New features of magnetoresistance in strongly anisotropic layered metals

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Does the standard theory of magnetoresistance is applicable to strongly anisotropic layered compounds (like all high-Tc superconductors), when the electron interlayer tunneling time is longer than the cyclotron period of motion in magnetic field or than in-layer mean scattering time)?

<u>Do we need a new theory to describe this regime?</u>

The answer is <u>we do need a new theory</u> because the way by which disorder is treated in 3D theory is inappropriate to 2D layers.

The new qualitative results of such theory are presented together with a detailed experimental test of the theory

Plan of the talk

1. Introduction. Motivation.
2. Interlayer transport in magnetic field: one-electron approach
3. Influence of coulomb e-e interaction on interlayer electron transport in magnetic field: quasiclassical nonperturbative approach.

Motivation

This question is rather general. Layered compounds arise very often: high-Tc cuprates, pnictides, organic metals, heterostructures, intercalated graphite, etc. Magnetoresistance (MQO and AMRO) is used to measure the quasi-particle dispersion, Fermi surface, effective mass, mean scattering time.. Recent observation of magnetic quantum and angular magnetoresistance oscillations makes a revolution in the understanding of the electronic structure of high-Tc superconductors.

Experimentally observed transitions coherent – weakly coherent – strongly incoherent interlayer coupling show many new qualitative feature: monotonic growth of interlayer magnetoresistance, different amplitudes of MQO and angular dependence of magnetoresistance, etc.

Why magnetoresistance studies are important?

There are only few methods to study electronic properties of metals, such as Fermi surface, electron dispersion, etc. These methods are

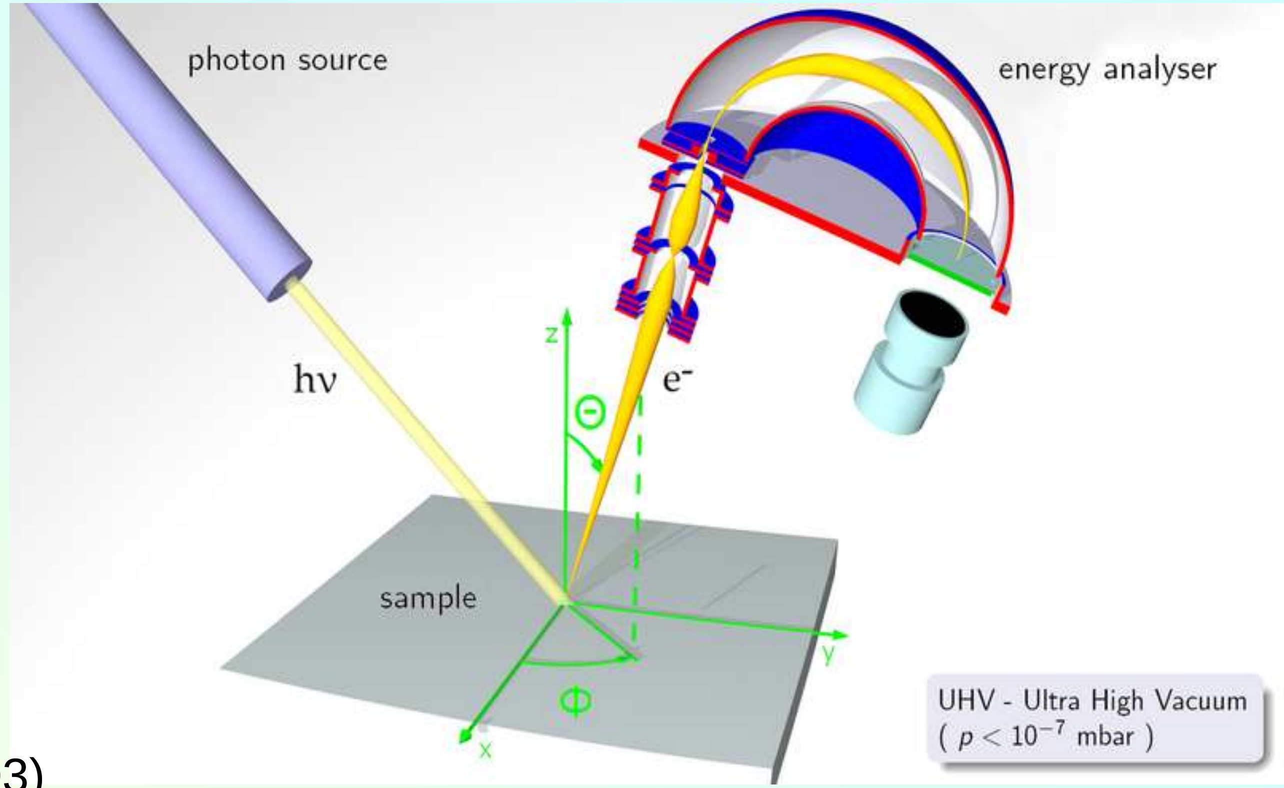
1. **Temperature dependence of conductivity**
2. **Anisotropic conductivity tensor** $\sigma_{ij} \propto e^2 \tau \langle v_i v_j \rangle_{FS}$
3. **ARPES (Angle resolved photoemission spectroscopy)**
4. **Angular dependence of magnetoresistance**
5. **Magnetic quantum oscillations**

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:

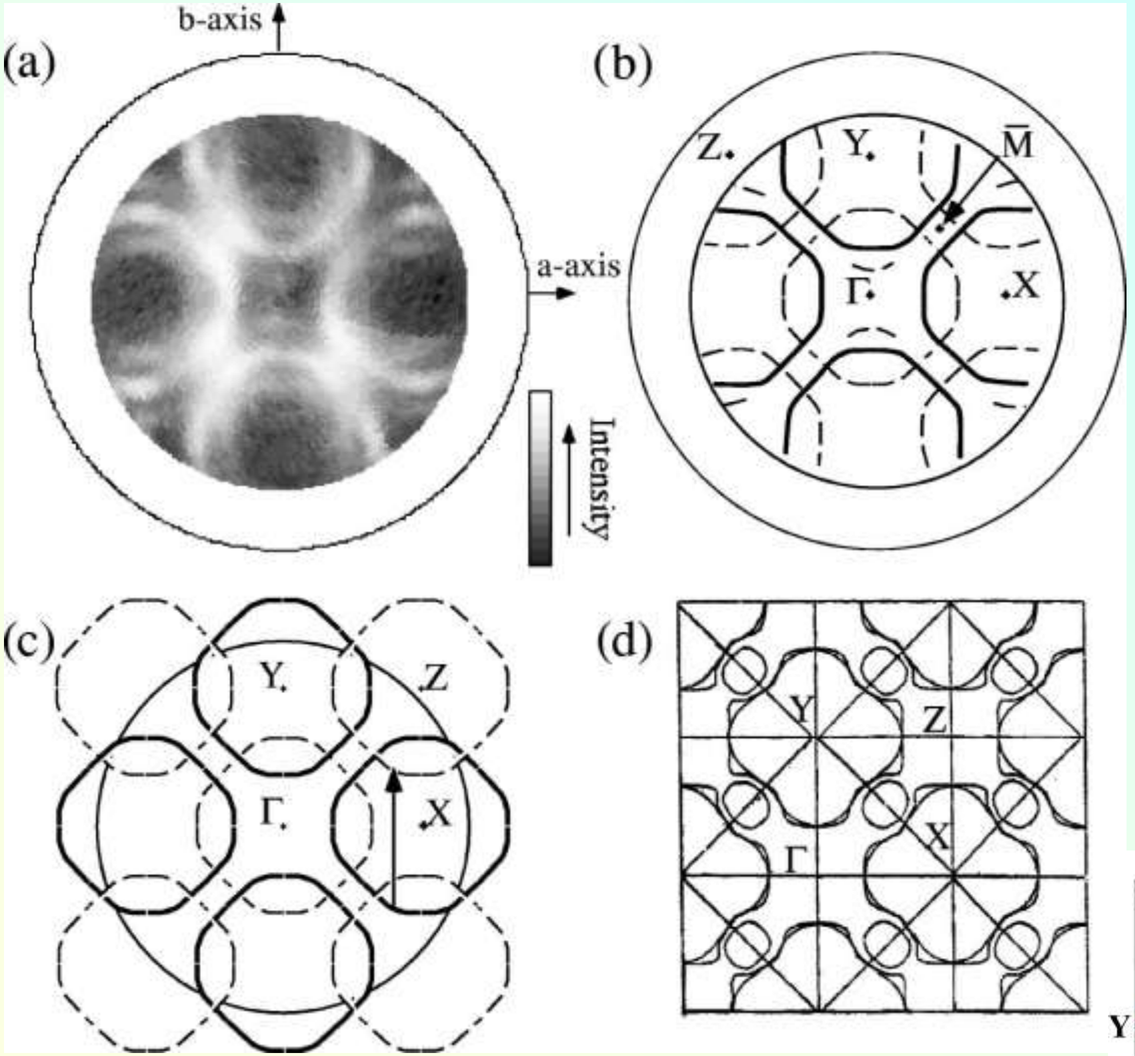
$$I(\mathbf{k}, \omega) = A(\mathbf{k}, \omega) f(\omega)$$

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

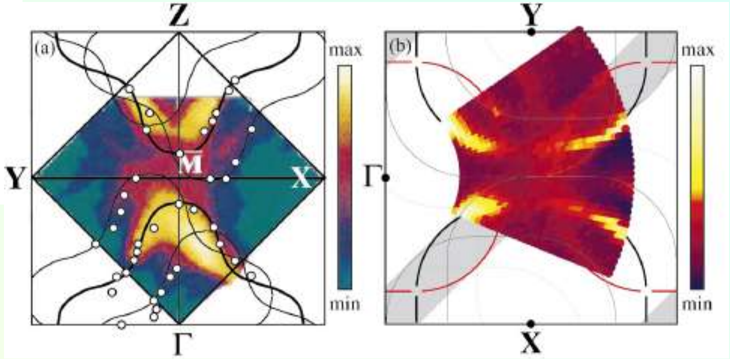
Therefore can find out information about *E(k)*

Drawback 1: Only surface electrons participate!

ARPES data and Fermi-surface shape



The Fermi surface of near optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (a) integrated intensity map (10-meV window centered at *EF*) 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.

Angular dependence of background magnetoresistance

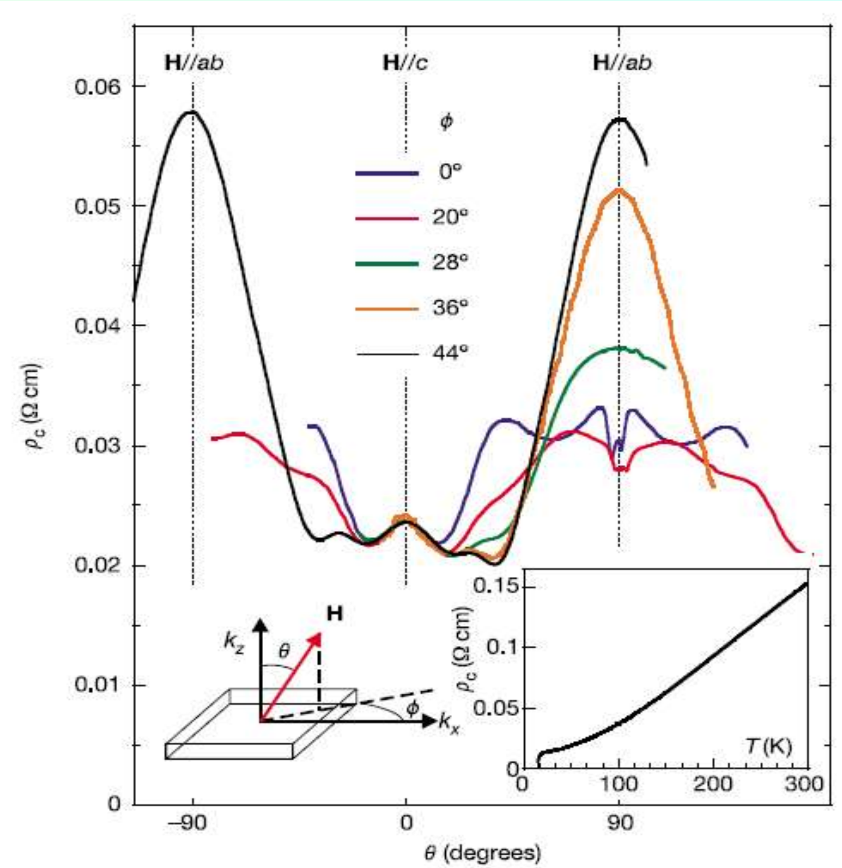
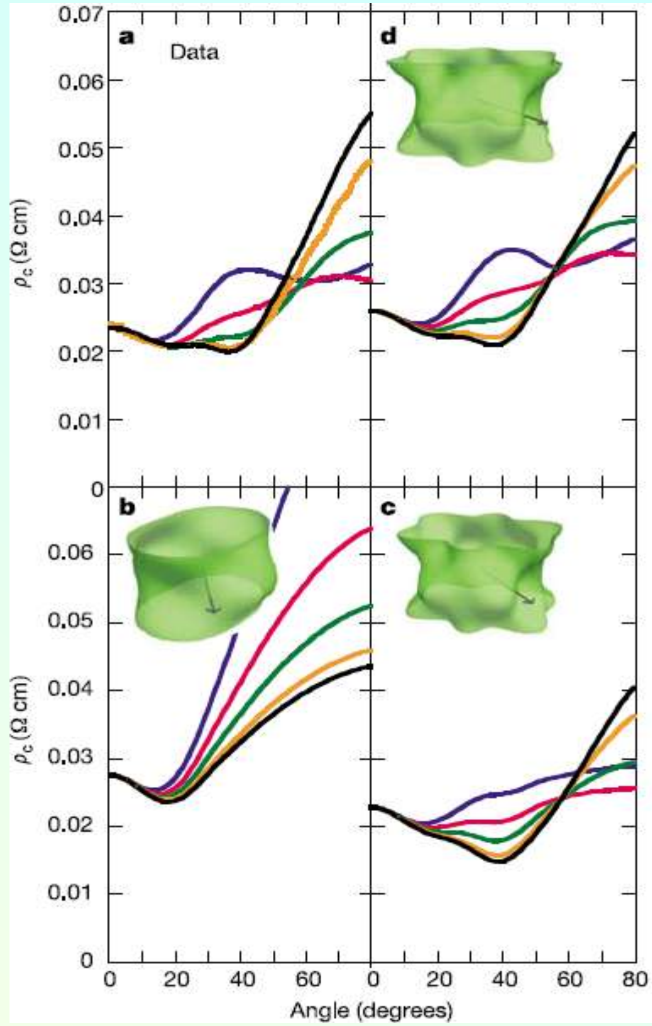


Figure 1 Polar AMRO sweeps in an overdoped Tl2201 single crystal ($T_c \approx 20$ K). The data were taken at $T = 4.2$ K and $H = 45$ T. The different azimuthal orientations ($\pm 4°$) of each polar sweep are stated relative to the Cu–O–Cu bond direction. The key features of the data are as follows: (1) a sharp dip in $\rho_\perp$ at $\theta = 90°$ 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 **H**||*ab* ($\theta = 90°$) that is maximal for $\phi \approx 45°$, consistent with previous azimuthal AMRO studies in overdoped Tl2201 (ref. 16), (3) a small peak at **H**||*c* ($\theta = 0°$), and (4) a second peak in the range $25° < \theta < 45°$ 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 $Tl_2Ba_2CuO_{6+d}$ from polar AMRO data.

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

Angular dependence of magnetoresistance

If the electron dispersion ε(*p*) is known, the background conductivity is given by the Shockley tube integral (solution of transport equation):

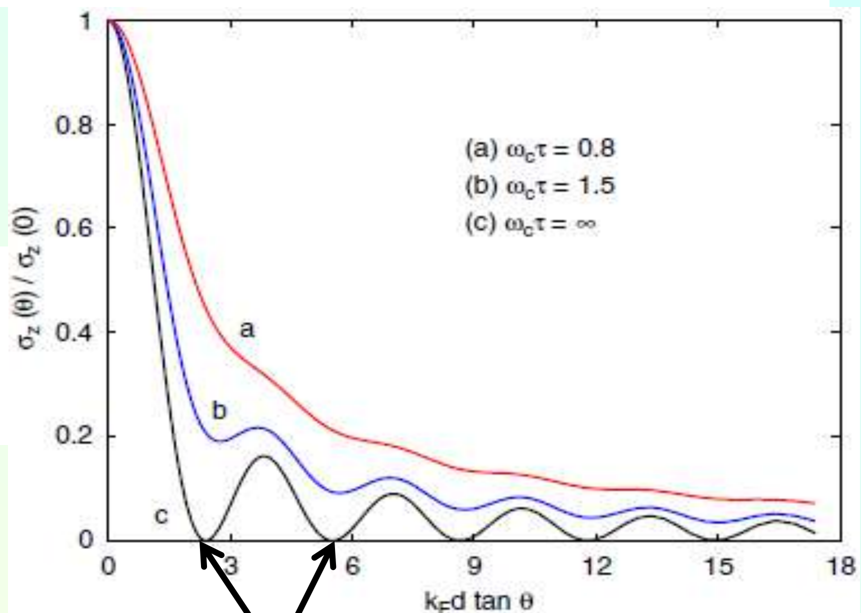
$$\sigma_{\alpha\beta}(\theta,\phi) = \frac{e^2}{4\pi^3\hbar^2}\int dk_{z0}\frac{m_H^*\cos\theta/\omega_H}{1-\exp(-2\pi/\omega_H\tau)} \times \int_0^{2\pi}\int_0^{2\pi} v_\alpha(\psi,k_{z0})\,v_\beta(\psi-\psi',k_{z0})\,e^{-\psi'/\omega_H\tau}d\psi' d\psi.$$

For axially symmetric dispersion and in the first order in t_z it simplifies to:

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

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

This gives angular magnetoresistance oscillations (AMRO):



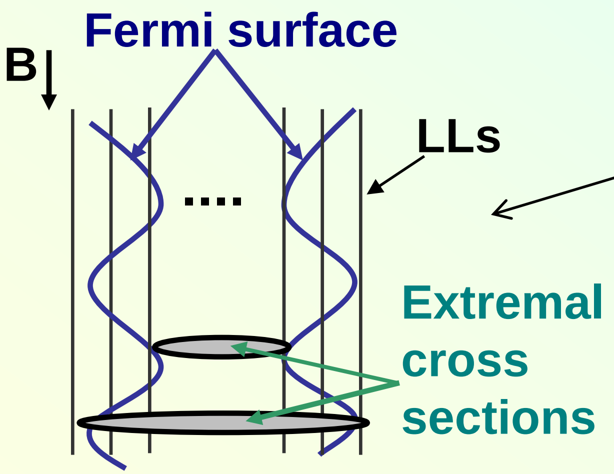
Yamaji angles

Geometrical interpretation of the angular magnetoresistance oscillations in q2D

Conductivity (very roughly) is proportional to the mean square velocity integrated over the whole Fermi surface : $\sigma_{zz} \propto e^2 \tau \left\langle v_z{}^2 \right\rangle_{FS}$

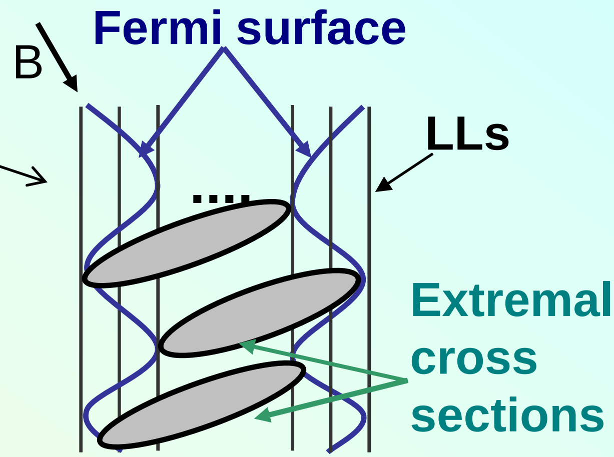
$v_z = \partial \varepsilon / \partial k_z \propto \partial A / \partial k_z ,$ where $\boldsymbol{A}$ is the cross-section area of the Fermi surface by the plane ⊥B

<u>***B***⊥conducting layers</u>



Geometrical interpretation of the Yamaji angles in quasi-2D metals

<u>Inclined magnetic field</u>



Cross section area and the electron dispersion have strong $\boldsymbol{k_z}$-dependence

Cross section area and the electron dispersion are almost $\boldsymbol{k_z}$-independent

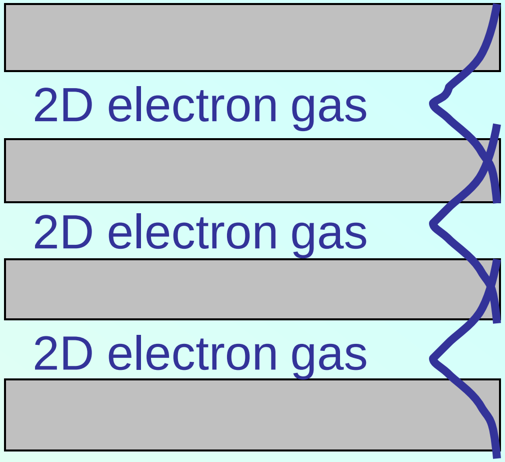
One can derive at $\omega_c \tau \gg 1$ [PG, PRB 81, 205122 (2010)]

$$\sigma_{zz}(\theta, \phi_0) = \frac{e^2 \tau \cos\theta}{8\pi^4 \hbar^2} \int \frac{dk_{z0}}{m_H^*} \left(\frac{\partial A(k_{z0}, \theta, \phi_0)}{\partial k_{z0}} \right)^2 .$$

The AMRO do not require 3D Fermi surface

They only require coherent interlayer tunneling in the Hamiltonian:

$$\underset{}{\hat{H} = \underbrace{\hat{H}_0}_{1} + \underbrace{\hat{H}_t}_{1} + \underbrace{\hat{H}_I}_{2}}$$



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:

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

The overlap of electron wave functions in tilted magnetic field

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

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

Magnetic quantum oscillations. Lifshitz-Kosevich formula.

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

Oscillations of conductivity $\tilde{\sigma} \sim \dfrac{d\tilde{M}(B)}{d(1/B)}$ **are easier to measure.**

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

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

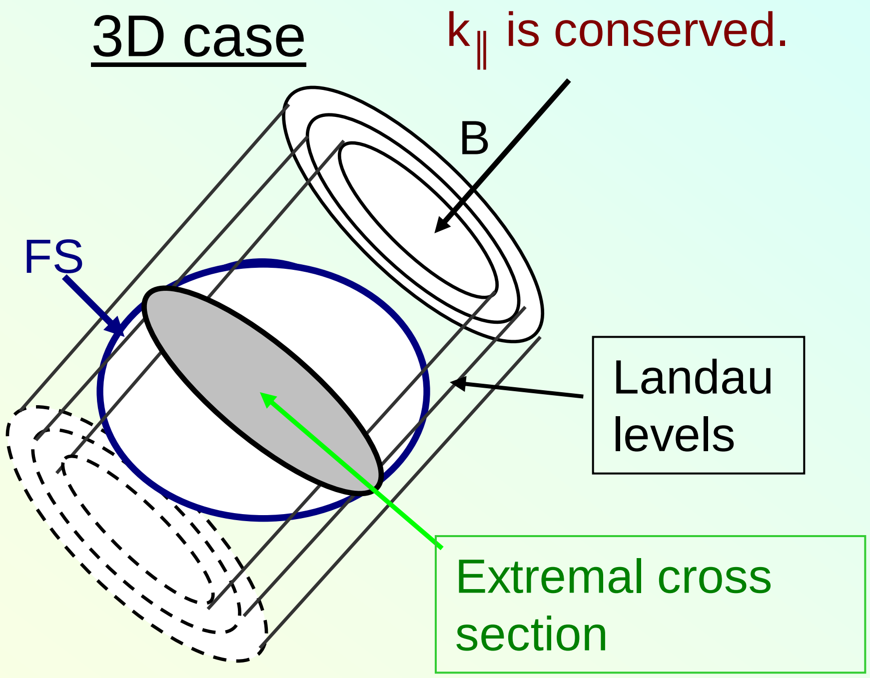
$$\kappa \equiv 2\pi k_B T / h\omega_C \, , \; \omega_C = eH / m^* c.$$

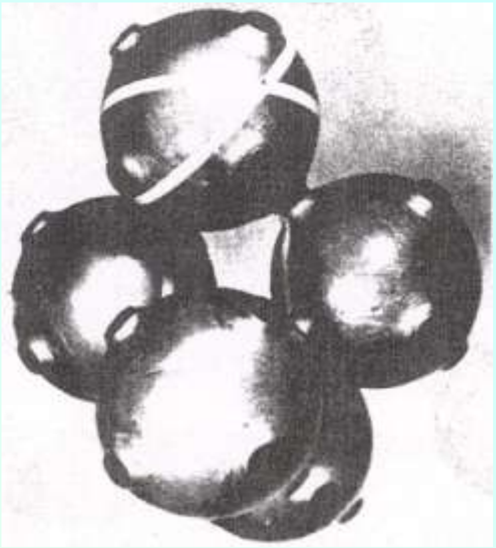
The scattering (Dingle) damping factor

$$R_D(p) = \exp\left(\frac{-\pi}{\tau\omega_C}\right),$$ $\tau = h / 2\pi k_B T_D$ is the mean free scattering time.

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

3D compounds in tilted magnetic field





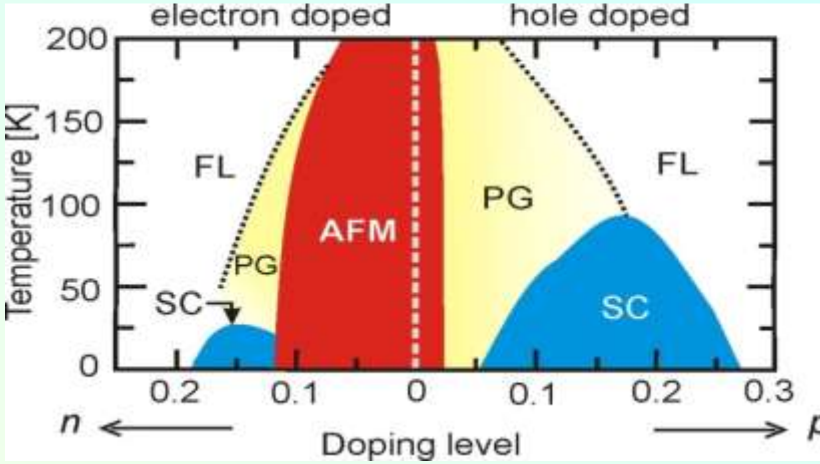
Fermi surface of gold

Extremal cross-section area of FS measured at various tilt angles of magnetic field allows to obtain the total Fermi surface of metals.

Phase diagram of high-Tc cuprate SC. High Tc and quantum phase transition

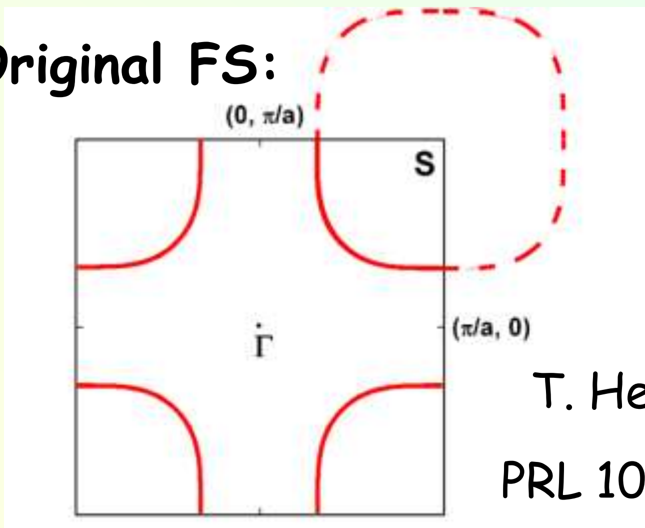
$Nd_{2-x}Ce_xCuO_4$

(NCCO)



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

Original FS:

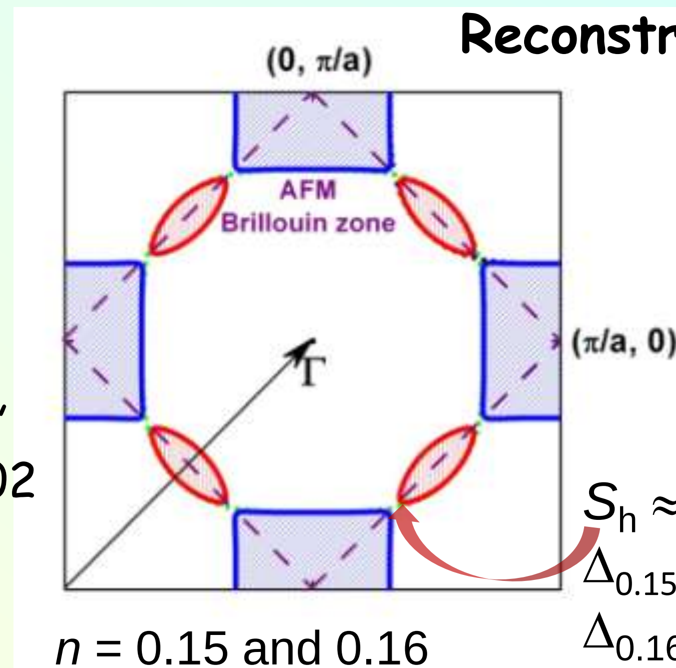


$n = 0.17$

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

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

Reconstructed FS:



$n = 0.15$ and 0.16

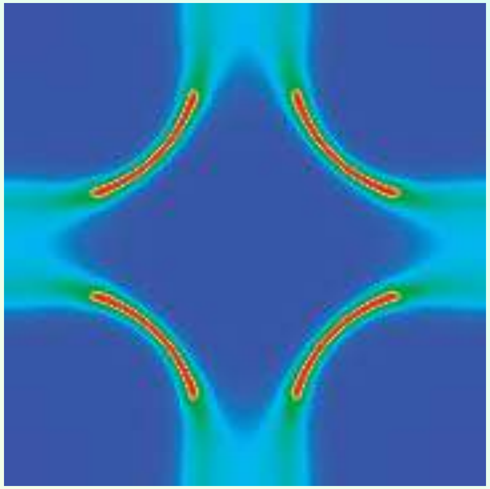
$S_h \approx 1.1\%$ of S_{BZ};

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

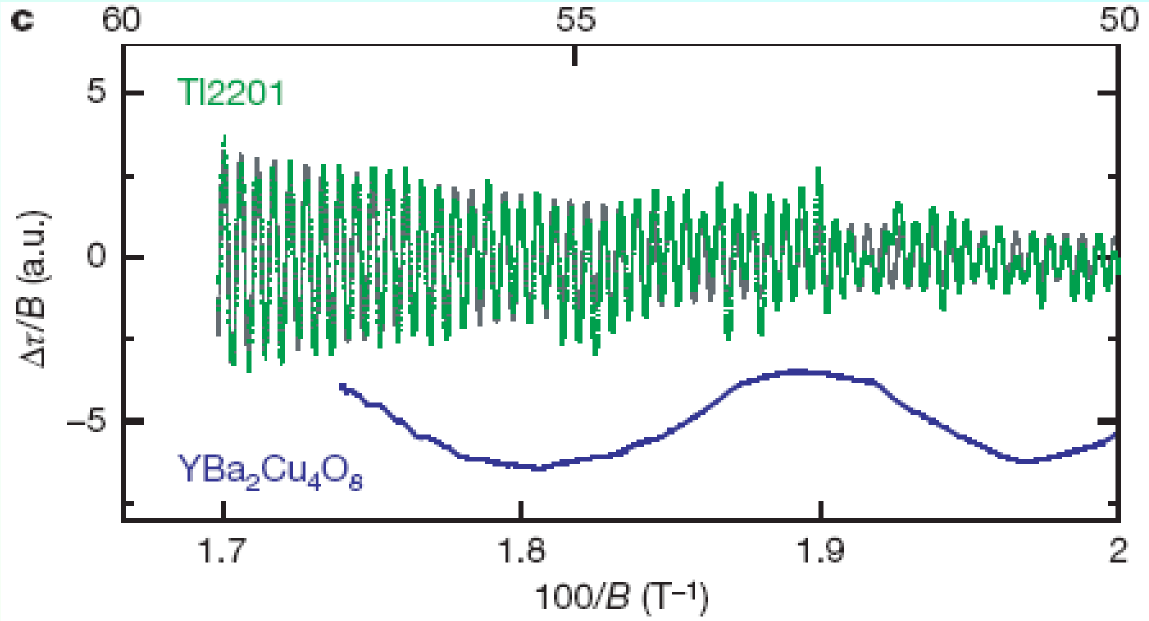
$\Delta_{0.16} \approx 36$ meV

Motivation

Quantum oscillations from Fermi arcs



ARPES image plot



T. Pereg-Barne et al., Nature Physics 6, 44 - 49 (2009)

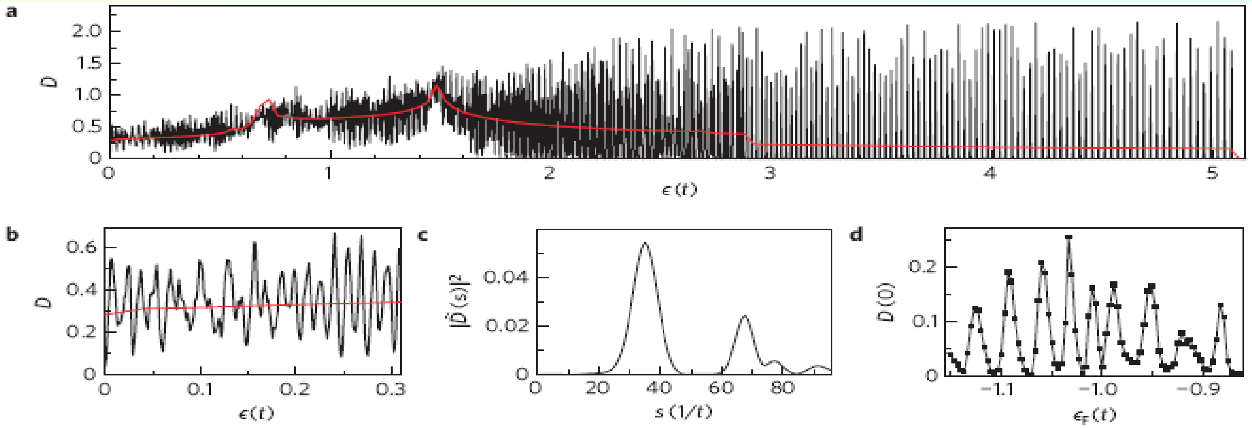


Figure 4 | Exact diagonalization of the lattice model. a, DOS as a function of energy in the FAM in zero (red) and non-zero (black) magnetic field corresponding to two vortices in a 20 × 20 magnetic unit cell. In YBCO with lattice constant $a_0 \simeq 4$Å this corresponds to the physical field of about 64 T. The parameters used are as follows: $\Delta_0/t = 1$, $\epsilon_F/t = -1.3$, $\nu = 0.6$ and $\tau = 0.1$. **b**, The low-energy DOS for the same parameters, in detail. **c**, The power spectrum of the low-energy DOS showing dominant frequency of oscillations $34t^{-1}$ and its second harmonic. **d**, DOS at the Fermi level as a function of ϵ_F.

Experiments on MQO in cuprates

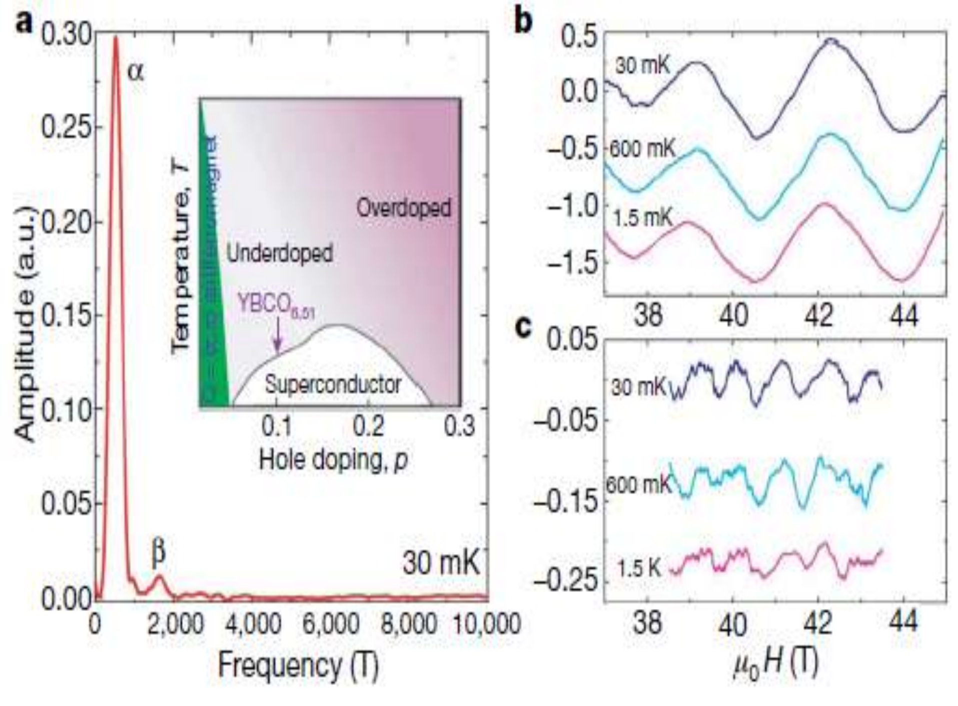


Figure 2 | de Haas-van Alphen oscillations in $YBa_2Cu_3O_{6.51}$. a, Fourier

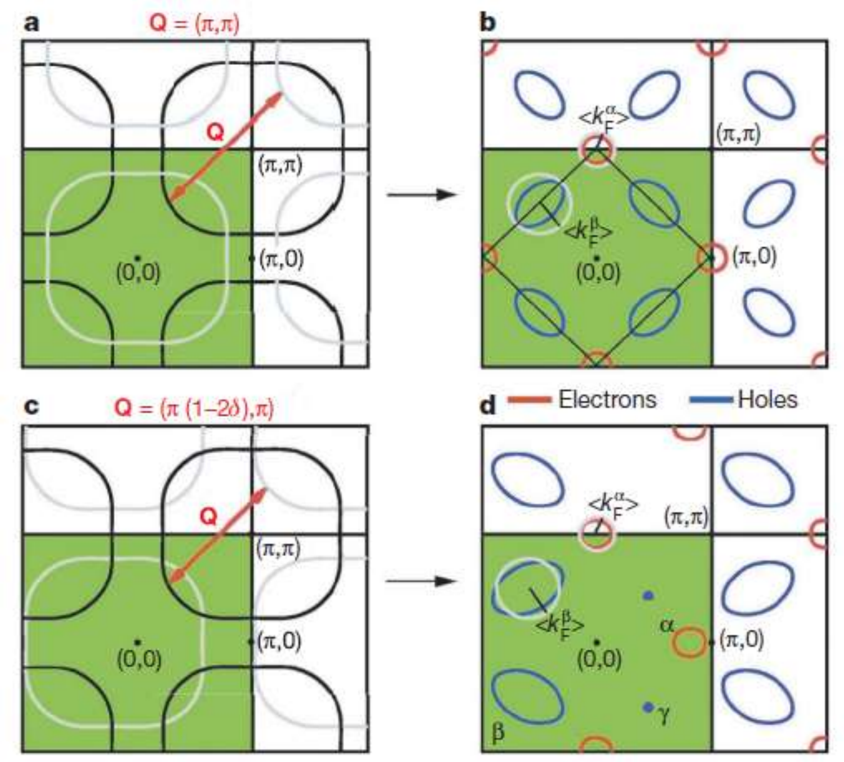


Figure 4 | Fermi surface reconstruction in $YBa_2Cu_3O_{6.51}$. a, Schematic Fermi surface reconstruction for a commensurate ordering wavevector $\mathbf{Q} = (\pi,\pi)$ and nominal doping $p_{nom} = 0.1$ in the extended Brillouin zone

S.E. Sebastian, N. Harrison, E. Palm et al., NATURE 454, 200 (2008)

PRL 101, 216402 (2008) PHYSICAL REVIEW LETTERS week ending 21 NOVEMBER 2008

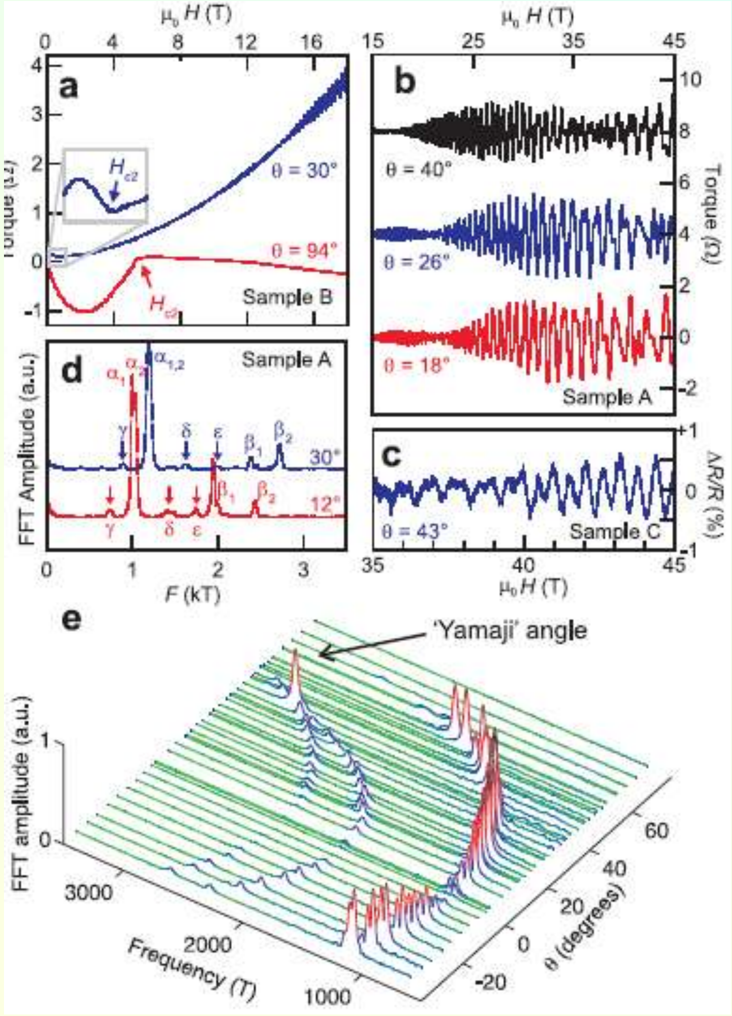
Motivation

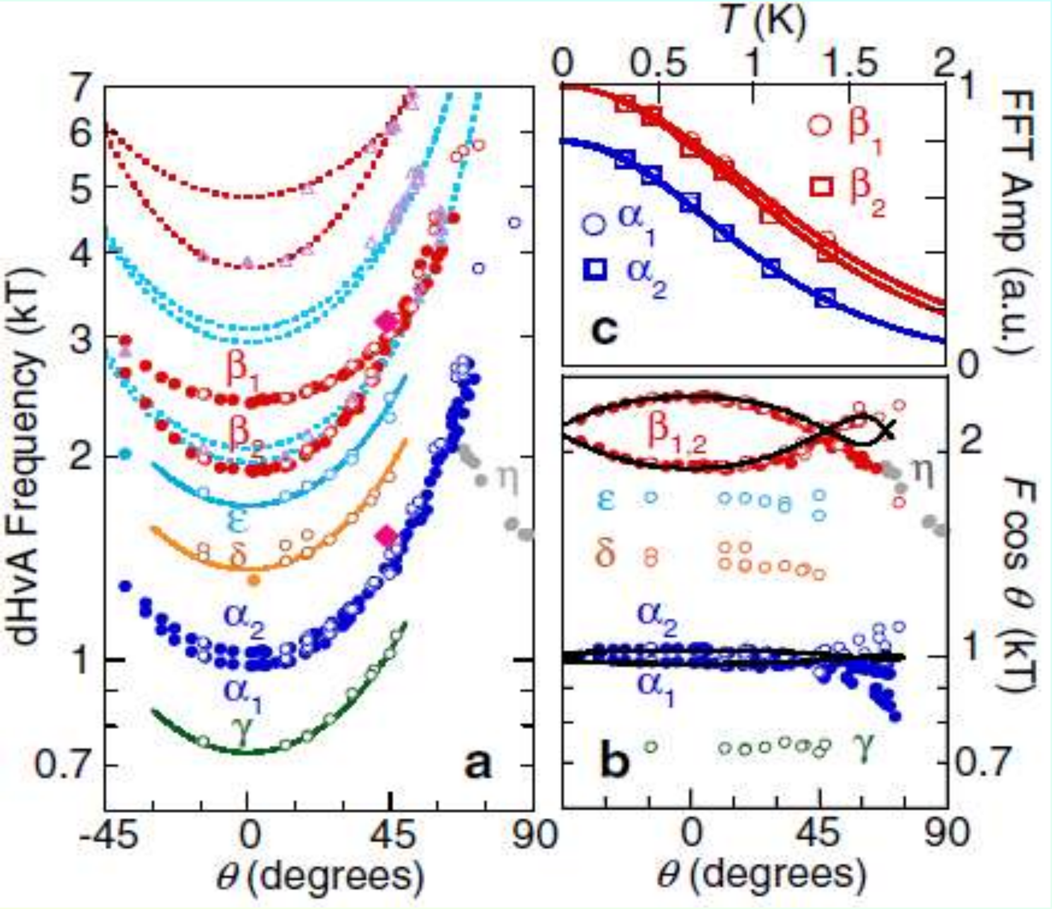
Fermi Surface of Superconducting LaFePO Determined from Quantum Oscillations

A. I. Coldea,[1] J. D. Fletcher,[1] A. Carrington,[1] J. G. Analytis,[2] A. F. Bangura,[1] J.-H. Chu,[2] A. S. Erickson,[2] I. R. Fisher,[2] N. E. Hussey,[1] and R. D. McDonald[3]

M8

Experiments on MQO in high-Tc





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. Wosnitza, *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:

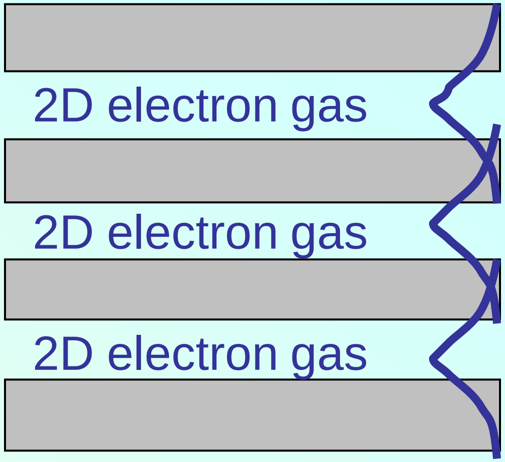
1. **D. Jérome and H.J. Schulz, Adv. Phys. 31, 299 (1982).**
2. **J. Singleton, Rep. Prog. Phys. 63, 1111 (2000).**
3. **M.V. Kartsovnik, *High Magnetic Fields: A Tool for Studying Electronic Properties of Layered Organic Metals*, Chem. Rev. 104, 5737 (2004).**
4. **M.V. Kartsovnik , V.G. Peschansky,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

One-electron approach
to the calculation of interlayer conductivity

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:

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

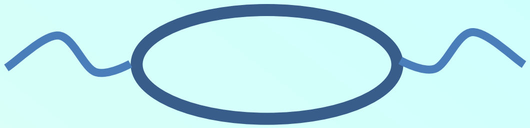
3. The coherent electron tunneling between any two adjacent layers:

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

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

Compare to calculation of conductivity in metals (standard theory, coherent 3D case)

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



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

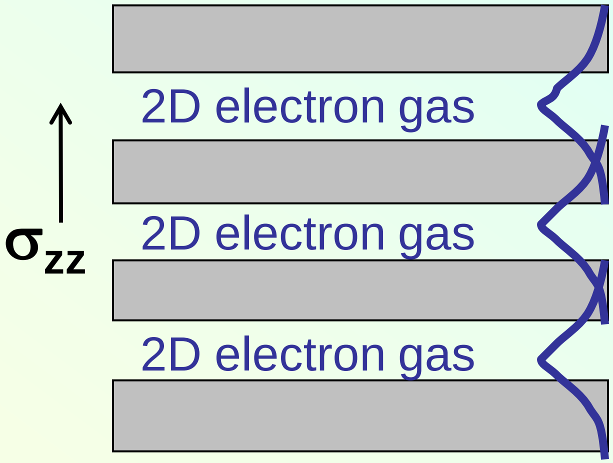
where $m=(n, k_y, k_z)$, the electron velocity $v_z(\varepsilon,n)=\partial\varepsilon/\partial k_z$, is determined by the 3D electron dispersion,

$G_R(m,\varepsilon)$ - retarded 3D electron Green's function, where scattering by impurities is taken in the lowest order (Born approx.),

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

- derivative of the Fermi distribution function.

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



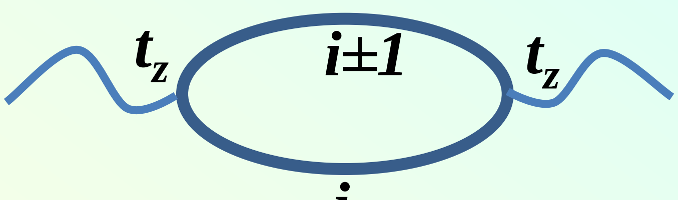
The interlayer transfer integral $t_z \ll \Gamma_0$ is the smallest parameter. We take it into account in the lowest order (after the magnetic field and impurity potential are included as accurately as possible). Interlayer conductivity is calculated as the <u>tunneling</u> between two adjacent layers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

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

where the Green's function $G_R(r,r',j,\varepsilon)$

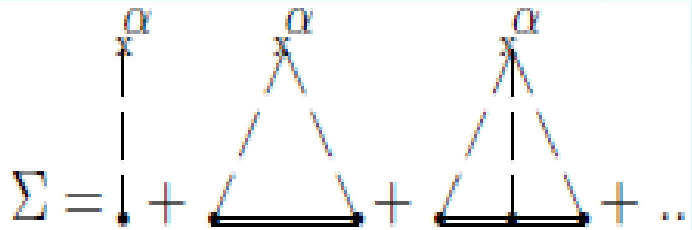
includes magnetic field and impurity scattering.

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



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

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



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

where

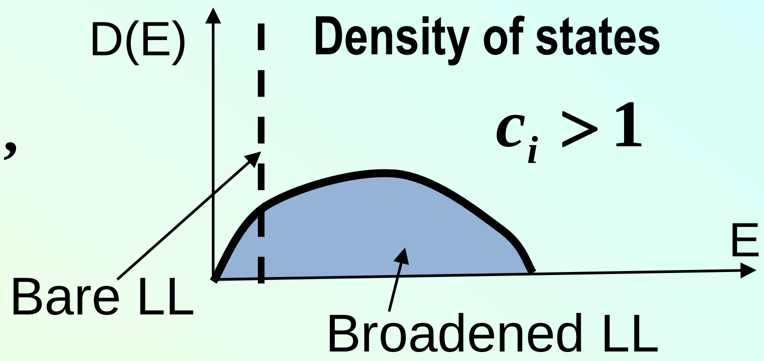
$$G_R(E,n) = \frac{E + E_g(1-c_i) \pm \sqrt{(E-E_1)(E-E_2)}}{2E\,E_g},$$

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

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

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

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



Landau level width

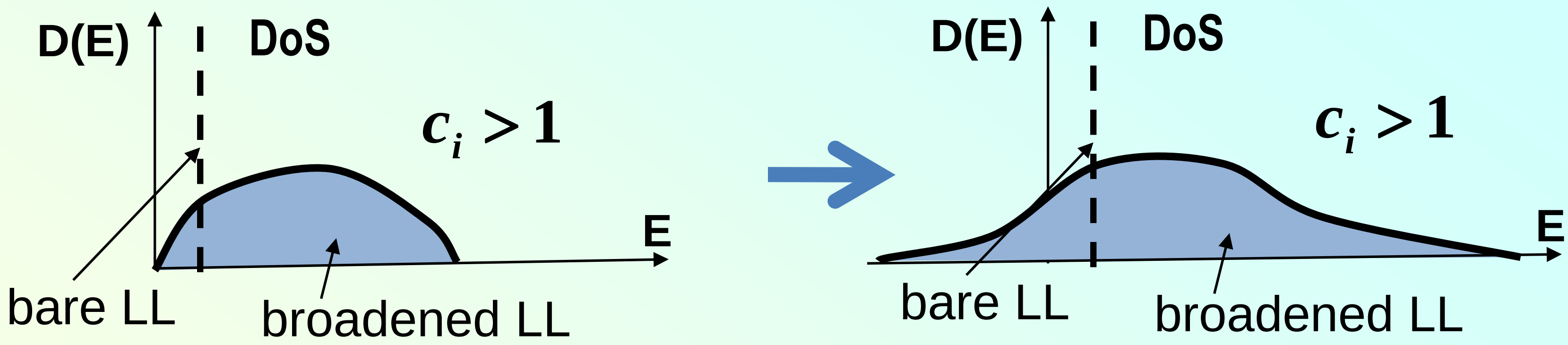
$$\Gamma_B \equiv (E_2 - E_1)/2 = 2E_g\sqrt{c_i} \propto \sqrt{B}.$$

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

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

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 ~$B_z^{1/2}$:



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

which gives $\overline{\sigma}_{zz} = \sigma_0 \sqrt{\pi \Gamma_0 / 4\omega_c} \approx 0.89 \sigma_0 \sqrt{\Gamma_0 / \omega_c}$.

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

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

In weak magnetic field this gives $\sigma_{zz}(B) = \sigma_0 \Gamma_0 / \left|\mathrm{Im}\Sigma(\mu, B)\right|$

In strong magnetic field we substitute the Green's function from the non-crossing approx. and obtain the monotonic part of interlayer conductivity

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

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 $\bar{\sigma}_{zz} \approx \dfrac{2\sigma_0\Gamma_0}{\pi E_g \sqrt{c_i}} = \sigma_0 \sqrt{\dfrac{4\Gamma_0}{\pi\hbar\omega_c}} \approx \sigma_0 \sqrt{\dfrac{\Gamma_0}{\omega_c}}\, 1.13.$

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

Result 1 Theoretical predictions on interlayer MR $R_{zz}(B)$

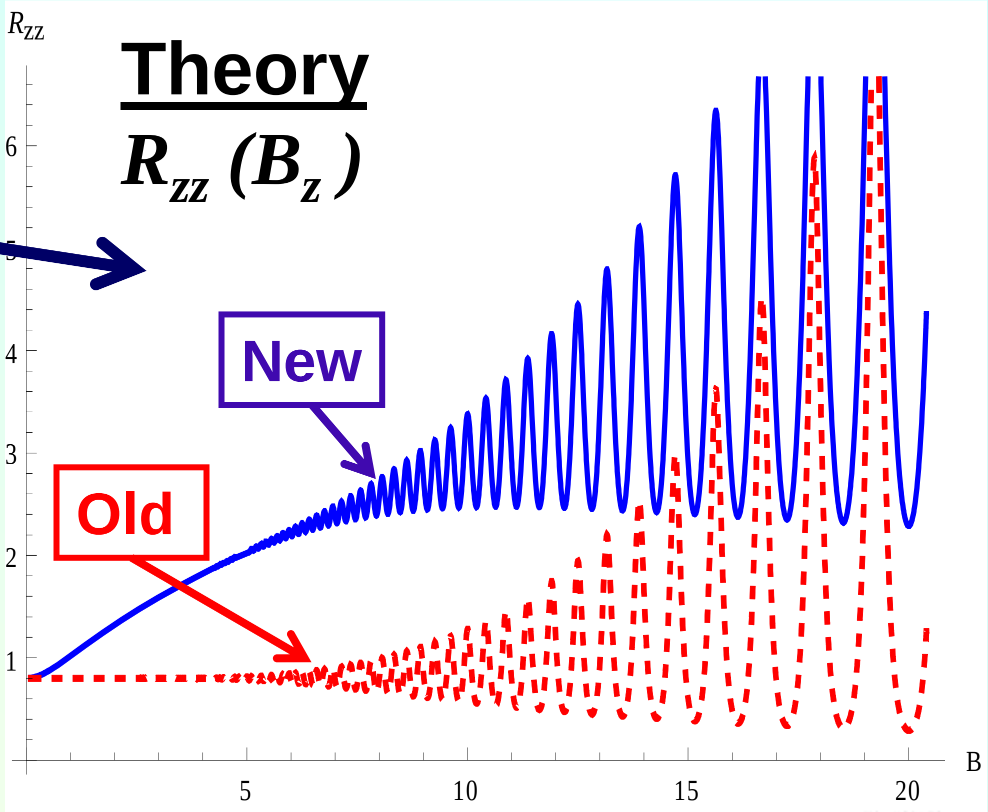
(magnetic field dependence: background and MQO)

Predictions of the new theory of MR:

1. Magnetoresistance (MR) grows with B_z at $\omega_C\tau > 1$: $R_{zz} \sim B_z^{1/2}$. (It grows even in the minima of MQO).

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.



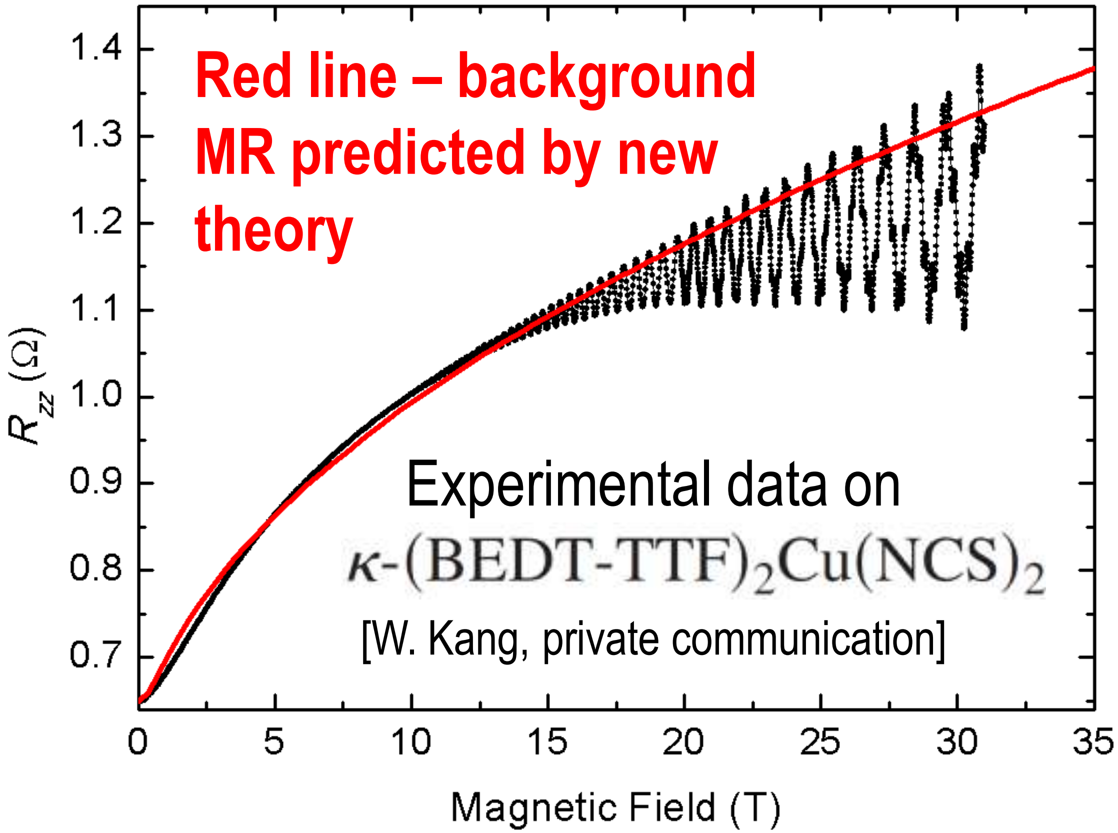
$$\bar{\sigma}_{zz}(B) \approx \sigma_0 \left[(2\omega_c\tau)^2 + 1 \right]^{-1/4}$$

The coefficient 2 slightly depends on the shape of Landau levels.

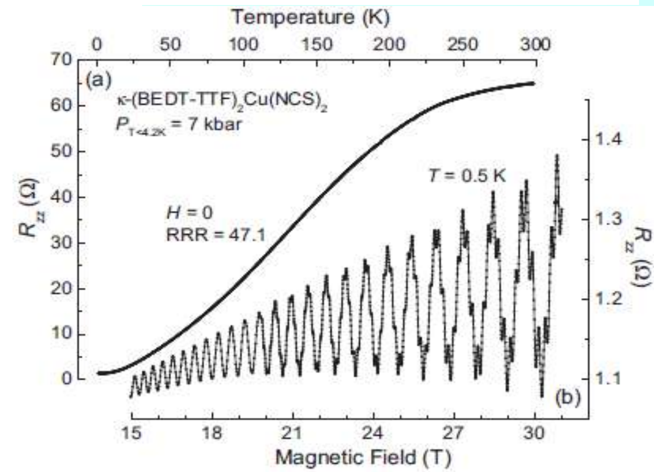
Details in P. D. Grigoriev, Phys. Rev. B 83, 245129 (2011).

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:



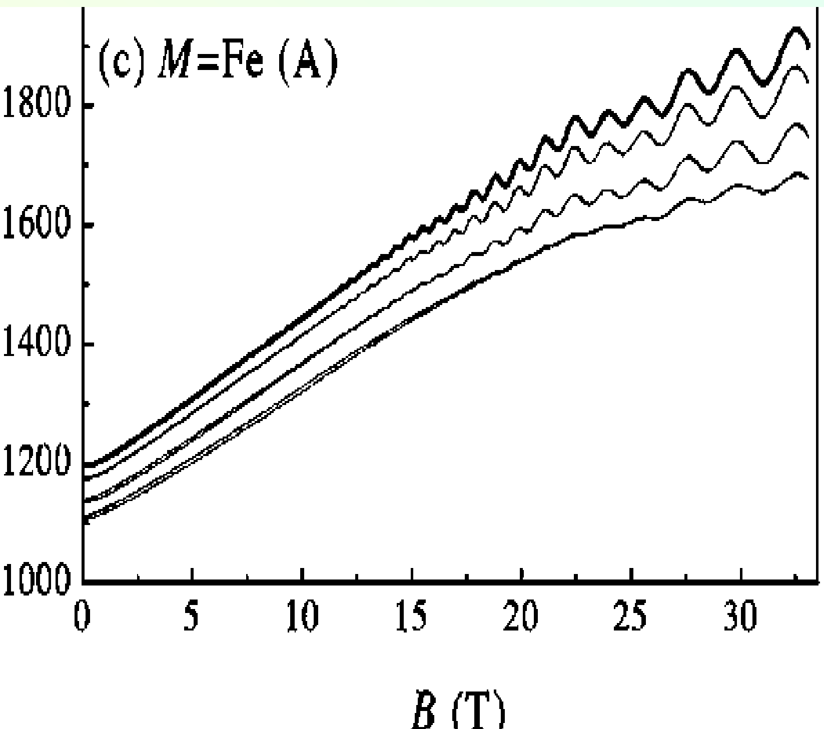
[W. Kang et al., PRB **80**, 155102 (2009)]

Comparison with experiments on interlayer MR $R_{zz}(B)$

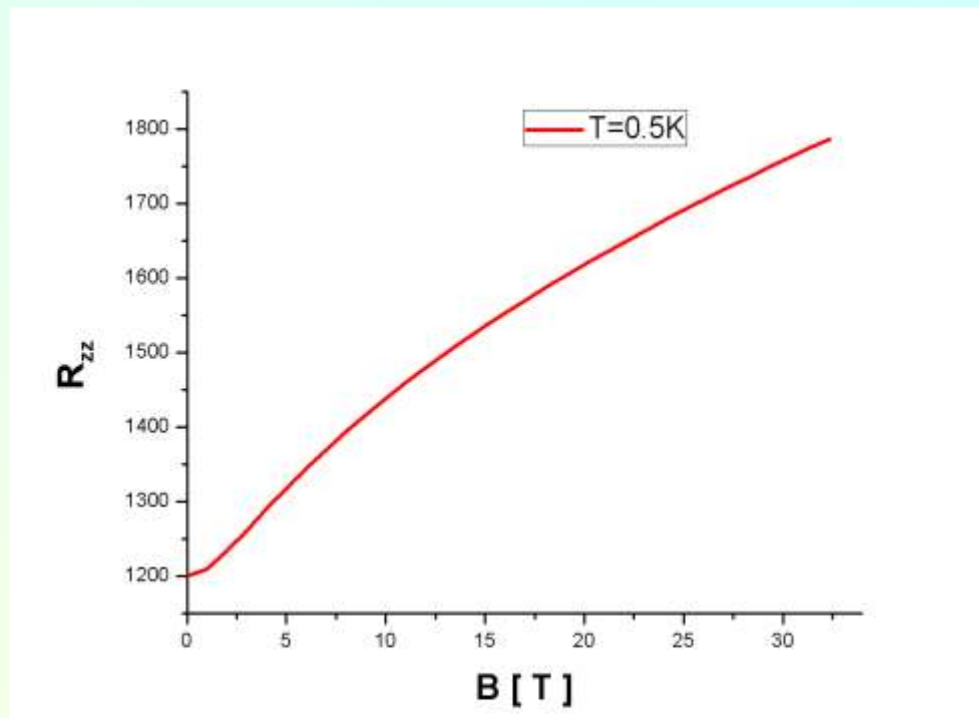
(magnetic field dependence: background and MQO)

measured field dependence of magnetoresistance in
$\beta'' - (BEDT-TTF)_4[(H_3O)Fe(C_2O_4)_3]C_5H_5N$

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

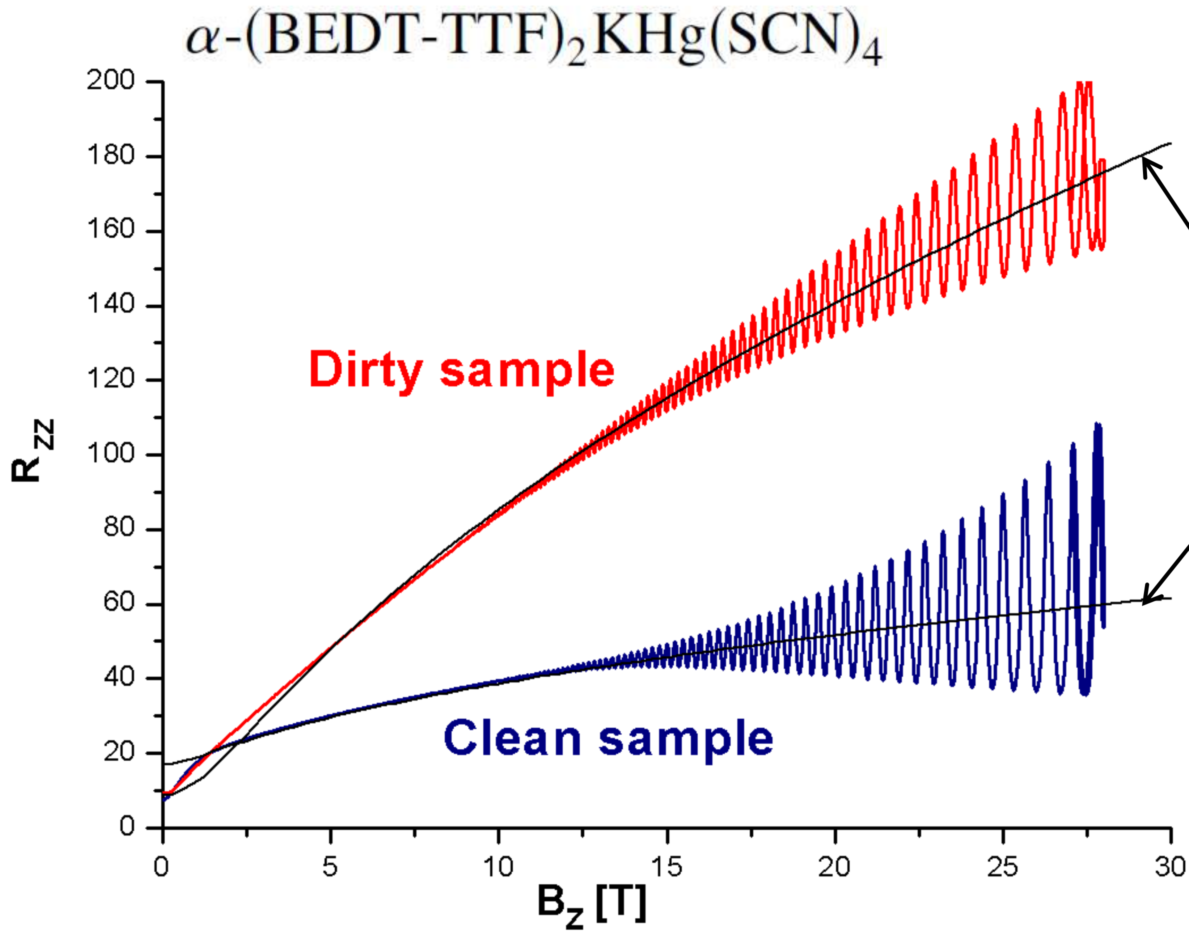


predicted field dependence of non-oscillating part of magnetoresistance



Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$

(magnetic field dependence: background and MQO)



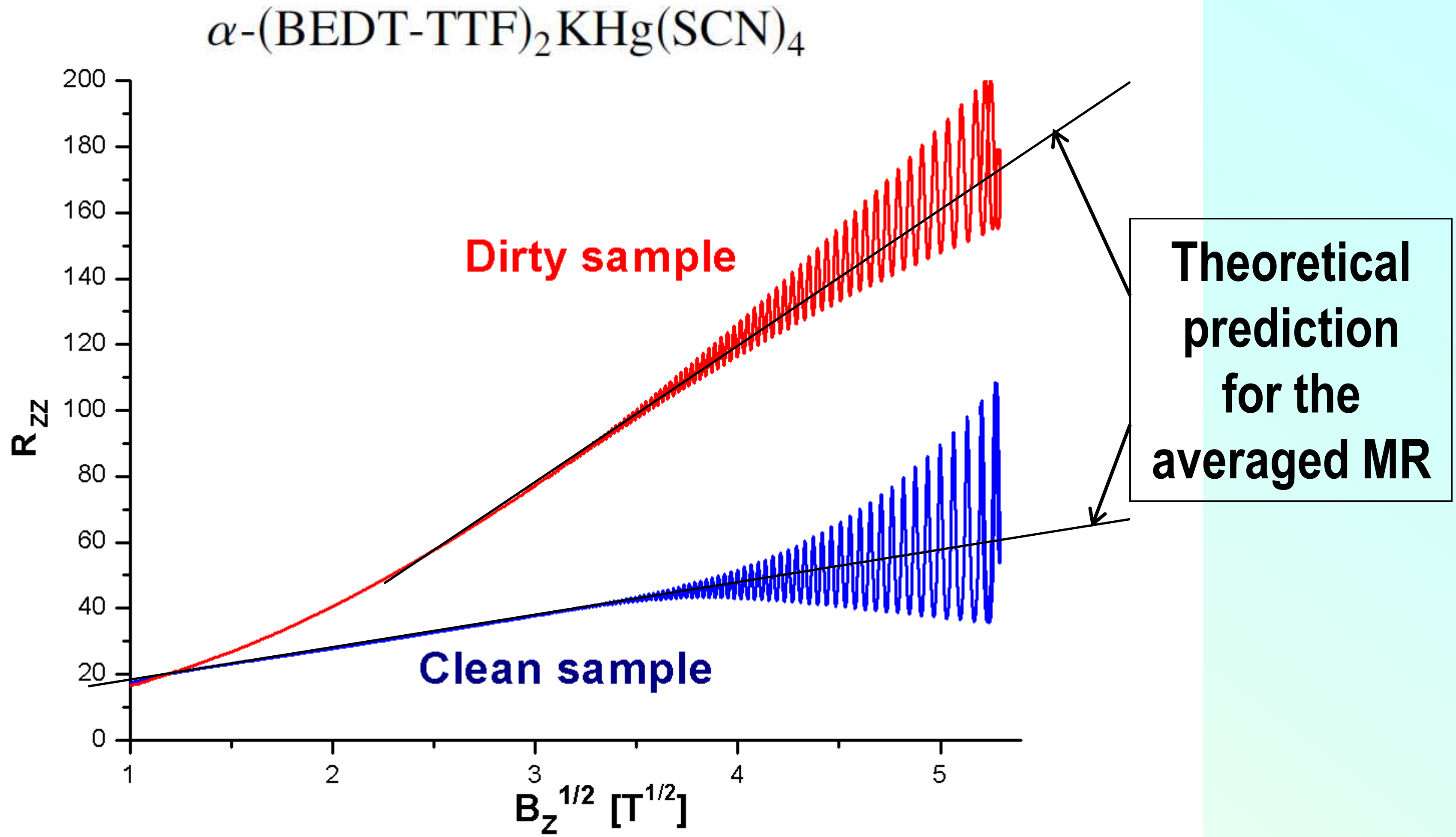
Theoretical prediction for the averaged MR

P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, arXiv:1205.0041

Agreement is excellent, especially in clean sample!

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$

(magnetic field dependence: background and MQO)



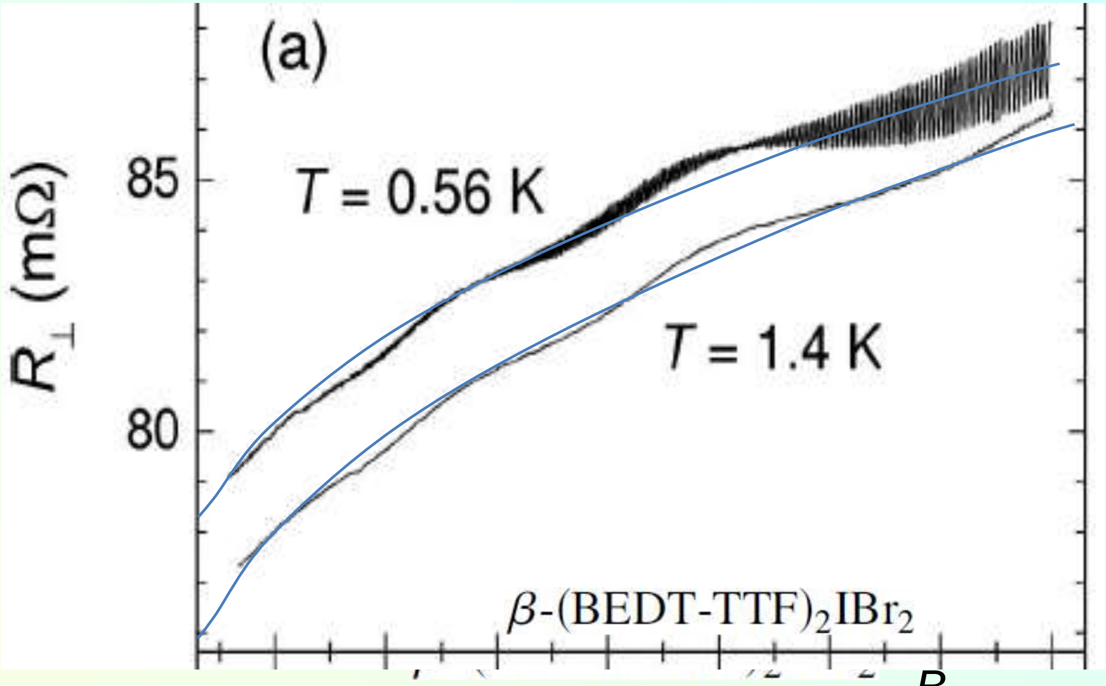
P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, arXiv:1205.0041

Agreement is excellent, especially in clean sample!

Result 1 Comparison with experiments on interlayer MR $R_{zz}(B)$

(magnetic field dependence: background and MQO)

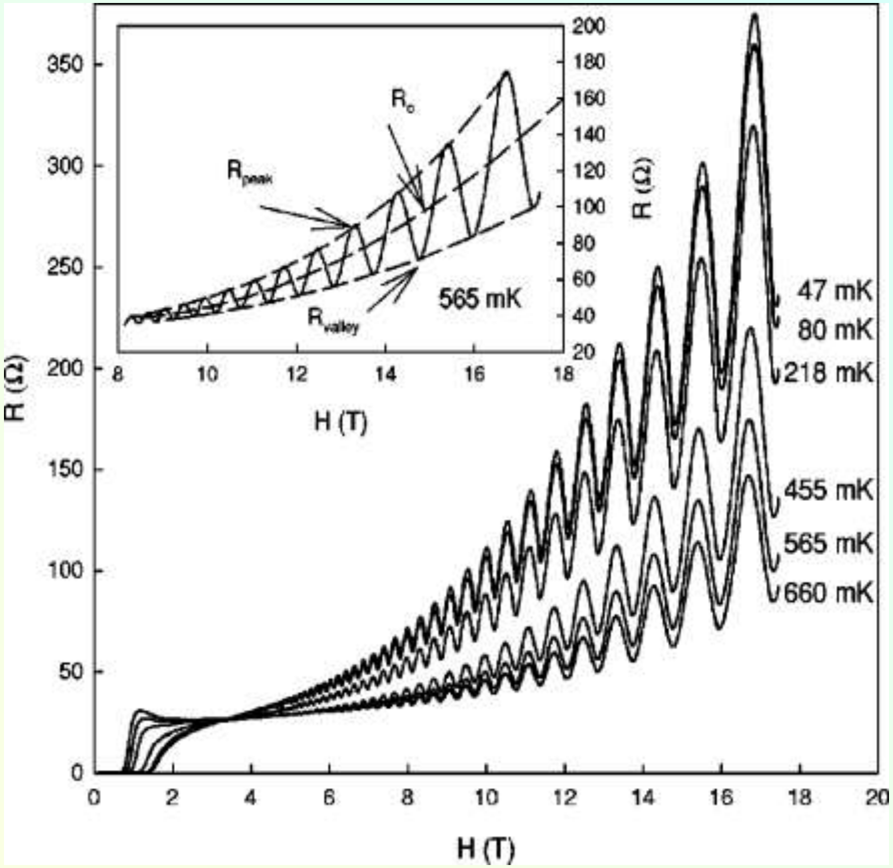
MR growth appears also at large $t_z \sim \Gamma$, as in β-(BEDT-TTF)$_2$IBr$_2$

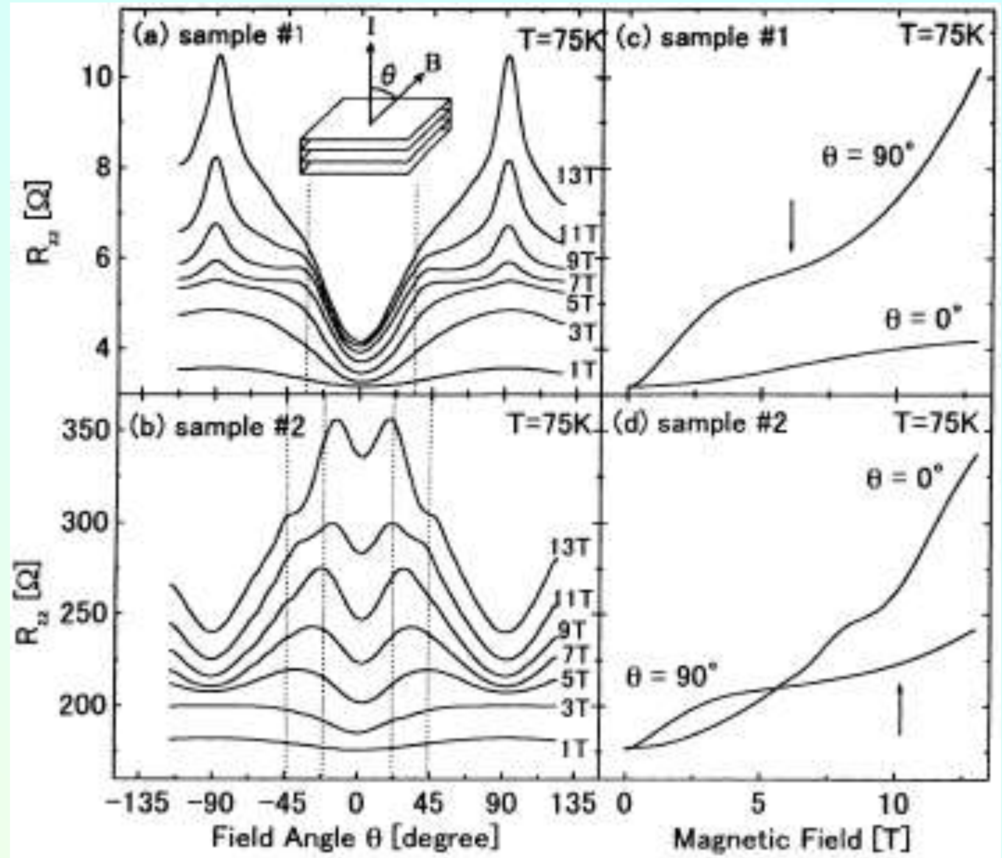


PRL 89, 126802 (2002);

Plan for future: consider MR at $t_z \sim \Gamma$

Interlayer MR in very anisotropic compounds





F. Zuo et al., PRB 60, 6296 (1999).
β-$(BEDT\text{-}TTF)_2SF_5CH_2CF_2SO_3$

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

Sometimes, MR grows too strongly with increasing B_z !

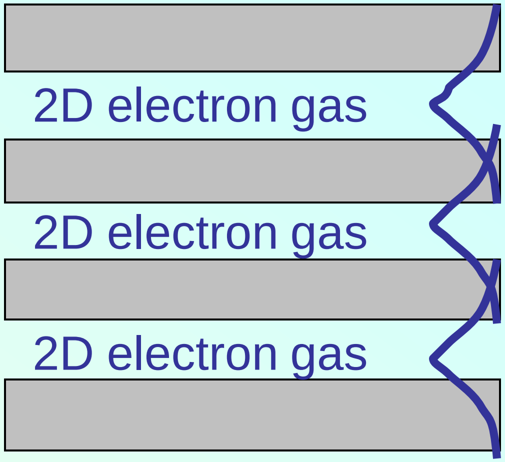
The model of weakly incoherent regime

is the same as in the coherent regime, but the parameters and approach to the solution differ.

The Hamiltonian contains 4 terms:

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

1 3 2 2



H_0 **- the 2D free electron Hamiltonian in magnetic field summed over all layers,**
H_I **– interaction with impurity potential,**
H_{int} **– e-e and e-ph interaction,**

H_t **– coherent electron tunneling between any two adjacent layers:**

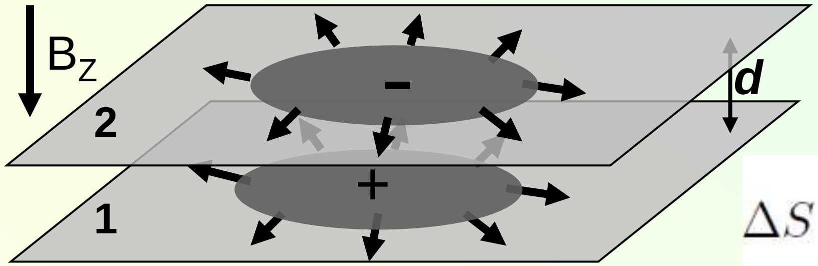
$$\hat{H}_t = 2t_z \sum_j \int dxdy[\Psi_j^\dagger(x,y)\Psi_{j-1}(x,y) + \Psi_{j-1}^\dagger(x,y)\Psi_j(x,y)],$$

Coulomb blocking of interlayer electron transport
(qualitative considerations)

Just after the jump the 2D electrons rapidly move on a distance $\xi \sim R_c$ or l_τ, where the Larmor radius $R_c = \hbar k_F c/eB_z$ and continue slow diffusive motion along the layer.

The Coulomb energy of charge separation between electron on one layer and a hole on another layer (see Fig) is $E_c\left(t\right) \approx 2\pi e^2 d/\varepsilon A\left(t\right)$

where $A\left(t\right) \approx \pi R^2\left(t\right)$ - is the time-dependent area of charge localization, $R\left(t\right) \approx R_c\sqrt{t/\tau+1}$, d – interlayer distance, ε - dielectric constant.



Due to Coulomb energy the quasiclassical action acquires additional term ($t_{\max} \sim \hbar/k_B T$):

$$\Delta S \approx \int_0^{t_{\max}} \frac{2e^2 d \cdot dt}{\varepsilon R_c^2\left(t/\tau+1\right)} = \frac{2\tau e^2 d}{\varepsilon R_c^2} \ln\left(1+\frac{t_{\max}}{\tau}\right)$$

This leads to Coulomb anomaly: $\sigma_{zz}\left(B_z\right)/\sigma_{zz}\left(0\right) \sim \exp\left(-\Delta S/\hbar\right)$

If ΔS>h, this gives Coulomb blockade of interlayer electron transport .

Calculation of Coulomb anomaly for interlayer electron transport

We follow Ref. 1 [L.S. Levitov, A.V. Shytov, JETP Lett. 66, 214 (1997)] and use semiclassical action, expanded up to quadratic terms in charge and current density deviation from equilibrium:

$$\mathcal{S} = \int\int d^4x_1 d^4x_2 \left[\mathbf{g}_1^T \hat{K}_{x_1-x_2} \mathbf{g}_2 + \delta_{12}\rho_1\rho_2 U\left(|r_1 - r_2|\right) \right]$$

Here $x_{1,2} \equiv (t_{1,2}, r_{1,2})$, integration over the interlayer coordinate z means the summation over two adjacent layers, $\delta_{12} \equiv \delta(t_1 - t_2)$,

$$\mathbf{g} = \mathbf{j} + \hat{D}\nabla\rho$$

is the external current, $D_{\alpha\beta}$ is the tensor of diffusion constants related to the conductivity tensor by the Einstein's formula: $\hat{\sigma} = e^2\nu\hat{D}$, where $\nu = dn/d\mu$ is compressibility, i.e. the density of states (DoS) at the Fermi level. The kernel $\hat{K}_{r,t}$ is related to the current-current correlator, yielding the correct Nyquist spectrum of current fluctuations in equilibrium:

$$(K^{-1}_{\omega,q})_{\alpha\beta} = \langle\langle \mathbf{g}^{\alpha}_{i\omega,q}\mathbf{g}^{\beta}_{-i\omega,-q}\rangle\rangle = \sigma_{\alpha\beta}|\omega| + \sigma_{\alpha\alpha'}D_{\beta\beta'}q_{\alpha'}q_{\beta'}$$

Calculation of quasiclassical action

The quasi-classical action is obtained by substitute the solution of classical electrodynamic equations :

$$\begin{array}{ll} \text{(i)} & \dot{\rho} + \nabla \cdot \mathbf{j} = \mathcal{J}(r,t)\ ; \\ \text{(ii)} & \mathbf{j} + D\nabla\rho = \hat{\sigma}(\omega,q)\mathbf{E}\ ; \\ \text{(iii)} & \mathbf{E}(r,t) = -\nabla_r \int dr' \rho(r',t) U(|r-r'|) \end{array}$$

The solution is obtained using the Fourier transform:

$$\begin{aligned} \rho(\omega,q) &= \frac{\mathcal{J}(\omega)}{|\omega| + Dq^2 + \sigma_{xx} q^2 U_q}\ , \\ \mathbf{j}(\omega,q) &= -i\mathbf{q}\rho(\omega,q)\left(D + \sigma_{xx} U_q\right)\ , \end{aligned}$$

! differs from that in Ref. 1, **where** $\mathbf{j}(\omega,q) = -i\hat{K}^{-1}(\omega,q)\mathbf{q}U_q\rho(\omega,q)$

However, the final action coincides with that in Ref. 1 [LSh]:

$$\mathcal{S}_0(\tau_1) = \sum_{\omega,q} \frac{|\mathcal{J}(\omega)|^2}{|\omega| + Dq^2} \frac{U_q}{|\omega| + Dq^2 + \sigma_{xx} q^2 U_q}$$

Application to double-layer system

We assume, that the charge and current densities on two adjacent layers differ by only the sign of the electric charge, i.e. the relaxation of the electron on the layer 2 and of the hole on layer 1 is identical. Then one can avoids the matrix notations and write the Coulomb interaction as a sum from two layers:

$$U\left(|r_1 - r_2|\right) = \frac{1}{\varepsilon |r_1 - r_2|} - \frac{1}{\varepsilon \sqrt{|r_1 - r_2|^2 + d^2}}$$

$$U_q \equiv \int e^{iqr} U\left(|r|\right) d^2 r = \frac{2\pi}{q\varepsilon}\left(1 - e^{-qd}\right)$$

The charge source on two layers than differ only by sign and becomes

$$\mathcal{J}(\boldsymbol{r}, t) = e\left|\Psi(\boldsymbol{r})\right|^2 \left[\delta(t + t_1) - \delta(t - t_1)\right],$$

Wave function Ψ is arbitrary (not only δ-function as in Ref. 1)

This charge source corresponds to the jump of an electron to adjacent layer at time $-t_1$ and jump back at time $+t_1$.
In imaginary time the Fourier transform of this source is $\mathcal{J}(\omega) = 2ie \sin \omega\tau_1$

Calculation of quasiclassical action (2)

$\sigma_{zz}/\sigma_{zz0} = \exp\left[-\mathcal{S}_1(T,V)/\hbar\right],$ **where** $\begin{array}{c}\mathcal{S}_1(T,V) = \mathcal{S}_0(T,\tau_1^*) - 2eV\tau_1^*, \\ \partial\mathcal{S}_0(T,\tau_1)/\partial\tau_1|_{\tau_1=\tau_1^*} = 2eV.\end{array}$

Since the distance between the molecular layers is usually *d* ~ 1*nm*, the voltage *V* = *Ed* applied between two conducting layers is usually much smaller than temperature and can be neglected. Then $\tau_1^*(T, V\to 0) = 1/4T.$

The action

$$\mathcal{S}_1(T,V \to 0) = \sum_{k=0}^{\infty}\int_0^{\infty}\frac{qdq}{\pi}\frac{4e^2T}{2\pi T(2k+1)+Dq^2} \times \frac{U_q}{2\pi T(2k+1)+Dq^2+\sigma_{xx}q^2U_q}.$$

Usually $d \ll 1/q \sim \sqrt{D\tau},$ **and** $U_q \approx 2\pi d$ **. Then**

$$\mathcal{S}_1(T,V\to 0) = \frac{e^2U_q}{\pi^2}\sum_{k=0}^{k_{\max}}\frac{\ln\left(1+\sigma_{xx}U_q/D\right)}{(2k+1)\,\sigma_{xx}U_q}.$$

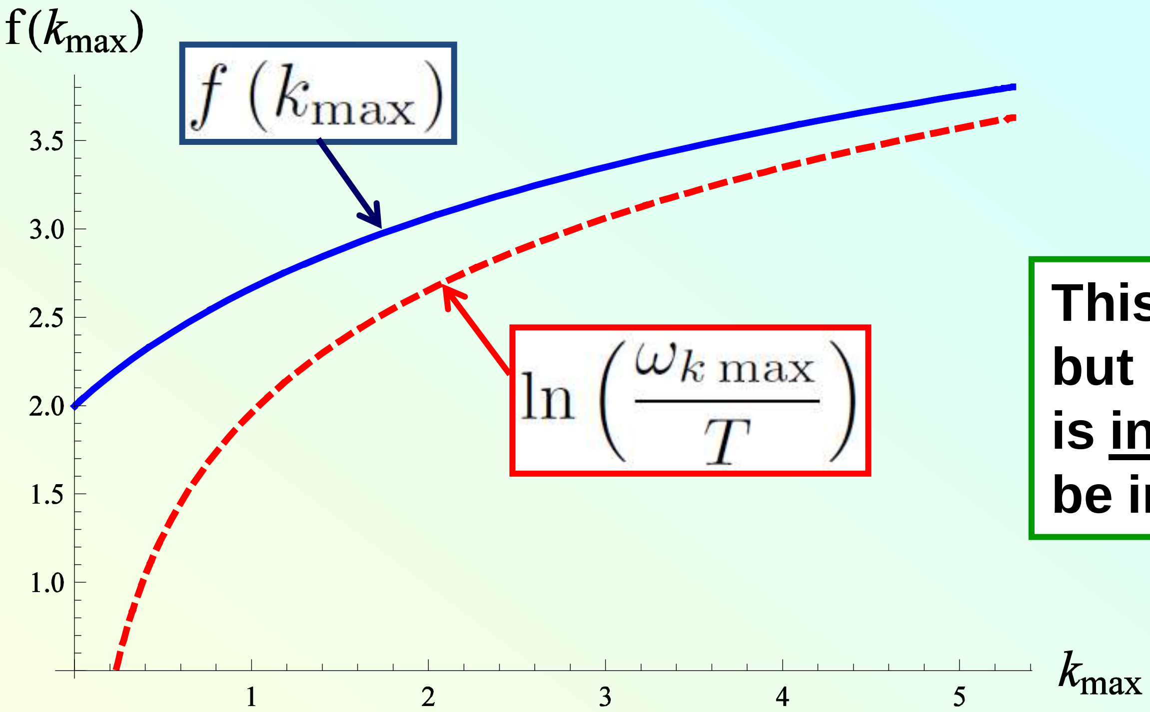
Finally $$\mathcal{S}_1(T) = \frac{e^2\ln\left(1+2\pi\sigma_{xx}d/D\right)}{2\pi^2\sigma_{xx}}\left[2\ln 2+\gamma+\psi\left(3/2+k_{\max}\right)\right]$$

where $k_{\max} \equiv \omega_{k\max}/4Te^{\gamma} \approx \max\left\{\hbar/\tau, \hbar\omega_c\right\}/4Te^{\gamma}$

Approximately $$\mathcal{S}_1(T) \approx \frac{e^2\ln\left(1+2\pi e^2\nu d\right)}{2\pi^2\sigma_{xx}}\ln\left(\frac{\omega_{k\max}}{T}\right)$$

Coincides with Ref. 1

Importance of the correction to $f(k_{max})$



This is a minor correction, but since in conductivity it is <u>in the exponent</u>, it may be important.

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

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

Calculation of Coulomb anomaly in the interlayer conductivity

The quasiclassical action due to Coulomb interaction

$$\mathcal{S}_1(T) = \frac{e^2 \ln\left(1 + 2\pi\sigma_{xx} d/D\right)}{2\pi^2 \sigma_{xx}} f\left(k_{\max}\right), \quad f\left(k_{\max}\right) \equiv 2\ln 2 + \gamma + \psi\left(3/2 + k_{\max}\right)$$

We use the diffusion coefficient in high magnetic field $\omega_c\tau >> 1$:

$D \approx R_c^2/2\tau$ **consistent with Drude formula** $D \approx D_0/\left[1 + (\omega_c\tau)^2\right]$

and Einstien's relation between conductivity and diffusion coefficient

$$\sigma_{xx} = e^2\nu D = \left(e^2/2\pi\hbar\right)\left[\nu\left(E_F, B\right)/\bar{\nu}\right]\left(2n_L + 1\right)/\omega_c\tau .$$

Finally

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

where $\sigma_{zz0}\left(B_z\right) \approx \sigma_{zz0}/\left[\left(2\omega_c\tau\right)^2 + 1\right]^{1/4}$

Usually, this is small correction

Thus, the Coulomb anomaly influences the interlayer electron transport only at low 2D electron concentration and in strong magnetic field, when $\omega_c\tau \gtrsim n_L$

Effect of finite interlayer hopping time

(phenomenological considerations)

The above calculation does not take into account finite interlayer transfer integral t_z, which broadens the 2D electron energy levels and limits the diffusive long-time electron dynamics in a 2D layer by the new time scale $\tau_{tz} \approx \hbar/2t_z$ The effect of finite t_z is similar to the effect of applied voltage V , because it also separates the energies on two layers by the energy up to $4t_z$.

$$\mathcal{S}_1(T,V) = \mathcal{S}_0(T,\tau_1^*) - 2eV\tau_1^*,$$

The voltage V enters the equation for τ_1:

$$\partial\mathcal{S}_0(T,\tau_1)/\partial\tau_1|_{\tau_1=\tau_1^*} = 2eV.$$

This reduces the Coulomb anomaly when $t_z > T$.

Finite t_z can be approximately taken into account by an effective increase of temperature according to the rule $T \to T^* \approx T + t_z$

Comparison with experiments in organic metals

Among layered organic metals he Coulomb effects are expected to be most important in $\beta\text{-}(BEDT\text{-}TTF)_2SF_5CH_2CF_2SO_3$ **because the FS area** $\pi k_{F1}k_{F2} = 0.0192\,\mathring{A}^{-2}$ **is only 5% of first Brillouin zone, which means low electron concentration and** $n_L \sim 10$.

Other parameters: $F = 200T$, $m^* = 2m_e$, $t_z \leq 18.5\mu eV = 0.21K$

$d \approx 17.5\mathring{A}$ $\varepsilon \approx 20$

Substitution of numbers assuming weak DoS oscillations gives

$$\sigma_{zz} \approx \frac{\sigma_{zz0}}{\left[(\omega_c\tau)^2 + 1\right]^{1/4}} \exp\left[-\frac{\omega_c\tau \ln(1 + 130/\varepsilon) \quad f(0.08\,B[T]/T^*[K])}{\pi(2F/B + 1)}\right]$$

Due to the weakly coherent theory of interlayer magnetotransport
[P. D. Grigoriev, PRB 83, 245129 (2011)]

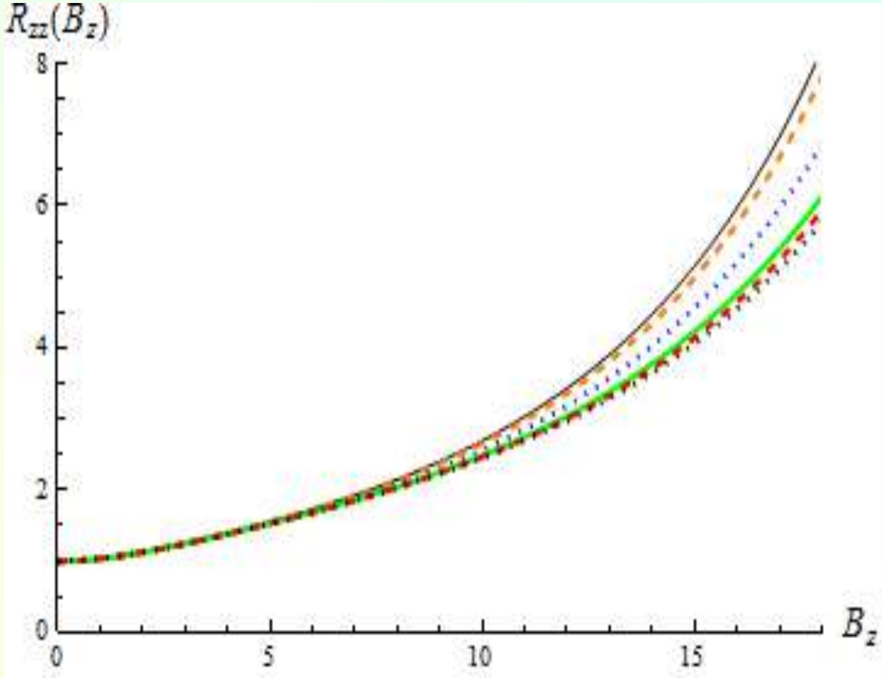
In this compound and experiment

$T_D \approx 0.5K$ **=>** $\tau_D = \hbar/2\pi T_D$

However, T_D **consists of contributions from short- and long-range disorder**

=> actual τ **may be longer** τ_D **.**

Comparison with experiments in organic metal β-(BEDT-TTF)$_2$SF$_5$CH$_2$CF$_2$SO$_3$



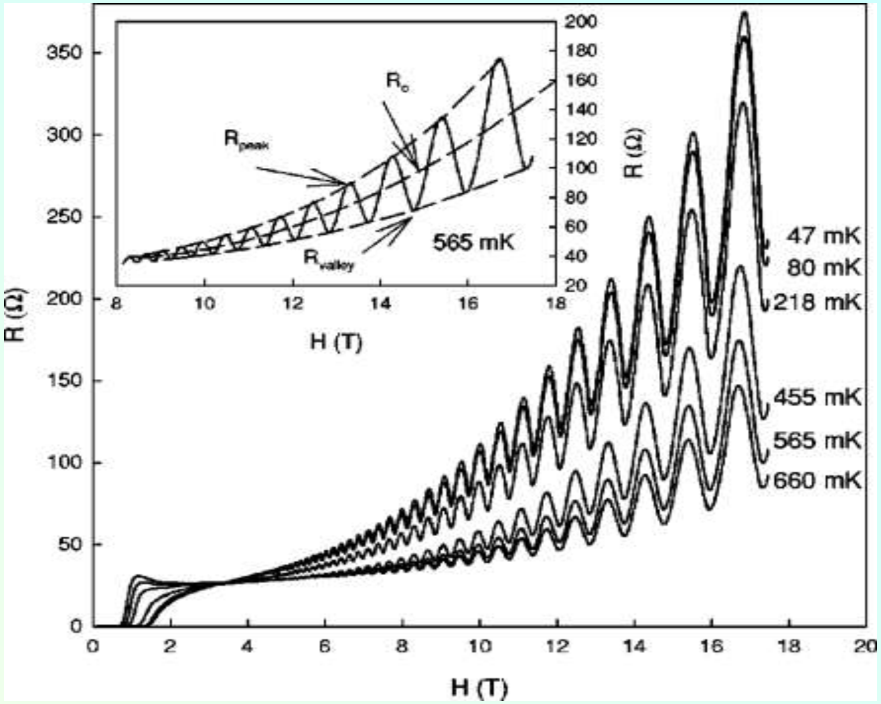
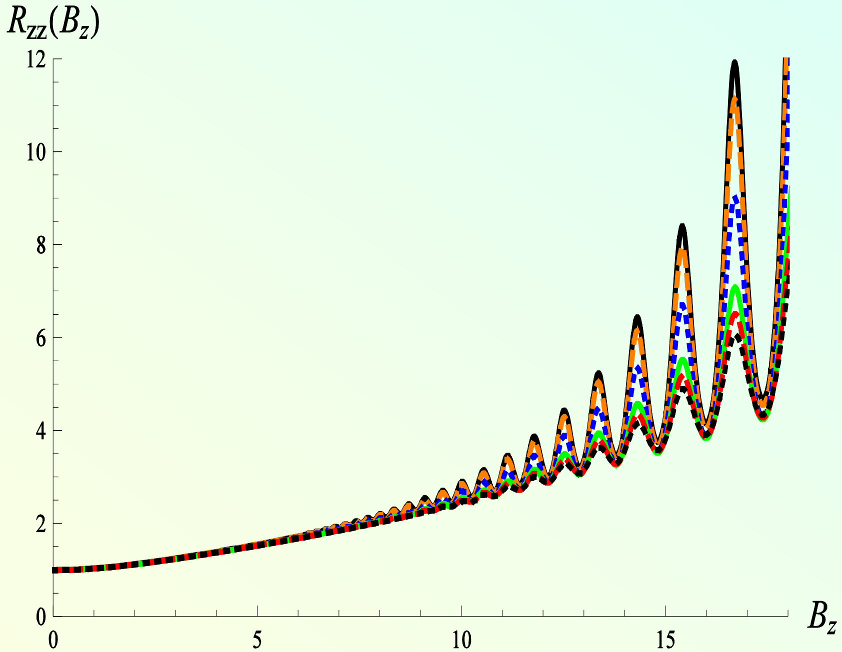
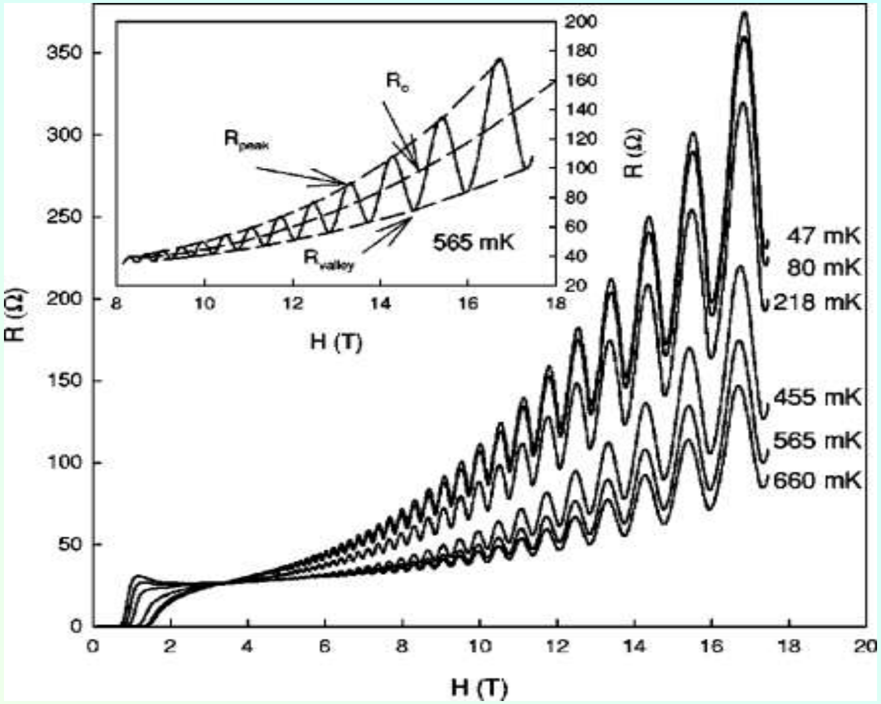


FIG. 3: The predicted field dependence of the background (non-oscillating) magnetoresistance $R_{zz}(B_z)/R_{zz}(0)$ in β-(BEDT-TTF)$_2$SF$_5$CH$_2$CF$_2$SO$_3$ at $t_z = 0.2K$ for six values of temperature: $T = 0.66$ K, 0.565 K, 0.455 K, 0.218 K, 80 mK, and 47 mK. The lower the temperature, the larger the magnetoresistance

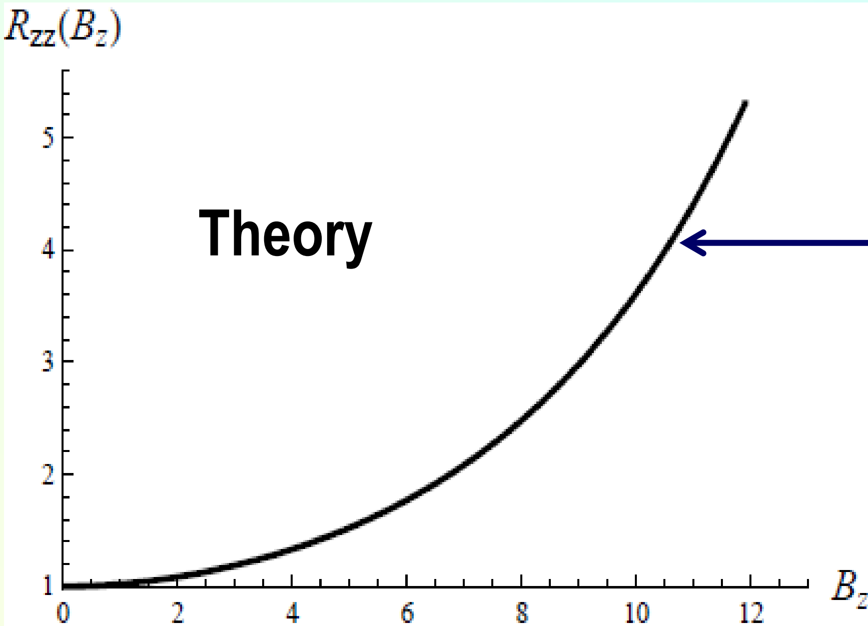
Agreement is reasonable. It improves after MQO are taken into account.

Effect of quantum oscillations

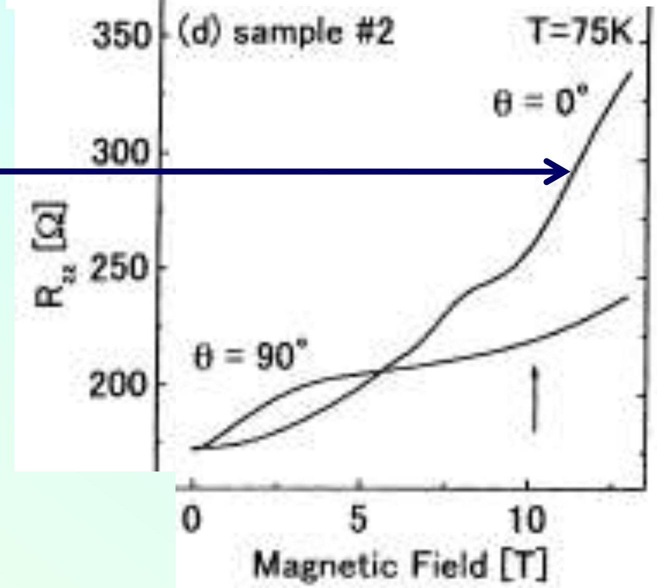




Comparison with experiments



Experiment GaAs/AlGaAs



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

Summary for Coulomb effects on interlayer magnetoresistance

- **The Coulomb anomaly for interlayer electron transport in magnetic field is approximately given by**

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

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

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

- **Usually, the Coulomb anomaly gives a small correction to interlayer conductivity of layered metals. But there are several compounds, as β-(BEDT-TTF)$_2$SF$_5$CH$_2$CF$_2$SO$_3$ and heterostructures, where Coulomb anomaly in strong magnetic field considerably suppresses interlayer conductivity σ_{zz}**

Conclusions

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

In one-electron approach the reduction of dimensionality + magnetic field increase the effect of impurities, which strongly modifies the magnetic-field dependence of interlayer conductivity

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

Thank you for attention!