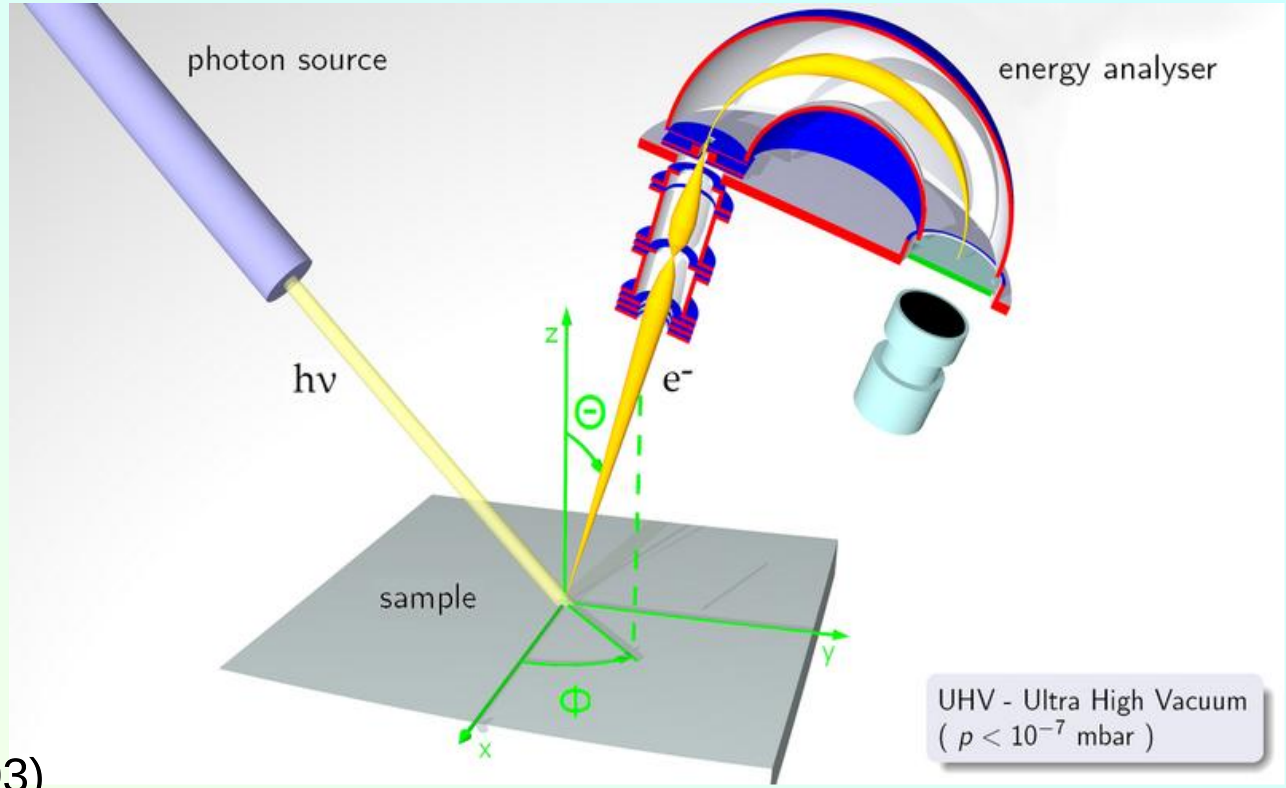
ARPES (Angle resolved photoemission spectroscopy)

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.



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

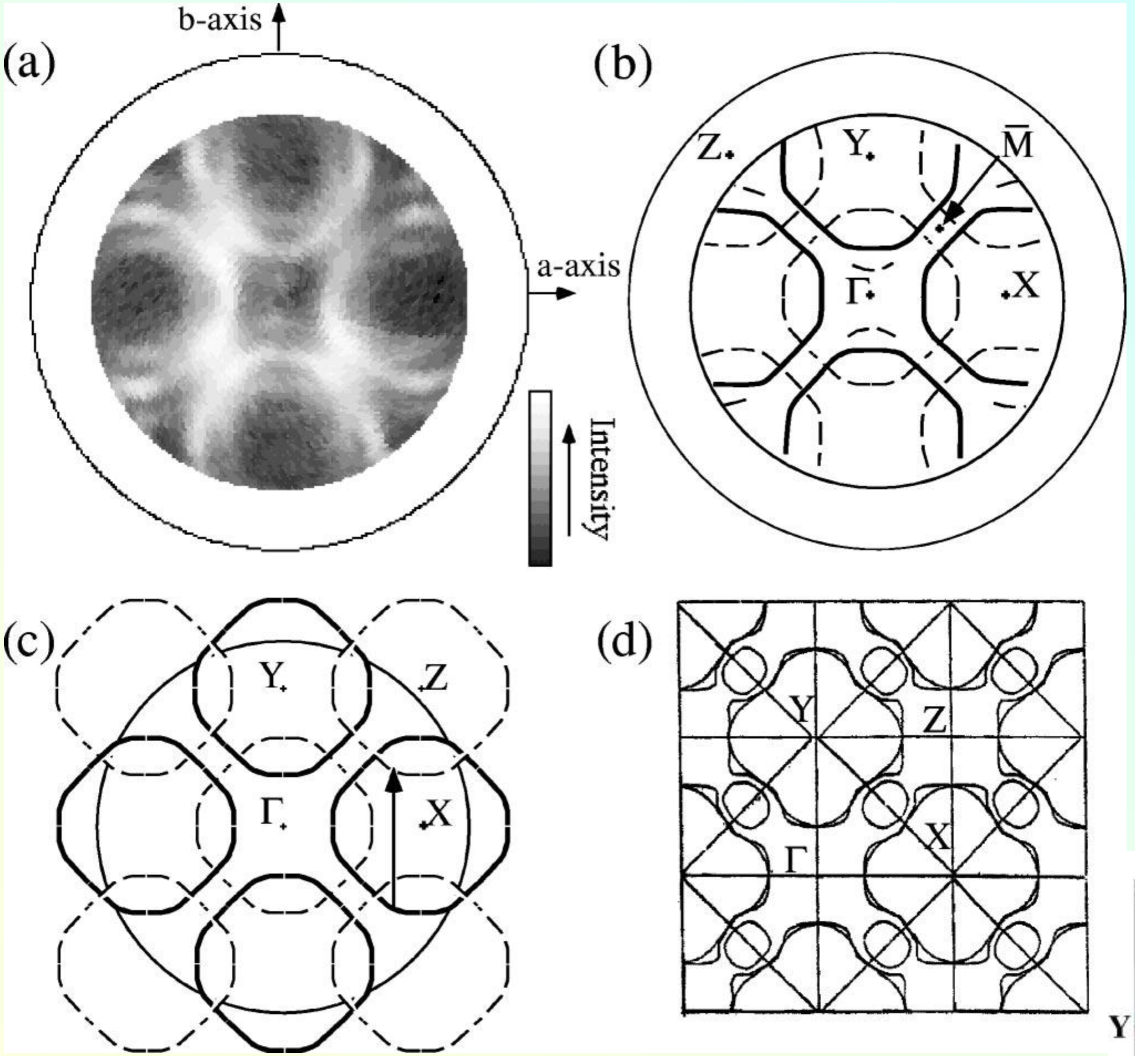
$$I(\mathbf{k},\omega) = A(\mathbf{k},\omega) f(\omega)$$

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

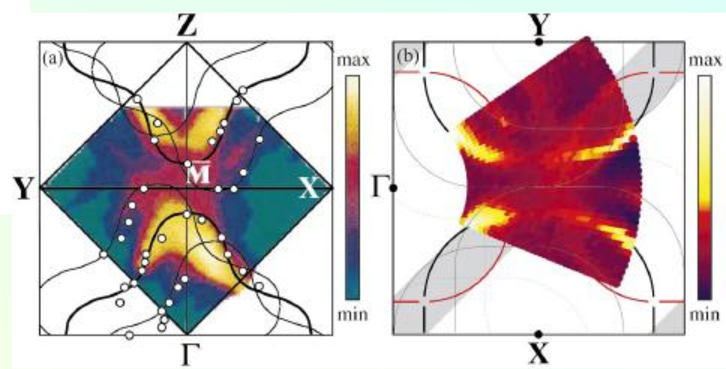
Therefore can find out information about *E(k)*

Drawbacks: 1) Often unavailable; 2) 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).

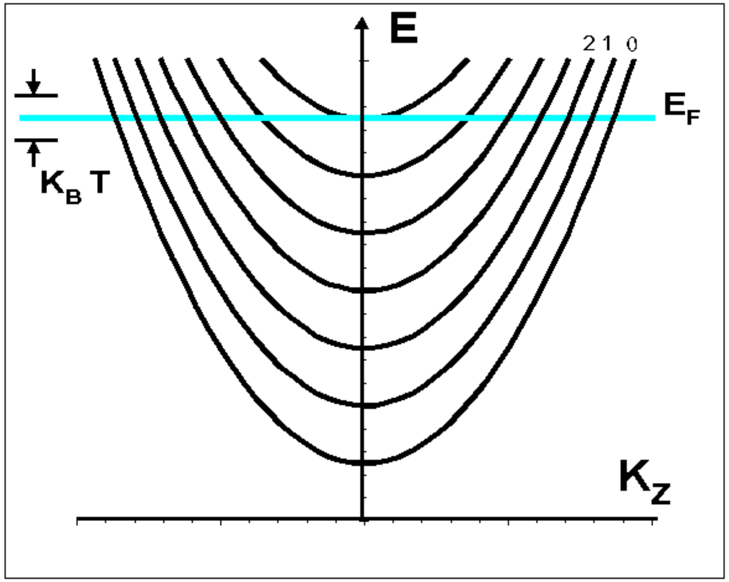


Drawback 2: Ambiguous interpretation.

Origin of magnetic quantum oscillations in metals

For parabolic electron dispersion in zero magnetic field
$\varepsilon(p)= p_x^2/2m_x + p_y^2/2m_y + p_z^2/2m_z$,

in magnetic field directed along z-axis the dispersion relation is
$\varepsilon(n,p_z)=\hbar\omega_c(n+1/2)+p_z^2/2m_z$,
where $\omega_c=eB/mc$
(Landau level quantization).



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

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

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

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

MQO of thermodynamic quantities

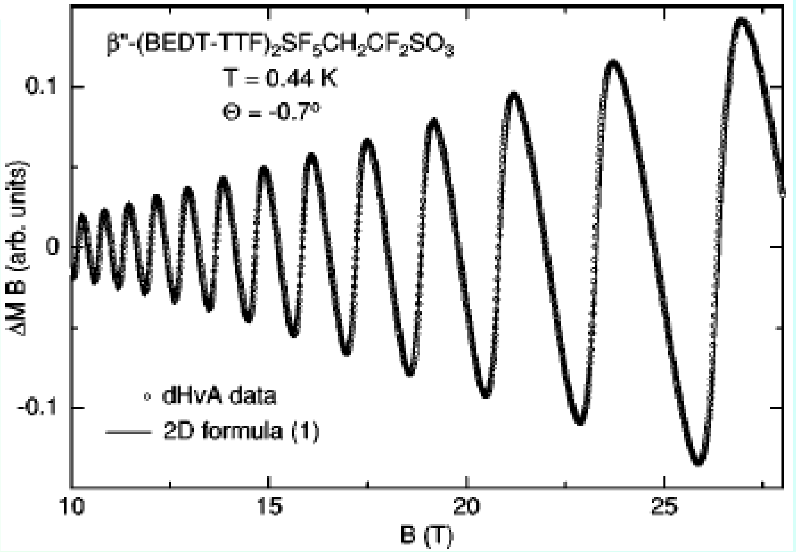
The thermodynamic potential is given by the integral of DoS:

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

where the density of electron states (DoS) is given by the sum over quantum states (Landau levels and p_z):

$$\rho(E, B) = \int dp_z \sum_n \delta\left(\varepsilon(n, p_z) - \mu\right) \frac{eB}{h^2 c}$$

Magnetization is given by the derivative $\tilde{M}(B) = -\frac{\partial \tilde{\Omega}}{\partial B}$



The transport quantities cannot be calculated so simply, but the main oscillating term in 3D metals comes from the scattering rate 1/τ which is proportional to the DoS (in Born approximation). Then

$$\frac{\Delta\tilde{\sigma}_{zz}}{\sigma_{zz}} \sim \frac{\Delta\tilde{\sigma}_{xx}}{\sigma_{xx}} \sim \frac{\Delta\tilde{\sigma}_{yy}}{\sigma_{yy}}, \sim \nu^{-1}(\mu) \sum_m \left(\frac{m_m^* S_m}{H}\right)^2 \frac{\partial \tilde{M}_m}{\partial H}, \quad (11.11)$$

Lifshitz-Kosevich formula for MQO

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

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

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

where the dHvA fundamental frequency $F = chA_{extr}/(2\pi)e$
allows to measure the Fermi-surface shape.

The temperature damping factor $R_T = \left(2\pi^2 k_B T/\hbar\omega_c\right)/\sinh\left(2\pi^2 k_B T/\hbar\omega_c\right)$
where $\omega_C = eH/m^*c$, allows to measure m*.

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

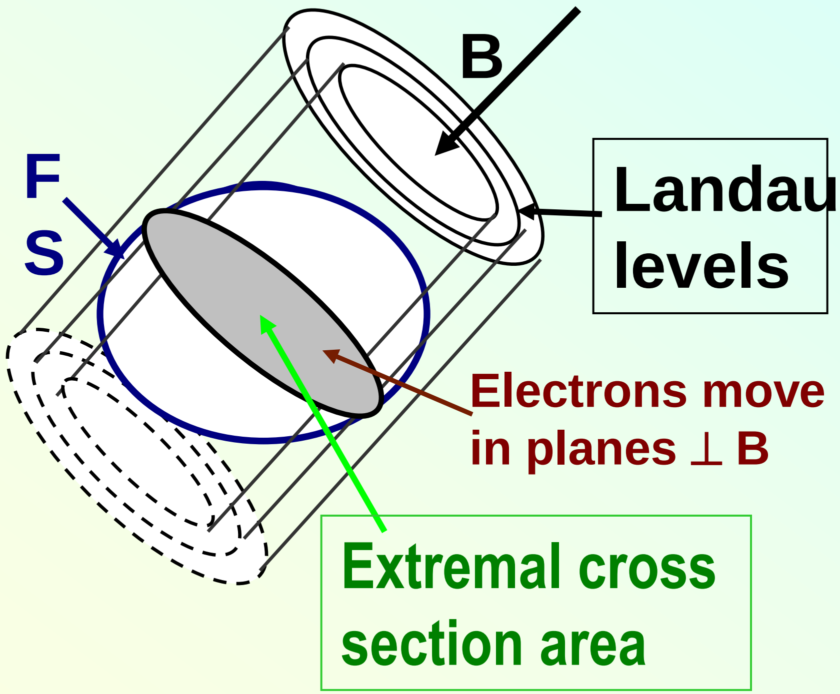
allows to measure the electron mean free time $\tau = h/(2\pi)^2 k_B T_D$

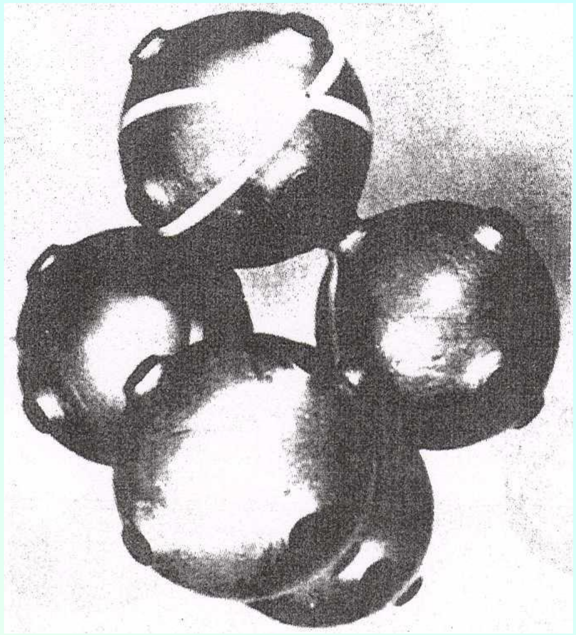
and the spin damping factor $R_s(p) = \cos\left(\frac{\pi p g m^*}{2m_0}\right)$ allows to measure the g-factor (if m* is known from T-dependence)

3D compounds in tilted magnetic field

3D case

$k_{\parallel}$ is conserved.





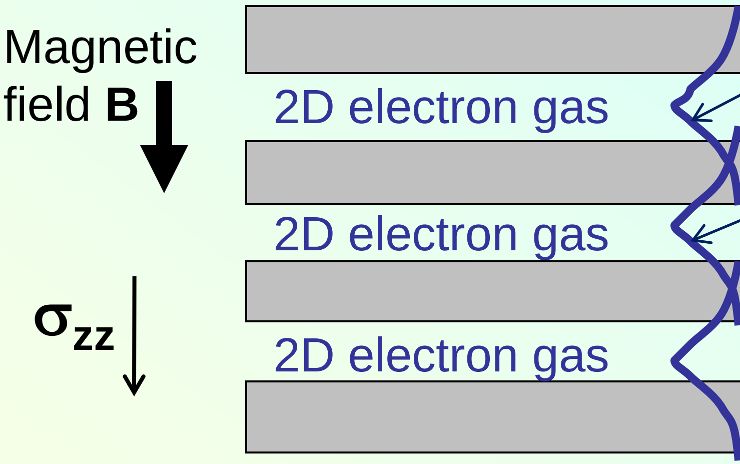
Fermi surface of gold

Extremal cross-section area of Fermi surface (FS), given by $F = \frac{chA_{extr}}{(2\pi)e}$, MQO frequency and measured at various tilt angles of magnetic field, allows to obtain the total FS geometry of metals.

MQO is a traditional tool to study FS geometry

Layered quasi-2D metals

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

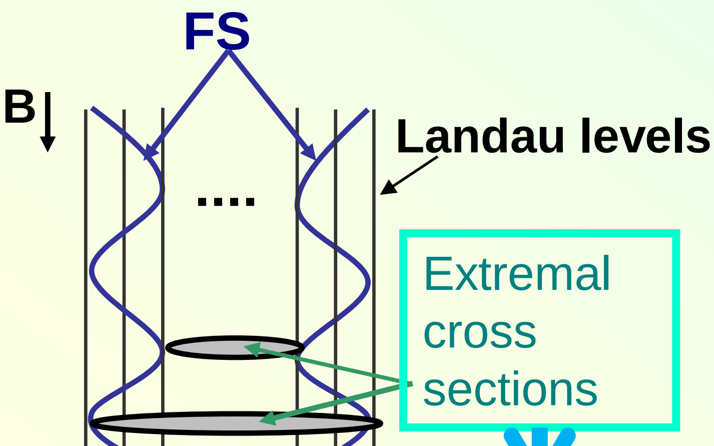


Electron wave functions overlap leads to the finite interlayer transfer integral t_z

Electron dispersion in the tight-binding approximation is highly anisotropic:
$\varepsilon(p)=\varepsilon_{||}(p_{||})+2t_z \cos(p_z d/\hbar)$, $t_z \ll E_F$

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

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



Extremal cross sections

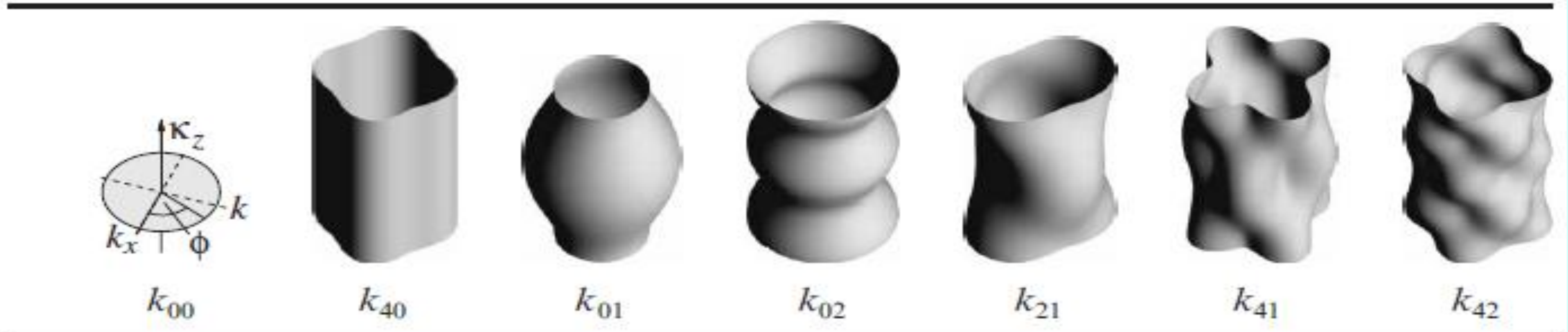
Two close frequencies => beats of MQO

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

Harmonic expansion for the angle-dependence of FS cross-section area (MQO frequency) in Q2D layered metals.

Harmonic expansion of Fermi momentum

$$k_F(\phi, k_z) = \sum_{\mu,\nu \geq 0} k_{\mu\nu} \cos(\nu k_z c^*) \cos(\mu\phi + \phi_\mu) .$$



Harmonic expansion of the angular dependence of FS cross-section area (measured as the frequency of magnetic quantum oscillations):

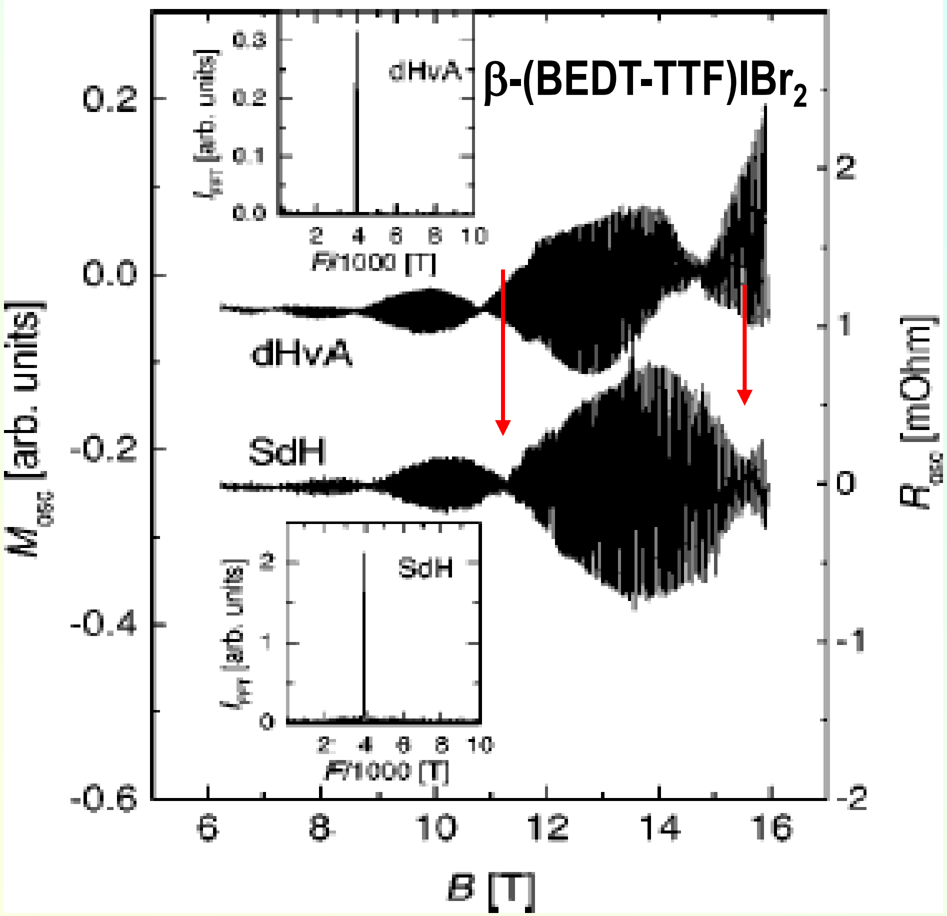
$$A(k_{z0}, \theta, \varphi) = \sum_{\mu,\nu} A_{\mu\nu}(\theta) \cos[\mu\varphi + \delta_\mu] \cos(\nu c^* k_{z0}) ,$$

One can derive the relation between the first coefficients $k_{\mu\nu}$ and $A_{\mu\nu}$!

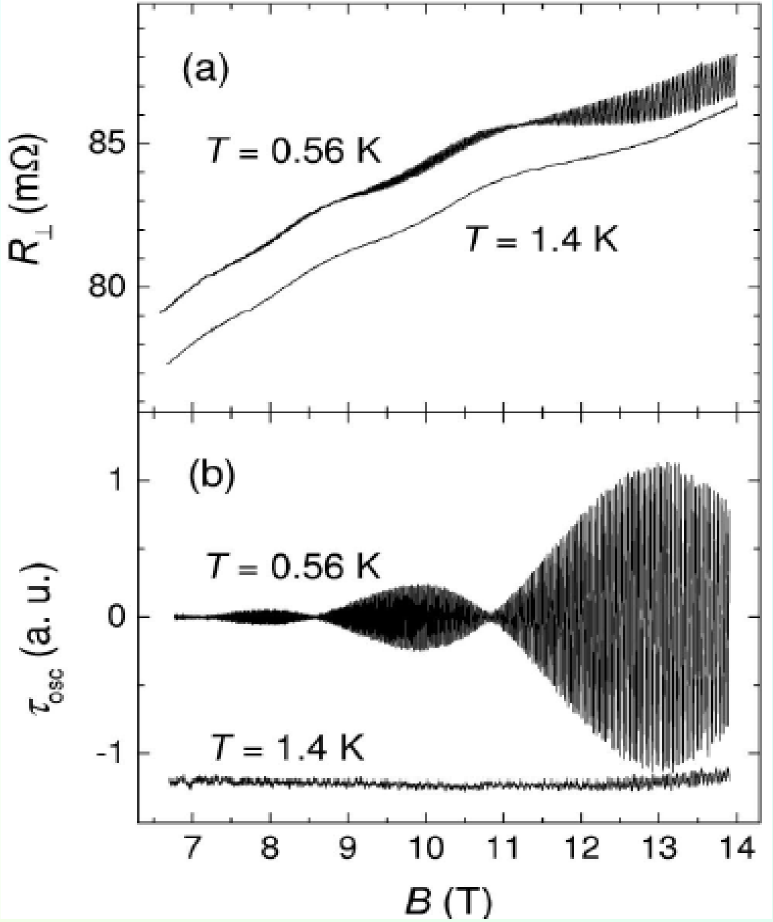
[First order: C. Bergemann et al., PRL 84, 2662 (2000); Adv. Phys. 52, 639 (2003).
Second order relation between $k_{\mu\nu}$ and $A_{\mu\nu}$: P.D. Grigoriev, PRB 81, 205122 (2010).]

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

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);

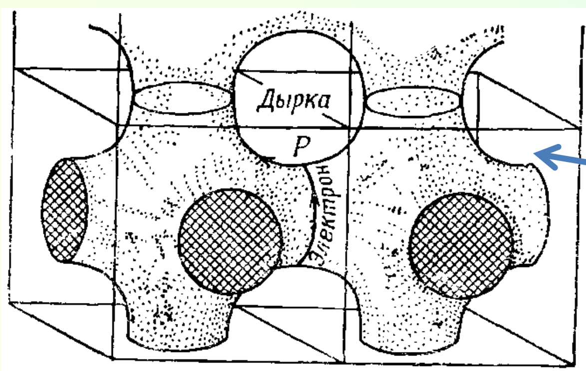
Rigorous calculation is performed in P.D. Grigoriev, PRB 67, 144401 (2003).

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⊥J gives MR.

For closed trajectories the conductivity tensor

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

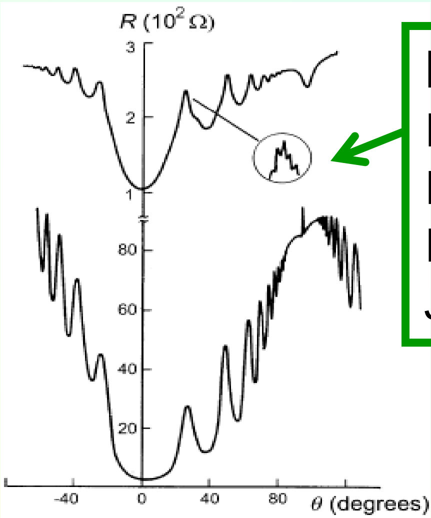


FS, containing open and closed trajectories

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

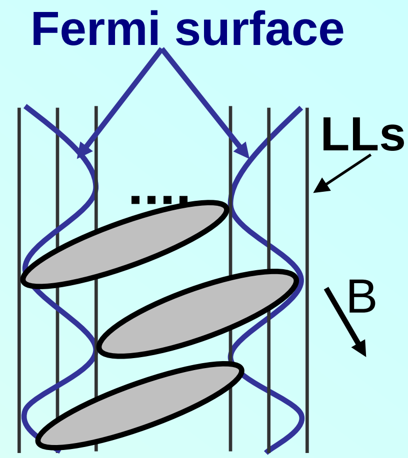
$$\sigma = \begin{pmatrix} B_{xx} & \frac{-A_{yx}}{H} & -B_{zx} \\ \frac{A_{yx}}{H} & \frac{A_{yy}}{H^2} & \frac{-A_{zy}}{H} \\ B_{zx} & \frac{A_{zy}}{H} & A_{zz} \end{pmatrix}$$

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



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

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



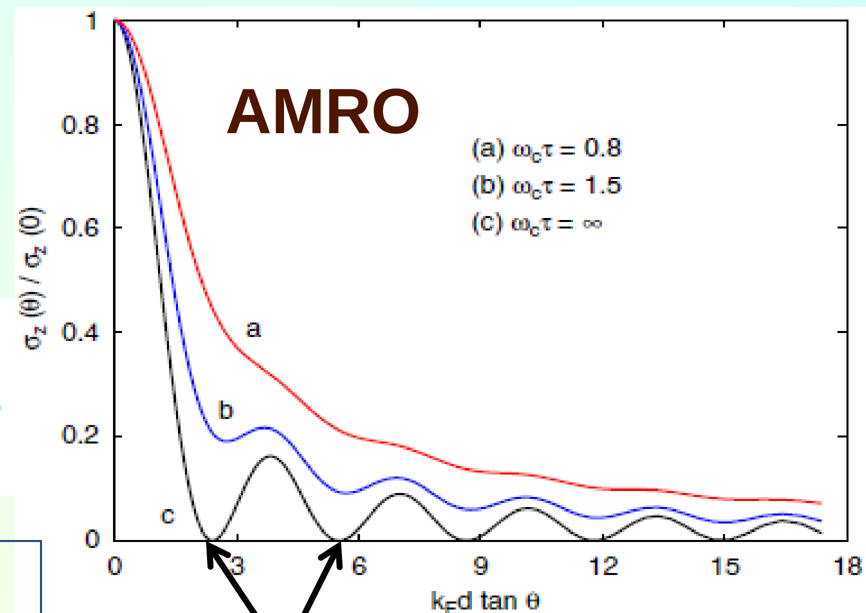
$$\sigma_{zz}^{3D} = e^2 \tau \sum_{FS} v_z^2, \quad v_z = \partial\varepsilon / \partial p_z$$

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

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

gives AMRO

gives damping of AMRO by disorder



Yamaji angles

Motivation

Angular dependence of background magnetoresistance

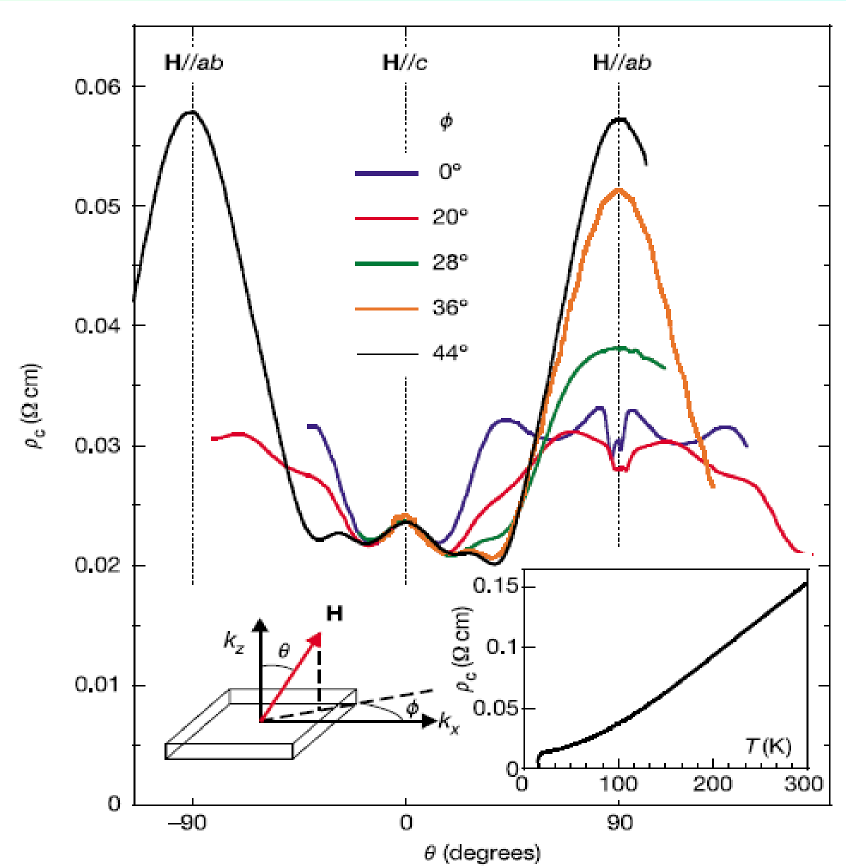
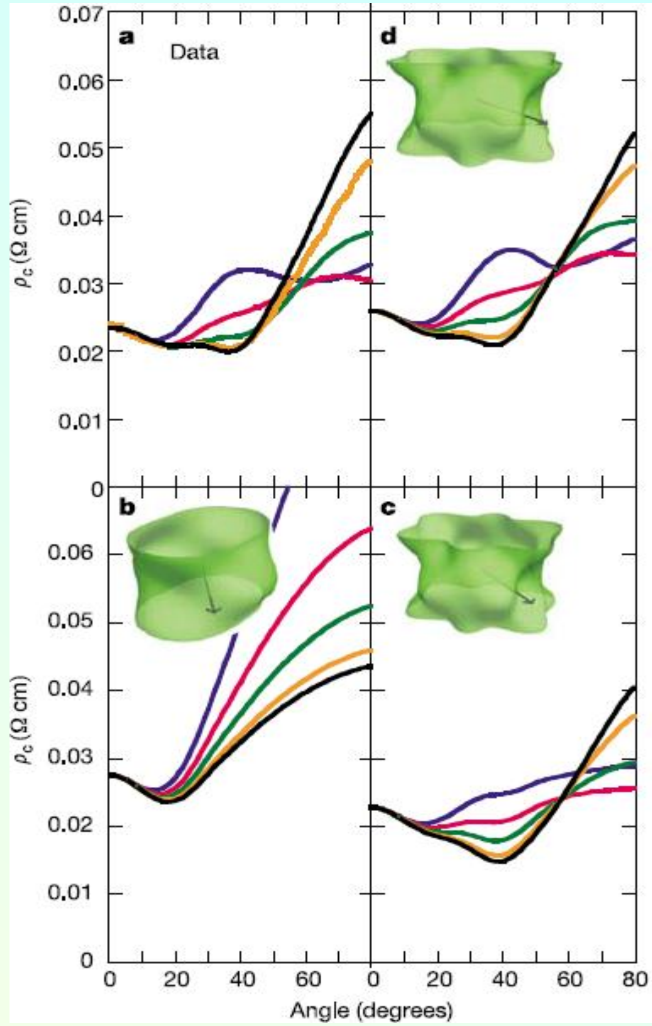


Figure 1 Polar AMRO sweeps in an overdoped Tl2201 single crystal ($T_c \approx 20$ K). The data were taken at $T = 4.2$ K and $H = 45$ T. The different azimuthal orientations ($\pm 4°$) of each polar sweep are stated relative to the Cu–O–Cu bond direction. The key features of the data are as follows: (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)