Magnetic quantum oscillations and angular dependence of magnetoresistance in layered high-Tc superconducting materials

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The goal:

1. To derive analytical formulas for MQO and AMRO, convenient for interpretation of experimental data.
2. To systemize the known previous results and to correct them or specify their applicability regions.
3. To perform numerical calculations to fit the data and to obtain information about high-Tc superconductors.

P.D. Grigoriev, Phys. Rev. B 81, 205122 (2010)

Motivation

All known high-Tc superconductors are layered quasi-2D compounds. The detailed knowledge of electron dispersion is very important for understanding the mechanisms of superconductivity: (How FS depends on doping and temperature? How close is SC Tc maximum to the quantum phase transition? How good is FS nesting? What are the Fermi arcs and hot spots?)

General opinion is that cuprate high-Tc superconducting materials are not metals and they do not possess Fermi surface. Hence, the observation of magnetic quantum oscillations or of typical magnetoresistance is impossible.

This is not true as many recent experiments show!

The only alternative to MQO to get experimental information about the electron spectrum is the angle-resolved photoemission spectroscopy (ARPES).

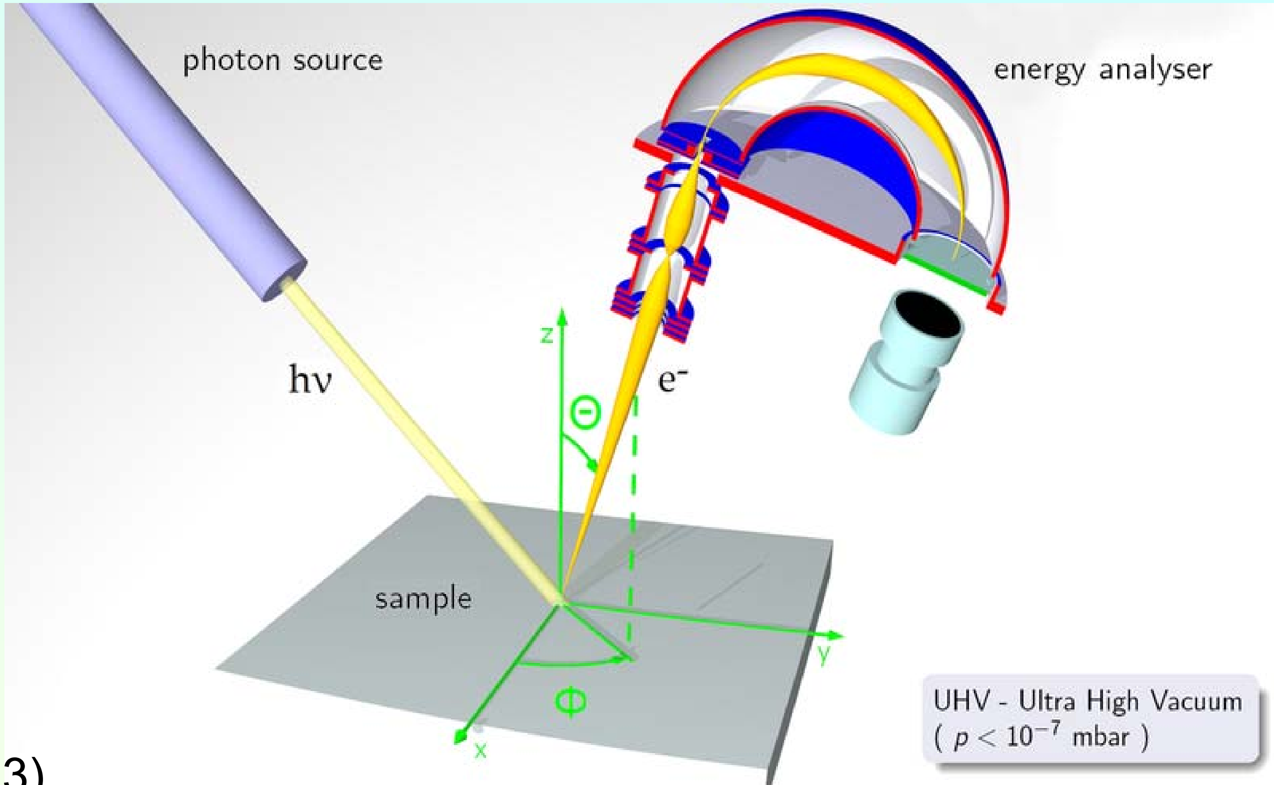
ARPES (Angle resolved photoemission spectroscopy)

M2

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:

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

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

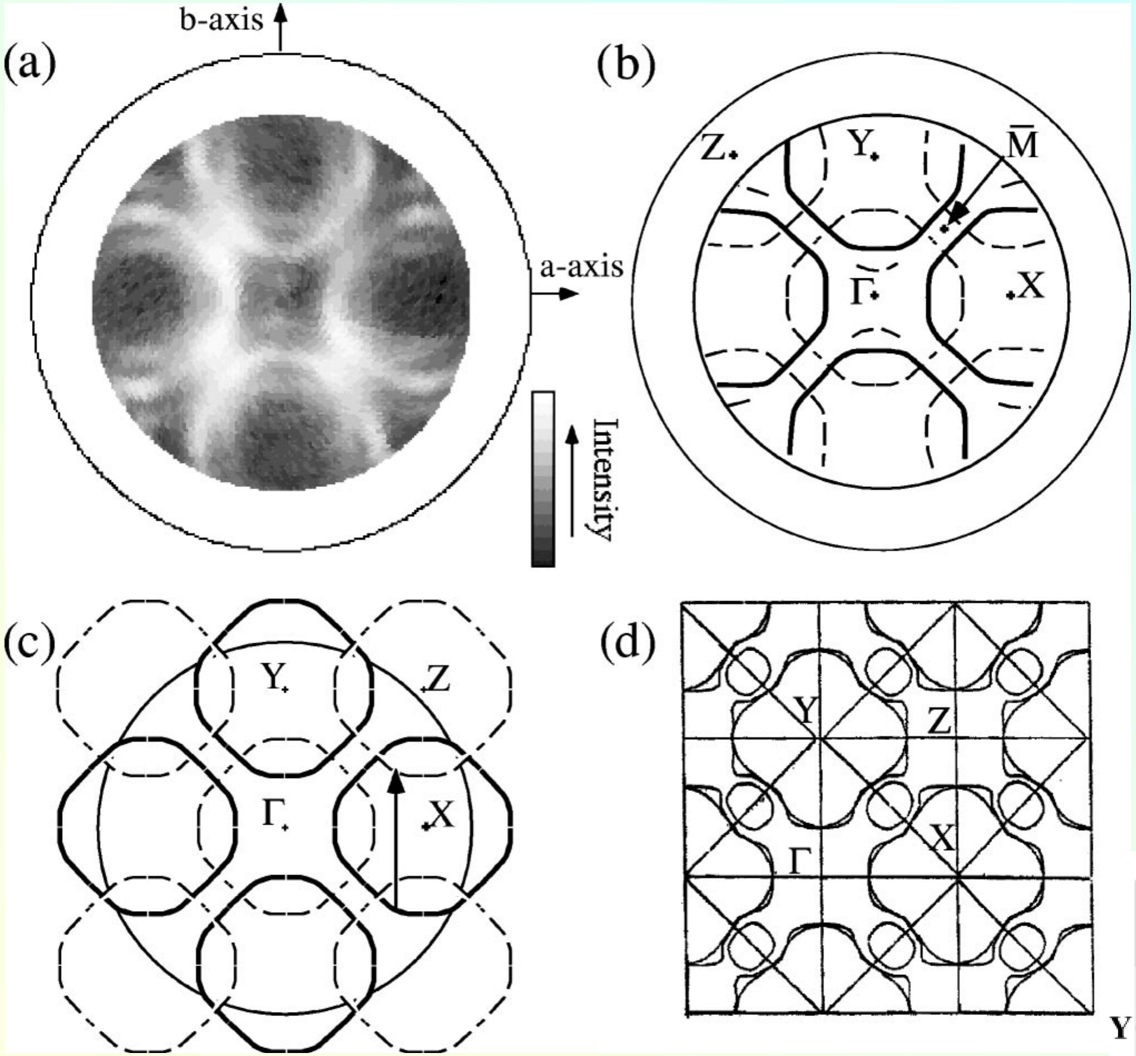
Therefore can find out information about *E(k)*

Drawback 1: Only surface electrons participate!

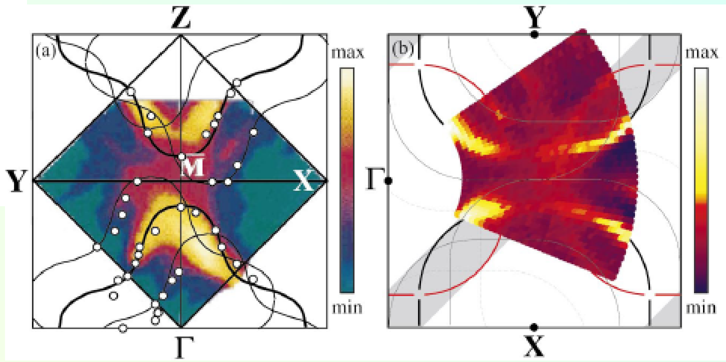
Motivation

Motivation

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).

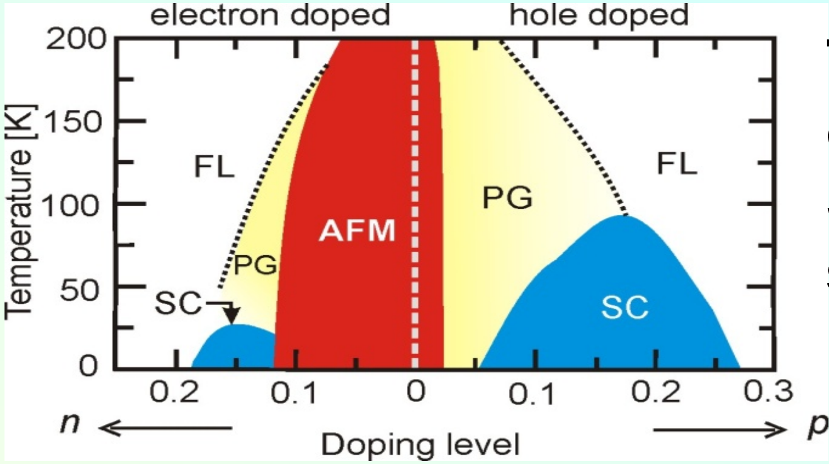


Drawback 2: Ambiguous interpretation.

Motivation

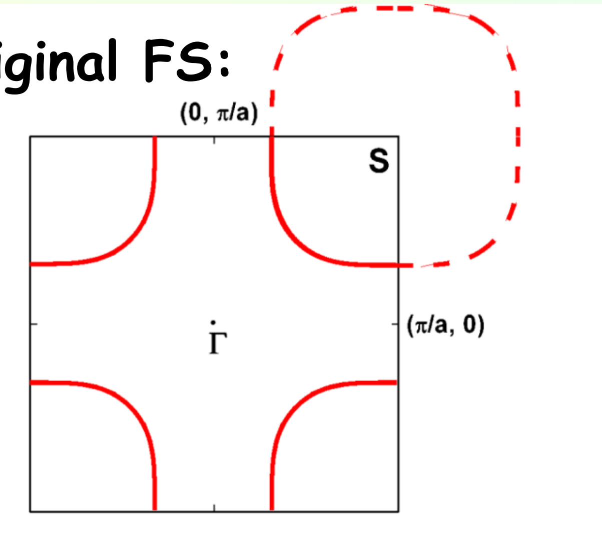
Phase diagram of high-Tc cuprate SC. High Tc and quantum phase transition

$Nd_{2-x}Ce_xCuO_4$ (NCCO)



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

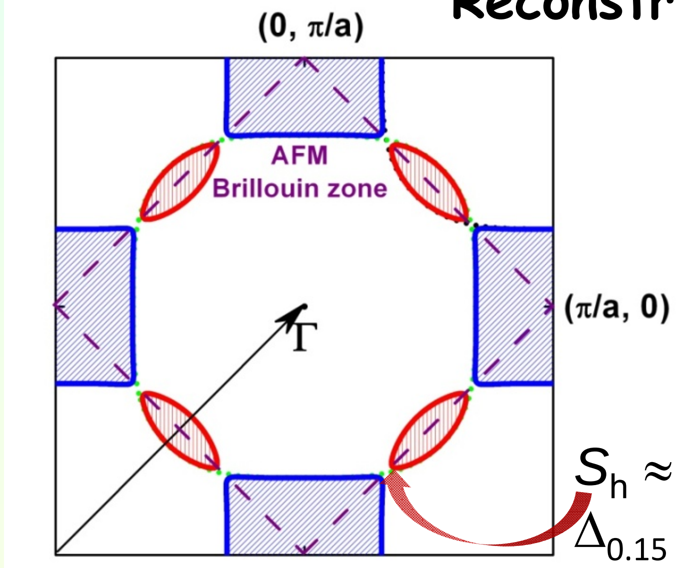
Original FS:



$\underline{n = 0.17}$

S_h = 41.5% of S_{BZ}

Reconstructed FS:



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

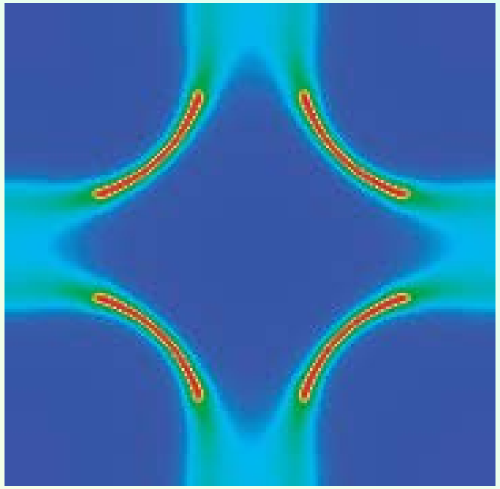
$S_h \approx$ 1.1% of S_{BZ};

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

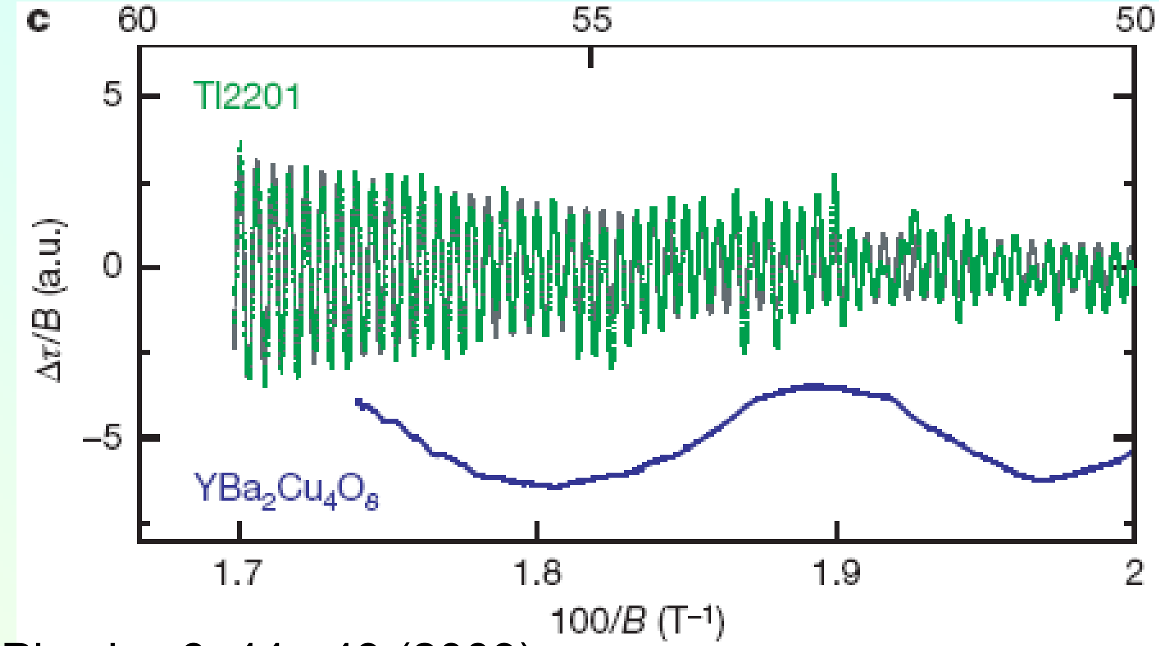
$\Delta_{0.16} \approx$ 36 meV

Motivation

Quantum oscillations from Fermi arcs



ARPES image plot



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

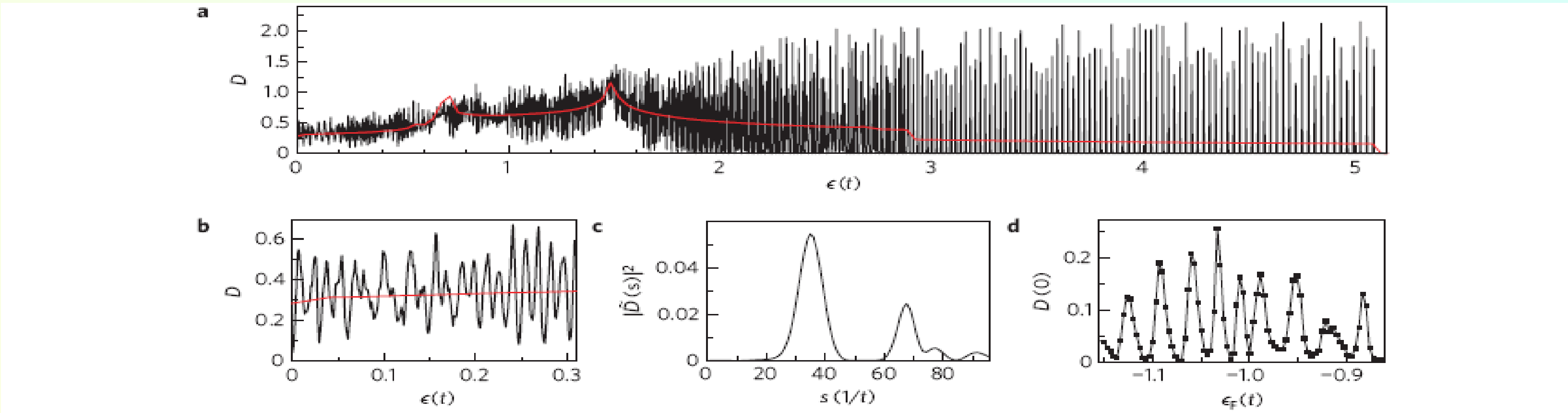


Figure 4 | Exact diagonalization of the lattice model. a, DOS as a function of energy in the FAM in zero (red) and non-zero (black) magnetic field corresponding to two vortices in a 20 × 20 magnetic unit cell. In YBCO with lattice constant $a_0 \simeq 4$Å this corresponds to the physical field of about 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

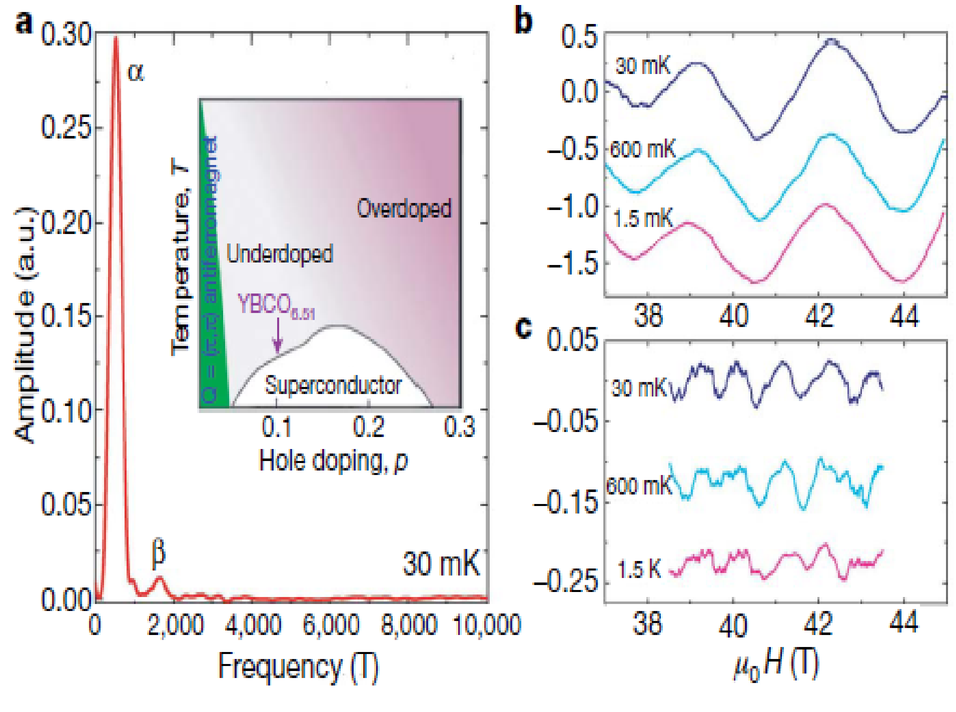


Figure 2 | de Haas-van Alphen oscillations in $YBa_2Cu_3O_{6.51}$. a, Fourier

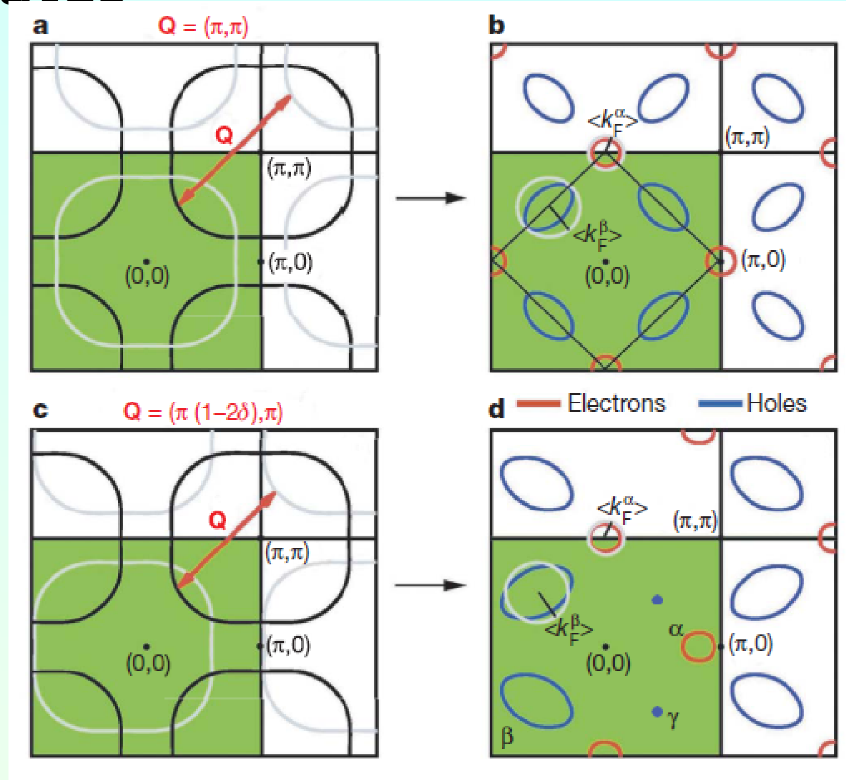


Figure 4 | Fermi surface reconstruction in $YBa_2Cu_3O_{6.51}$. a, Schematic Fermi surface reconstruction for a commensurate ordering wavevector **Q** $= (\pi,\pi)$ and nominal doping $p_{nom} = 0.1$ in the extended Brillouin zone

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

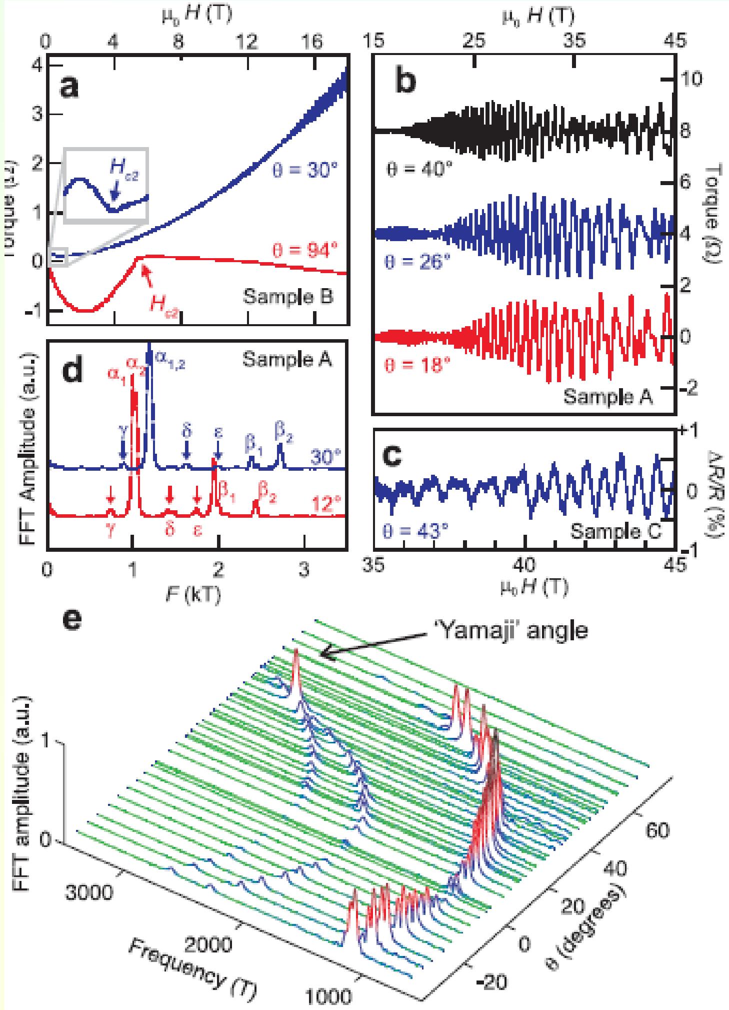
PRL **101,** 216402 (2008) PHYSICAL REVIEW LETTERS week ending 21 NOVEMBER 2008

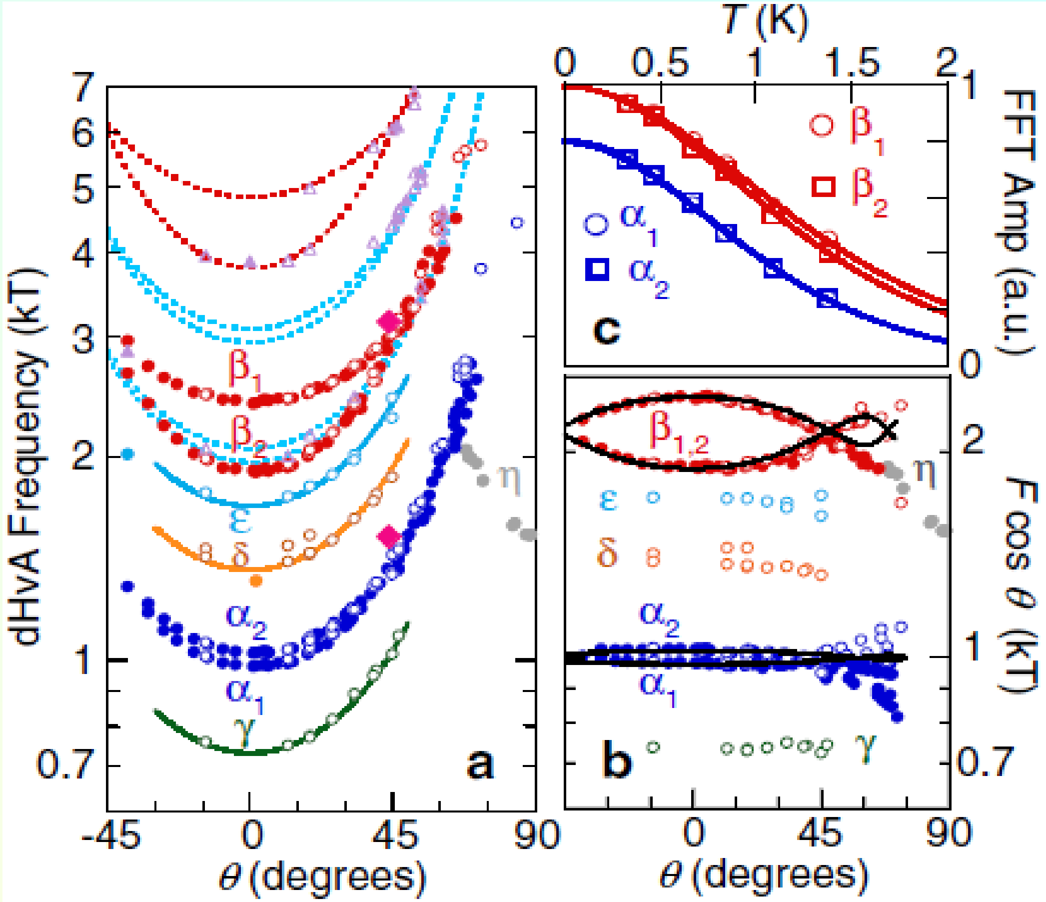
Fermi Surface of Superconducting LaFePO Determined from Quantum Oscillations

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]

M4

Experiments on MQO in high-Tc





Motivation

Lifshitz-Kosevich formula for MQO

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

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

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

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

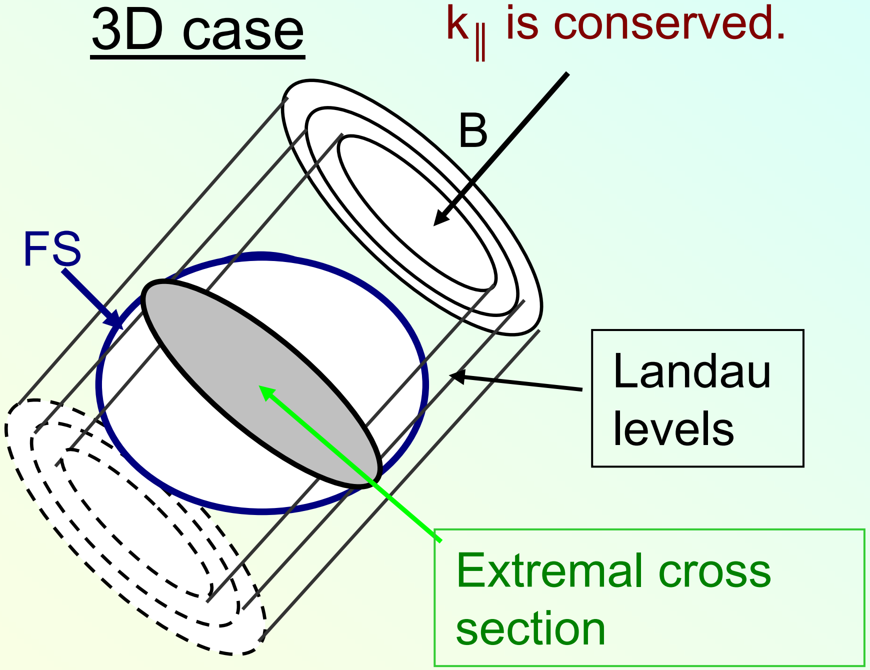
$$\kappa \equiv 2\pi k_B T / h\omega_C \, , \; \omega_C = eH / m^* c.$$

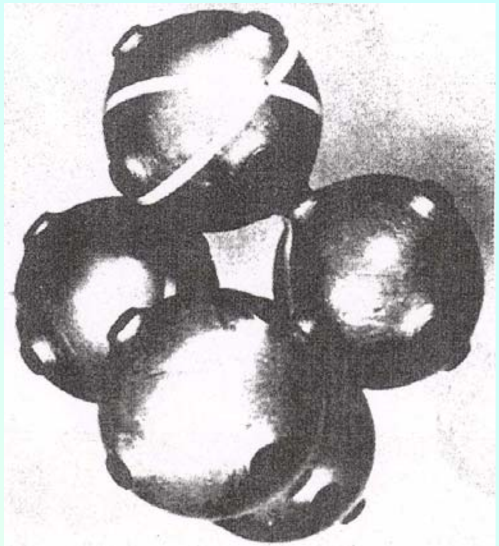
The scattering (Dingle) damping factor

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

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

3D compounds in tilted magnetic field





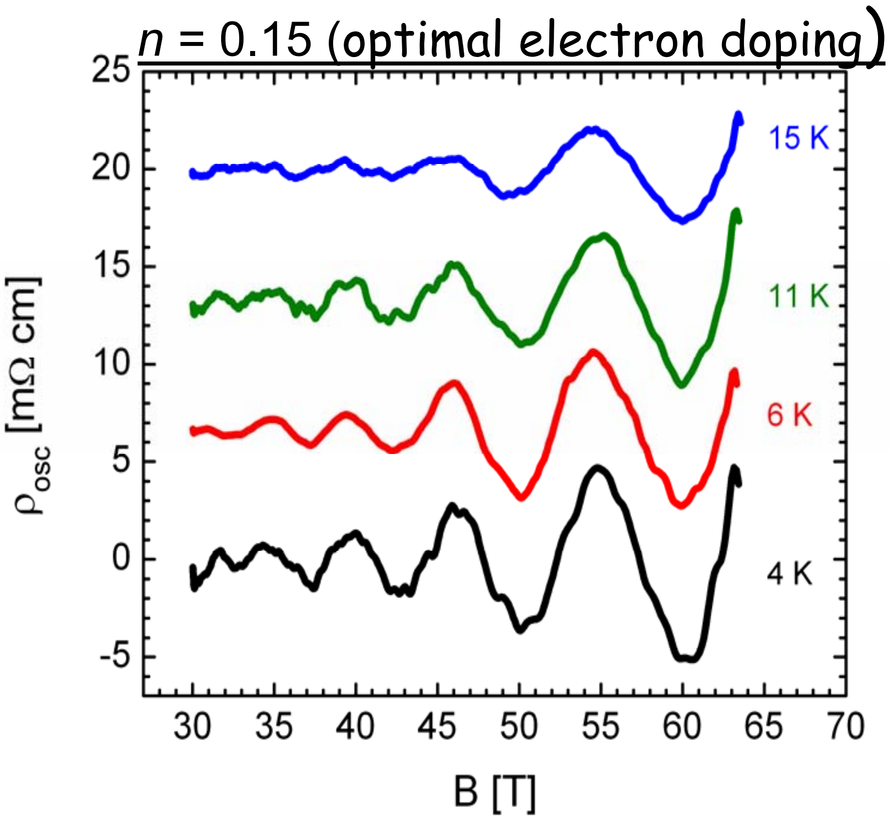
Fermi surface of gold

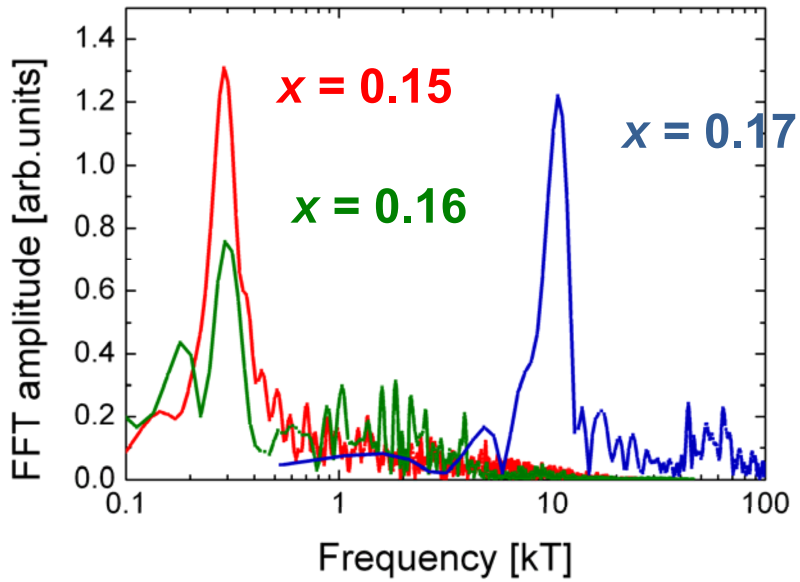
Extremal cross-section area of FS measured at various tilt angles of magnetic field allows to obtain the total Fermi surface of metals.

MQO is a traditional tool to study FS geometry

Problems with MQO in high-Tc materials

1. High-Tc cuprate are very dirty (doping is necessary for SC), and the MQO signal is weak and noisy.
2. The Fermi surface in these materials depends on doping level, temperature and magnetic field => much more work is need.
3. Magnetic field must be strong enough to suppress SC.

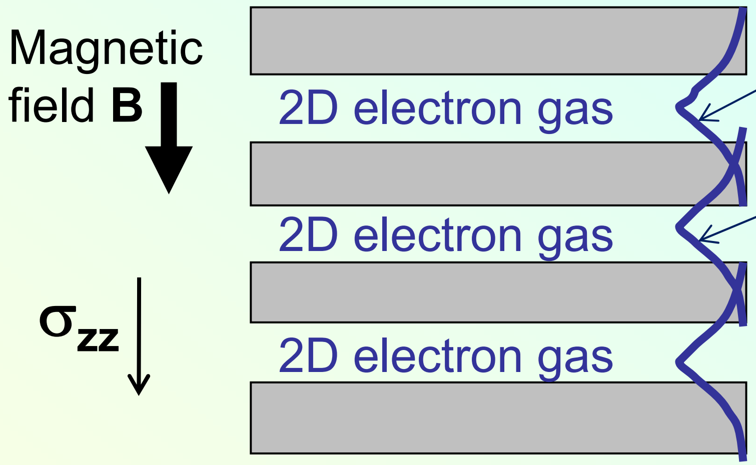




Can one simplify the processing of MQO data?

Layered quasi-2D metals

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



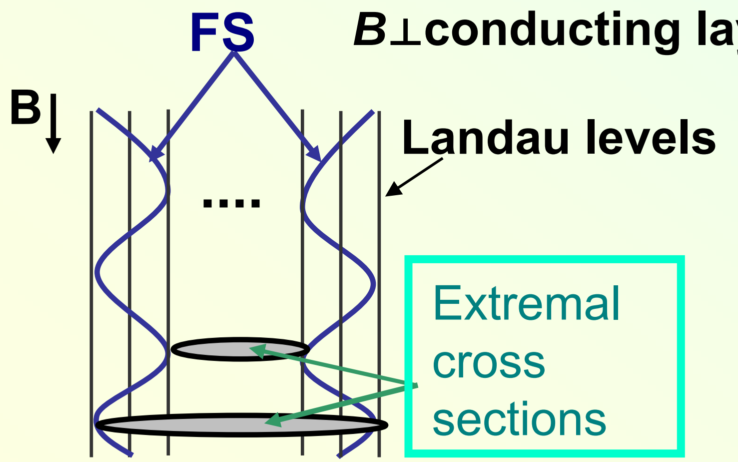
Electron wave functions overlap leads to the finite interlayer transfer integral t_z

Electron dispersion in the tight-binding approximation is highly anisotropic:
$\varepsilon(p) = p_{||}^2/2m_{||} + 2t_z \cos(k_z d)$, $t_z << E_F$

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

Fermi surface in quasi-2D metals is a warped cylinder

***B*⊥conducting layers**



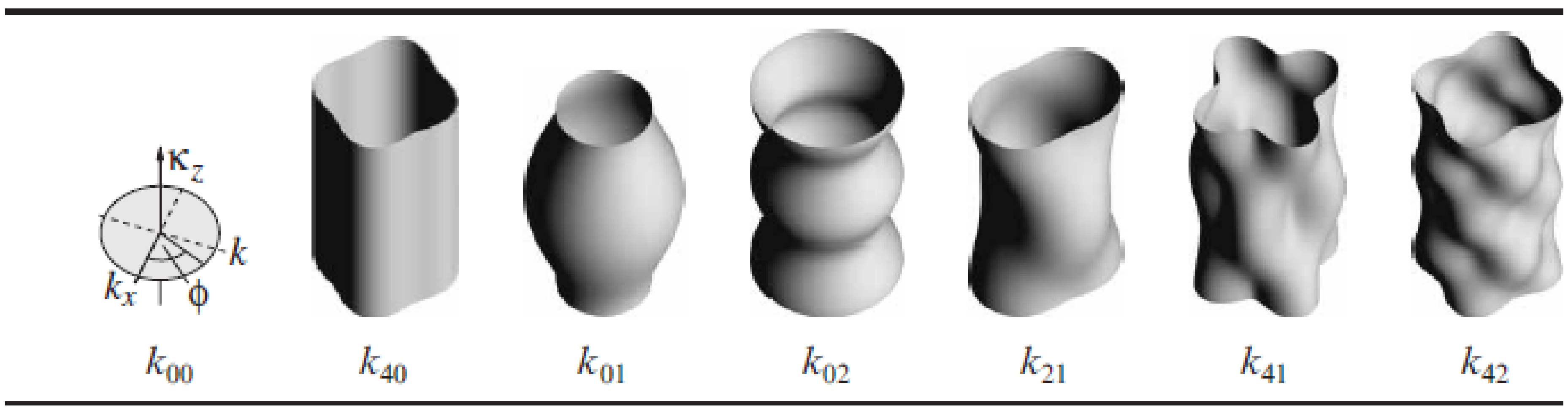
The extremal FS cross-section areas are measured by magnetic quantum oscillations. Their difference gives the value of interlayer transfer integral t_z

Harmonic expansion of Fermi momentum

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

The coefficients $k_{\mu\nu}$ fall down rapidly with increasing μ and ν:
$k_{\mu 0}/k_{00} << 1$, $k_{0\nu}/k_{00} << 1$, $k_{\mu\nu}/k_{00} \sim k_{\mu 0} k_{0\nu}/k_{00}^2$.

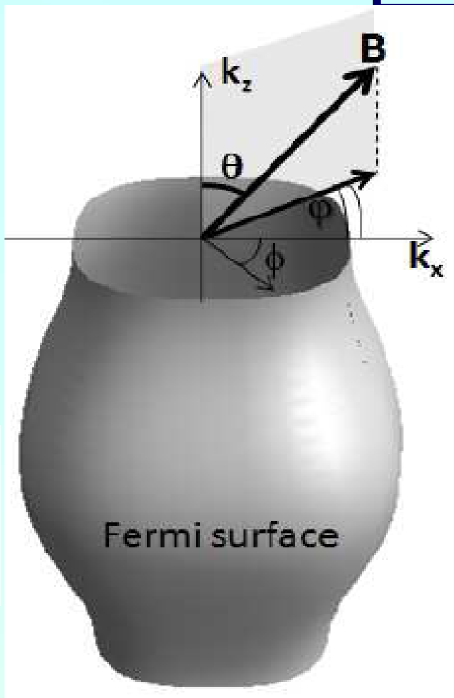
Illustration how different harmonics affect the FS shape



[C. Bergemann et al., Adv. Phys. (2003)]

H1

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

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

We only need to write down the relation between the first few coefficients $k_{\mu\nu}$ and $A_{\mu\nu}$!

First-order harmonic expansion result. Why it is bad?

$$A^{(1)} = \frac{2\pi k_{00}}{\cos\theta} \sum_{\mu,\nu\geq 0}{}' (-1)^{2\mu} k_{\mu\nu} \cos\left[\mu\phi + \phi_\mu\right] \cos\left(\nu k_{z0} c^*\right) J_\mu\left(\nu\kappa\right)$$

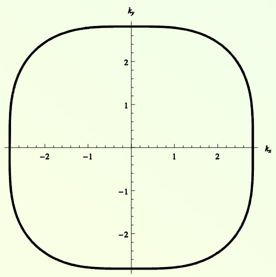
[C. Bergemann et al., PRL 84, 2662 (2000).]

Since $J_\mu(0)=0$ for $\mu\neq 0$, all terms ~$k_{\mu 0}$ vanish in $A^{(1)}$. Hence, the φ-dependence of the cross-section area A(θ,φ) starts from the term $k_{\mu 1}$, which is of the same order as the neglected second-order term $k_{\mu 0}k_{01}/k_F$.

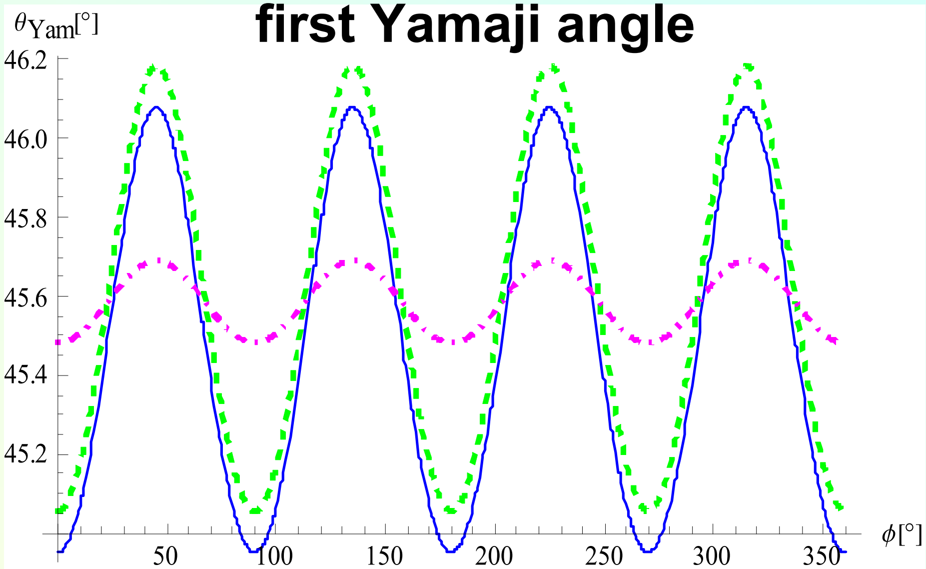
Therefore, the first-order result in $k_{\mu\nu}$ for the cross-section area does not give the correct φ-dependence even in the lowest order!

In fact, the error is very large.

For the in-plane Fermi surface with tetragonal symmetry (as in high-Tc cuprates) the amplitude of the φ-oscillations of the first Yamaji angle is 6 times less than the exact result.

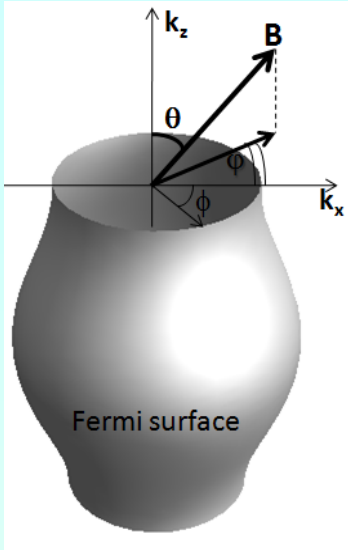


φ-dependence of the first Yamaji angle



New result 1A: Corrected analytical formula for the main ϕ-dependent term in the cross-section area

(straight interlayer hopping)



This formula is obtained in the second order in coefficients $k_{\mu\nu}$ from the Fermi momentum expansion

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

The main ϕ-dependent term in the cross-section area is

$$A^{(1)} = \frac{4\pi k_F^2 t_c C_1}{E_F} \frac{\cos[c^* k_{z0}]}{\cos\theta} \times$$

$$\times \left\{ J_0(\kappa) + \beta (-1)^{m/2} \cos(m\phi) \left[(1 + \beta_1/\beta + m) J_m(\kappa) - \kappa J_{m+1}(\kappa) \right] \right\}$$

these terms were absent

where $\beta \equiv k_{\mu 0}/k_{00}$, $\beta_1 = k_{\mu 1}/k_{01}$, $\kappa \equiv c^* k_F \tan\theta$

For the typical electron dispersion $\varepsilon(k, \phi) = k^\alpha g(\phi)$, $\beta_1/\beta = 1$

New result 1B: Corrected analytical formula for the main ϕ-dependent term in the cross-section area

inclined (φ-dependent) interlayer hopping

Fermi momentum is given by $k_F(\phi, k_z) = \sum_{\nu \geq 0} k_\nu(\phi)\cos(\nu k_z c^*)$

where

$$k_0(\phi) \approx (1 + \beta\cos 2m\phi)\, k_F,$$
$$k_1(\phi) \approx \frac{2t_c}{E_F} k_F C_1 \sin(m\phi)(1 + \beta_1\cos 2m\phi)$$

The main ϕ-dependent term in the cross-section area in the second order in coefficients $k_{\mu\nu}$ is

$$A(k_{z0}, \theta, \varphi) \approx \frac{\pi k_F^2}{\cos\theta} + \frac{4\pi k_F^2 t_c C_1}{E_F\cos\theta}\cos[c^* k_{z0}] \times$$
$$\times \left\{ J_m(\kappa)\sin(m\varphi) + \frac{\beta}{2}(-1)^{3m/2}\left[\left(1 + \frac{\beta_1}{\beta} + 3m\right) J_{3m}(\kappa) - \kappa J_{3m+1}(\kappa)\right]\sin(3m\varphi)\right\}$$

these terms were absent

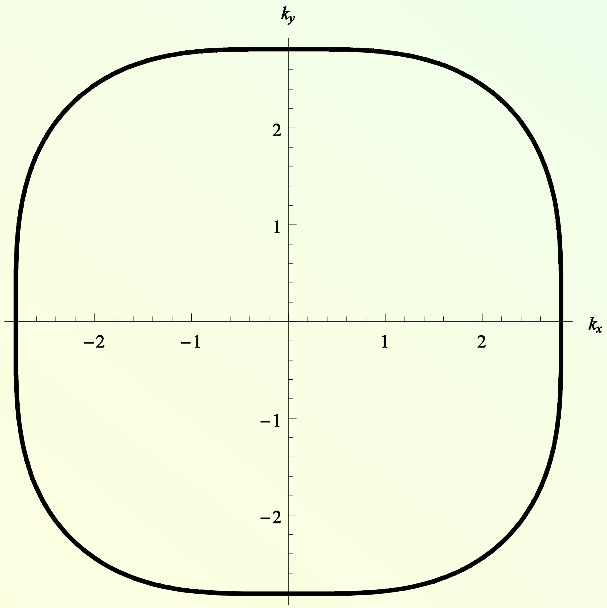
where $\beta \equiv k_{\mu 0}/k_{00}$, $\beta_1 = k_{\mu 1}/k_{01}$, $\kappa \equiv c^* k_F \tan\theta$

For the typical electron dispersion $\varepsilon(k, \phi) = k^\alpha g(\phi)$, $\beta_1/\beta = 1$

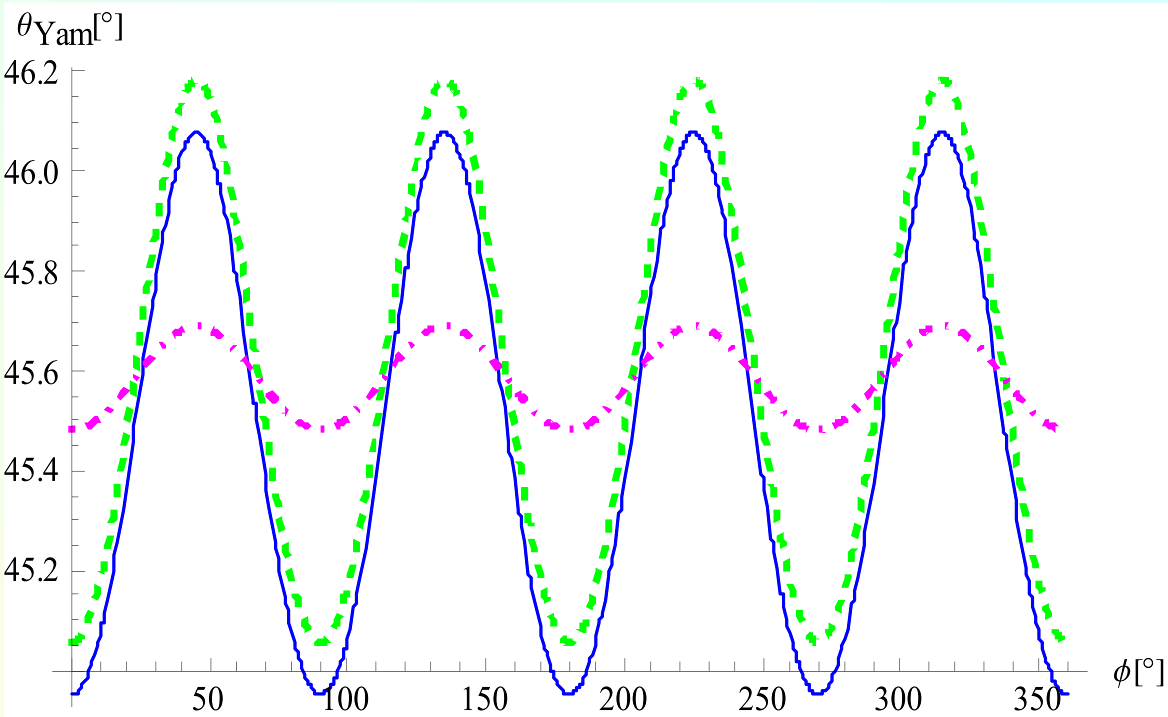
The difference between first- and second-order results is very large.

For the in-plane Fermi surface with tetragonal symmetry (as in high-Tc cuprates) the amplitude of the φ-oscillations of the first Yamaji angle is 6 times less than the exact result.

In-plane Fermi surface for $\beta=k_{40}/k_{00}=0.07$

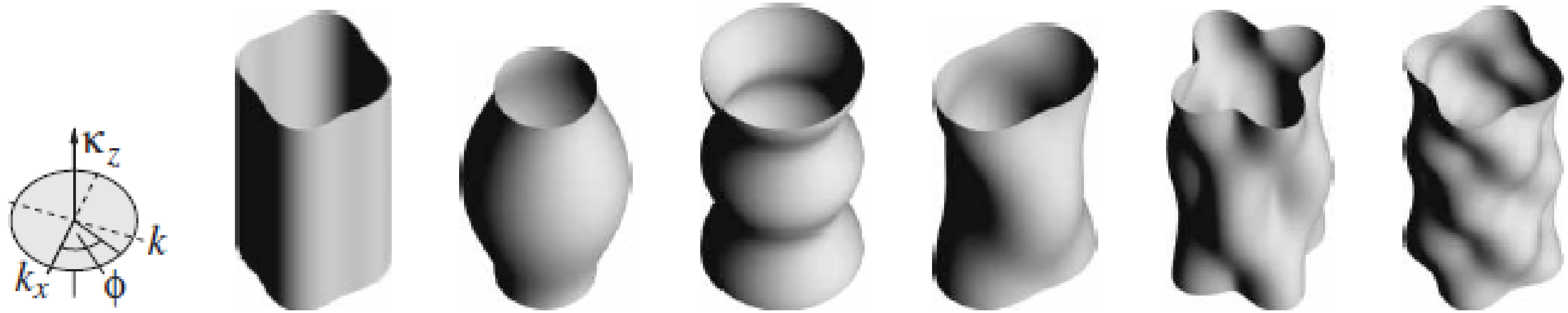


φ-dependence of the first Yamaji angle



What results obtained from the first-order harmonic expansion are valid and what can be corrected ?

Extracted warping parameters k [$10^7 m^{-1}$] of the three Fermi surface sheets of Sr_2RuO_4 [data from C. Bergemann et al., Adv. Phys. (2003).**]**



	k_{00}	k_{40}	k_{01}	k_{02}	k_{21}	k_{41}	k_{42}
α	304	−10	—	0.31	1.3	—	−1.0
β	622	−45	3.8	small	—	−0.6	small
γ	753	small	small	0.53	—	small	0.5

Probably, correct

Wrong, but can be easily corrected using new formula

Why do we need experiments to get the FS geometry. If band-structure calculation are enough?

Sr_2RuO_4

Table 9. Warping parameters $k_{\mu\nu}$ from table 4, compared with LDA band structure calculations. The units are in $10^7\,m^{-1}$, as usual. For more details, refer to the text.

Sheet	Parameter	DHvA	LDA (Oguchi)	LDA (Singh)
α	k_{00}	304	328.2	334.4
	k_{40}	−10	−22.0	−27.0
	k_{02}	0.31	0.9	−1.0
	k_{21}	1.3	0.3	0.8
	k_{42}	−1.0	2.1	2.1
β	k_{00}	622	653.1	649.4
	k_{40}	−45	−43.1	−45.0
	k_{01}	3.8	8.5	9.6
	k_{02}	small	−2.9	−2.8
	k_{41}	−0.6	−1.8	−4.0
	k_{42}	small	1.0	1.9
γ	k_{00}	753	723.5	724.0
	k_{40}	small	−3.7	0.4
	k_{01}	small	−1.2	−1.5
	k_{02}	0.53	2.0	1.9
	k_{41}	small	−3.3	−1.9
	k_{42}	0.5	0.7	−0.4

Application of the obtained formulas to analyze MQO and angular dependence of background MR

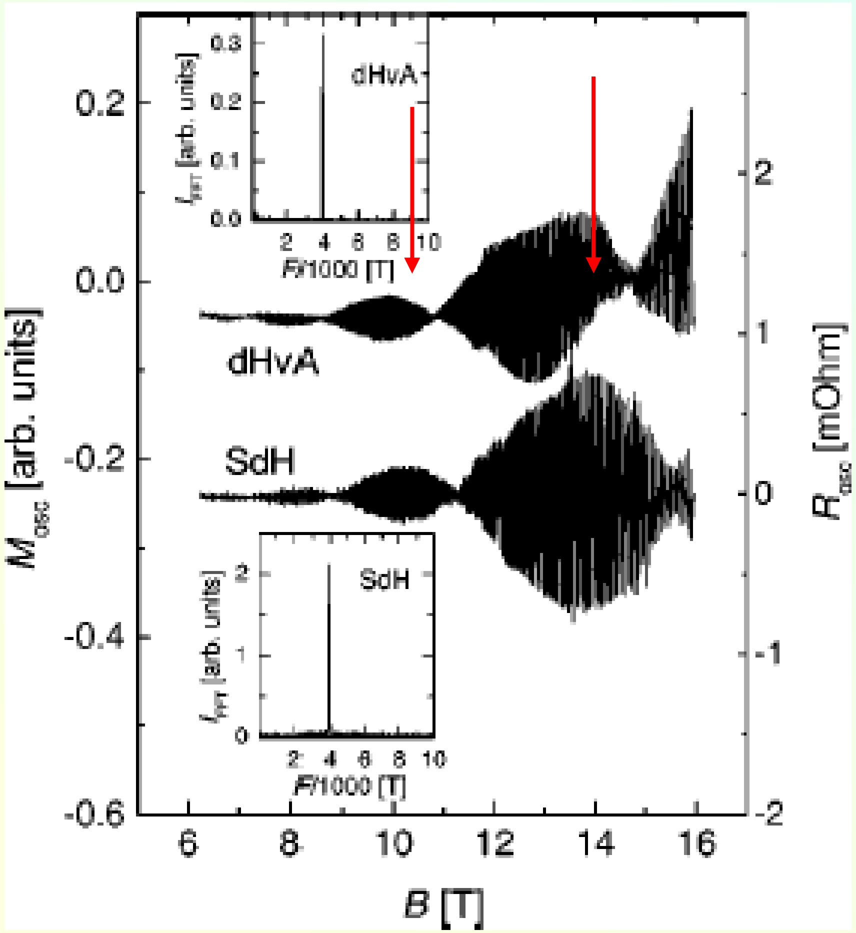
The above formulas can be used to:

1. **Determine the optimal magnetic field direction for the observation of the φ-dependence of MQO frequency.**
2. **Extract the Fermi-surface shape and electron dispersion from the angular dependence of the MQO frequency.**
3. **Determine the optimal magnetic field direction for the observation of beats of MQO. Their observation mean the existence of 3D Fermi surface.**
4. **Determine the optimal magnetic field direction for the observation of Yamaji angles and to extract electron dispersion parameters from the φ-dependence of the Yamaji angles.**
5. **Check the numerical fittings when the large number of fitting parameters makes the numerical procedure to be ambiguous.**

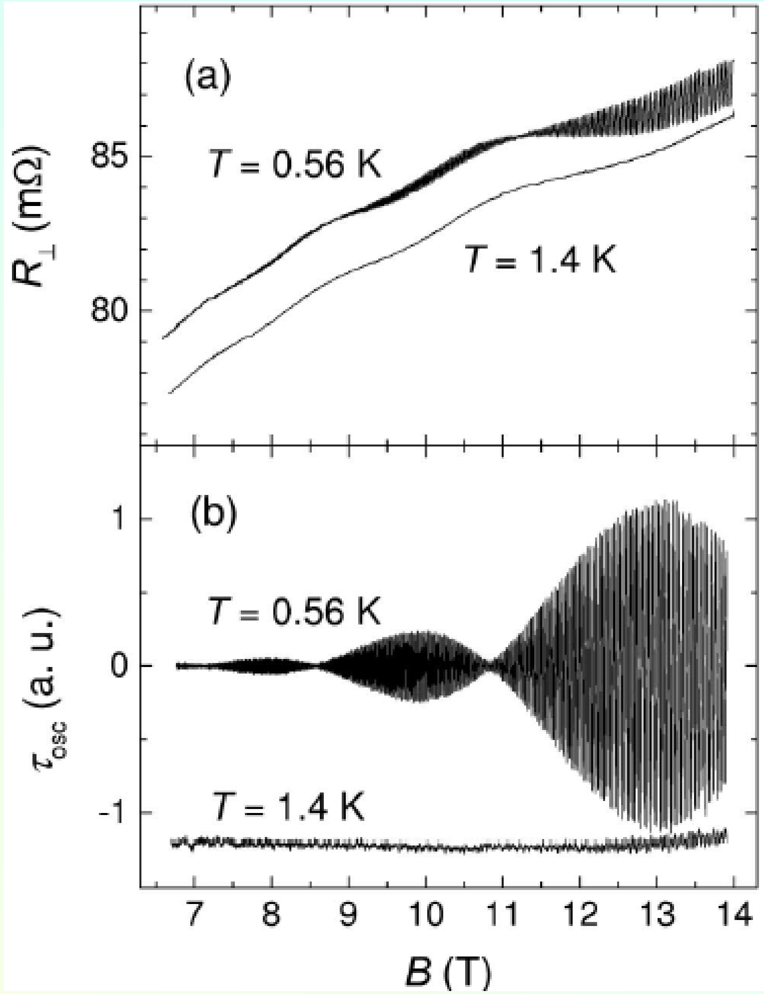
A8

Problems with the standard (L-K) description of quasi-2D magneotresistance oscillations

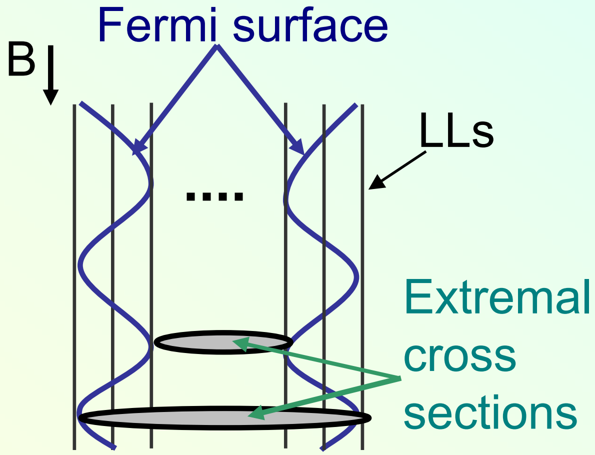
Phase shift of beats between MQO of conductivity and magnetization in the organic metal β-(BEDT-TTF)IBr_2



Slow oscillations in β-(BEDT-TTF)IBr_2 and other q2D metals, 10-year puzzle!



Magnetic quantum oscillations in quasi-2D compounds



$\hbar\omega c < 4t << E_F$

Quasi-2D compounds include heterostructures, layered organic metals, intercalated graphite compounds, high-Tc cuprates and many others.

Electron dispersion in the tight-binding approximation

$\varepsilon(n,p_z)=\hbar\omega_c(n+1/2)+2t\cos(k_z d)$, $t<<E_F$.

The dHvA frequency is related to the extremal cross section of the Fermi surface as $\mathbf{F_{dHvA} = c\hbar A_{ext} /2\pi e}$

Two extremal cross sections of the Fermi surface => two close fundamental frequencies in MQO:

$\mathbf{M \sim \sin(2\pi(F-\Delta F)/B) + \sin(2\pi(F+\Delta F)/B) = 2\sin(2\pi F/B)\cos(2\pi\Delta F/B)}$

beats

The theory of magnetic quantum oscillations in Q2d and the quantitative description of the slow oscillations and the phase-shift of beats has been given in the papers:

1. P.D. Grigoriev, M.V. Kartsovnik, W. Biberacher, N.D. Kushch, P. Wyder, "Anomalous beating phase of the oscillating interlayer magnetoresistance in layered metals", Phys. Rev. B 65, 60403(R) (2002).

2. M.V. Kartsovnik, P.D. Grigoriev, W. Biberacher, N.D. Kushch, P. Wyder, "Slow oscillations of magnetoresistance in quasi-two-dimensional metals", Phys. Rev. Lett. 89, 126802 (2002).

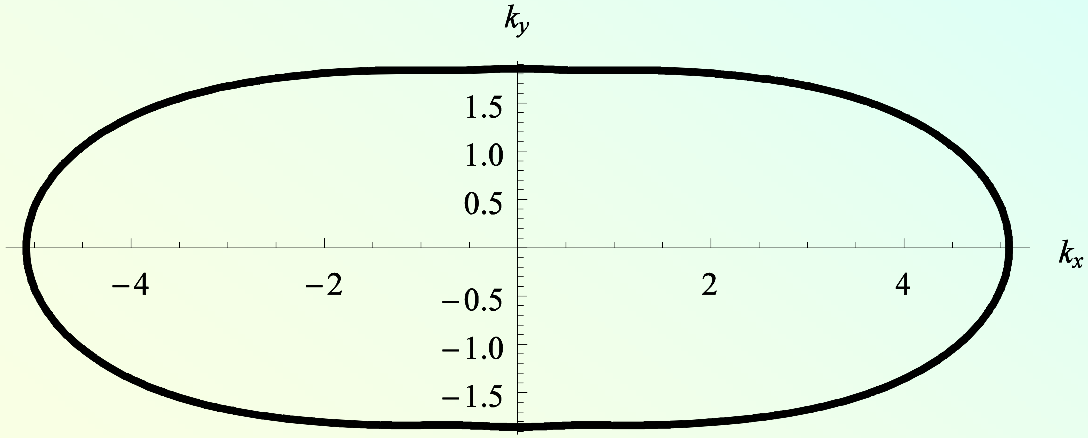
3. P.D. Grigoriev, "Theory of the Shubnikov-de Haas effect in quasi-two-dimensional metals", Phys. Rev. B 67, 144401 (2003).

Main idea: the traditional expansion (in the Lifshitz-Kosevich formula) in the small parameter - the ratio of the Landau level separation and the band width, $h\omega_c / t_z$, is not valid in quasi-2D metals because the band width in k_z in q2D metals is too small.

What to do when the harmonics do not fall down rapidly with increasing their order?

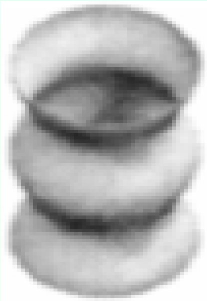
$$k_F(\phi, k_z) = \sum_{\mu,\nu \geq 0} k_{\mu\nu} \cos(\nu k_z c^*) \cos(\mu\phi + \phi_\mu).$$

For elongated in-plane Fermi surface $\beta = k_{20}/k_{00} \sim 1$.



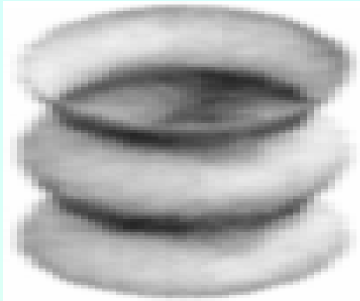
F5

Yamaji angles for elliptic in-plane FS



dilation Λ_x :

$\mathbf{x} \rightarrow \lambda\, \mathbf{x}$



axially-symmetric Fermi surface

elliptic in-plane Fermi surface

Yamaji angles θ_m are known. Being independent of ϕ, they satisfy the equation:

$$J_0\left(c^* k_F \tan\theta_m\right) = 0$$

The magnetic field direction

$$\mathbf{n} \rightarrow \Lambda_x(\mathbf{n}) = \frac{(n_x/\lambda, n_y, n_z)}{\sqrt{(n_x/\lambda)^2 + n_y^2 + n_z^2}}.$$

New Yamaji angle is ϕ-dependent:

$$\frac{\tan\theta^*_{Yam}}{\tan\theta_{Yam}} = \frac{\sqrt{n_x^2/\lambda^2 + n_y^2}}{n_z \tan\theta_{Yam}} = \sqrt{\frac{\cos^2\varphi}{\lambda^2} + \sin^2\varphi}.$$

Substituting azimuth angle after the dilation, $\tan\varphi_1 = \lambda\tan\varphi$, we obtain the new Yamaji angles:

$$\frac{\tan\theta^*_{Yam}}{\tan\theta_{Yam}} = \frac{1}{\sqrt{\lambda^2\cos^2\varphi_1 + \sin^2\varphi_1}}.$$

F6

New result 2: Exact formula for the ϕ-dependence of Yamaji angles for the elliptic in-plane Fermi surface:

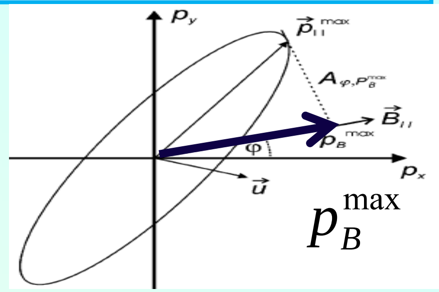
For the elliptic Fermi surface $\varepsilon(k_x, k_y) \equiv k_x^2/2m_x + k_y^2/2m_y$

the Yamaji angles θ_n are given by the equation:

$$J_0\left[c^* p_B^{\max}(\phi) \tan\theta_n\right] = 0. \quad (3)$$

where $p_B^{\max} = \sqrt{(p_1 \cos\phi)^2 + (p_2 \sin\phi)^2},$

and $p_1^2 = 2m_x\varepsilon_F$ and $p_2^2 = 2m_y\varepsilon_F.$



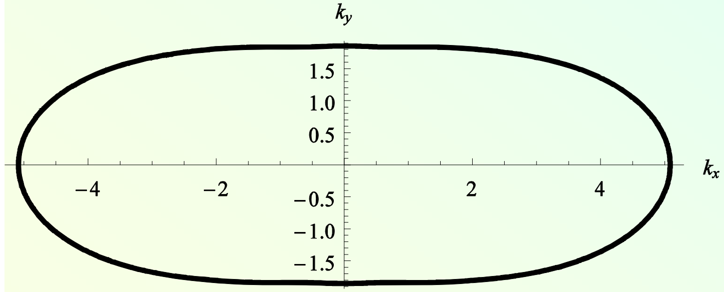
For the low-symmetry electron dispersion (triclinic or monoclinic with the elongated FS), this formula allows to extract the ratio of the main axes of the FS ellipse (or how elongated FS is).

Comparison of the new analytical formula for elliptic FS with the numerical results for other shapes of FS

F7

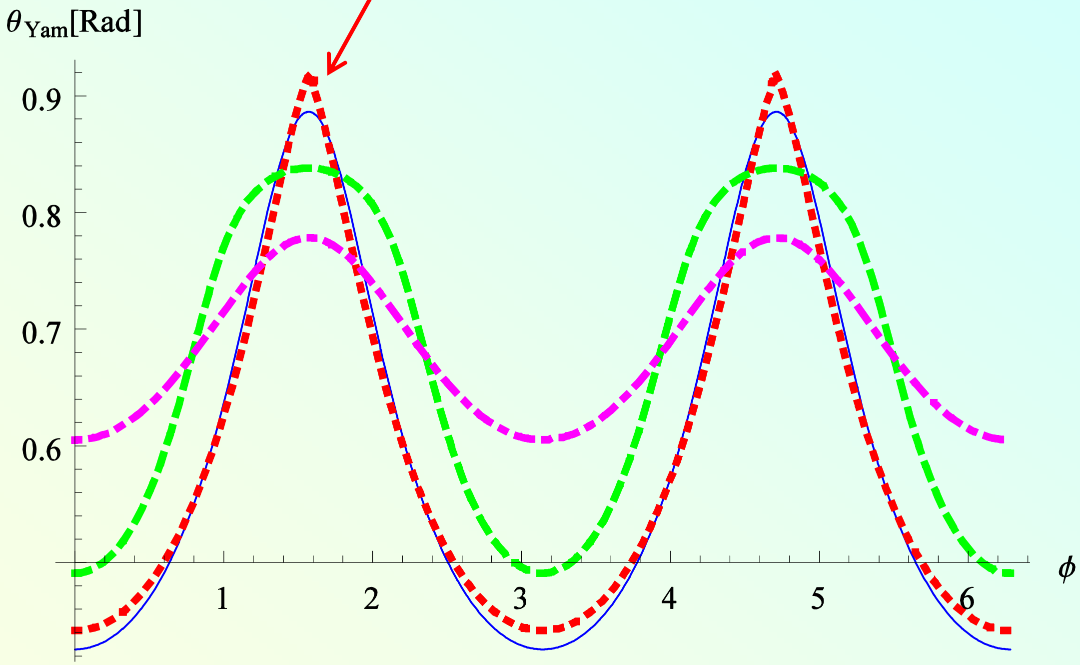
Conclusion: For any elongated FS it gives good agreement !

Very elongated but not elliptic Fermi surface:



$$J_0 \left[c^* p_B^{\max} (\phi) \tan \theta_n \right] = 0.$$

φ-dependence of the first Yamaji angle

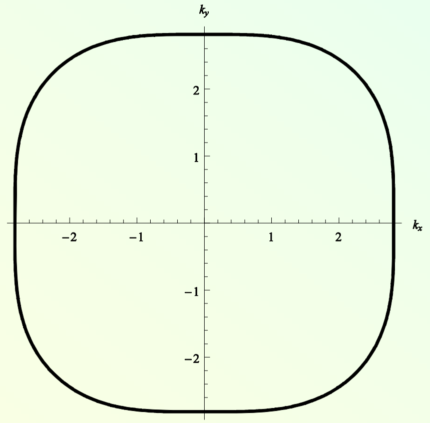


Red line – result of the new formula,
it almost coincides with exact result (**blue line**);
Green line – new harmonic expansion result;
Magenta – old harmonic expansion result;

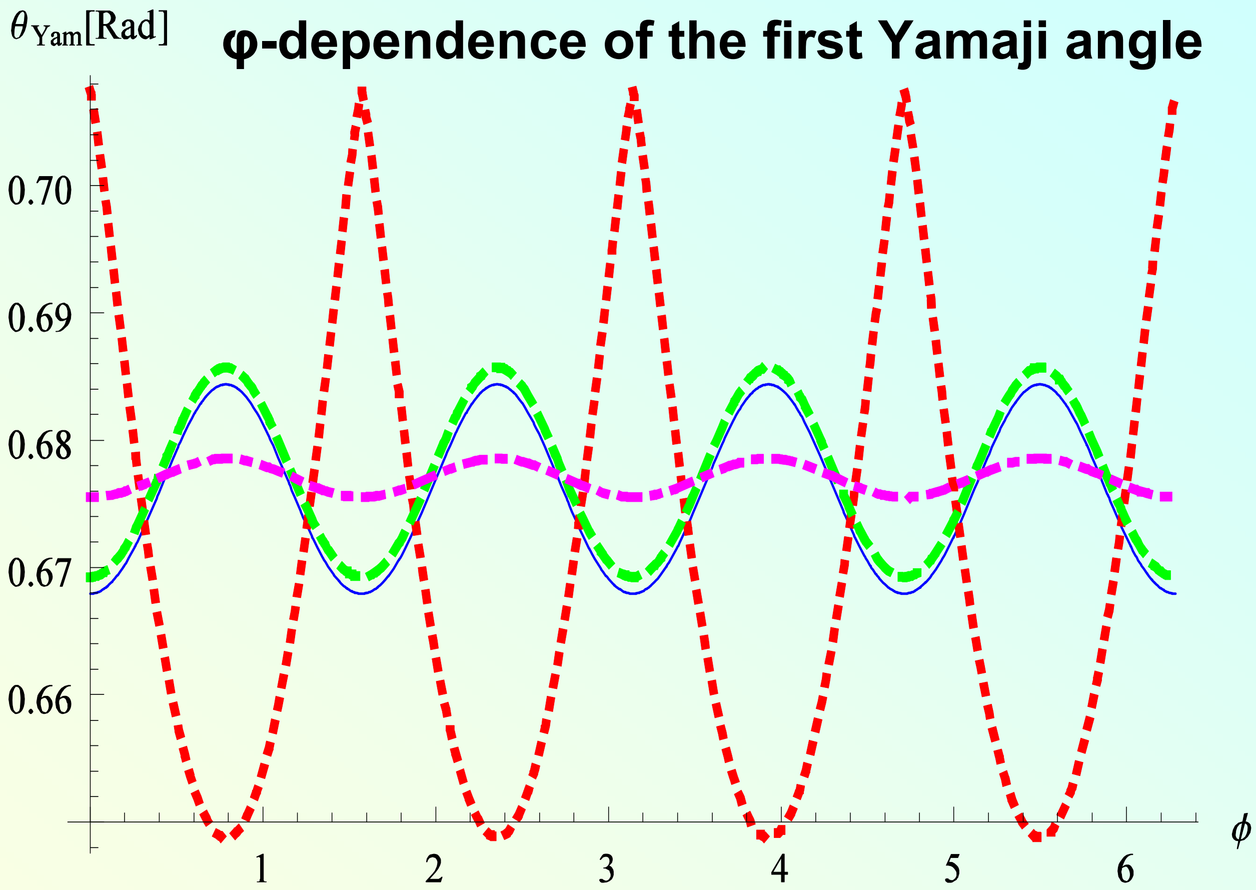
Comparison of the analytical formulas with numerical results for FS with tetragonal symmetry

<u>Conclusion:</u> formula fails for tetragonal or hexagonal symmetries, where harmonic expansion is rather accurate.

Fermi surface



φ-dependence of the first Yamaji angle



Green line – new result; it coincides with exact result (blue line); Magenta – old harmonic expansion result;

Red line – result of formula

$$J_0\left[c^* p_B^{\max}(\phi)\tan\theta_n\right] = 0.$$

Comparison with previous results

New formula for the Yamaji angles

$$J_0\left[c^* p_B^{\max}(\phi)\tan\theta_n\right] = 0.$$

approximately coincides with the previous result of Yakovenko:

$$|\tan\,\theta| = [\pi\hbar(n - {}^{1}/_{4}) \pm (\mathbf{p}_{||}^{\max}\cdot\mathbf{u})]/p_B^{\max}d \qquad \textbf{(4)}$$

The derivation of (4) is not applicable, but the formula works well for many compounds!

This explains why Eq. (4) was successfully used to determine the elongation parameters of the Fermi surface in organic metals.

F3

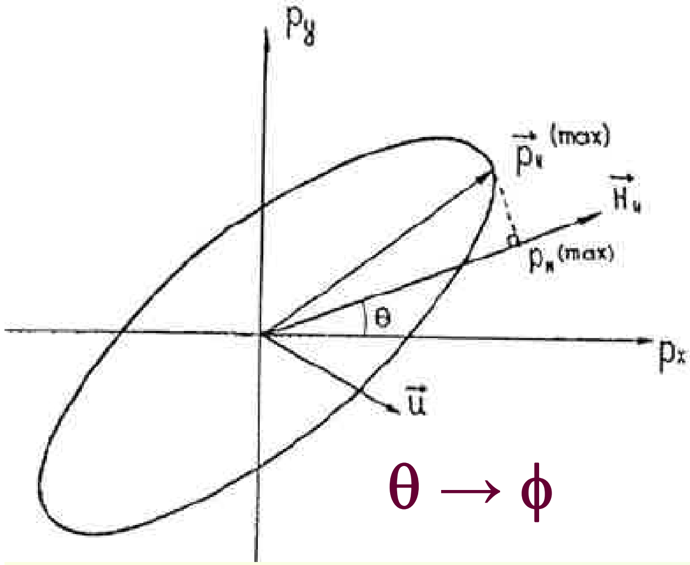
Derivation of the formula (1) in Ref. M. V. Kartsovnik, V. N. Laukhin, S. I. Pesotskii, I. F. Schegolev, V. M. Yakovenko, J. Phys. I 2, 89 (1992).

At $\omega_c\tau \gg 1$ from the S-T integral $\sigma_{zz}^{(0)} = \sigma_{HH}^{(0)} \sin^2\varphi \propto \langle \bar{v}_z^2 \rangle$

where the velocity, averaged over the electron orbit

$$\bar{v}_z = \overline{\partial E/\partial p_z} = \frac{2td}{T\hbar}\int_0^T d\xi \sin\left\{\left[p_z(\xi)d + (\mathbf{p}_\parallel(\xi)\mathbf{u})\right]/\hbar\right. \quad \mathbf{(2)}$$

and $p_z(\xi) = P_z - p_H(\xi)\cot\varphi,$



The integral over is assumed to be rapidly oscillating and is taken in the saddle-point approximation, which gives

$$\bar{v}_z(P_z) \propto \sin\left(\frac{P_z d}{\hbar}\right)\cos\left(\frac{|dp_H^{(max)}\cot\varphi - (\mathbf{p}_\parallel^{(max)}\mathbf{u})|}{\hbar} - \frac{\pi}{4}\right).$$

This gives the condition for the N-th Yamaji angle (minimum of averaged velocity):

$$|\cot\varphi_c| = [\pi\hbar(N - 1/4) \pm (\mathbf{p}_\parallel^{(max)}\mathbf{u})]/p_H^{(max)}d, \quad \mathbf{(1)}$$

Problem: the integral (2) is not rapidly oscillating even at high tilt angle as in the first Yamaji angle, where it makes only one oscillation.

First analytical result on the azimuth-angle dependence of magnetoresistance in quasi-2D metals $R_{zz}(\theta,\phi)$

F2

[M. V. Kartsovnik, V. N. Laukhin, S. I. Pesotskii, I. F. Schegolev, V. M. Yakovenko, J. Phys. I 2, 89 (1992).]

The ϕ-dependent Yamaji angles (maxima of $R_{zz}(\theta,\phi)$ are given by equation:

$$|\tan\theta| = [\pi\hbar(n - {}^{1}/_{4}) \pm (\mathbf{p}_{||}^{\max}\cdot\mathbf{u})]/p_B^{\max}d$$

where the sign in the $\pm$ is the same as the sign of $\tan\theta$ and the meaning of $\mathbf{p}_{||}^{\max}$ and $p_B^{\max}$ is illustrated in Figure 4: $\mathbf{p}_{||}^{\max}$ is the in-plane Fermi momentum whose projection on the field rotation plane, determined by angle φ, takes the maximum value, denoted as $p_B^{\max}$. From the periods of AMROs measured at various azimuthal angles φ, one can determine $p_B^{\max}(\varphi)$ and graphically deduce the shape and size of the FS cross section in the $p_x p_y$ plane.

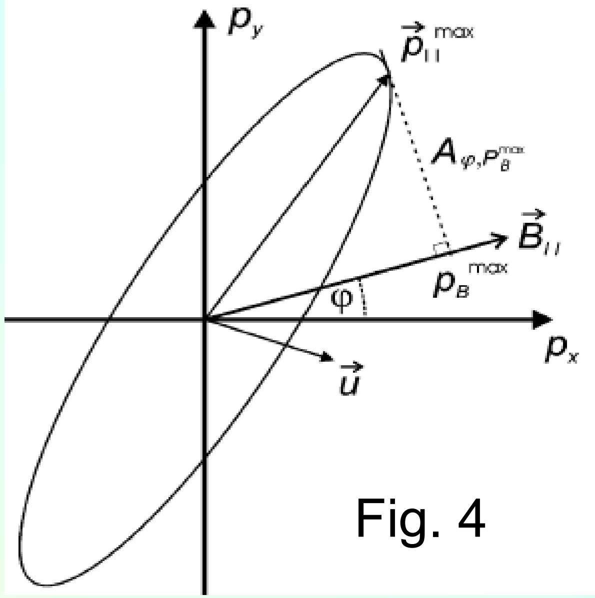


Fig. 4

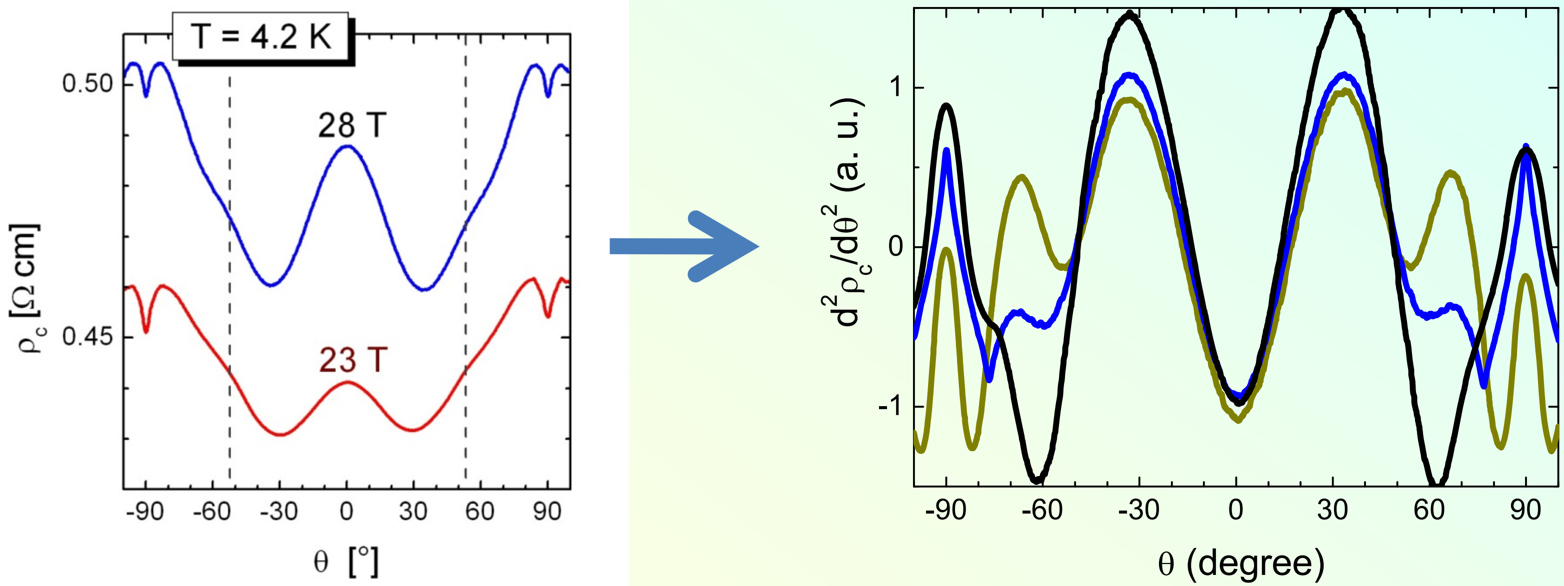
This simple formula is widely used to extract the in-plane FS shape

Other results (AMRO):

1. **Derivation and investigation of the applicability region of the relation between the angular dependence of magnetoresistance and of the FS cross-section area at $\omega_c\tau$ >>1 in quasi-2D compounds (t_c/E_F<<1):**

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

2. **Angular magnetoresistance oscillations and their fit by numerical calculations:**



Summary (MQO)

P.D. Grigoriev, Phys. Rev. B 81, 205122 (2010).

Analytical formulas are obtained for the θ,ϕ -dependence of the cross-section area (MQO frequency), which can be used to extract the FS shape from experimental data on MQO in various layered high-Tc superconductors. We also suggests the optimal B-direction for the observation of the angular dependence of MQO.

1. **Harmonic expansion:**

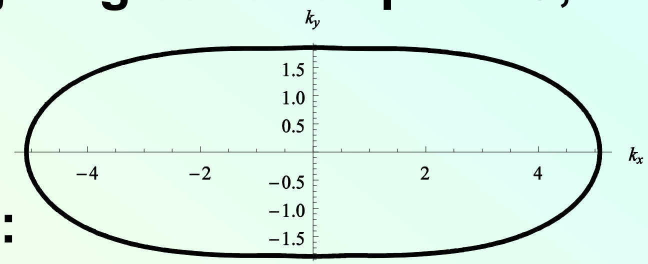
$$k_F(\phi, k_z) = \sum_{\mu,\nu \geq 0} k_{\mu\nu} \cos(\nu k_z c^*) \cos(\mu\phi + \phi_\mu) .$$

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

2. **The formula for the ϕ - dependence of Yamaji angles for elliptic FS, which also works well for any elongated FS.**

$$J_0 [c^* p_B^{\max}(\phi) \tan\theta_n] = 0.$$

Applicable to elliptic and elongated in-plane FS:



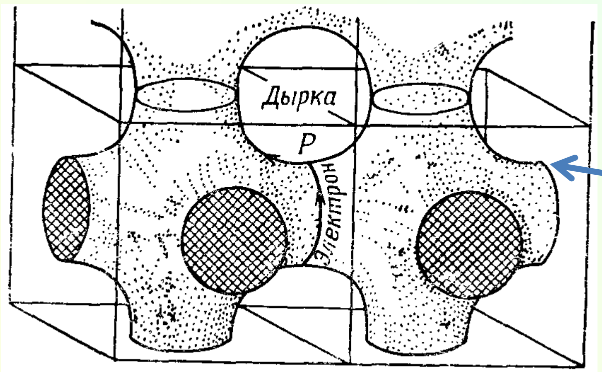
Thank you for the attention!

Background (classical) magnetoresistance in normal 3D metals (strong fields)

In strong magnetic field the magnetoresistance depends on the shape and topology of the Fermi surface (FS), because at $\omega_c\tau \gg 1$ the electrons can encircle the FS before being scattered.

The conductivity tensor for closed trajectories

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



FS, containing open and closed trajectories

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

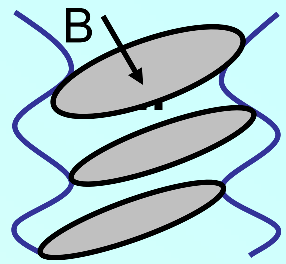
$$\sigma = \begin{pmatrix} B_{xx} & \frac{-A_{yx}}{H} & -B_{zx} \\ \frac{A_{yx}}{H} & \frac{A_{yy}}{H^2} & \frac{-A_{zy}}{H} \\ B_{zx} & \frac{A_{zy}}{H} & A_{zz} \end{pmatrix}$$

Introduction

A10

Background magnetoresistance in q2D. Shockley tube-integral formula for conductivity.

The convenient coordinates for electrons in magnetic field in momentum space are: energy E, momentum along magnetic field k_H and the phase along the closed electron trajectory ϕ)



Kinetic equation for electron distribution function *g* in magnetic field in the τ–approximation in Q2D metals is

$$e\mathbf{E}\cdot\mathbf{v}\left(-\frac{\partial f^0}{\partial \mathscr{E}}\right)=\frac{g}{\tau}+\omega_H\frac{\partial g}{\partial \phi}.$$

The solution of this equation is

$$g(\mathscr{E},k_{\mathrm{H}},\phi)=\frac{e}{\omega_H}\left(-\frac{\partial f^0}{\partial \mathscr{E}}\right)\int_{-\infty}^{\phi}\mathbf{v}(\mathscr{E},k_{\mathrm{H}},\phi)\,e^{(\phi''-\phi)/\omega_H\tau}\,d\phi''\cdot\mathbf{E}.$$

Integration of this distribution function over the momentum space gives the Shockley tube-integral formula for conductivity

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

Introduction

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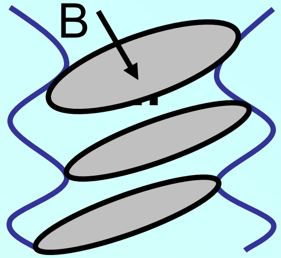

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Introduction

A12

Many papers are devoted to the analytical theory on the polar-angle θ-dependence of magnetoresistance and MQO frequency for the axially-symmetric electron dispersion

$\varepsilon(\boldsymbol{p}) = p_{||}^2/2m_{||} + 2t_z \cos(k_z d).$

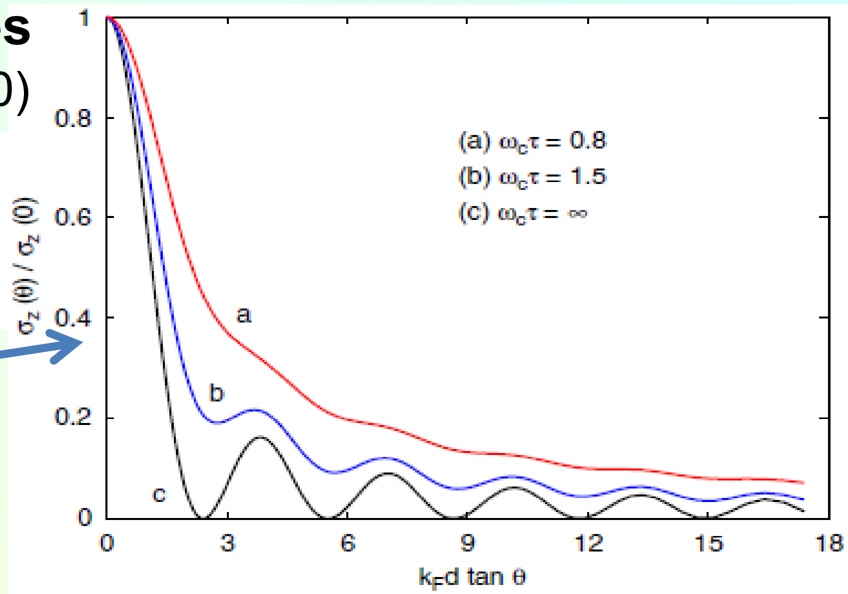
Then Shockley tube integral

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

simplifies and in the first order in t_z gives

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

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



which gives AMRO:

From AMRO one determines k_F, which is compared with the MQO data.

Introduction

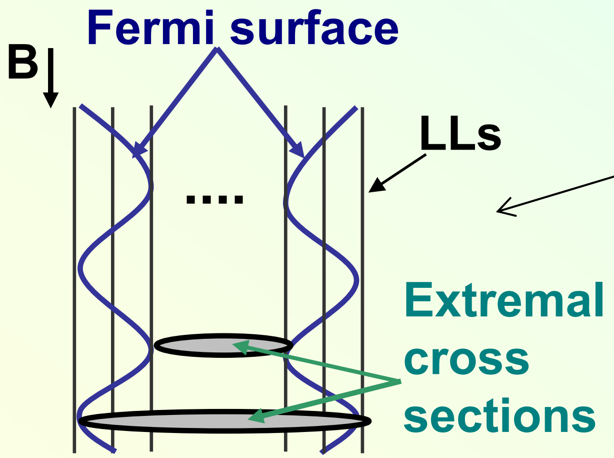
A11

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

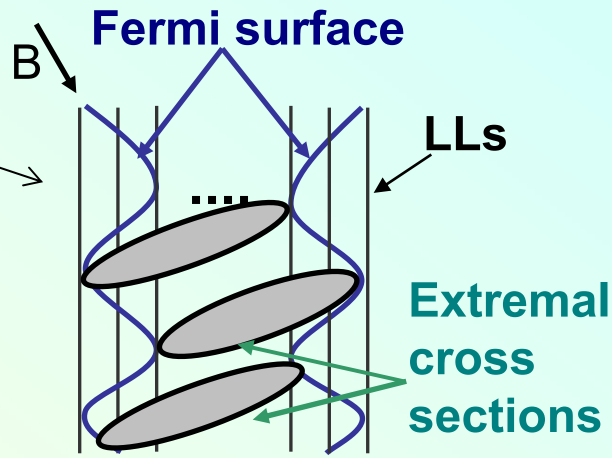
B⊥conducting layers



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

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

Inclined magnetic field



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

Below I will derive that at $\omega_c \tau$ >>1

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

M5

Angular dependence of background magnetoresistance

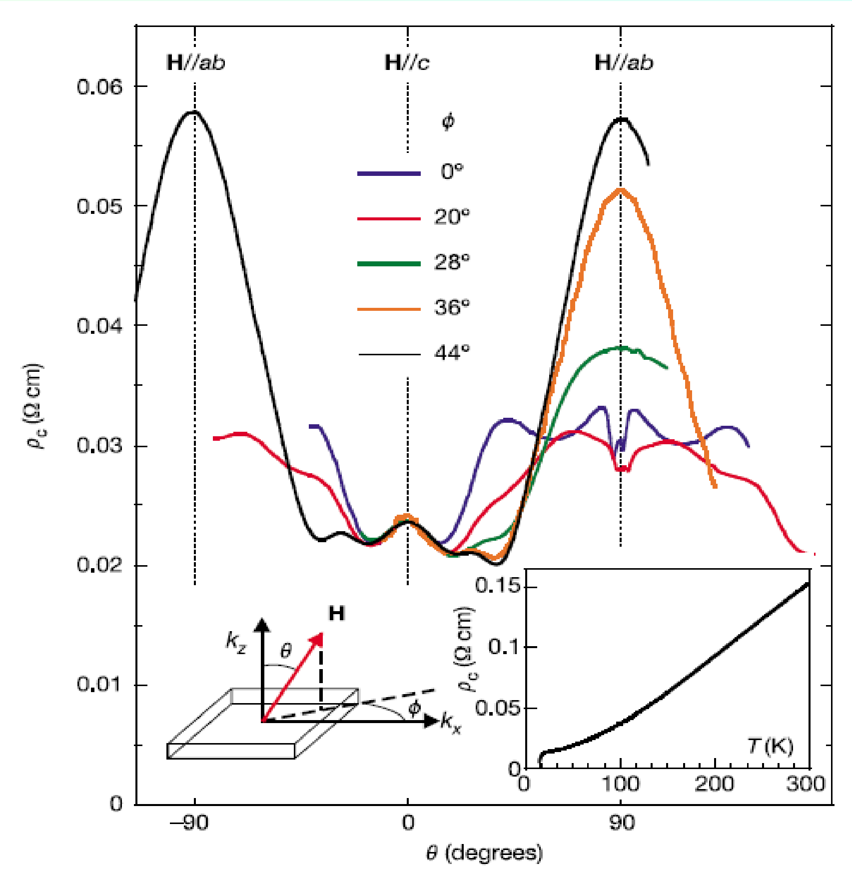
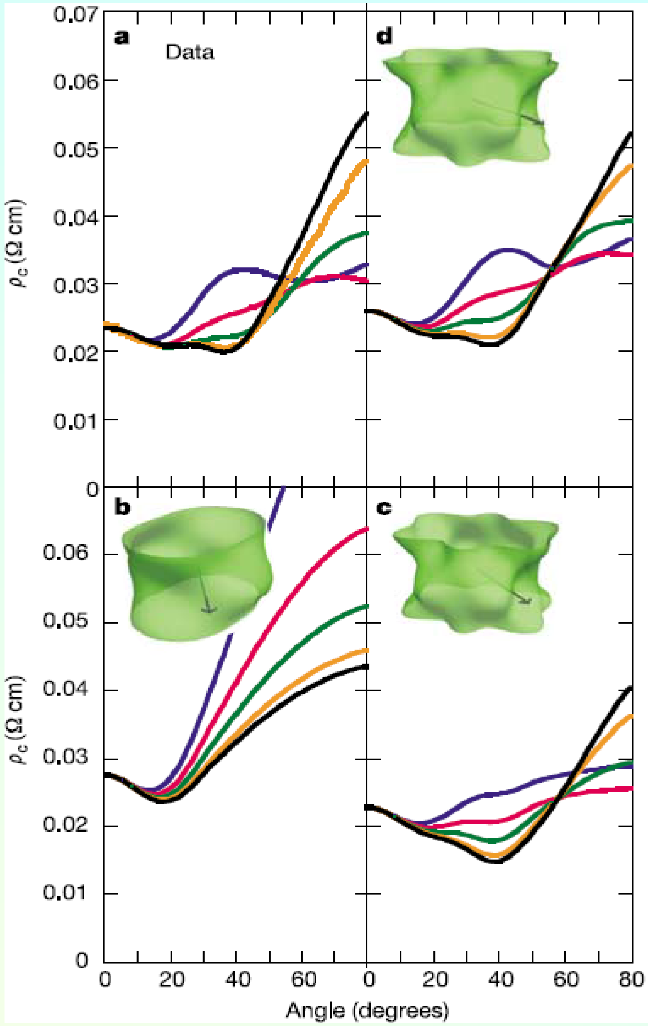


Figure 1 Polar AMRO sweeps in an overdoped Tl2201 single crystal ($T_c \approx 20$ K). The data were taken at $T = 4.2$ K and $H = 45$ T. The different azimuthal orientations ($\pm 4°$) of each polar sweep are stated relative to the Cu–O–Cu bond direction. The key features of the data are as follows: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

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

Difficulties with the numerical calculation of AMRO

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

! The numerical calculation of the S-T integral is hard, because

1)At high tilt angle the FS cross section includes additional closed pockets due to multiple intersection with FS.

2)The integration variable ψ differs from the azimuth angle ϕ. This difference must be thoroughly taken into account.

3)At each step of 3D integration one needs to solve the nonlinear algebraic equation to determine k_z at the point on the FS intersection with the plane $\perp$ B.

4)The calculation gives $\sigma_{zz}(\theta,\phi)$ for the known electron dispersion, while we need to solve the inverse problem. The fitting procedure takes too many fitting parameters and becomes ambiguous.

Can we avoid these complications?

Derivation of relation (5) between magnetoresistance and FS cross-section area

B3

We start from the Shockley tube integral:

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

At $\omega_c\tau$ >>1 it simplifies to

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

The integral

$$I \equiv \int_0^{2\pi} d\psi v_z(\psi,k_{z0}) = \int_0^{2\pi} d\phi \frac{k_F(\phi,k_z)}{m_H^*\cos\theta}\frac{\partial k_F(\phi,E)}{\partial E}\frac{\partial E}{\partial k_z} = \int_0^{2\pi} d\phi \frac{k_F(\phi,k_z)}{m_H^*\cos\theta}\frac{\partial k_F(\phi,k_z)}{\partial k_z}$$

The derivative $\frac{\partial k_F(\phi,k_z)}{\partial k_z} = \frac{\partial k_F[\phi,k_z(k_{z0},\phi)]}{\partial k_{z0}\cdot(\partial k_z/\partial k_{z0})}$ and $\partial k_z/\partial k_{z0} = 1$ from $k_z = k_{z0} - k_F(\varphi+\phi',k_z)\tan\theta\cos\phi'$

Combining this we get $$I = \int_0^{2\pi}\frac{d\phi}{m_H^*\cos\theta}\frac{\partial k_F^2(\phi,k_z)}{2\partial k_{z0}} = \frac{\partial A(k_{z0},\theta,\varphi_0)}{\partial k_{z0}\, m_H^*}$$

B1

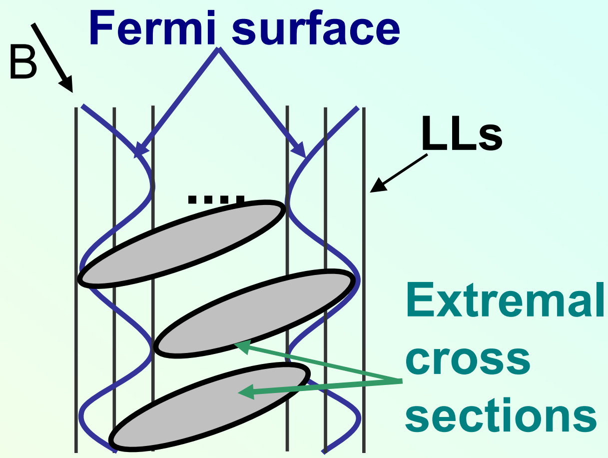
<u>New result 1:</u> Derivation of relation between the angular dependence of magnetoresistance and of the FS cross-section area Its applicability region.

At $\omega_c \tau$ >>1(strong magnetic field and in pure samples) and t_z<<E_F, the interlayer conductivity $\sigma_{zz}(\theta,\phi)$ is related to the k_z-dependence of the FS cross-section area A as

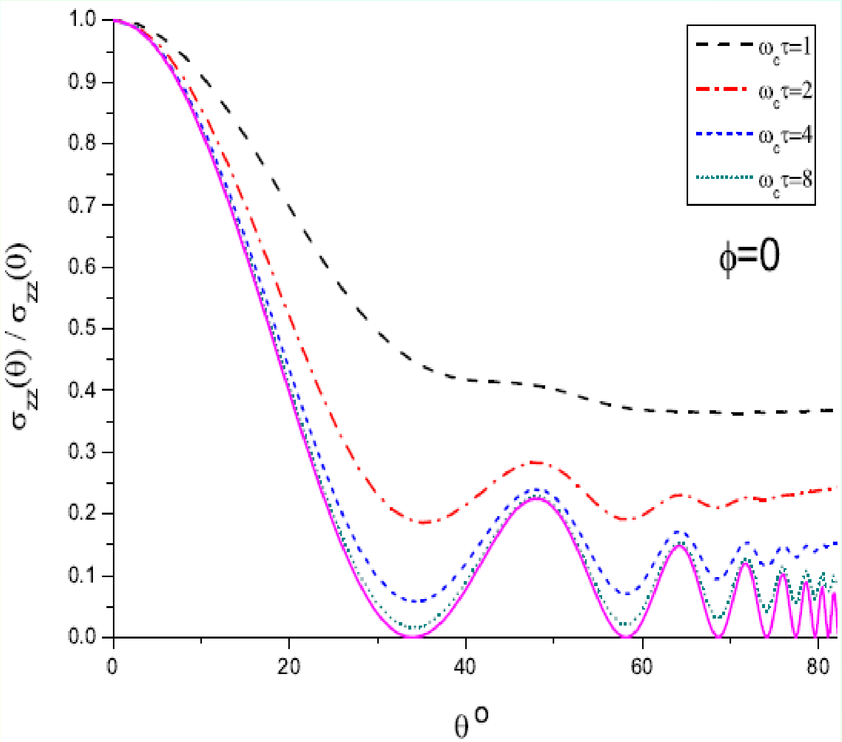
$$\sigma_{zz}\left(\theta,\phi_0\right) = \frac{e^2\tau\cos\theta}{8\pi^4\hbar^2}\int\frac{dk_{z0}}{m_H^*}\left(\frac{\partial A\left(k_{z0},\theta,\phi_0\right)}{\partial k_{z0}}\right)^2. \qquad (5)$$

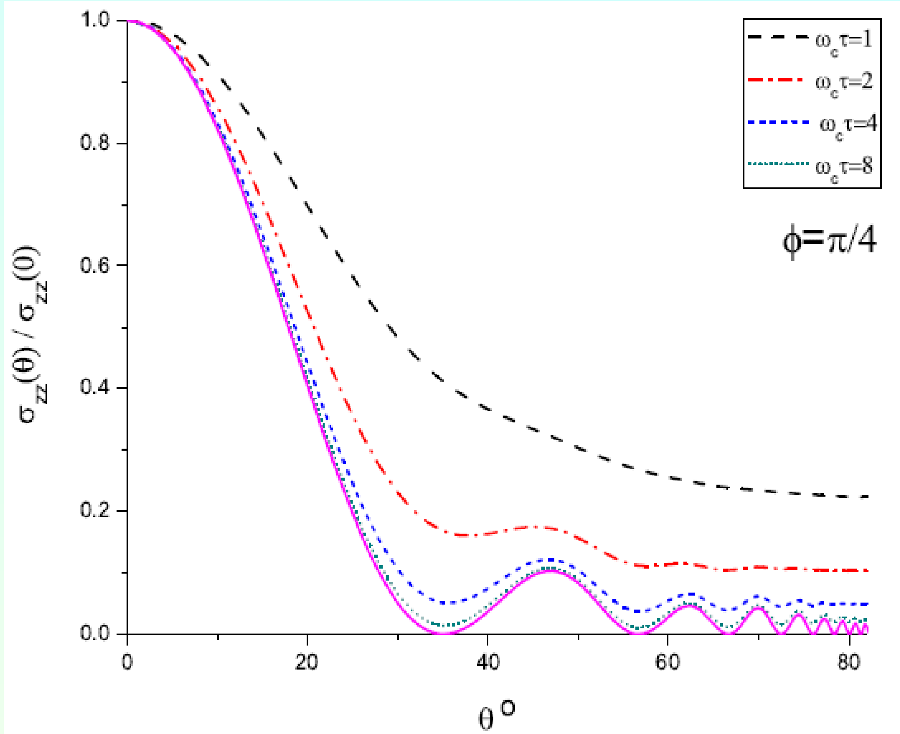
This result relates the calculations of the θ,ϕ - dependence of cross-section area with the magnetoresistance. The positions and the ϕ-dependence of the Yamaji angles are the same.

This relation works well even at $\omega_c \tau$ ~1, as show numerical calculations.



Numerically calculated angular dependence of conductivity $\sigma_{zz}(\theta,\phi)$ for several $\omega_c\tau$ at two different azimuth angles.



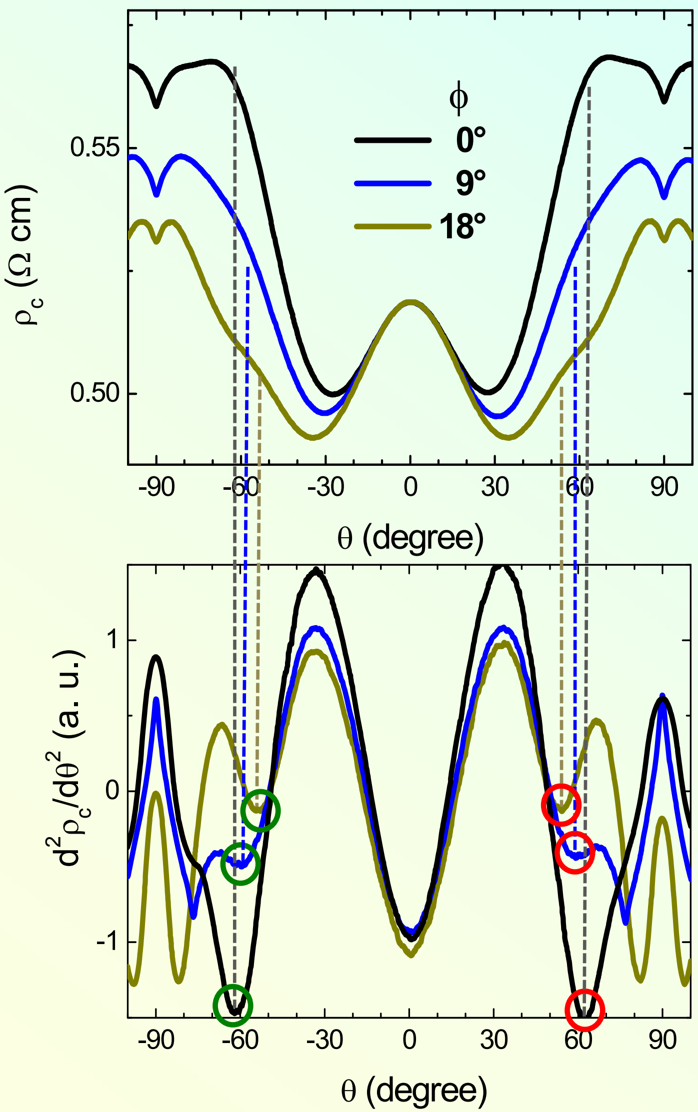


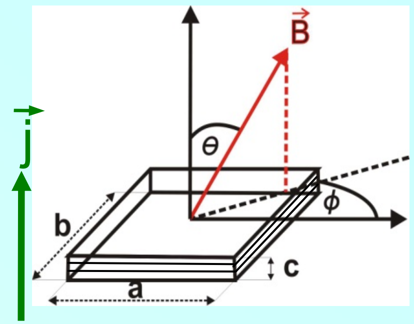
These plots show that the relation between the angular dependence of magnetoresistance and of cross-section area works well at $\omega_c\tau >\approx 2$.

They also show that the saturation value of conductivity at $\theta \to \pi/2$ is strongly ϕ-dependent and can be used to extract the in-plane FS shape.

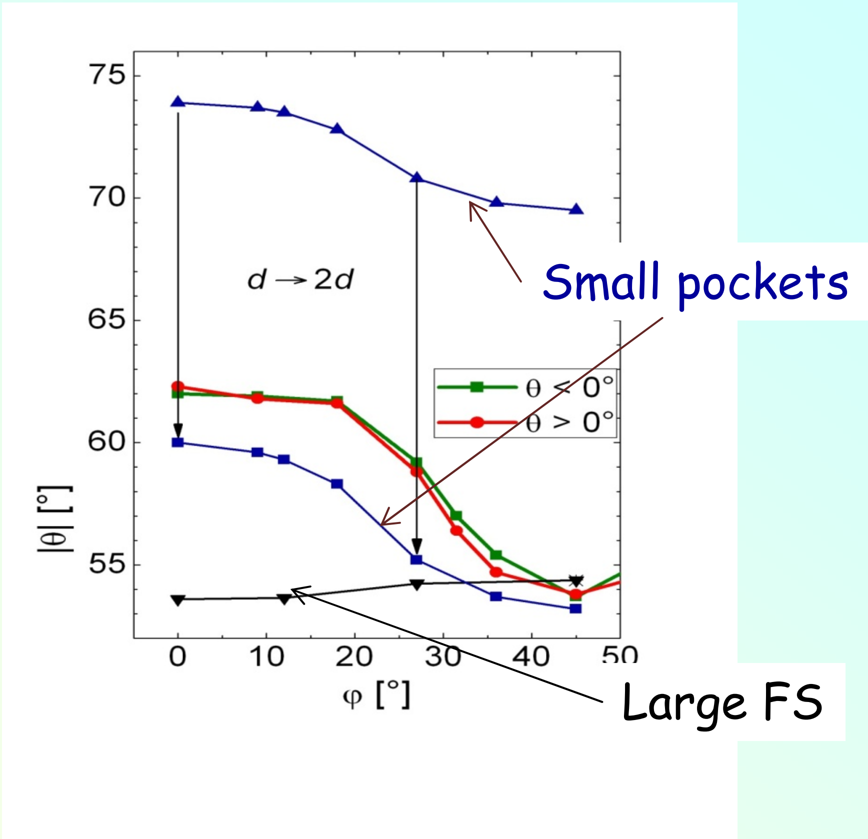
AMRO in NCCO

x = 0.17



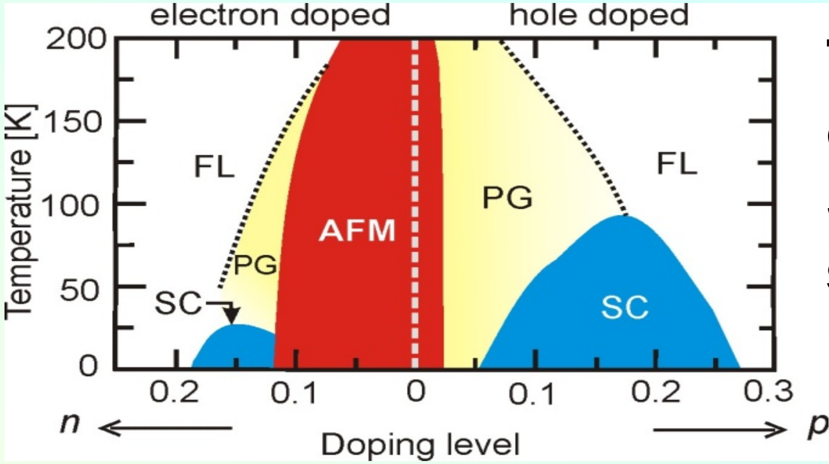


AMRO position is a function of $k_F(\varphi)d$



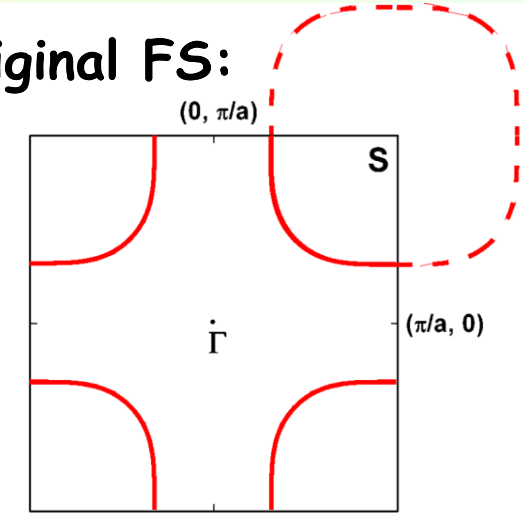
Phase diagram of high-Tc cuprate SC. High Tc and quantum phase transition

$Nd_{2-x}Ce_xCuO_4$ (NCCO)



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

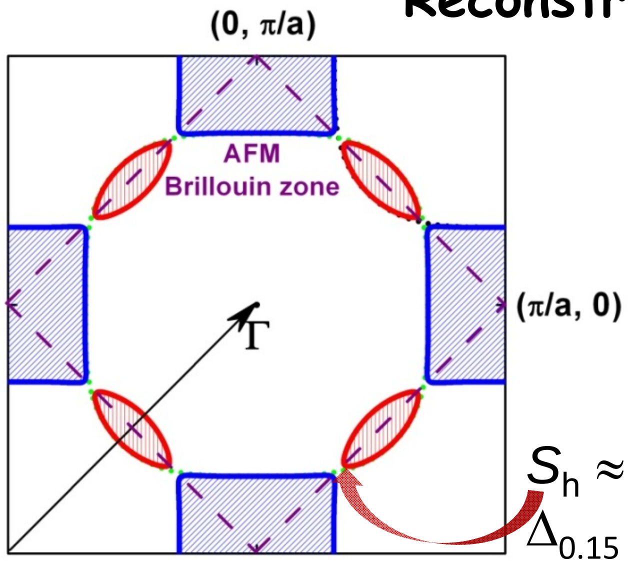
Original FS:



n = 0.17

S_h = 41.5% of S_{BZ}

Reconstructed FS:



n = 0.15 and 0.16

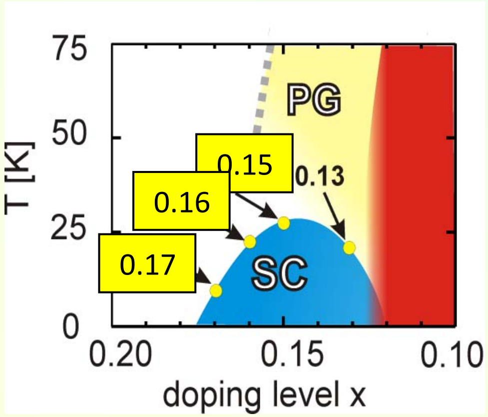
$S_h \approx 1.1\%$ of S_{BZ};

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

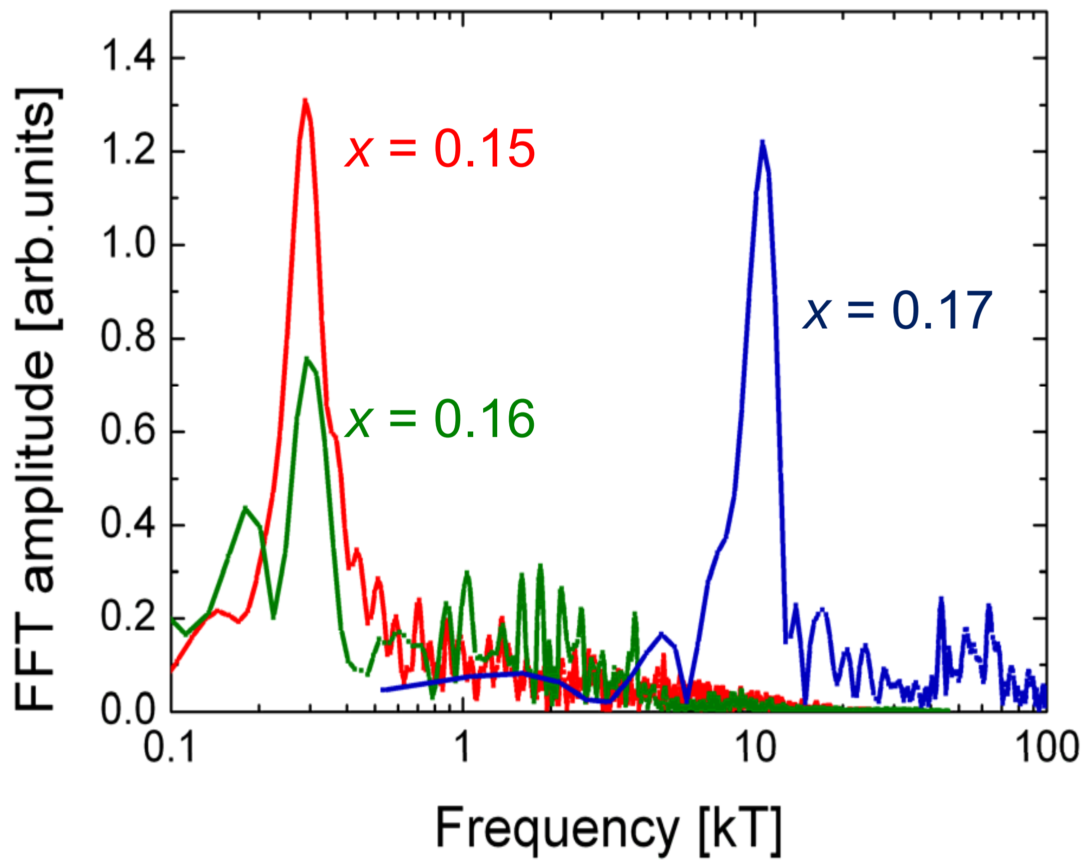
$\Delta_{0.16} \approx 36$ meV

Doping dependence of the Fermi surface (experimental data obtained from MQO)

Phase diagram of electron-doped superconductor
$Nd_{2-x}Ce_xCuO_4$

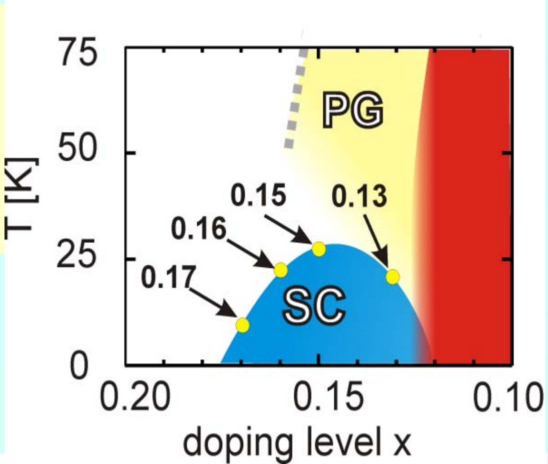


Fourier transform of MQO data

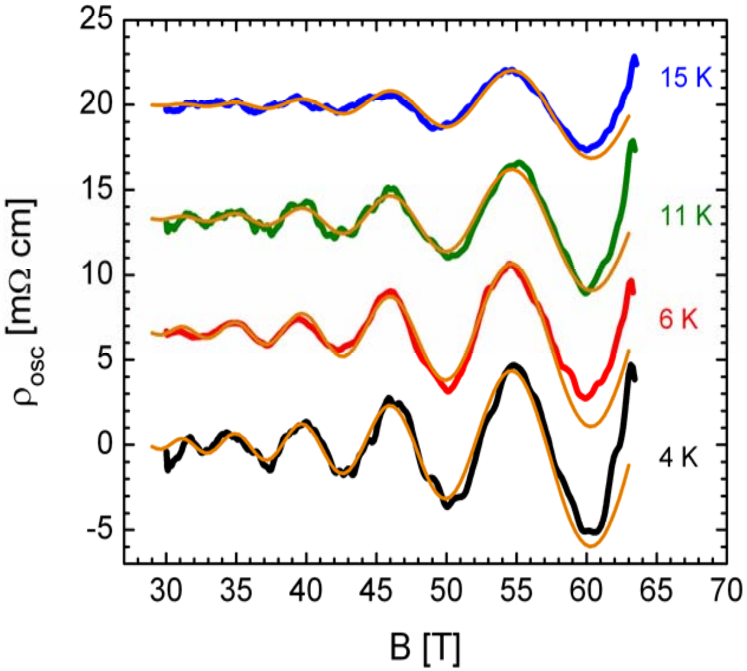


Fermi surface for x = 0.15 and 0.16 appears to be very different from that for x = 0.17

SdH oscillations in $Nd_{2-x}Ce_xCuO_4$



n = 0.15 (optimal doping)

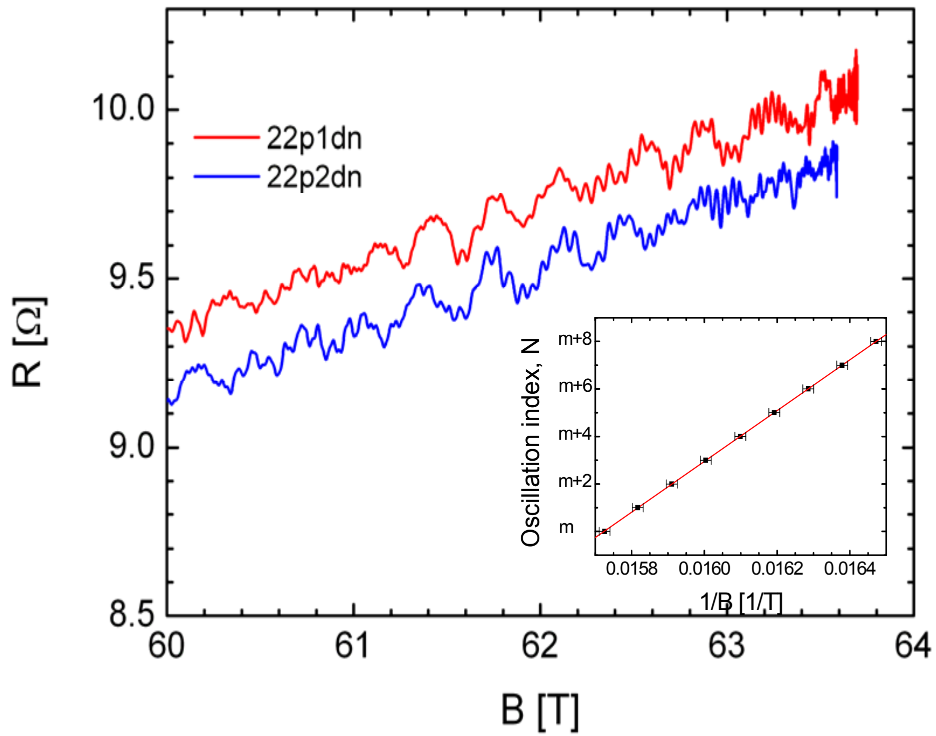


F = 290 T

$\Rightarrow$ $S_{FS} = 2\pi eF/h = 0.011 S_{BZ}$

very small FS!

n = 0.17, strong overdoping



F = 10700 ±300 T $S_{FS} = 0.405 \pm 0.01\ S_{BZ}$

Summary (MQO)

P.D. Grigoriev, Phys. Rev. B 81, 205122 (2010).

Analytical formulas are obtained for the θ,ϕ -dependence of the cross-section area (MQO frequency), which can be used to extract the FS shape from experimental data on MQO in various layered high-Tc superconductors. We also suggests the optimal B-direction for the observation of the angular dependence of MQO.

1. **Harmonic expansion:**

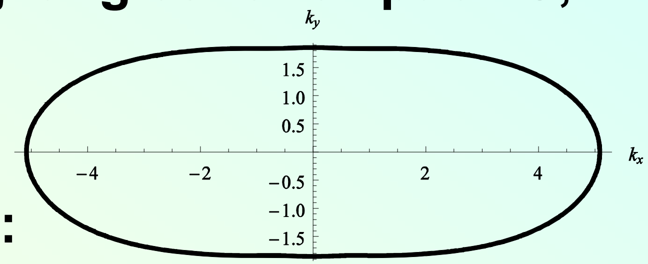
$$k_F(\phi, k_z) = \sum_{\mu,\nu\geq 0} k_{\mu\nu}\cos(\nu k_z c^*)\cos(\mu\phi + \phi_\mu).$$

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

2. **The formula for the ϕ - dependence of Yamaji angles for elliptic FS, which also works well for any elongated FS.**

$$J_0\left[c^* p_B^{\max}(\phi)\tan\theta_n\right] = 0.$$

Applicable to elliptic and elongated in-plane FS:



Thank you for the attention!

Other results (AMRO):

1. **Derivation and investigation of the applicability region of the relation between the angular dependence of magnetoresistance and of the FS cross-section area at $\omega_c\tau$ >>1 in quasi-2D compounds (t_c/E_F<<1):**

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

2. **Angular magnetoresistance oscillations and their fit by numerical calculations:**