp(\pi^2 g_0^2)$$

where the

Larmor radius

$$R_c = \hbar k_F c / eB = k_F l_H^2 = (2N_{LL} + 1) / k_F,$$

and dimensionless conductivity

$$g_0 = (h/e^2) \sigma_{xx} \approx (2N_{LL} + 1) / \pi$$

Hence the localization length $\xi \sim R_c \exp\{(2N_{LL} + 1)^2\}$

where N_{LL} is the number of filled Landau levels; usually $N_{LL} \gg 1$.

In organic metals for highest available fields $N_{LL} > 10$ (usually $N_{LL} \sim 100$)

No electron localization at $N_{LL} \gg 1$ and Kubo formula works!

Because $T, \hbar/\tau, t_z \gg [\omega_c / (2N_{LL} + 1)] \exp[-(2N_{LL} + 1)^2]$!

Landau level broadening in 2D case depends on the range of impurities

For a white-noise or Gaussian correlator of the impurity potential $U(\mathbf{r})$:

$$Q(\mathbf{r}) \equiv \langle U(\mathbf{0}) U(\mathbf{r}) \rangle \propto \exp(-r^2/2d^2)$$

one obtains dome-like (“non-crossing” approx.) and **Gaussian** LL shape (in better approx.):

$$D(\varepsilon) = \frac{\exp(-\varepsilon^2/2\Gamma_N^2)}{2\pi l_H^2 \sqrt{2\pi}\Gamma_N}$$

with the LL width:

$$\begin{aligned} \Gamma_N^2 &= \int Q_{\mathbf{k}} \exp\left(-\frac{k^2 l_H^2}{2}\right) \left[L_N\left(\frac{k^2 l_H^2}{2}\right) \right]^2 \frac{d^2 k}{(2\pi)^2} \\ &= \int Q(\mathbf{r}) \exp\left(-\frac{r^2}{2l_H^2}\right) \left[L_N\left(\frac{r^2}{2l_H^2}\right) \right]^2 \frac{d^2 r}{2\pi l_H^2}, \end{aligned}$$

and L_N is a Laguerre polynomial

For a long-range impurity potential, when $d \ll l_H$, the LL width Γ is independent of B (but may depend on LL number N), while for short-range disorder in strong field $\omega_c \tau \gg 1$ the LL width $\Gamma \propto \sqrt{B}$ as in the “non-crossing” approximation.

The exactly solvable models, applicable to the lowest LL, prove Gaussian LL shape

$$\rho(E) \underset{E \rightarrow \infty}{\simeq} \sqrt{\frac{2}{w}} \frac{\kappa}{\pi^2} \pi \nu^2 e^{-\nu^2} \left(1 + O\left(\frac{1}{\nu^2}\right) \right), \quad \text{where} \quad \nu = \sqrt{\frac{2\pi}{w\kappa^2}} \left(E - \frac{1}{2} \frac{\hbar e B}{m} \right)$$

[E. Brezin, D.I. Gross, C. Itzykson. Nucl. Phys. B 235, 24 (1984)]

$$\frac{D(E)}{n_L} = \begin{cases} 0, & E < 0, \\ \frac{1}{E_0} S_f \left(f \ln \frac{E_0}{E} \right), & 0 \leq \frac{E}{E_0} \ll e^{-1/f}, \\ \frac{f}{E}, & e^{-1/f} \ll \frac{E}{E_0} \ll 1, \\ \frac{2\pi^{-1/2} E^2}{(f_1 E_1^2)^{3/2}} \exp\left(-\frac{E^2}{f_1 E_1^2}\right), & E_0 \ll E, \end{cases}$$

where $f_1 = \frac{n_{\text{imp}} z_1}{n_L}$ $E_1 = \frac{n_L u_0}{z_1}$

I.S. Burmistrov, M.A. Skvortsov,
JETP Lett. 78, 156 (2003)

Result 2.

Magnetic quantum oscillations of conductivity in the weakly coherent regime

MQO of interlayer conductivity:

$$\sigma_{zz} = \sigma_0(B) \sum_{k=-\infty}^{\infty} (-1)^k \exp\left[\frac{2\pi(ik\mu)}{\omega_c}\right] \frac{2k\pi^2 T / \omega_c}{\sinh(2k\pi^2 T / \omega_c)} \left[1 + \frac{2\pi|k|\Gamma_B}{\omega_c}\right] R_D\left(\frac{|k|\Gamma_B}{\omega_c}\right).$$

background MR

$$\sigma_0(B) = \frac{e^2 t_z^2 v_F d}{\Gamma_B} \propto \frac{1}{\sqrt{B}},$$

where

$$\Gamma_B \approx \Gamma_0 \left[\left(\frac{4\omega_c}{\pi\Gamma_0} \right)^2 + 1 \right]^{1/4} + \Gamma_{LR} \propto \sqrt{B_z}.$$

Dingle factor

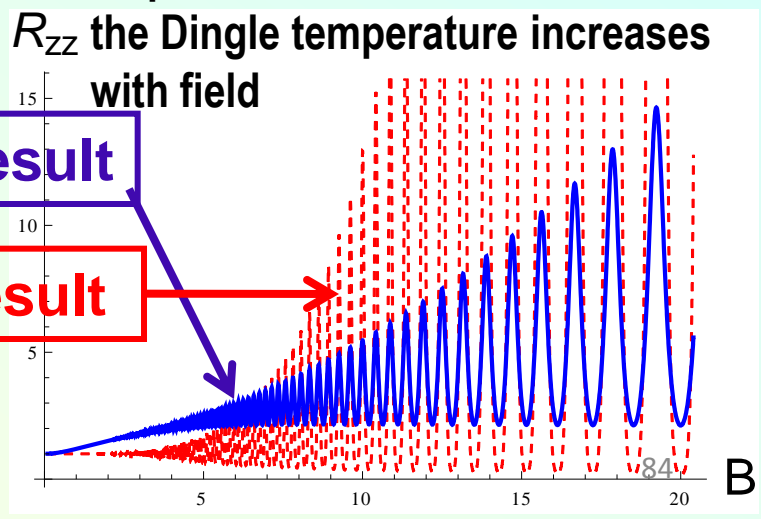
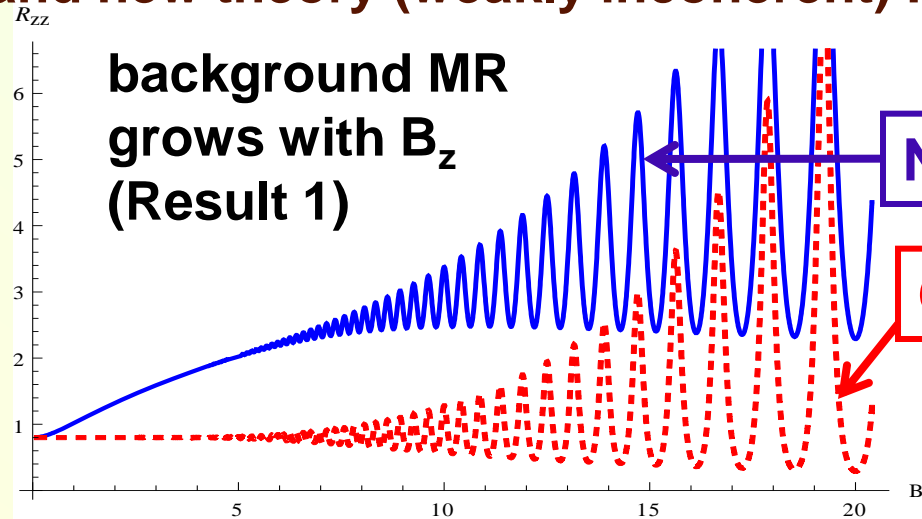
$$R_D(k) = \frac{\Gamma}{\pi} \int_{-\infty}^{\infty} \exp\left(\frac{2\pi ikE}{\hbar\omega_c}\right) |D(E)|^2 dE$$

and the Dingle factor depends on LL shape:

Comparison of the results on R_{zz} of standard theory (coherent regime) and new theory (weakly incoherent):

amplitude of MQO reduces because

the Dingle temperature increases with field



New result

Old result

Landau level shape and harmonic damping in 3D

In 3D the electron Green's function has the form

$$G_R^0(r_1, r_2, j, \varepsilon) = \sum_{n, k_y, k_z} \frac{\Psi_{n, k_y, j}^{0*}(x_2, y_2) \Psi_{n, k_y, j}^0(x_1, y_1) e^{ik_z(z_1 - z_2)}}{\varepsilon - \varepsilon_{3D}(n, k_y, k_z) - \Sigma_R(\varepsilon, B)},$$

impurity effect

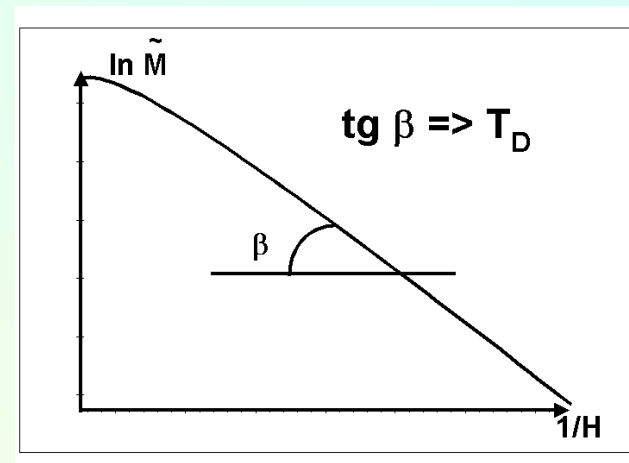
This corresponds to the Lorentzian shape of electron levels:

$$\text{Im } G_R(n, k_y, k_z, \varepsilon) = \frac{\text{Im } \Sigma_R(\varepsilon)}{[\varepsilon - \varepsilon(n, k_y, k_z) - \text{Re } \Sigma_R(\varepsilon)]^2 + [\text{Im } \Sigma_R(\varepsilon)]^2}$$

that gives exponential Dingle factor of MQO:

$$R_D(k, \varepsilon) = \exp\left(\frac{-2\pi k |\text{Im } \Sigma_R(\varepsilon)|}{\omega_c}\right).$$

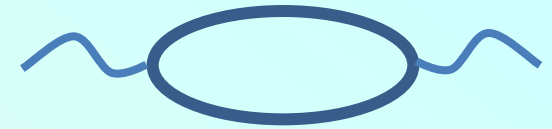
(k - harmonic number)



Calculation of conductivity in metals (standard theory, coherent 3D case)

Conductivity (the linear response to external electric field) is calculated from the Kubo formula:

$$\sigma_{zz} = \frac{e^2}{V} \sum_m v_z^2(m) \int \frac{d\varepsilon}{2\pi} [2 \operatorname{Im} G_R(m, \varepsilon)]^2 [-n'_F(\varepsilon)],$$



where $m=(n, k_y, k_z)$, the electron velocity $v_z(\varepsilon, n) = \partial\varepsilon / \partial k_z$, is determined by the 3D electron dispersion,

$G_R(m, \varepsilon)$ - retarded electron Green's function, where scattering by impurities is taken in the lowest order (Born approx.),

$$n'_F(\varepsilon) = -1 / \left\{ 4T \cosh^2 [(\varepsilon - \mu) / 2T] \right\}$$

- derivative of the Fermi distribution function.

Evaluation of the Kubo formula

We now substitute $\text{Im } G_R(m, \varepsilon) = \frac{\text{Im } \Sigma_R(\varepsilon)}{[\varepsilon - \varepsilon(m) - \text{Re } \Sigma_R(\varepsilon)]^2 + [\text{Im } \Sigma_R(\varepsilon)]^2}$

Change integration variable ($k_z \rightarrow \varepsilon'$):

$$\sigma_{ZZ} = e^2 N_{LL} \int \frac{d\varepsilon'}{2\pi} \sum_n |v_z(\varepsilon', n)| \int \frac{d\varepsilon}{2\pi} [2 \text{Im } G_R(\varepsilon', \varepsilon)]^2 [-n'_F(\varepsilon)]$$

where $v_z(\varepsilon, n) = \partial\varepsilon / \partial k_z = d \sqrt{4t^2 - [\varepsilon - \omega_c(n + 1/2)]^2}$

Applying Poisson summation formula after integrations we get

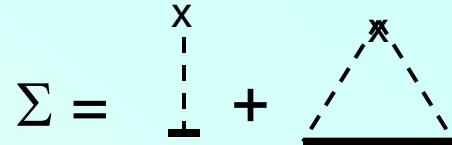
$$\sigma_{ZZ} = e^2 N_{LL} \int \frac{d\varepsilon}{2\pi} [-n'_F(\varepsilon)] \sum_{k=-\infty}^{\infty} (-1)^k \frac{2td^2}{k} J_1\left(\frac{4\pi k t}{\omega_c}\right) \times$$

$$\times \left(\frac{1}{|\text{Im } \Sigma_R(\varepsilon)|} + \frac{2\pi k}{\omega_c} \right) \exp\left(\frac{2\pi i k \varepsilon^*}{\omega_c}\right) R_D(k, \varepsilon),$$

where the Dingle factor $R_D(k, \varepsilon) = \exp\left(\frac{-2\pi k |\text{Im } \Sigma_R(\varepsilon)|}{\omega_c}\right)$.

Evaluation of the Kubo formula (2)

Scattering on point-like impurities in self-consistent Born approximation:



$$\Sigma^R(m, \epsilon) = \left\langle \sum_i U^2 G(r, r, \epsilon) \right\rangle = \Sigma^R(\epsilon) = C_i U^2 \int d^3 r G(r, r, \epsilon)$$

We assume the harmonic damping is strong and keep only first harmonics in the expression for conductivity:

$$\sigma_{ZZ} = \sigma_0 \int d\epsilon [-n'_F(\epsilon)] \times \left[\frac{1 - \frac{\omega_c}{\pi t} J_1\left(\frac{4\pi t}{\omega_c}\right) \cos\left(\frac{2\pi \epsilon^*}{\omega_c}\right) R_D(\epsilon)}{1 - 2J_0\left(\frac{4\pi t}{\omega_c}\right) \cos\left(\frac{2\pi \epsilon^*}{\omega_c}\right) R_D(\epsilon)} + \frac{2\pi k_B T_D}{t} J_1\left(\frac{4\pi t}{\omega_c}\right) \cos\left(\frac{2\pi \epsilon^*}{\omega_c}\right) R_D(\epsilon) \right]$$

This term cannot be obtained from the Boltzmann transport equation

Observable consequences

For $4\pi t \gg \hbar\omega_c$ the expression for conductivity simplifies:

$$\sigma_{ZZ} = \sigma_0 \left[1 + 2 \sqrt{\frac{\omega_c (1+a^2)}{2\pi^2 t}} \cos\left(\frac{2\pi \mu}{\omega_c}\right) \cos\left(\frac{4\pi t}{\omega_c} - \frac{\pi}{4} + \phi_b\right) R_D^{tot} R_T + \frac{\omega_c}{2\pi^2 t} R_D^2 \sqrt{1+a_s^2} \cos 2\left(\frac{4\pi t}{\omega_c} - \frac{\pi}{4} + \phi_s\right) \right],$$

Phase shift of beats

where the phase shift of beats

$$\phi_b = \arctan(a), \quad a = \frac{\omega_c}{2\pi t} \left(1 + \frac{\pi}{\omega_c \tau} \right)$$

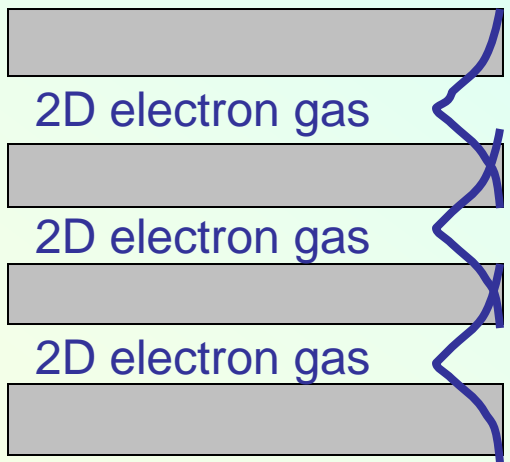
Slow oscillations

and

$$\phi_s = \arctan(a_s), \quad a_s = \omega_c / 2\pi t.$$

The temperature damping factor $R_T = \frac{2\pi^2 k_B T / \omega_c}{\sinh(2\pi^2 k_B T / \omega_c)}$

Coherent and incoherent interlayer electron transport



The coherent regime gives the well-defined 3D electron dispersion $\epsilon(p) = \epsilon_{||}(p_{||}) + 2t_z \cos(k_z d)$ and Fermi surface as a warped cylinder. It assumes $t_z \tau \gg \hbar$, where τ is the in-plane mean free time.

Theory of magnetoresistance in coherent regime is developed and works well.

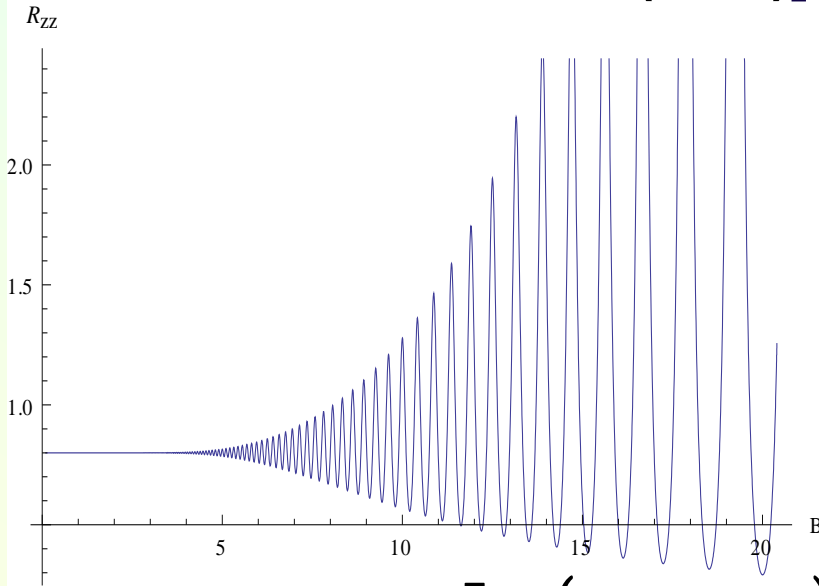
“Weakly incoherent” interlayer magnetotransport:

$p_{||}$ is conserved in interlayer tunneling, but the tunneling time is longer than the cyclotron and/or mean free times. The 3D FS and electron dispersion are smeared. Examples - all layered metals with small t_z in strong magnetic field: organic metals, heterostructures, high-Tc cuprates, pnictides, intercalated graphite.

Are the standard formulas for magnetoresistance applicable in this case? Does this regime contains new physics?

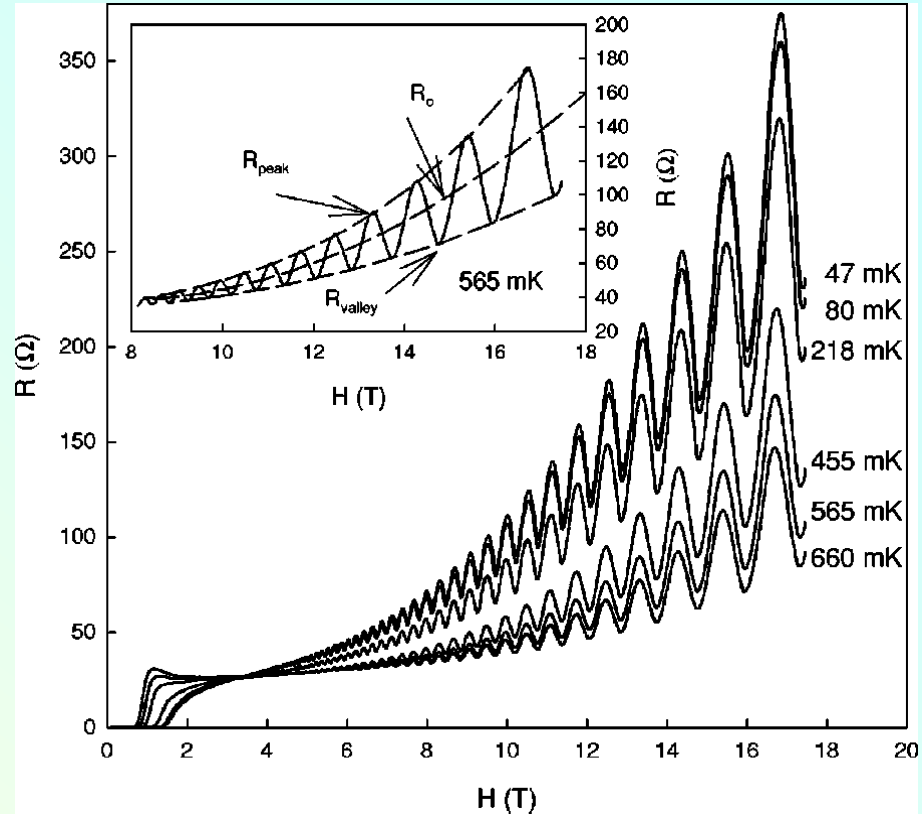
MQO in the weakly incoherent regime ($B_z || \sigma_{zz}$)

Theory [T. Champel and V. P. Mineev, PRB 66, 195111 (2002)]



$$\sigma_{zz} = \sigma_0 \sum_{k=-\infty}^{\infty} (-1)^k \exp\left[\frac{2\pi(ik\mu - |k|\Gamma_B)}{h\omega_c}\right] \times \frac{2k\pi^2 T / h\omega_c}{\sinh(2k\pi^2 T / h\omega_c)} \left[1 + \frac{2\pi|k|\Gamma_B}{h\omega_c}\right].$$

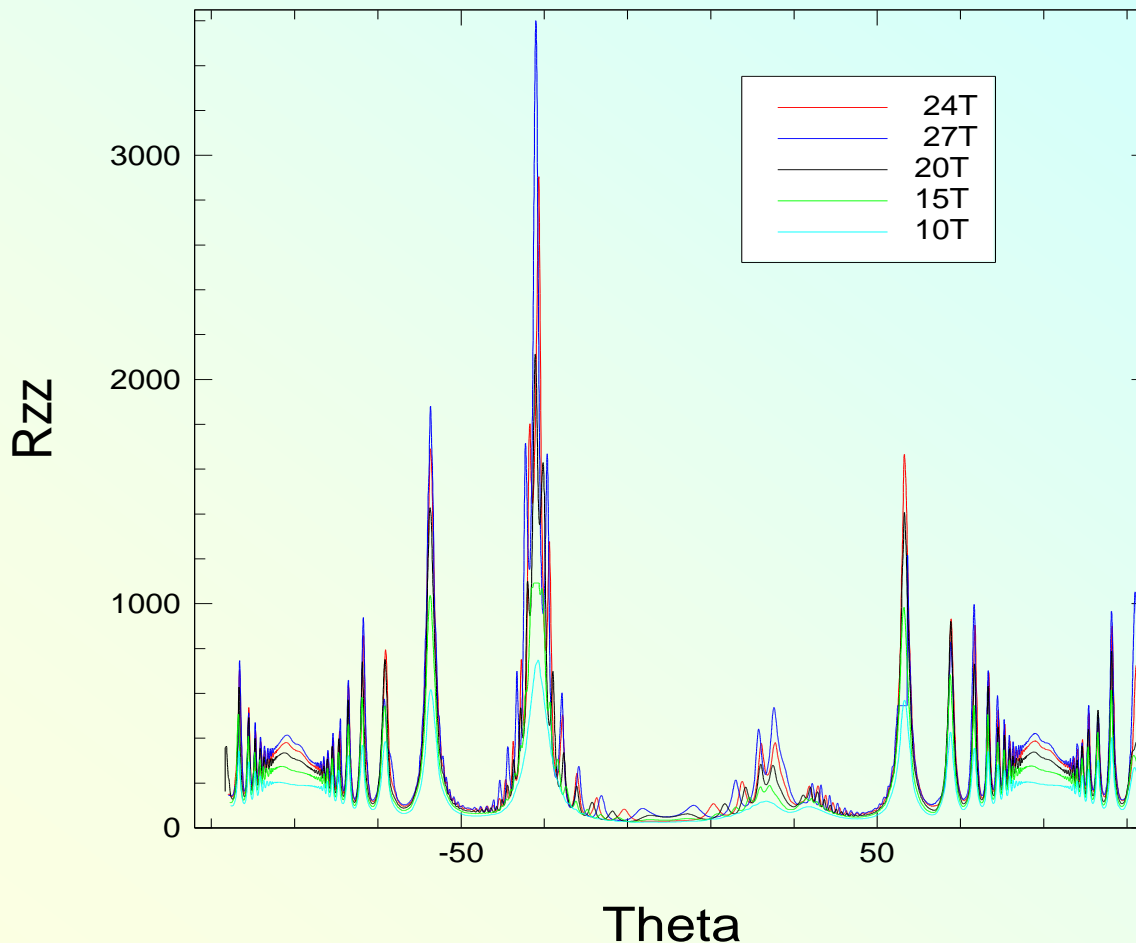
Experiment



β -(BEDT-TTF)₂SF₅CH₂CF₂SO₃
F. Zuo et al., PRB 60, 6296 (1999).

According to the 3D standard theory, in the minima of MQO the magnetoresistance decreases, while on experiment it increases.

Observed angular dependence of MR

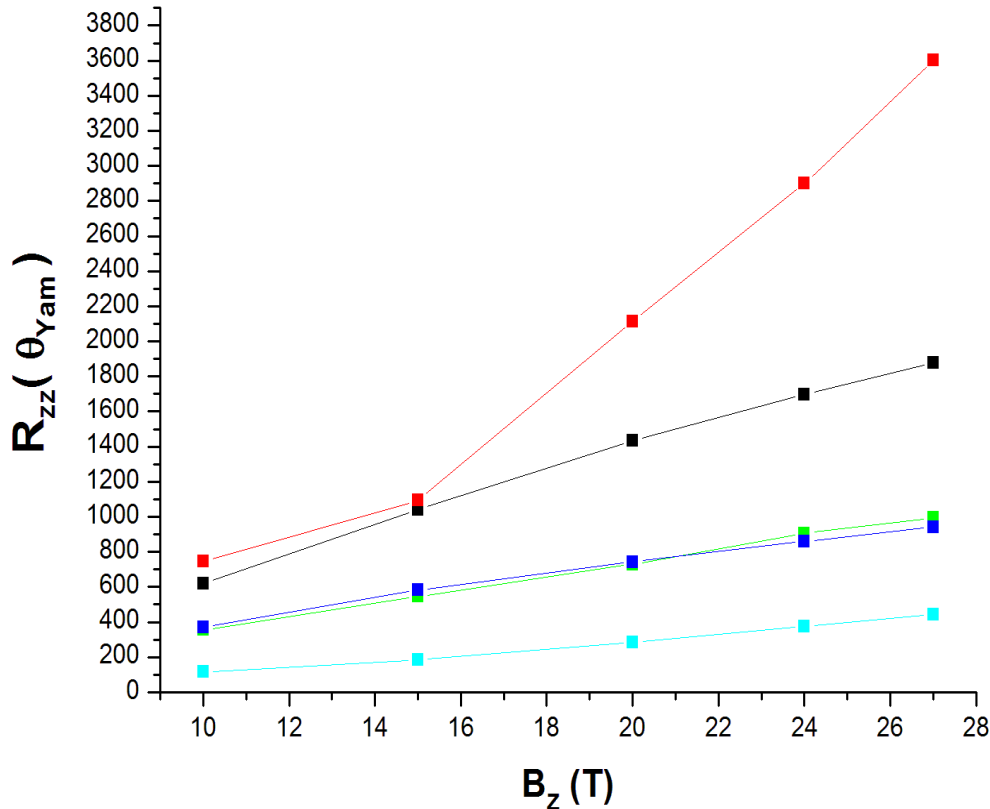


The positions of AMRO maxima coincide with Yamaji angle for given Fermi surface and triclinic symmetry.

The overlap with MQO gives noise to AMRO.

One can compare $R_{zz}(B)$ with theory in the AMRO maxima. The old theory predicts $R_{zz}(\theta_{Yam}, B) \sim B^2$

Magnetic field dependence of MR in the AMRO maxima (Yamaji angles)



Observed linear dependence $R_{zz}(\theta_{Yam}, B) \sim B$ contrary to the $R_{zz}(\theta_{Yam}, B) \sim B^2$ predicted by the old 3D-like theory

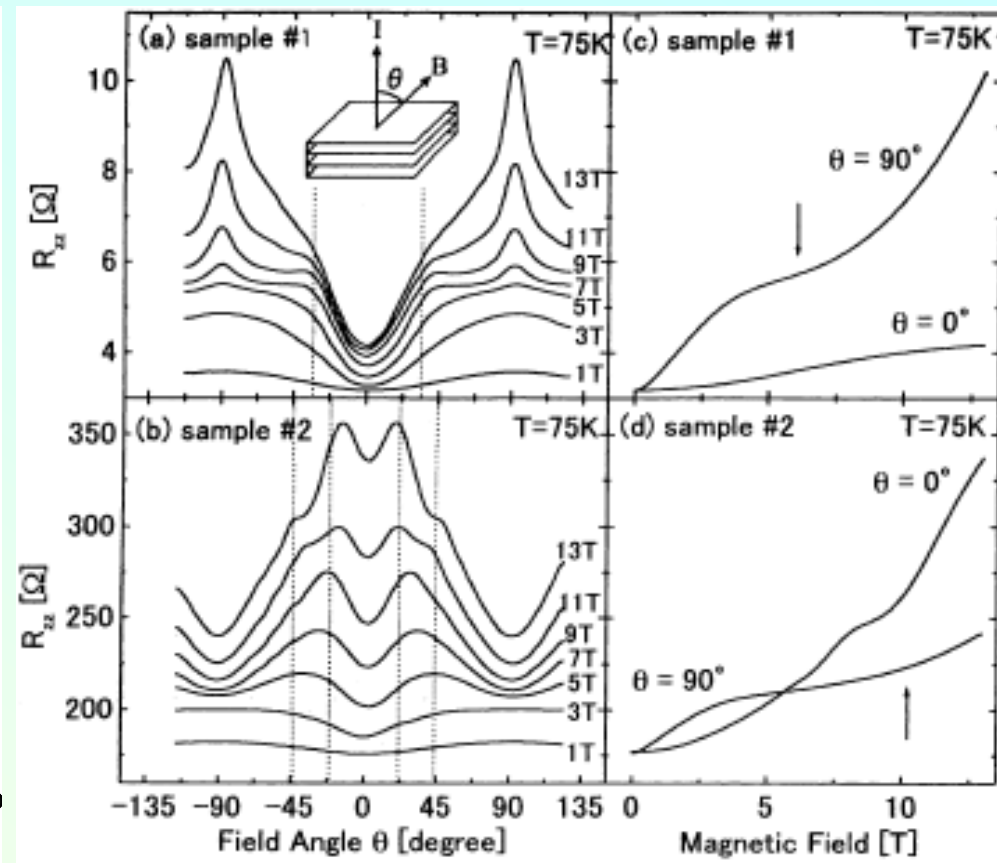
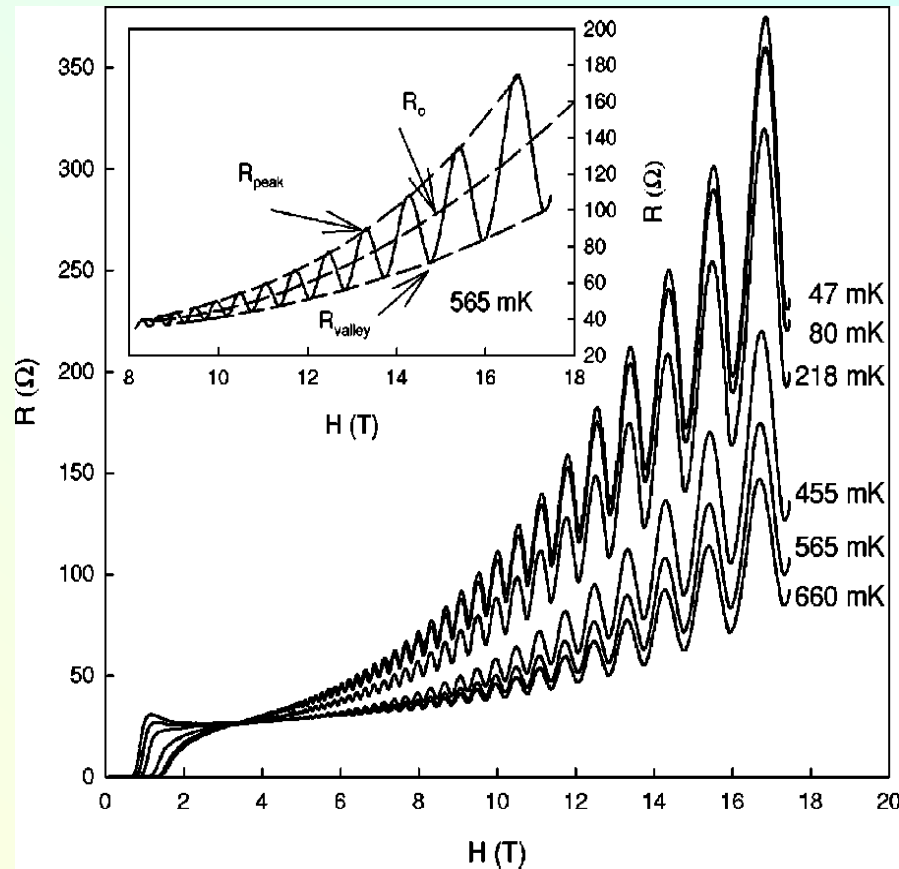
$$\frac{\sigma_z(B)}{\sigma_z(0)} = J_0^2(k_F d \tan \theta) + 2 \sum_{j=1}^{\infty} \frac{J_j^2(k_F d \tan \theta)}{1 + (j\omega_c \tau)^2}$$

suggest that it does not work

For Lorentzian LL shape and neglecting the quantum term the new weakly coherent theory predicts $R_{zz}(\theta_{Yam}, B) \sim B^{3/2}$, giving slightly better agreement, however other LL shapes may give different result.

More accurate calculation based on newly proposed weakly coherent model is planned for nearest future.

Interlayer MR at very strong magnetic field



F. Zuo et al., PRB 60, 6296 (1999).
 β -(BEDT-TTF) $_2$ SF $_5$ CH $_2$ CF $_2$ SO $_3$

GaAs M. Kuraguchi et al.,
 Synth. Met. 133-134, 113 (2003)

Sometimes, MR grows too strongly with increasing B_z !

Summary

- Applying the method of [L.S. Levitov, A.V. Shytov, JETP Lett. 66, 214 (1997)] the Coulomb anomaly of interlayer electron transport in strong magnetic field is analyzed and compared to the experimental data on layered organic metals.

- The Coulomb anomaly is given by

$$\frac{\sigma_{zz}}{\sigma_{zz0}(B)} \approx \exp \left[-\frac{\omega_c \tau \ln(1 + 2\pi e^2 \bar{\nu} d / \epsilon) f(k_{\max})}{\pi (2n_L + 1) [\nu(E_F, B) / \bar{\nu}]} \right]$$

where $f(k_{\max}) \equiv 2 \ln 2 + \gamma + \psi(3/2 + k_{\max})$

- This generalizes the result of [L.S. Levitov, A.V. Shytov, JETP Lett. 66, 214 (1997)] for finite temperature and finite upper cutoff

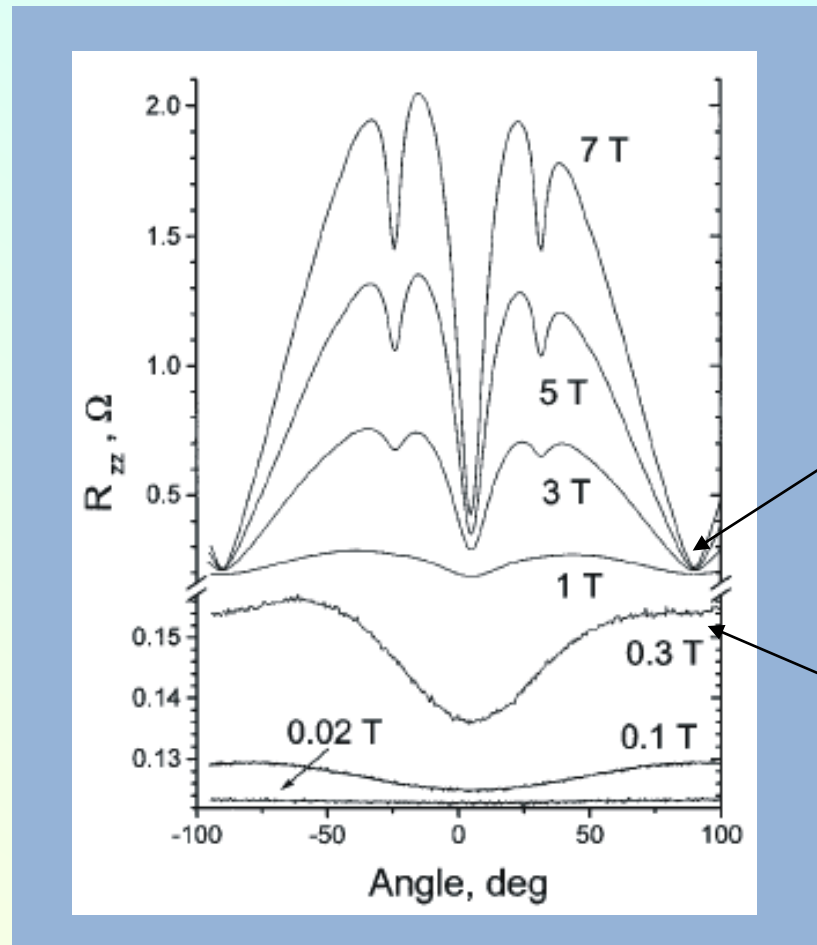
$$k_{\max} \equiv \omega_{k_{\max}} / 4T e^\gamma \approx \max \{ \hbar / \tau, \hbar \omega_c \} / 4T e^\gamma$$

- Usually, the Coulomb anomaly gives a small correction to interlayer conductivity of layered metals. But there are several compounds, as β -(BEDT-TTF)₂SF₅CH₂CF₂SO₃ where the Coulomb anomaly in strong magnetic field considerably suppresses interlayer conductivity σ_{zz}

Similar behaviour: $(\text{TMTSF})_2\text{PF}_6$ in the metallic state

Plan for future:

apply similar arguments to quasi-1D organic metals, where magnetic field also localizes conducting electrons, and the polarons may also prevent interlayer electron transport.



E. Chashechkina & P. Chaikin,
PRL **80**, 2181 (1998)

Experimental observations of MQO enhancement

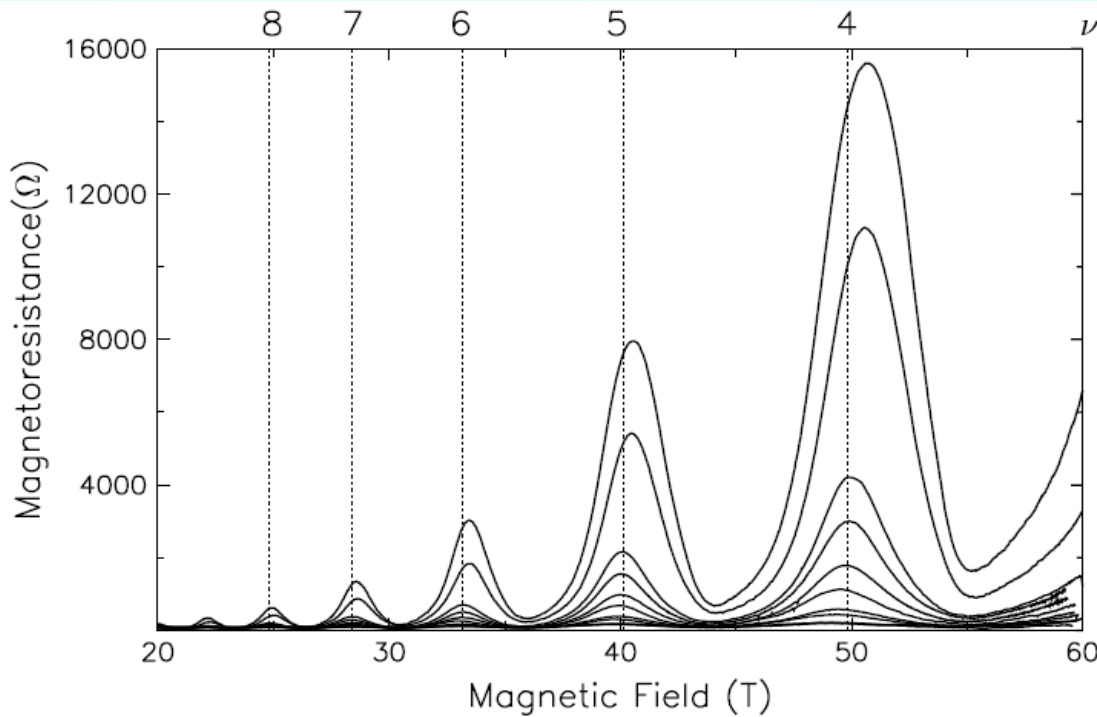
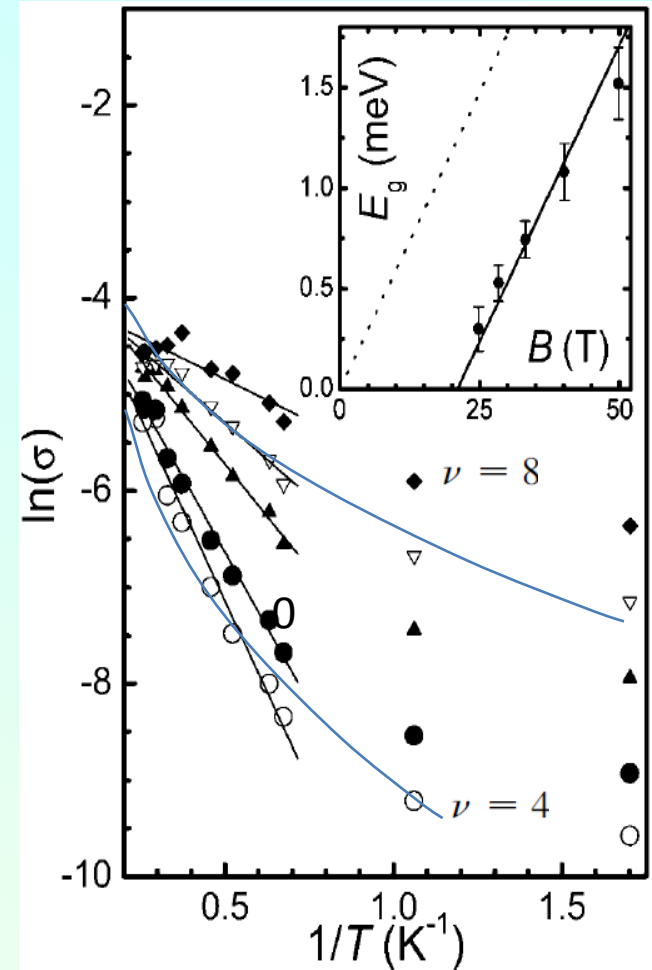


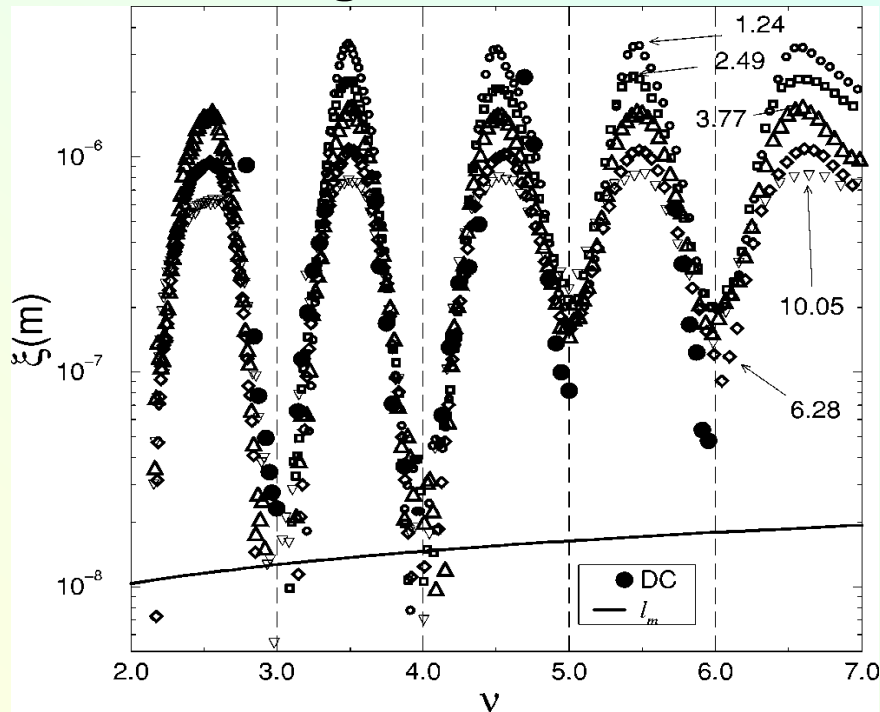
FIG. 1. The temperature dependent magnetoresistance in β'' -(BEDT-TTF) $_2$ SF $_5$ CH $_2$ CF $_2$ SO $_3$ (from the top, 0.59, 0.94, 1.48, 1.58, 1.91, 2.18, 2.68, 3.03, 3.38, 3.80, and 4.00 K). The dotted lines and numbers indicate integer Landau-level filling factors $\nu = F/B$.



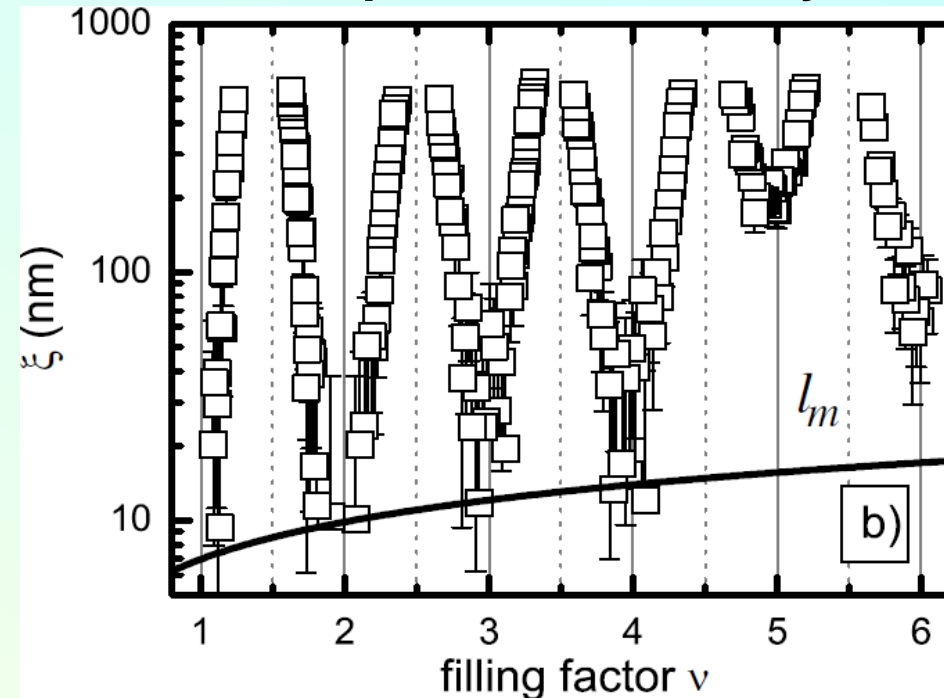
These magnetoresistance peaks were interpreted to be due to the gaps between LL in electron spectrum [M.-S. Nam et al., PRL 87, 117001 (2001)], **but there is another explanation that the contribution to conductivity from the Coulomb blockade**

Electron localization length depends on the Landau level filling factor ν

If $\nu \sim 1$, electron localization length ξ has oscillating dependence on the LL filling factor ν , which is extracted from in-plane conductivity:



R. M. Lewis and J. P. Carini,
PRB 64, 073310 (2001).

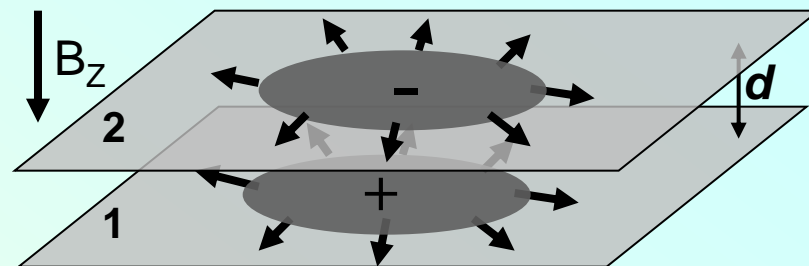


F. Hohls, U. Zeitler, and R.J. Haug,
Phys. Rev. Lett. 86, 5124 (2001).

This leads to the enhancement of MQO of interlayer conductivity, when Coulomb energy from the formation of polaron is larger than t_z .

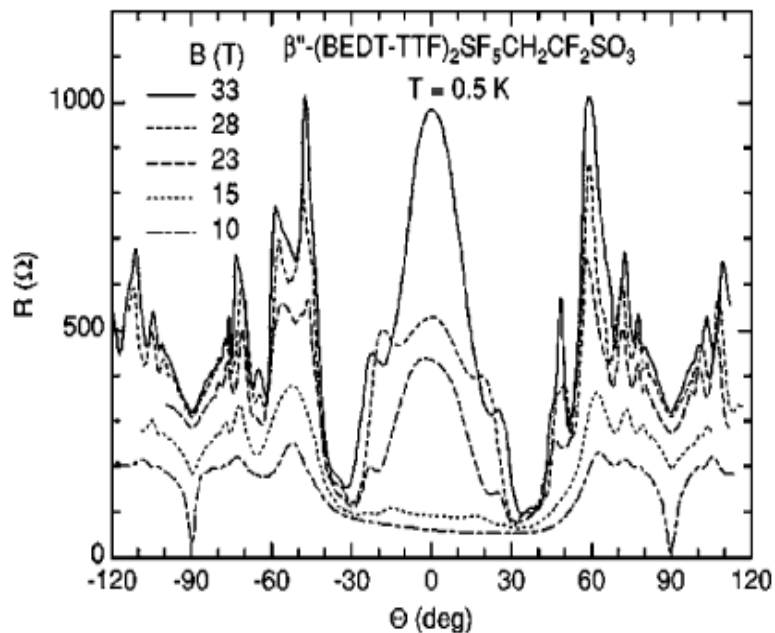
Differences of interlayer conductivity from electron transport in doped semiconductors

1. No variable range hopping (all electrons jump on interlayer distance d).
2. Electron localization length ξ depends on time (due to charge relaxation) and on magnetic field
3. $\xi \gg d$.
4. Exciton relaxation time is longer than the electron hopping time.



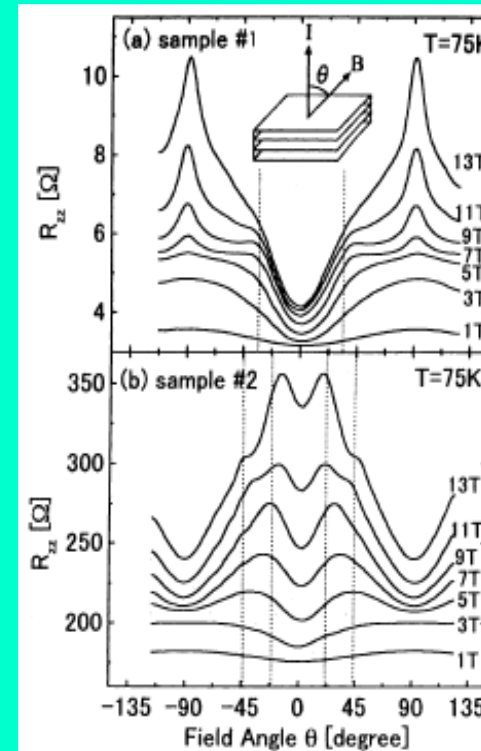
The polaron and activation interlayer electron transport also change the angular dependence of magnetoresistance

β'' -(BEDT-TTF)₂SF₅CH₂CF₂SO₃



J. Wosnitza et al., **65**, 180506(R) (2002)

GaAs/AlGaAs superlattice



coherent

incoherent

M. Kuraguchi et al.,
Synth. Met. **133-134**, 113 (2003)

Transition (or crossover) from the coherent to the weakly incoherent regime

We have considered two limit cases:

1. Weak magnetic field, when the electron level width does not depend on magnetic field: $\Gamma_B \approx \Gamma_0$
2. Strong field, when the Landau level broadening increases with field and becomes much larger than without field:

$$\Gamma_B \approx \Gamma_0 \sqrt{4\omega_c / \pi \Gamma_0} \propto \sqrt{B} \gg \Gamma_0.$$

What is the behavior in the transition region is not clear yet (there is no quantitative theory).

In the calculations the LL width of the form $\Gamma_B \approx \Gamma_0 \left[\left(4\omega_c / \pi \Gamma_0 \right)^2 + 1 \right]^{1/4}$ has been used, which is valid only in limit cases.

Almost all layered materials with weak interlayer coupling in strong magnetic field are in the weakly incoherent limit!

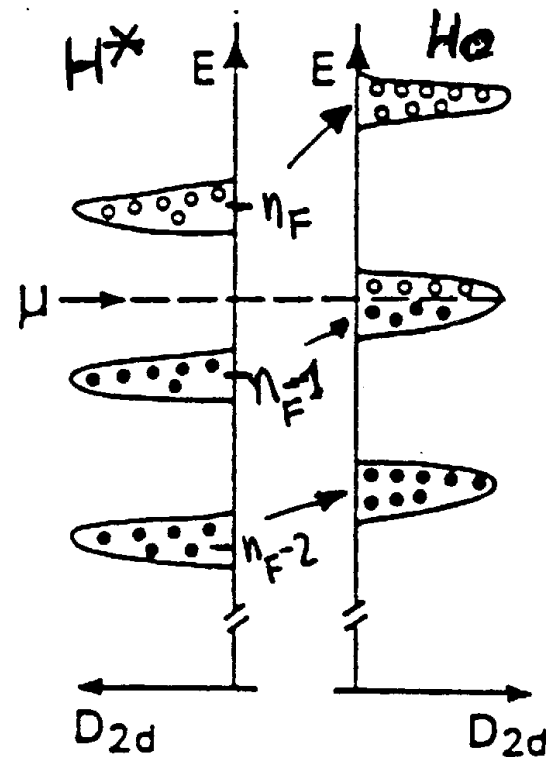
Chemical potential oscillations

The origin of the oscillations of chemical potential in 2D electron gas in magnetic field:

the total electron density is a sum over occupied Landau levels:

$$g(B) \sum_{n=0}^{\infty} f_n(n) = N$$

$$f_n(n) = \frac{1}{1 + \exp\left(\frac{\hbar\omega_c(n + \frac{1}{2}) - \mu(B)}{k_B T}\right)}$$



If the Landau levels are sharp, the chemical potential periodically jumps between adjacent Landau levels as magnetic field changes.

The chemical potential remains fixed in many quasi-2D metals

PHYSICAL REVIEW B

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Two-dimensional Fermi liquid with fixed chemical potential

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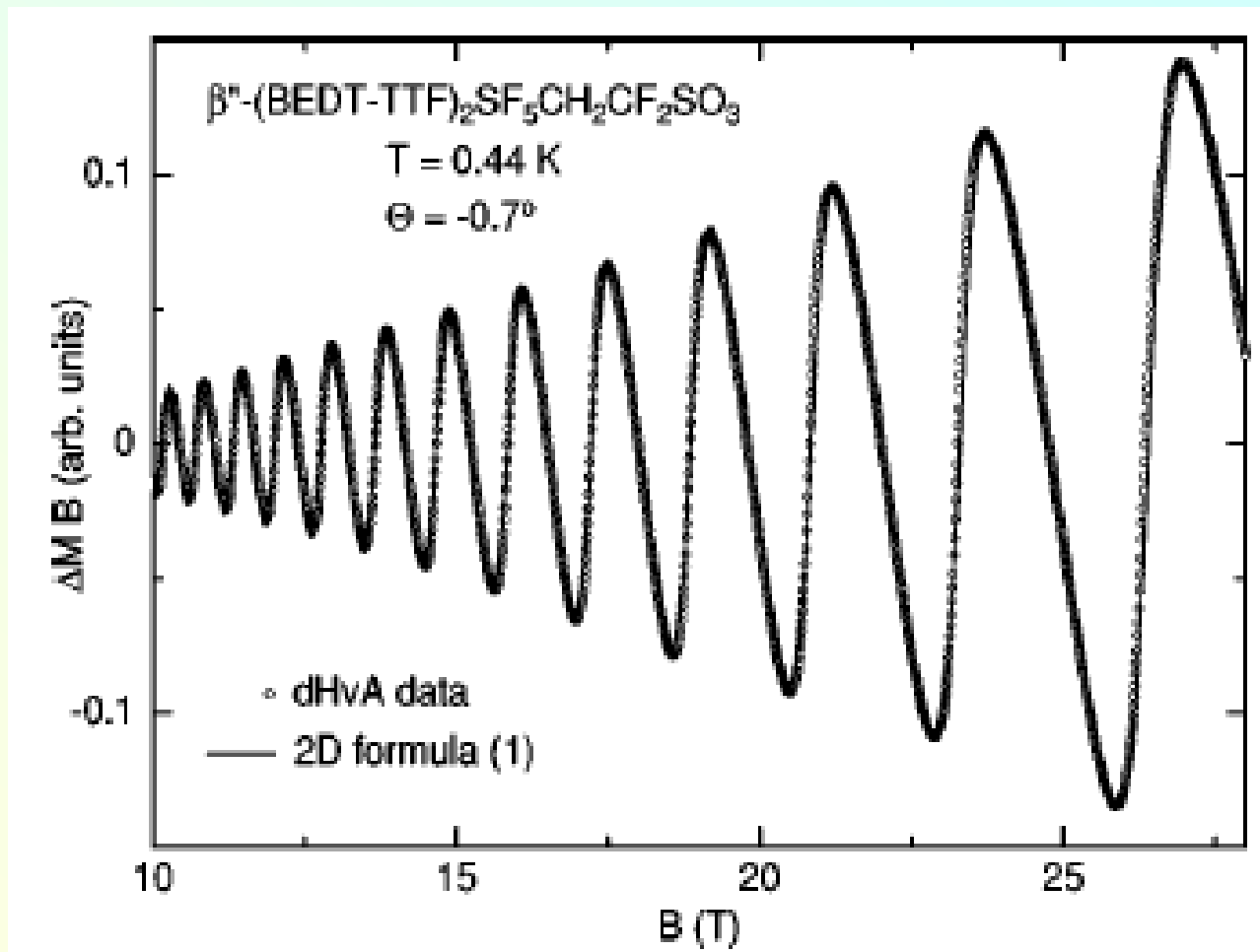
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(Received 28 October 1999)

de Haas-van Alphen measurements made on the organic metal β'' -(BEDT-TTF)₂SF₅CH₂CF₂SO₃ reveal the existence of an ideal two-dimensional (2D) Fermi surface, but rather than having the conventional sawtooth wave form that is normally observed in all other 2D electron gases, instead, an “inverse sawtooth” wave form is observed, which is to be expected when the chemical potential is pinned at a constant value. While this proves the existence of the theoretically predicted quasi-one-dimensional band, it further implies that this band has an exceptionally large density of states.

Shape of dHvA oscillations corresponds to fixed chemical potential



The chemical potential oscillations are absent because of the magnetostriction, which leads to MQO of electron density, leading to the grand canonical ensemble.

Oscillations of the chemical potential and the equation of state for beryllium

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(Submitted 18 October 1984)

Zh. Eksp. Teor. Fiz. **88**, 1771–1779 (May 1985)

An attempt was made to detect oscillations of the chemical potential of beryllium associated with variations in the density of states in a quantized magnetic field. No oscillations were detected from voltage traces recorded across a measuring capacitor with a Be single crystal as one of its plates, and it is deduced that their amplitude is at least an order of magnitude less than expected. The result is attributed to cancellation of the changes in the chemical potential associated with oscillations in the density of states and with magnetostriction (volume changes). Such cancellation can occur if the compressibility of beryllium is determined primarily by the conduction electrons.

For coherent limit these two approaches are equivalent and give similar results

For example, without magnetic field one easily obtains from

$$\sigma_{zz} = \frac{e^2 t_z^2 d}{L_x L_y} \left\langle \int d^2 r d^2 r' \int \frac{d\varepsilon}{2\pi} 4 \operatorname{Im} G_R(r, r', j, \varepsilon) \operatorname{Im} G_R(r', r, j+1, \varepsilon) \left[-n'_F(\varepsilon) \right] \right\rangle,$$

that conductivity is proportional to in-plane mean free time τ .

This fact has direct physical meaning. If electron at $t=0$ is on the layer 0, its wave function amplitude on layer 1 is $f \approx t_z t / h$. After time τ electron scatters on impurity on layer 0, and since the impurity potential is different on two layers, the coherence between two layers is lost. After time τ the probability that the electron tunnels to the next layer is $f^2(\tau) \approx (t_z \tau / h)^2$ and the mean velocity is $f^2(\tau) d / \tau \approx (t_z / h)^2 \tau d$.

The standard model of interlayer electron transport

The Hamiltonian contains 3 terms:

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

1
1
2

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

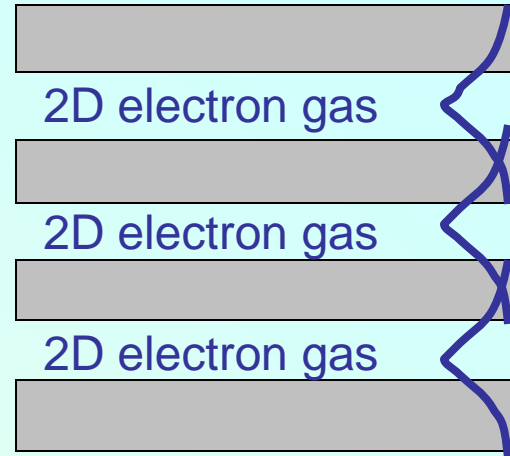
$$\hat{H}_0 = \sum_{m,j} \varepsilon_{2D}(m) c_{m,j}^+ c_{m,j},$$

the coherent electron tunneling between any two adjacent layers:

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

and the point-like impurity potential:

$$\hat{H}_I = \sum_i V_i(r) \quad \text{where} \quad V_i(r) = U \delta^3(r - r_i)$$



The electron-electron and electron-phonon interactions are included in the renormalization of electron effective mass (Fermi liquid theory). 107

Strongly incoherent interlayer magnetotransport is very model-dependent

Usually, the conductivity in this regime has non-metallic exponential temperature dependence (thermal activation or Mott-type). It has very weak or no angular dependence of background magnetoresistance (contrary to the coherent case)

1. Interlayer hopping by resonant impurities [A. A. Abrikosov, *Physica C* 317-318, 154 (1999); D. B. Gutman and D. L. Maslov, *PRL* 99, 196602 (2007) ; *PRB* 77, 035115 (2008);]
2. Boson-assisted interlayer tunneling [U. Lundin and R. H. McKenzie, *PRB* 68, 081101(R) (2003); A. F. Ho and A. J. Schofield, *PRB* 71, 045101(2005);]
3. Complete localization of electrons and variable-range hopping between localized states [V. M. Gvozdkov, *PRB* 76, 235125 (2007); etc.]

Hopping conductivity and metal-insulator phase transition

PHYSICAL REVIEW B 76, 235125 (2007)

Incoherence, metal-to-insulator transition, and magnetic quantum oscillations of interlayer resistance in an organic conductor

V. M. Gvozdkov

Idea: all electronic states are localized as in QHE

IV. VARIABLE RANGE HOPPING, MAGNETORESISTANCE OSCILLATIONS, AND METAL-TO-INSULATOR TRANSITION

**A. Integer quantum Hall effect
regime and variable range hopping**

$$\sigma_{\tau}(T_0/T) = \sigma_{\tau}(0)\exp(-\sqrt{T_0/T}).$$

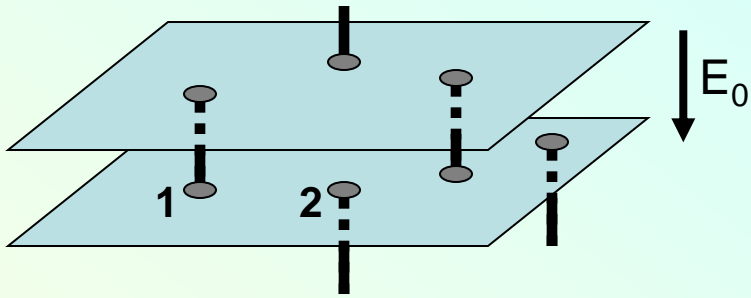
C. Scaling and the metal-to-insulator transition

$$\sigma_{\tau}(B, T) = \sigma_{\tau}(0)\exp[-A(|B - B_0|/T^{0.65})^{0.77}]$$

V. M. Gvozdkov, PRB **76**,
235125 (2007)

! However, metallic in-plane conductivity and good angular magnetoresistance oscillations do not support this scenario

Incoherent conductivity channel [PRB 79, 165120 (2009)]



The resistance through each hopping center contains two in-series elements:

$$R_{\perp} = R_{hc} + R_{\parallel}.$$

The hopping-center resistance R_{hc} is almost independent of magnetic field and has nonmetallic temperature dependence.

The in-plane resistance R_{\parallel} depends on the magnetic field \perp to the conducting layers, and has the metallic temperature dependence. It can be calculated in the limit when the concentration of hopping centers $n_i = 1/l_i^3$ is much less than the concentration of normal impurities $n_{\tau} = 1/l_{\tau}^3$. Then the resistance R_{\parallel} is determined by the in-plane conductivity:

$$R_{\parallel} = \ln(l_i/l_{\tau}) / \pi \sigma_{\parallel} d.$$

The total incoherent part of conductivity:

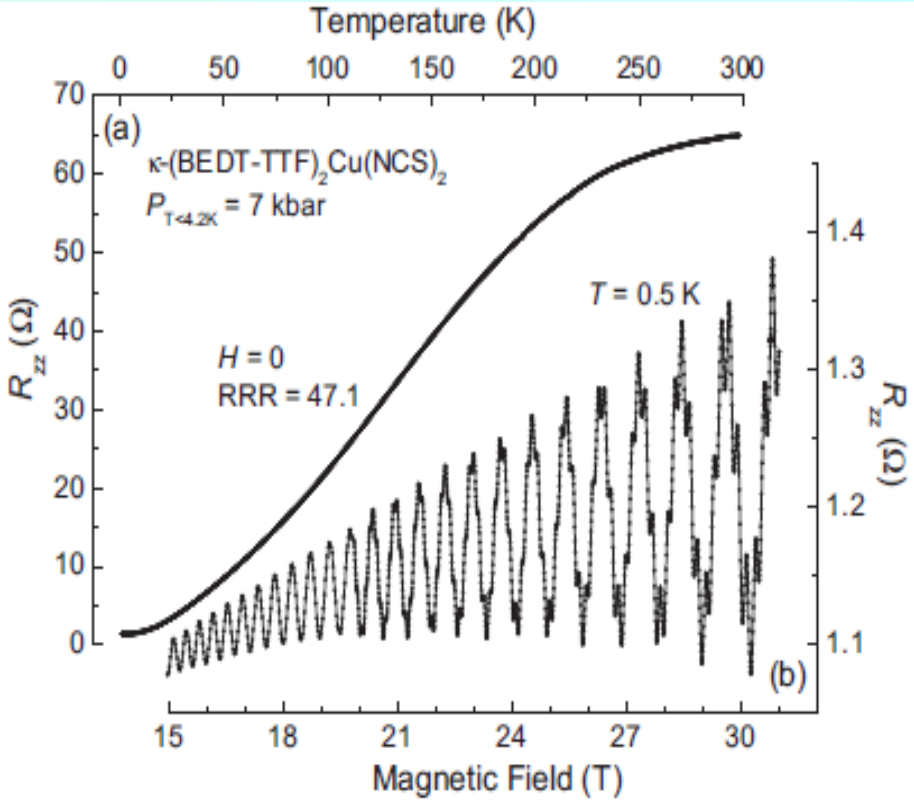
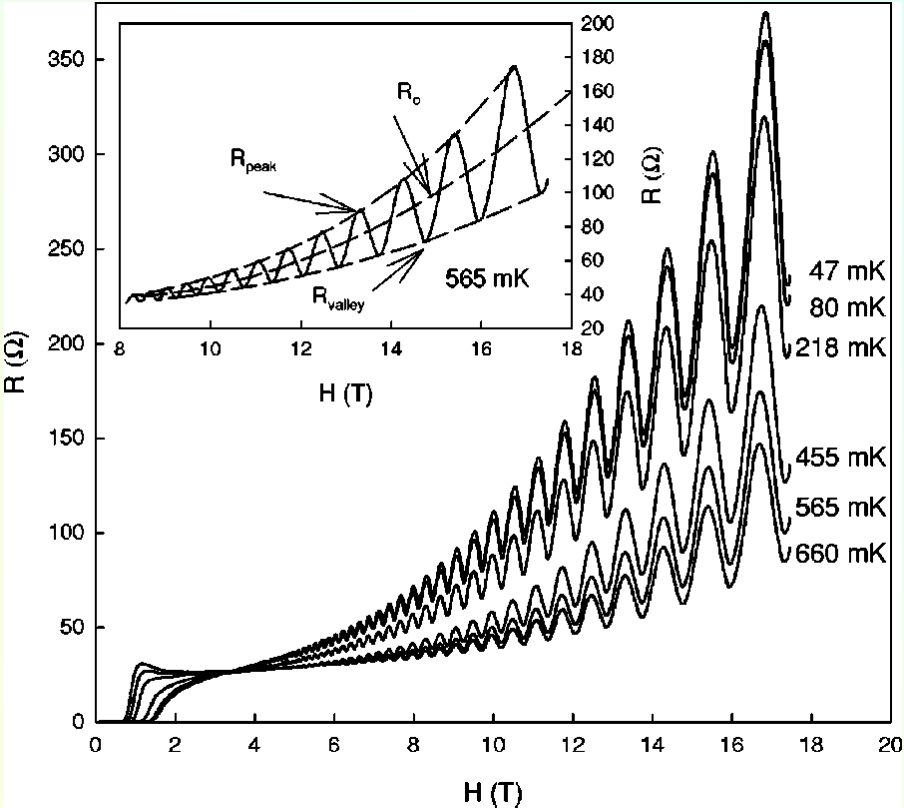
σ_{\parallel} depends on magnetic field \perp layers and has metallic T-dependence.

$$\sigma_i = \frac{\pi \sigma_{\parallel} n_i d^3}{\pi d \sigma_{\parallel} R_{hc} + \ln(l_i/l_{\tau})}.$$

Motivation

Strongly incoherent models can explain the monotonic growth of MR

when magnetic field is \perp layers (parallel to electric current)



β -(BEDT-TTF) $_2$ SF $_5$ CH $_2$ CF $_2$ SO $_3$
F. Zuo et al., PRB 60, 6296 (1999).

W. Kang et al., PRB 80, 155102 (2009)