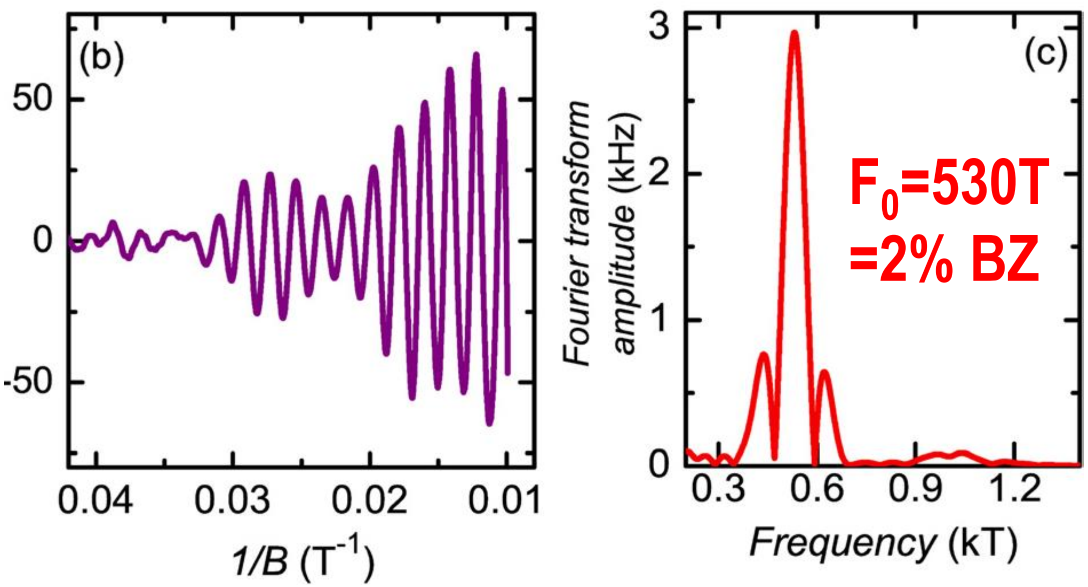
On the origin of magnetic quantum oscillations in YBCO high-Tc superconductors

Pavel D. Grigoriev[1] & Tim Ziman[2]

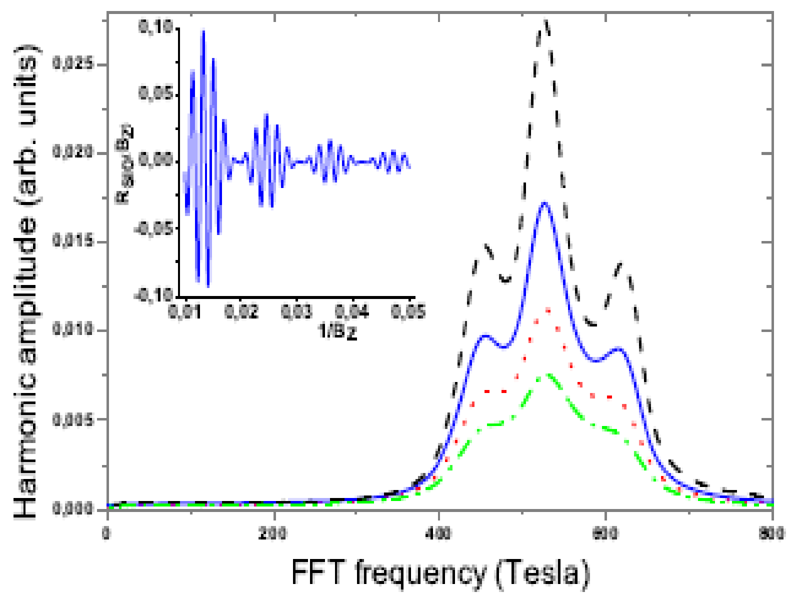
[1] Landau Institute for Theoretical Physics, Chernogolovka, Russia
[2]Institut Laue-Langevin, Grenoble, France

Aim is to explain the observed unusual set of oscillation frequencies of magnetoresistance, consisting of low-frequency peak + two side peaks.

Observed MQO of contactless resistivity in YBCO



Theoretical prediction



P.D. Grigoriev, T. Ziman, JETP Lett. 106, 361; Phys. Rev. B 96, 165110 (2017)

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* is related to the FS extremal cross-section area: $F = chA_{extr}/(2\pi)e,$

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

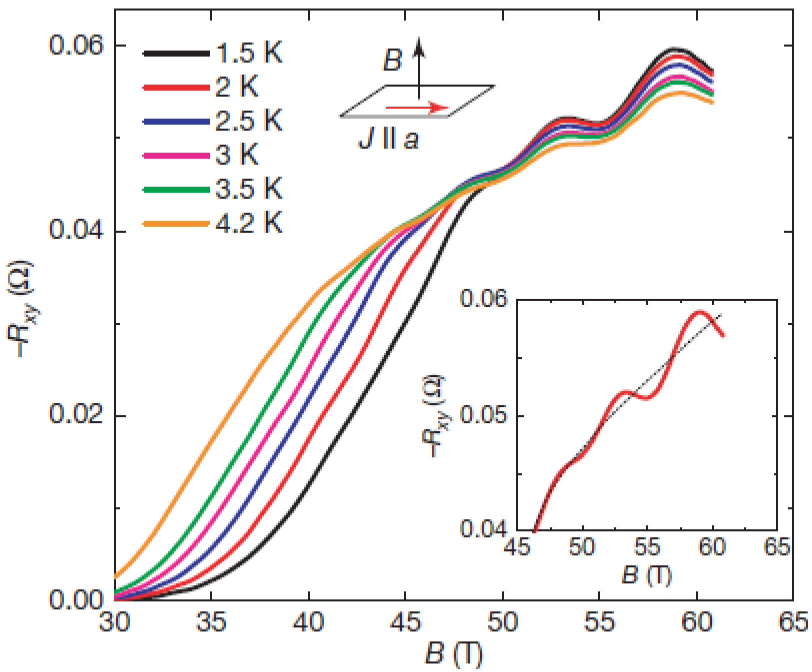
$\kappa \equiv 2\pi k_B T/\hbar\omega_C\,,\ \omega_C = eH/m^*c.$

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

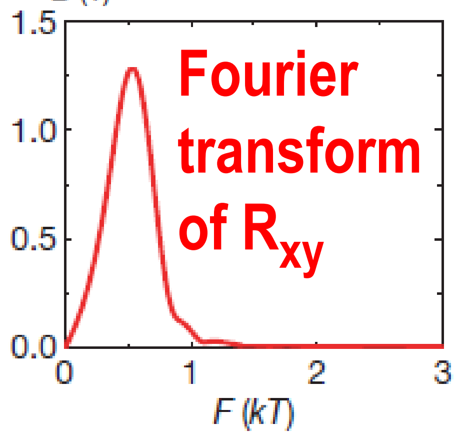
$\tau = \hbar/2\pi k_B T_D$ is the mean free scattering time.

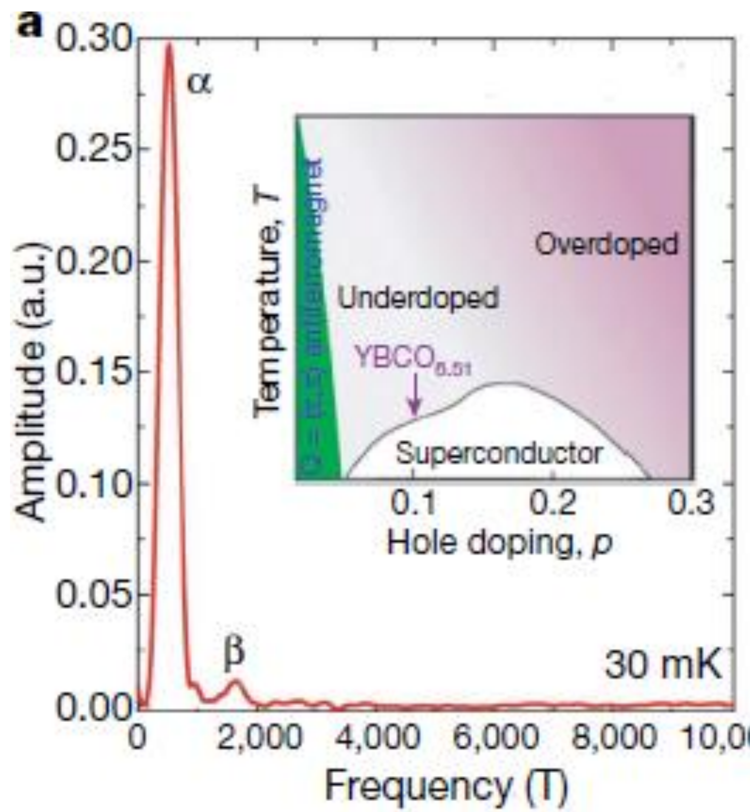
The spin factor $R_s(p) = \cos\left(\frac{\pi p g m^*}{2m_0}\right).$

First observations of MQO in YBCO



N.Doiron-Leyraud et al., Nature 447, 565 (2007)



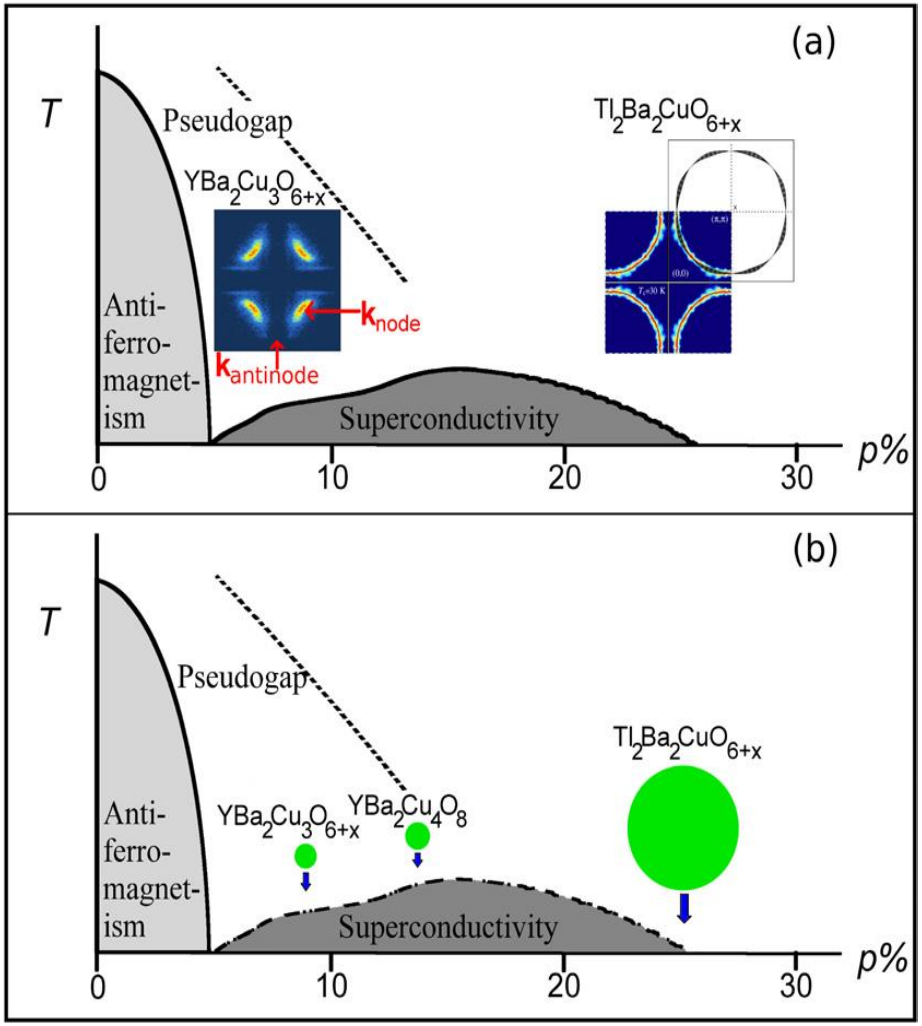


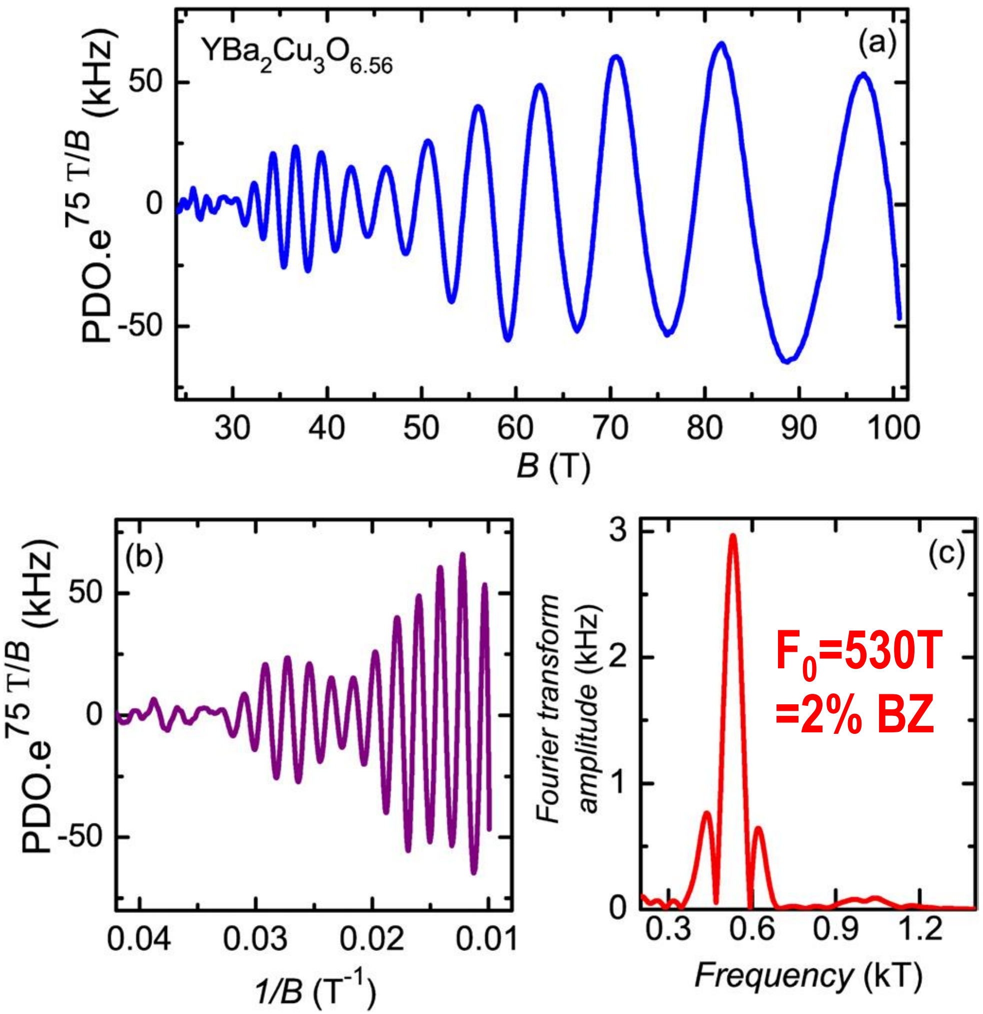
dHvA effect; S.E. Sebastian et al., Nature 454, 200 (2008).

$$F = c\hbar A_{extr} / e,$$

According to the Lifshitz-Kosevich formula any MQO frequency *F* is related to the Fermi-surface extremal cross-section area.

Quantum oscillations observed in YBCO cuprates high-Tc superconductors

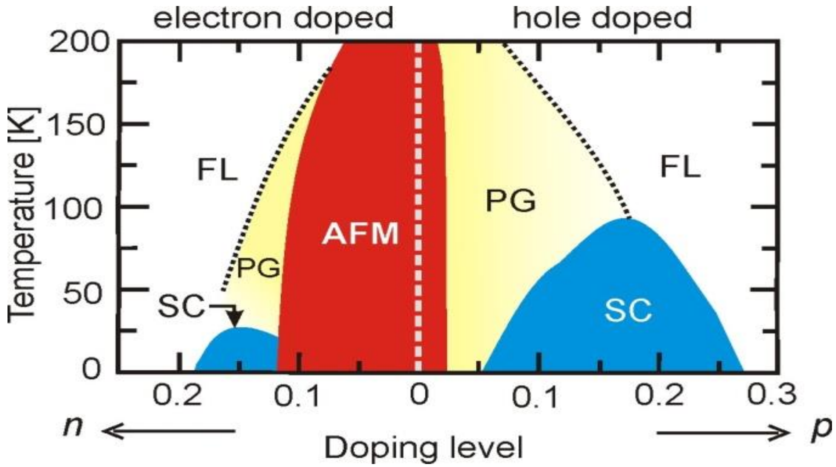




Phase diagram and magnetic quantum oscillations of YBCO cuprate superconductors [Figs. are taken from review S.E. Sebastian et al., Rep. Prog. Phys. 75, 102501 (2012)]

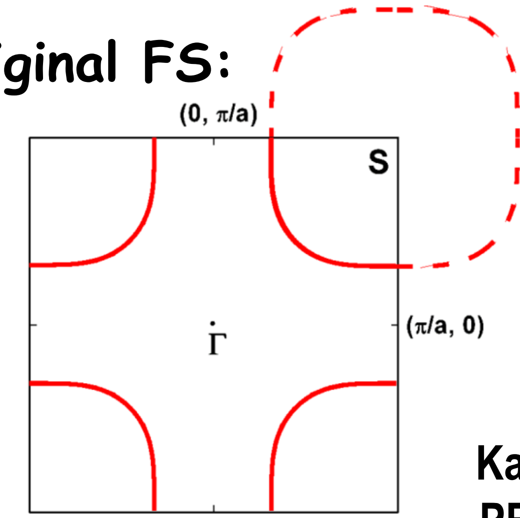
Fermi-surface reconstruction in electron-doped cuprate superconductors

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



For hole-doped YBCO it does not work, because (1) size of hole pocket is larger than 2% of BZ 2) AFM order is absent at doping level p>0.03.

Original FS:

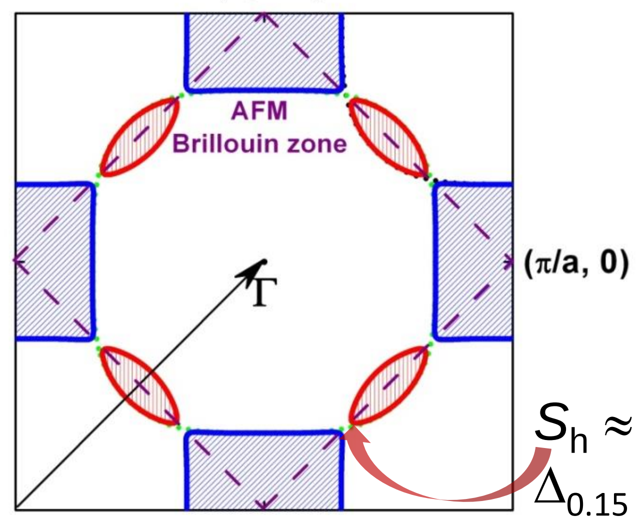


<u>n = 0.17</u>

S_h = 41.5% of S_{BZ}

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

Reconstructed FS:



<u>n = 0.15 and 0.16</u>

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

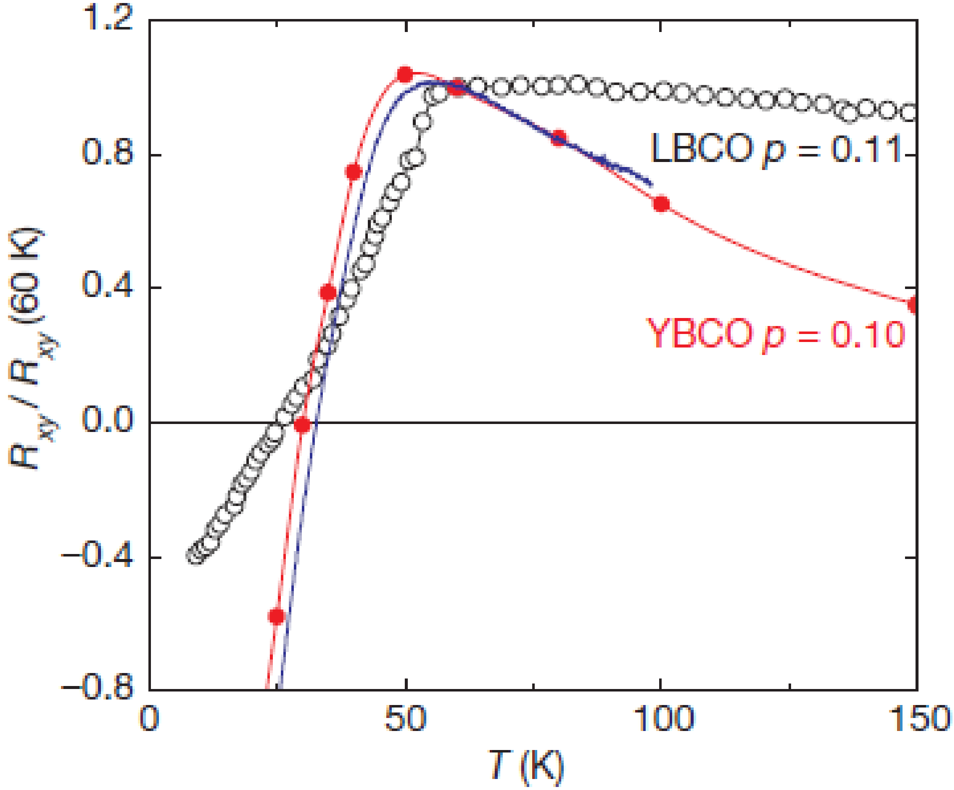
$\Delta_{0.15} \approx 64$ meV;

$\Delta_{0.16} \approx 36$ meV

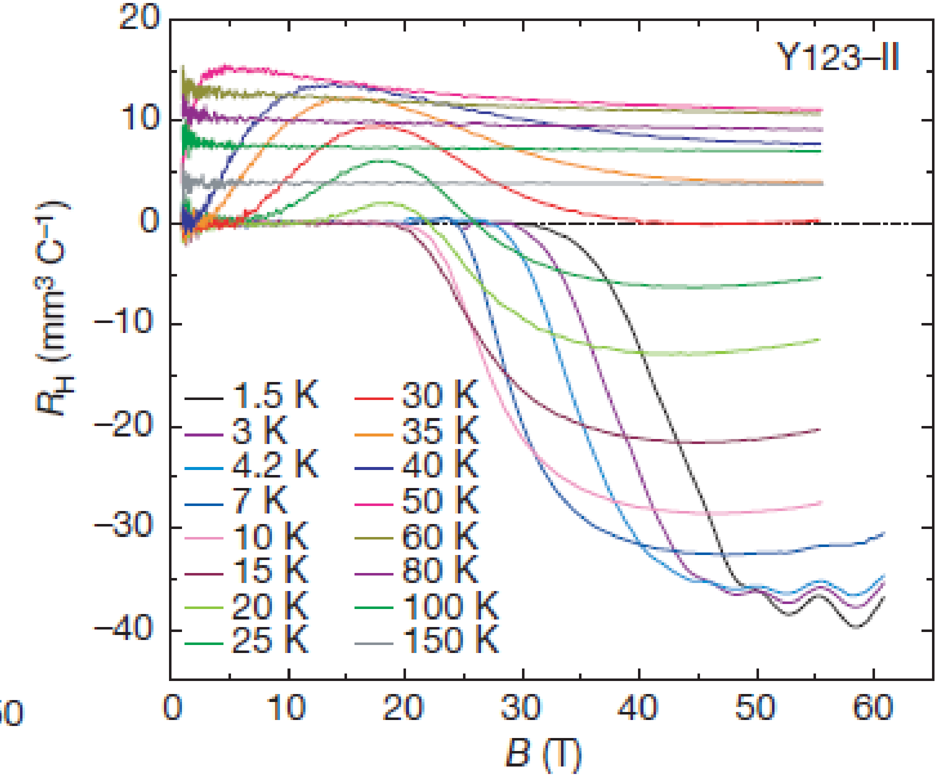
Negative Hall effect

Does it come from electron pockets, superconducting vortex drift or other effects?

Temperature dependence of Hall resistance

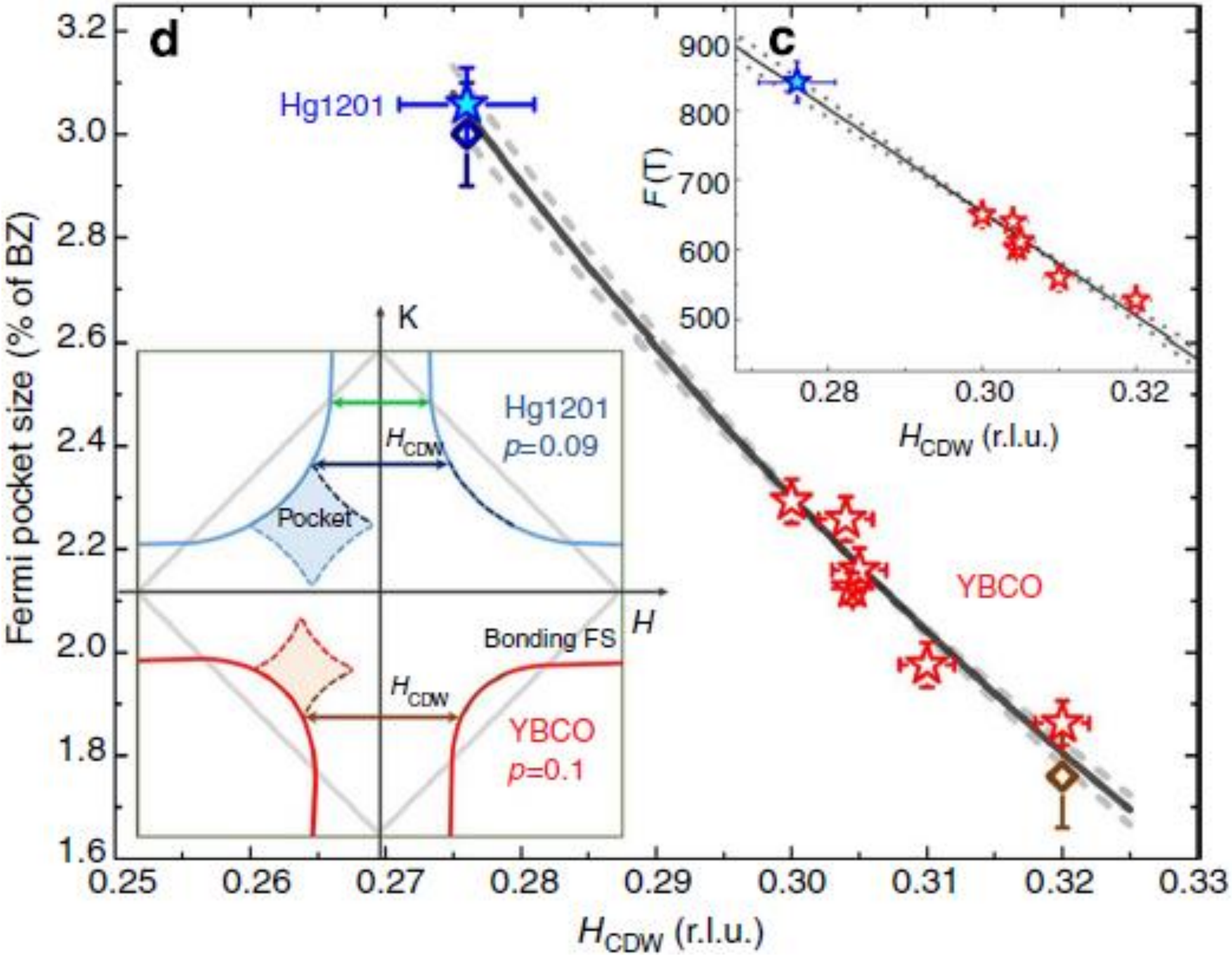


Field dependence of Hall resistance



D. LeBoeuf et al., *Nature* **450**, 533 (2007)

Main-stream explanation of MQO in YBCO:



W. Tabis et al., Nature Comm. **5**, 5875 (2014)

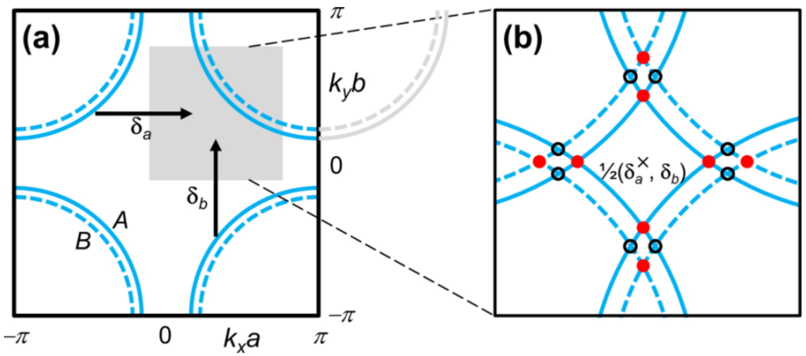
Fermi-surface reconstruction due to charge-density wave

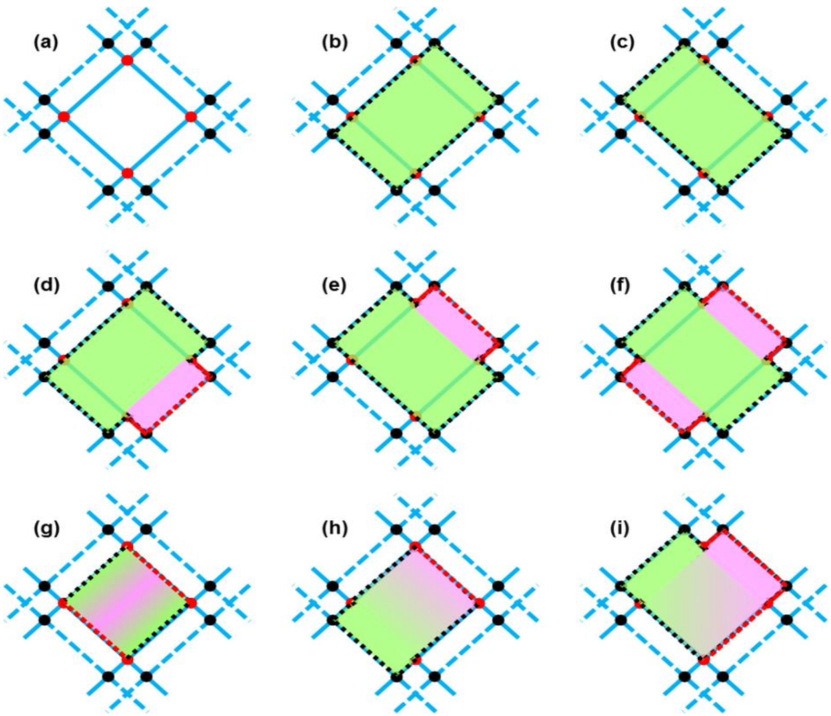
Main drawbacks:

1). Does not predict 3-peak structure of Fourier transform. It gives 2 pockets of bilayer-split FS => two close FFT frequencies.

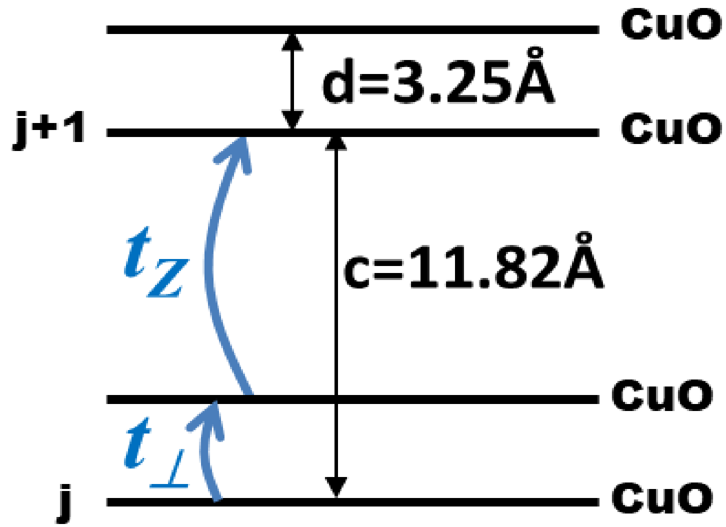
2) Dependence of split frequencies on tilt angle of B.

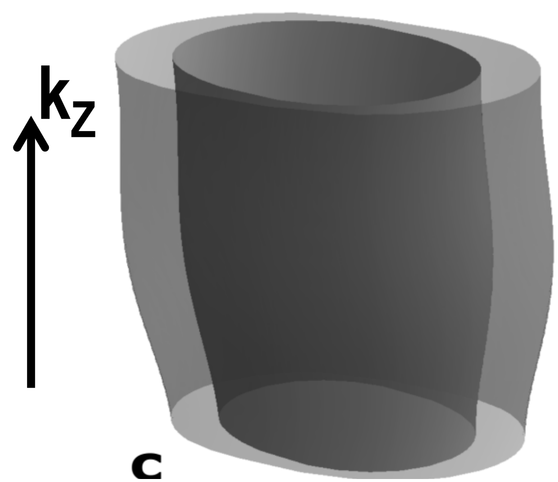
FS reconstruction by CDW predicts 2 closed pockets due to bilayer splitting





A.K.R.Briffa et al., Phys. Rev. B 93, 094502 (2016)

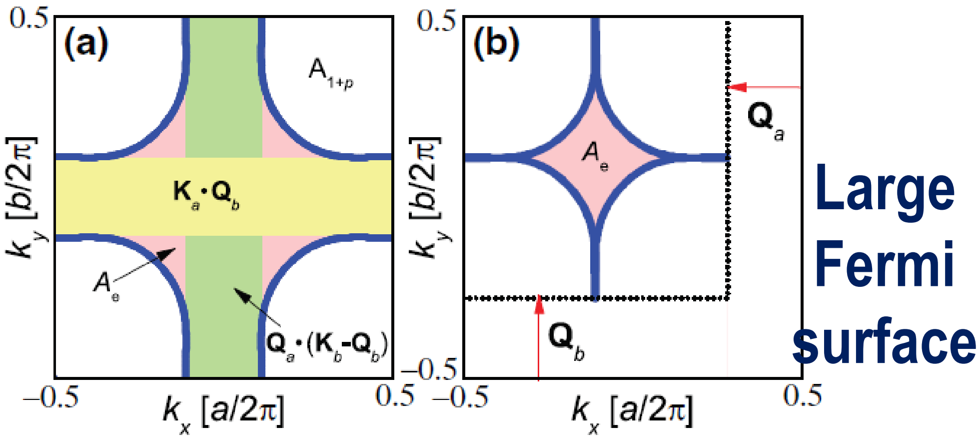


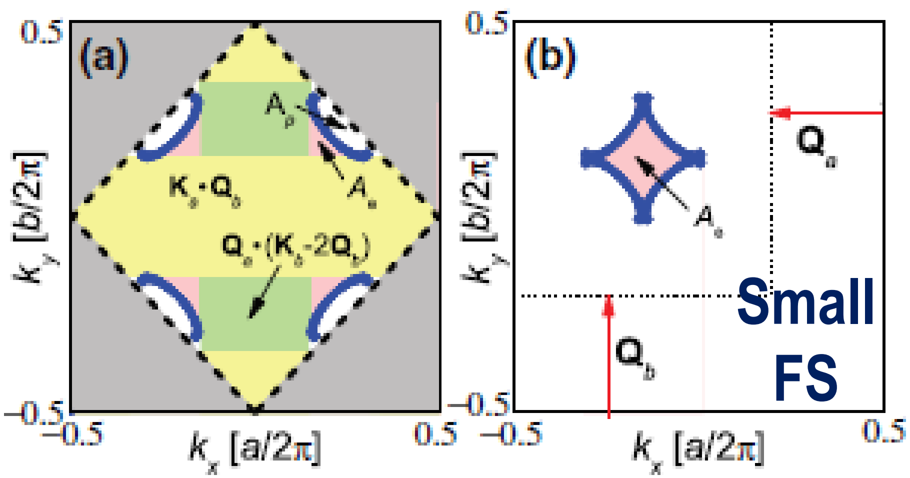


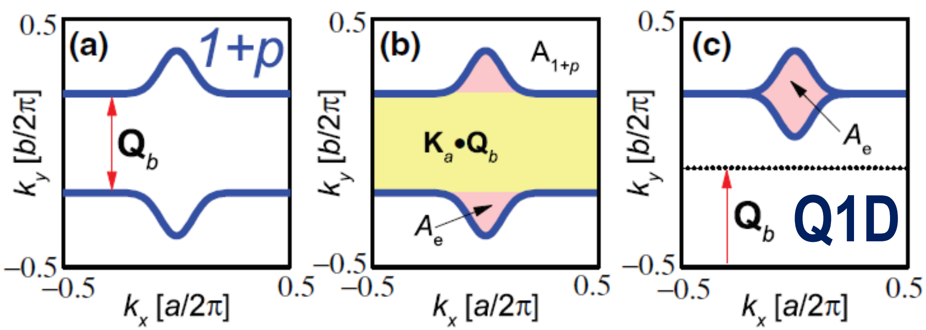
Schematic FS view

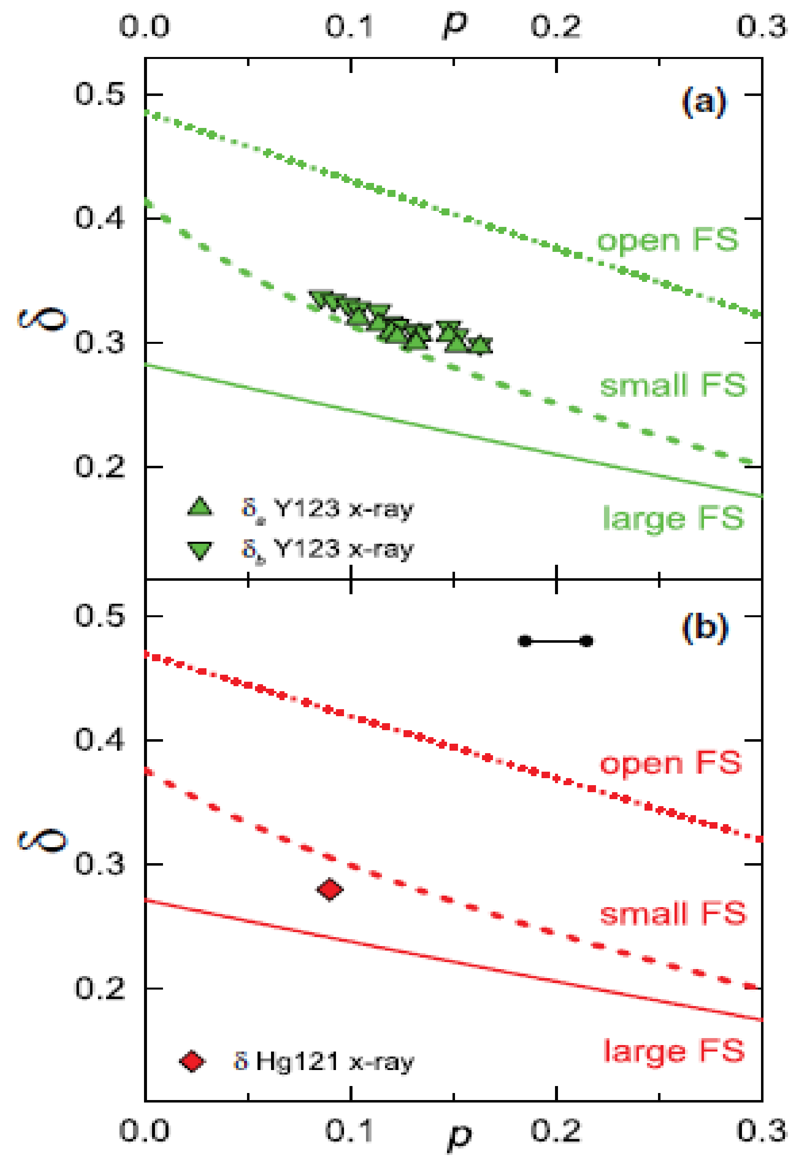
Bilayer-split Fermi surface [PG&TZ, JETP Lett. 106, 361 (2017)]

Main-stream explanation of MQO in cuprates (2)







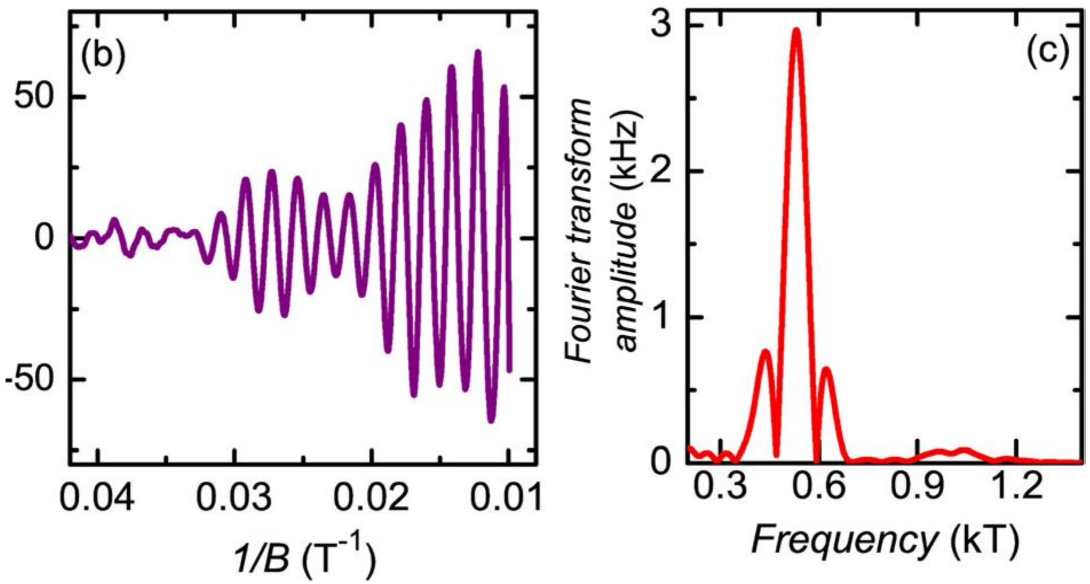


N. Harrison, Phys. Rev. B 94, 085129 (2016)

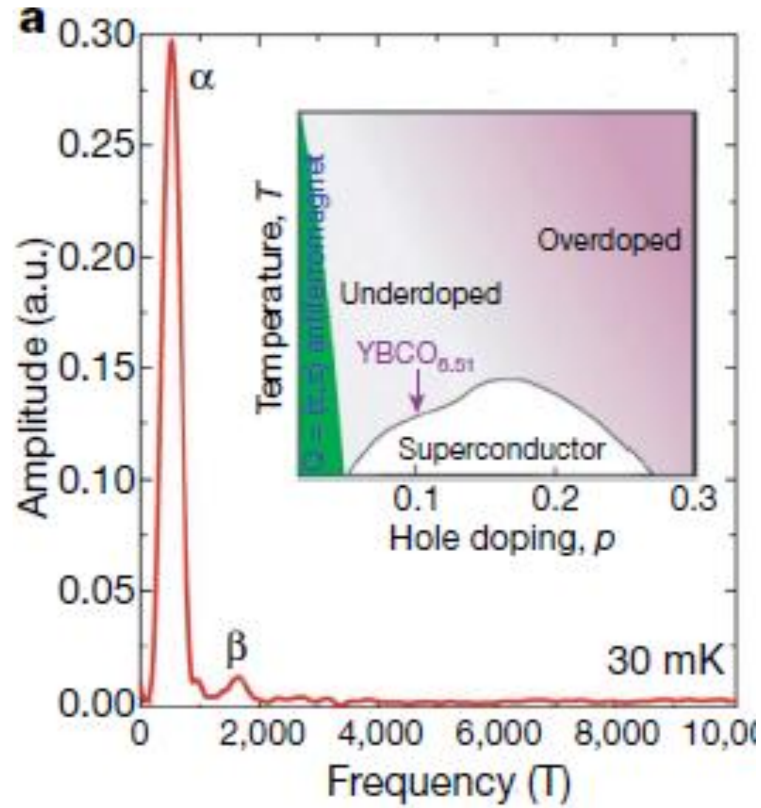
Main drawbacks of standard MQO scenario

1. ! FS reconstruction predicts (many) other MQO frequencies which are not observed in experiment, e.g. due to bilayer splitting.
2. ! In the scenario of FS reconstruction even a small change of doping leads to strong relative change of small FS pocket areas and of F_α. However, in experiment, the $F_\alpha \approx 530T$ and $F_\alpha \pm 90T$ frequencies do not depend considerably on doping level.
3. No agreement with ARPES data
4. How a weak fluctuating CDW ordering leads to "strong" FS reconstruction, i.e. creates a large gap, so that the magnetic breakdown at field B=100T cannot overcome it?
5. ! The angular dependence of $\Delta F_\alpha = 90T$ frequency is described by standard formula $\Delta F_c \cos\theta \propto J_0(k_F c^\star \tan\theta)$. It corresponds to the FS area $\sim \pi k_F^2$ = 6% of BZ and to $F_\beta \approx 1.6kT$ rather than $F_\alpha \approx 530T$.
6. Strong spatial inhomogeneity in YBCO, leading to variations of Fermi level along the sample, should strongly suppress MQO.
7. In $YBa_2Cu_4O_8$ no CDW has been detected, but the MQO are similar.
8. There are too many fitting parameters in FS reconstruction scenario, suggesting that something simple and important is missing.

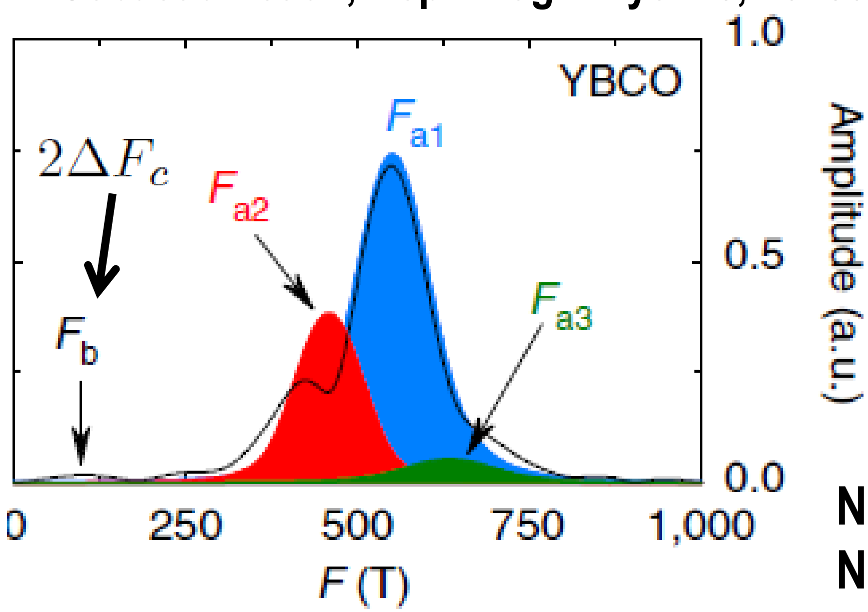
Dominance of the $F_\alpha \approx 530T$ and $F_\alpha \pm 90T$ frequencies



S.E. Sebastian et al., Rep. Prog. Phys. 75, 102501 (2012)

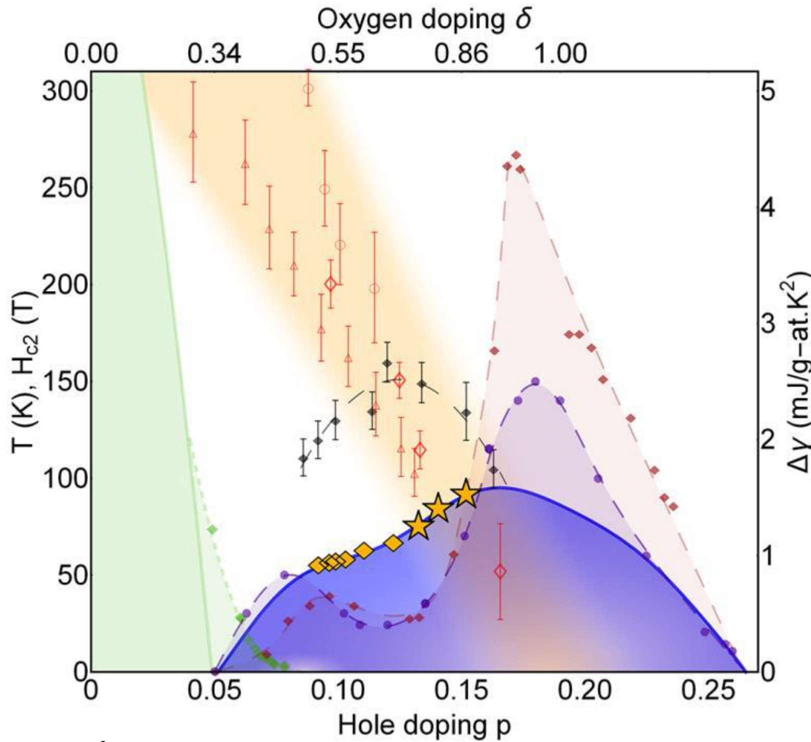


dHvA effect; S.E. Sebastian et al., Nature 454, 200 (2008).

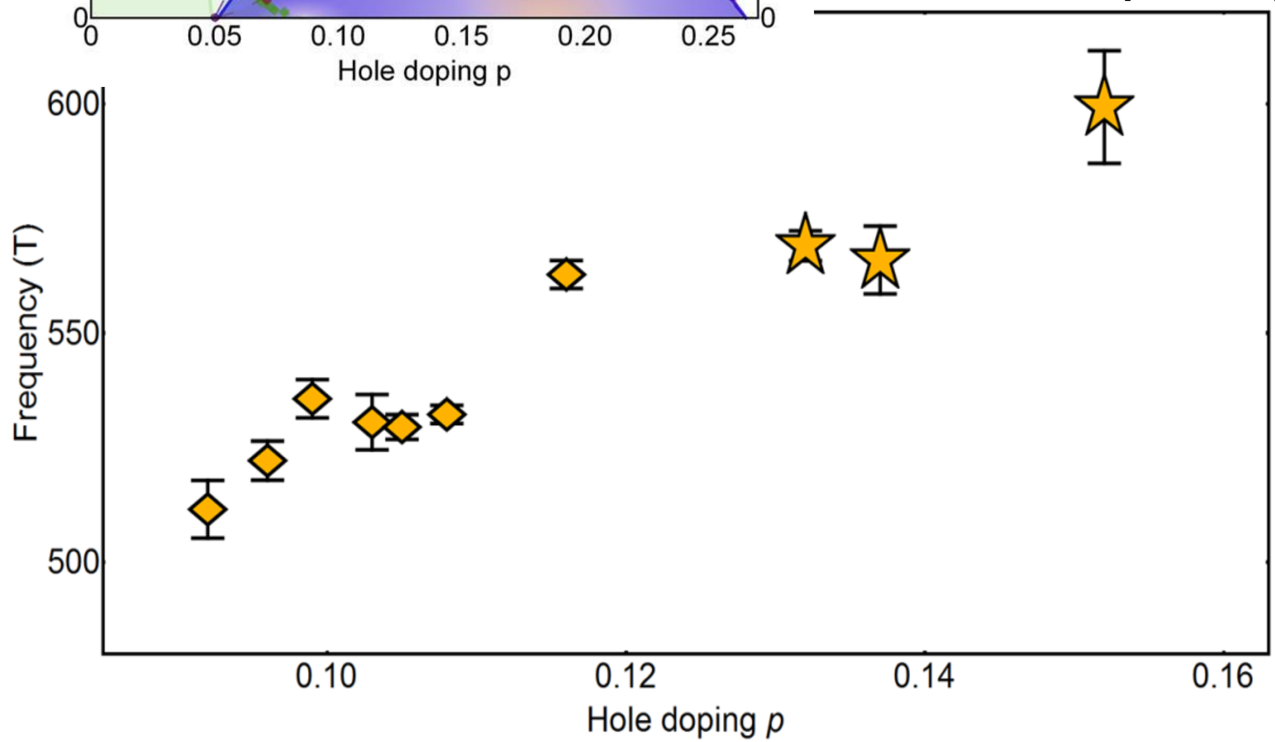


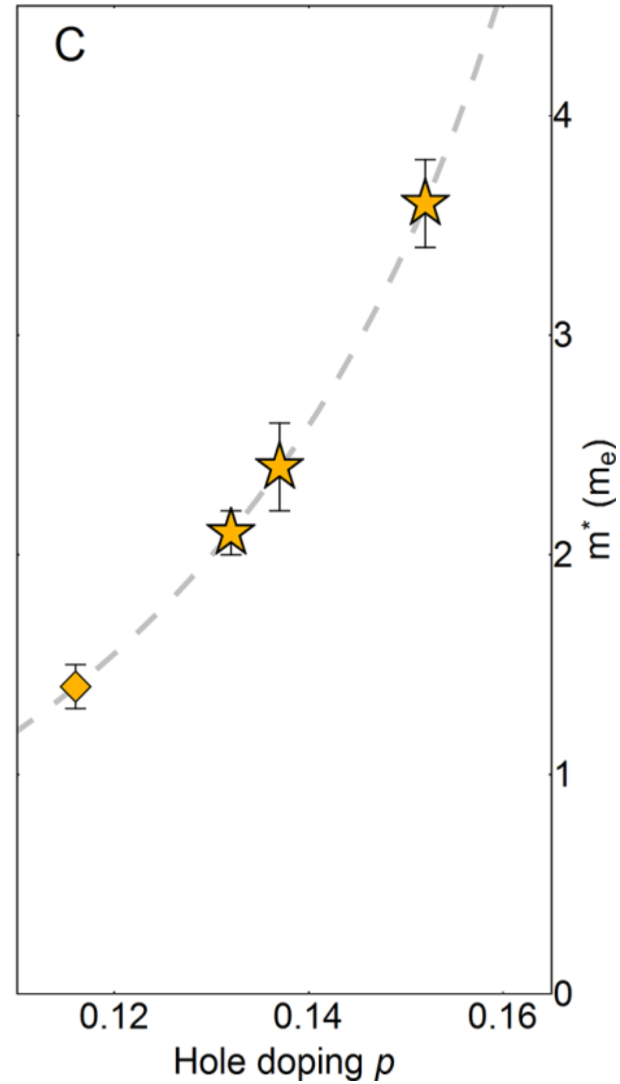
N. Doiron-Leyraud et al., Nature Comm. 6, 6034 (2015).

Doping-dependence of MQO frequencies in YBCO is weak, contrary to m*



B. J. Ramshaw, S. E. Sebastian, et al., Science **348**, 317 (2015)





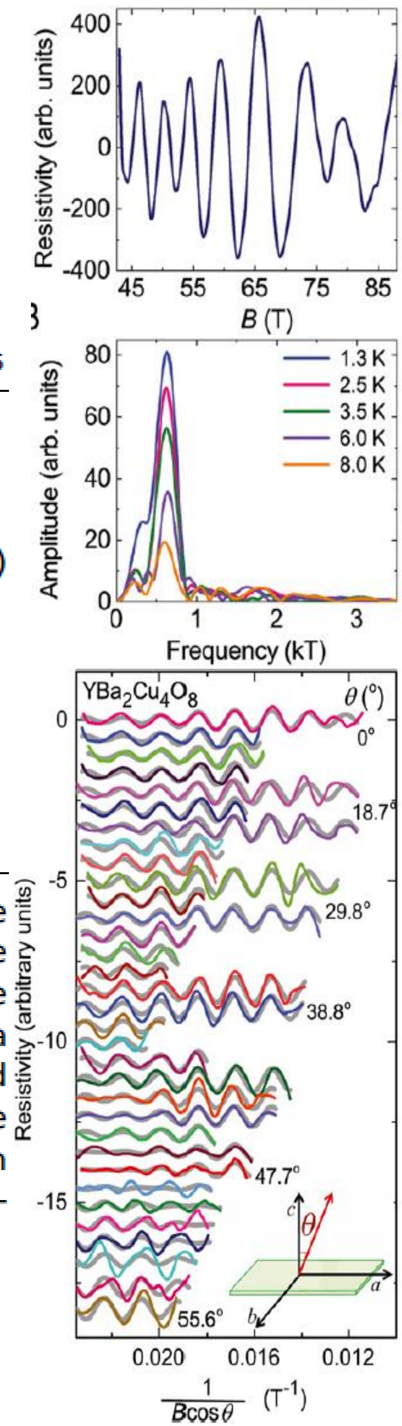
MQO in $YBa_2Cu_4O_8$ (without CDW?)

Table 1. Parameters used to simulate the oscillatory waveform for a quasi-2D split Fermi surface model shown in Fig. 4 represented by the equation $\Psi_{\mathrm{twofold}} \approx \sum_{j=1}^{6} N_j [R_{\mathrm{MB}} R_s R_D R_T]_j \cos(2\pi F_j / B\cos\theta - \pi + \phi)$

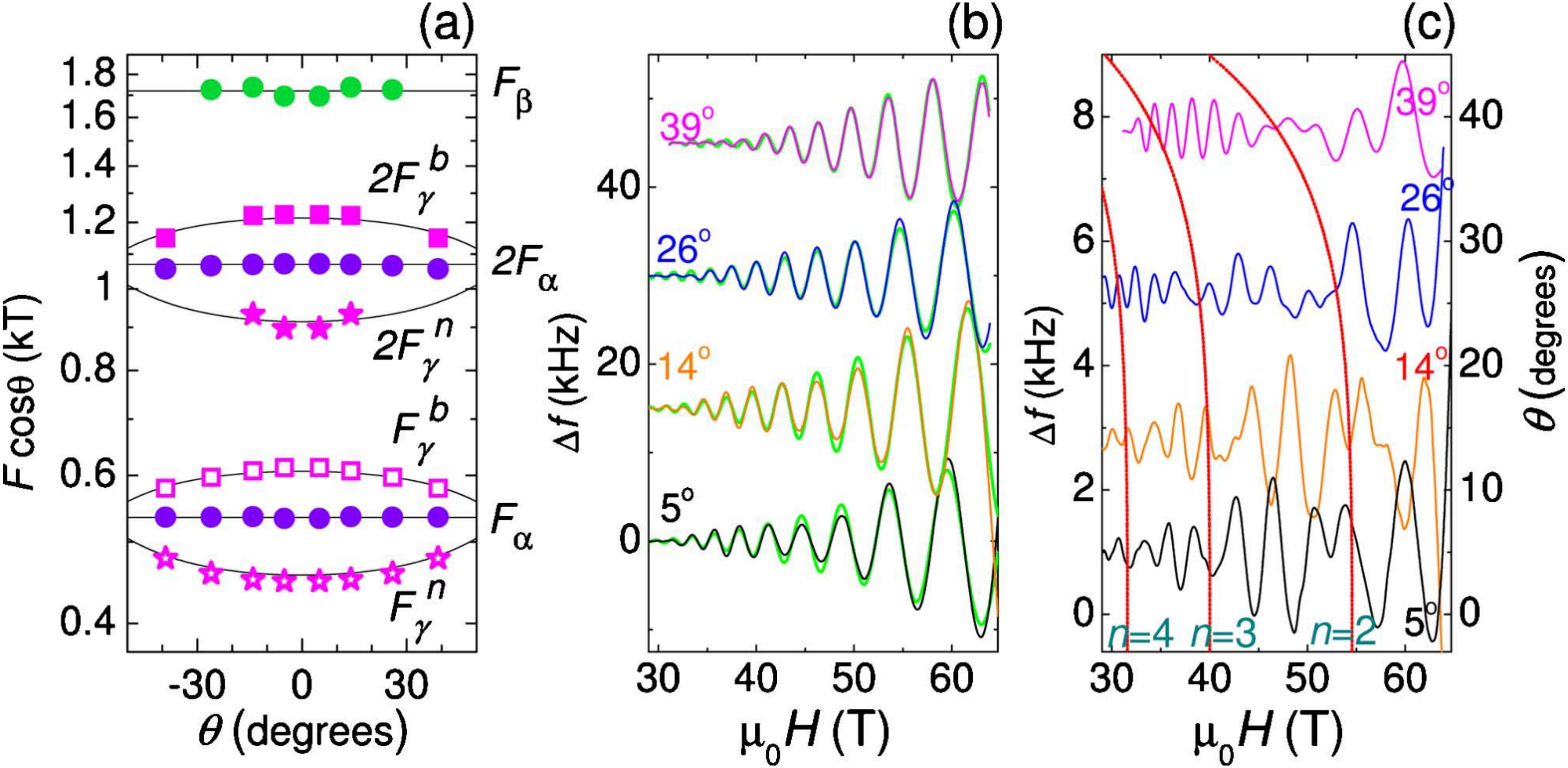
Parameter	Description	$YBa_2Cu_4O_8$	$YBa_2Cu_3O_{6.56}$
F_0	Quantum oscillation frequency	639 T	534 T
$\Delta F_{\mathrm{twofold}}$	Staggered twofold warping frequency	—	15 T
$\Delta F_{\mathrm{split}}$	Bilayer splitting frequency	91 T	90 T
$m^*_{\parallel}$	Quasiparticle effective mass	1.8 m_e (fixed)	1.6 m_e (fixed)
B_0	Magnetic breakdown field	4.2 T	2.7 T
$g^*_{\parallel\square}$	*g*-Factor 1	2.0	2.1
$g^*_{\parallel\diamond}$	*g*-Factor 2	0.1	0.4
$\xi_{\square}$	*g*-Factor anisotropy 1	1.6	1.4
$\xi_{\diamond}$	*g*-Factor anisotropy 2	0.8	0.2
ϕ	Phase	-1.6^c	0 (fixed)

Here, R_{MB} is the magnetic breakdown amplitude reduction factor (defined in *Methods*), and N_j counts the number of instances that the same orbit is repeated within the magnetic breakdown network. R_D is the Dingle damping factor, R_T is the thermal damping factor, and R_s is the spin damping factor (defined in *Methods*). The tabulated values used to simulate the quantum oscillation waveform yield good agreement with experiment as a function of B and θ (Figs. 2 and 3). The effective mass is taken to be a fixed quantity, having been determined independently from temperature-dependent measurements (9). The parameters are the same for all of the orbits, except for those denoted by subscripts $\square$ and $\diamond$, which correspond to subsets of orbits as defined in the text. The values of $g^*_{\parallel j}$ and ξ_j here represent parameters used for simulation rather than unique identifications. The parameters used for $YBa_2Cu_3O_{6.56}$ shown for comparison are taken from ref. 16.

B.S. Tan et al., PNAS **112**, 9568 (2015).



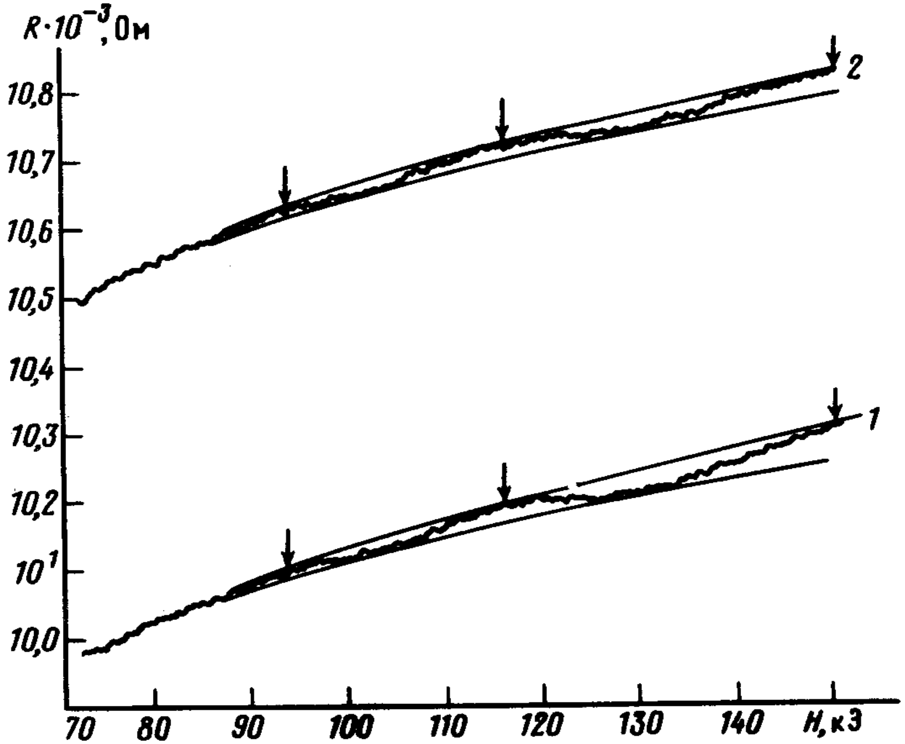
Angular dependence of MQO frequencies



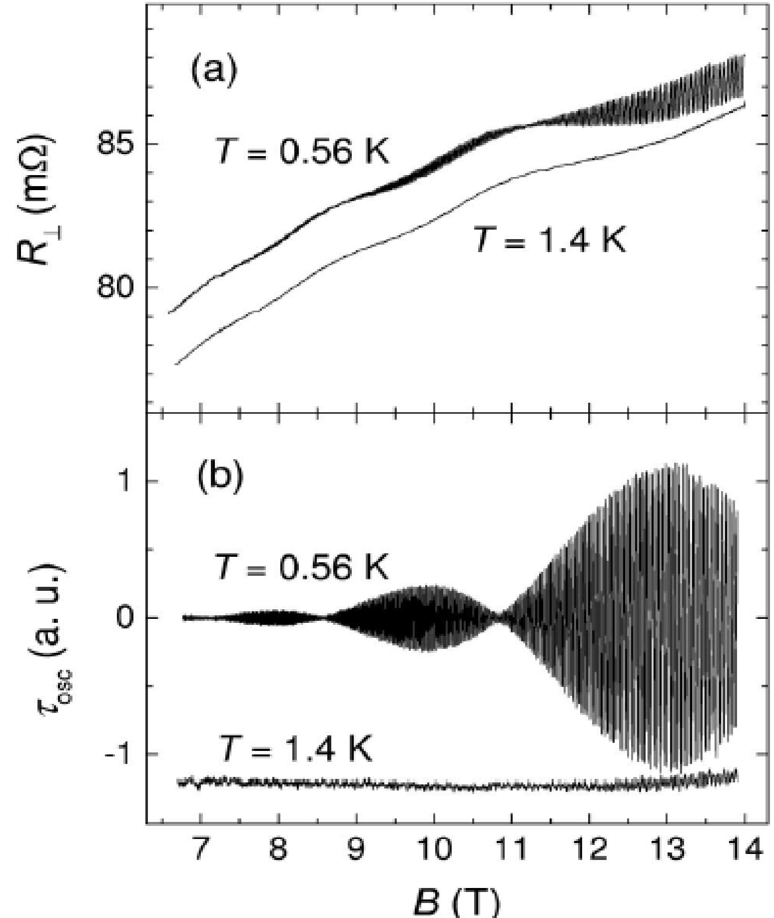
S.E. Sebastian et al., PRB 81, 214524 (2010)

The angular dependence of ΔF_α=90T frequency, described by standard formula, $\Delta F_c \cos\theta \;\propto\; J_0(k_F c^\star \tan\theta)$ corresponds to the FS area $\sim\pi k_F^2$ = 6% of BZ and to $F_\beta \approx$1.6kT rather than $F_\alpha \approx$530T.

Slow oscillations of conductivity in Q2D organic metals appear not from small Fermi-surface pockets but from the splitting due to interlayer transfer integral



M.V. Kartsovnik *et al.*, *Pis'ma Zh. Eksp. Teor. Fiz.* **47,** 302 (1988) [JETP Lett. **47, 363 (1988)]**



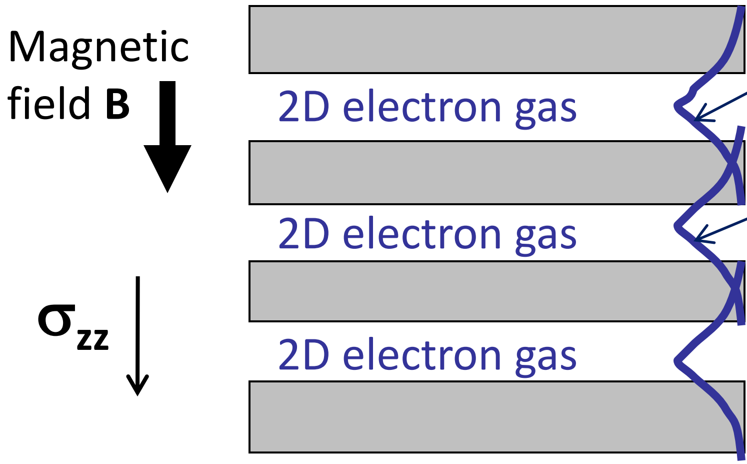
First they were erroneously attributed to small pockets of the Fermi surface, but later explained by FS warping due to interlayer electron dispersion.

M.V. Kartsovnik, P.D. Grigoriev et al., Phys. Rev. Lett. 89, 126802 (2002);

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

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

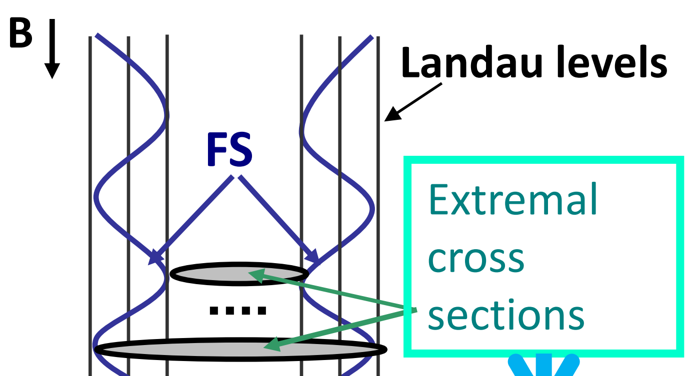
Electron dispersion in the tight-binding approximation is highly anisotropic:

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

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

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

In momentum space:

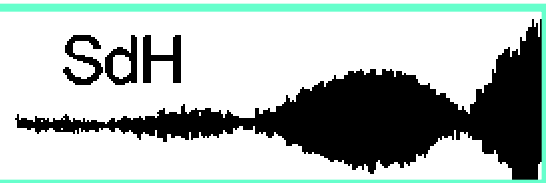


Extremal cross sections

Two close frequencies => beats of MQO

Fermi surface in layered Q2D metals is a warped cylinder.

The size of warping $W=4t_z \sim \hbar\omega_c$



Qualitative explanation of slow oscillations in Q2D metals

Conductivity is a product of density of states (DoS) and diffusion coefficient:

$$\sigma_i(\varepsilon) = e^2 g(\varepsilon) D_i(\varepsilon)$$

The oscillating DoS at the Fermi level is

$$g(\varepsilon)/g_0 = 1 + 2A\cos\left(2\pi\left(\varepsilon + t_z\right)/\omega_c\right) + 2A\cos\left(2\pi\left(\varepsilon - t_z\right)/\omega_c\right)$$

and the diffusion coefficient is

$$D_i(\varepsilon)/D_0 = 1 + B\cos\left(2\pi\left(\varepsilon + t_z\right)/\omega_c\right) + B\cos\left(2\pi\left(\varepsilon - t_z\right)/\omega_c\right)$$

The product $g(\varepsilon) D_{i,\beta}(\varepsilon)$ **contains**

$$\frac{D_i(\varepsilon) g(\varepsilon)}{D_0 g_0} = 1 + .. + 2AB\cos\left(2\pi\left(\varepsilon + t_z\right)/\omega_c\right)\cos\left(2\pi\left(\varepsilon - t_z\right)/\omega_c\right)$$

$$+ AB\left[\cos^2\left(2\pi\left(\varepsilon + t_z\right)/\omega_c\right) + \cos^2\left(2\pi\left(\varepsilon - t_z\right)/\omega_c\right)\right]$$

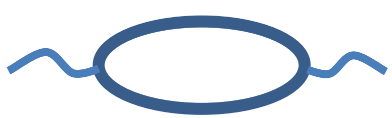
slow oscillations $\cos(4\pi t_z/\hbar\omega_c)$

$$\cos(x-y)\cos(x+y) = [\cos(2x) + \cos(2y)]/2$$

Second harmonic of quantum oscillations

$$\Rightarrow \boxed{AB\cos\left(4\pi t_z/\omega_c\right)}$$ **(slow oscillations!)**

Slow oscillations can also be calculated using the Kubo formula:
[P.D. Grigoriev, PRB 67, 144401 (2003)]



Results of our calculations of magnetic oscillations using Kubo formula

Intralayer conductivity

$$\sigma_{xx}(\mu, T) \approx \overline{\sigma}_{xx}^{(0)}(\mu) + \sigma_{xx}^{\mathrm{QO}}(\mu) R_T R_W + \sigma_{xx}^{\mathrm{SO}}(\mu),$$

$$\overline{\sigma}_{xx}^{(0)}(\varepsilon) \approx \frac{e^2}{2\pi\hbar d}\frac{\overline{\alpha}\gamma_0}{\gamma_0^2+\pi^2}.$$

$$\sigma_{xx}^{\mathrm{SO}}(\varepsilon) \approx 2\pi^2 \overline{\sigma}_{xx}^{(0)} R_D^2 J_0^2(\lambda) \frac{\pi^2 - 3\gamma_0^2}{\left(\gamma_0^2+\pi^2\right)^2}$$

$$\sigma_{xx}^{\mathrm{QO}}(\varepsilon) \approx -2\overline{\sigma}_{xx}^{(0)} R_D R_S \left[\frac{2\pi^2 J_0(\lambda)}{\gamma_0^2+\pi^2}\cos(\overline{\alpha}) - \frac{\lambda}{\overline{\alpha}} J_1(\lambda)\sin(\overline{\alpha})\right]$$

$$R_D = \exp(-\gamma)$$

where $\alpha \equiv \alpha(\varepsilon_*) \equiv 2\pi\varepsilon_*/(\hbar\omega_c)$ $\lambda = 4\pi t_z/(\hbar\omega_c)$, $\gamma = 2\pi\Gamma/(\hbar\omega_c)$

T. I. Mogilyuk, P. D. Grigoriev, Phys. Rev. B 98, 045118 (2018).

Interlayer conductivity

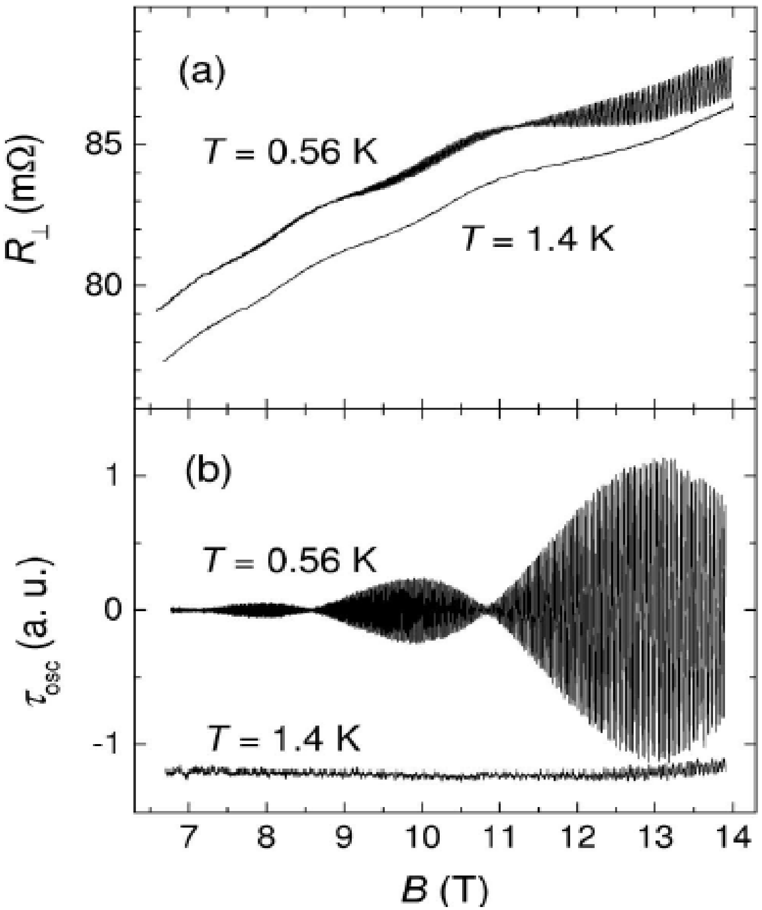
$$\sigma_{zz}^{\mathrm{QO}}(\mu) \approx 2\overline{\sigma}_{zz}^{(0)} \cos(\overline{\alpha}) R_D \left[J_0(\lambda) - \frac{2}{\lambda}(1+\gamma_0) J_1(\lambda)\right]$$

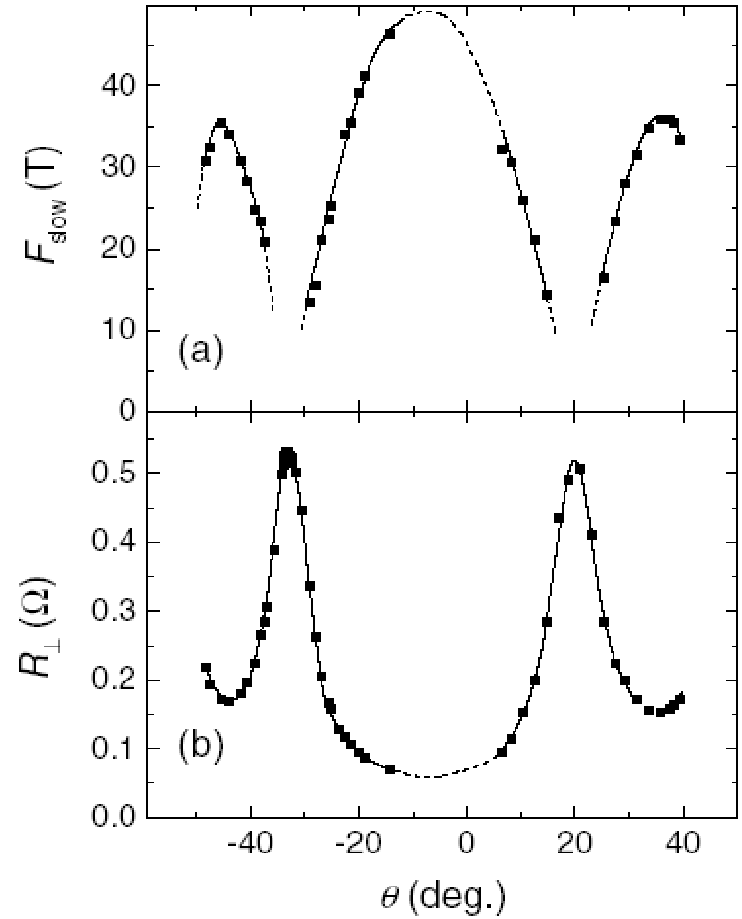
$$\sigma_{zz}^{\mathrm{SO}}(\mu) \approx 2\overline{\sigma}_{zz}^{(0)} R_D^2 J_0(\lambda)\left[J_0(\lambda) - \frac{2}{\lambda} J_1(\lambda)\right]$$

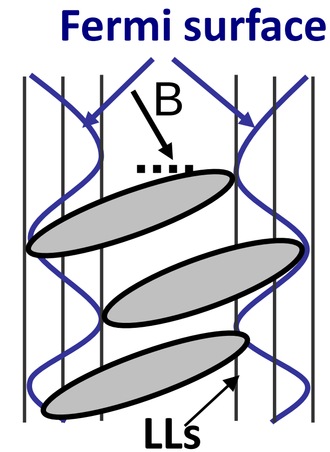
P. D. Grigoriev, Phys. Rev. B 67, 144401 (2003).

Slow oscillations (angular dependence of frequency)

[M. V. Kartsovnik, P. D. Grigoriev et al., Phys. Rev. Lett. 89, 126802, (2002)]







General view of quantum & slow oscillations of magnetoresistance

Angle dependence of the frequency of slow oscillations is similar to that of *t(θ)*

$$F_{slow} = \frac{2t_z B}{\hbar\omega_c} = \frac{2t_z m^* c}{e\hbar\cos\theta} \propto \frac{t_z(\theta)}{\cos\theta} \propto \frac{J_0\left(k_F d\tan\theta\right)}{\cos\theta}$$

Useful properties of differential (slow) oscillations

At $4\pi t_z >> \hbar\omega_c$ the frequency of slow oscillations is given by

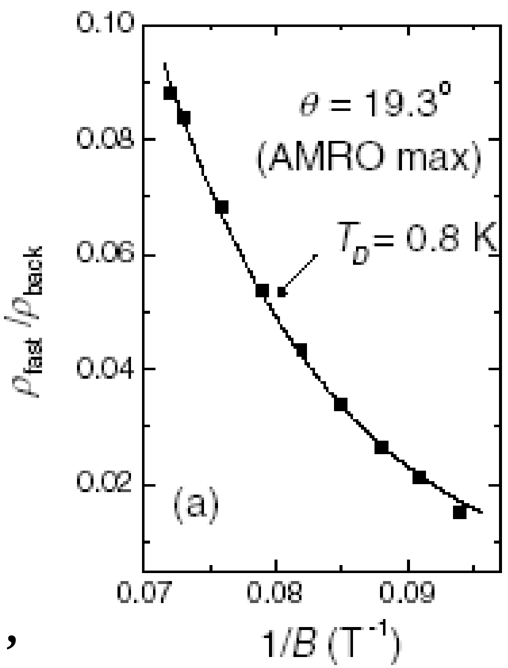
$$F_{slow} = \frac{2t_z B}{\hbar\omega_c} = \frac{2t_z m^* c}{e\hbar\cos\theta} \propto \frac{t_z(\theta)}{\cos\theta} \propto \frac{J_0\left(k_F d\tan\theta\right)}{\cos\theta}$$

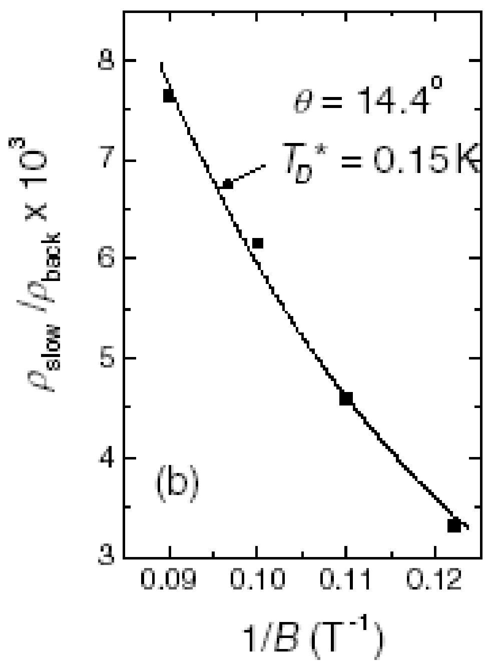
1. **It allows measuring interlayer transfer integral t_z.**
2. **The angular dependence of this frequency allows measuring the Fermi momentum $k_F d$.**

3. The Dingle temperatures of slow and quantum oscillations differ strongly: T_D^{Slow} contains only short-range disorder and is not affected by sample inhomogeneity. =>

a) Their amplitude is much larger.

b) Allows to determine contribution from different types of disorder.

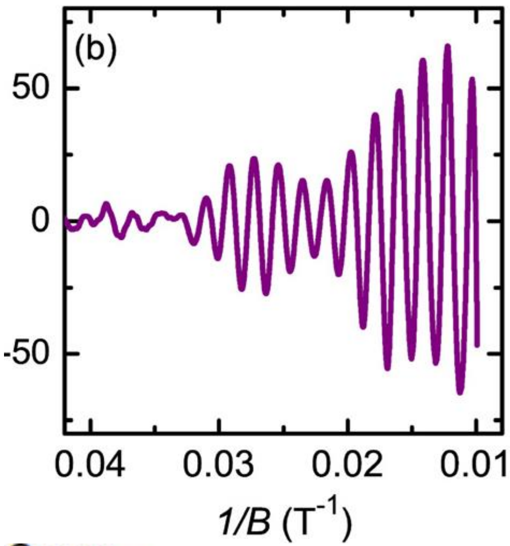


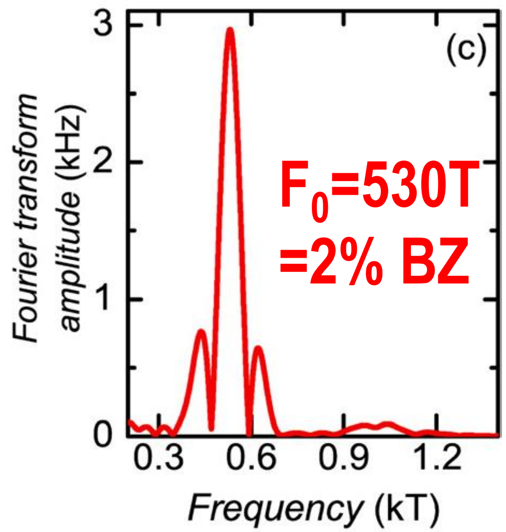


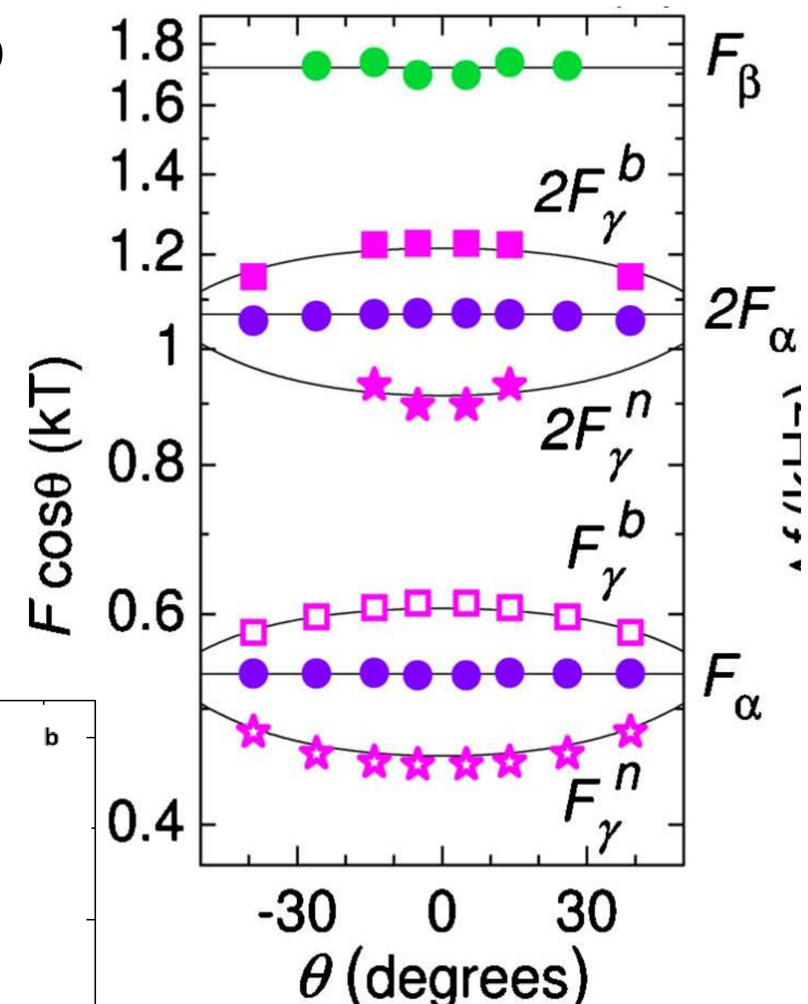
Dingle factor: $R_D(p) = \exp\left(\frac{-\pi}{\tau\omega_C}\right) = \exp\left(\frac{-2\pi^2 T_D}{\hbar\omega_C}\right),$

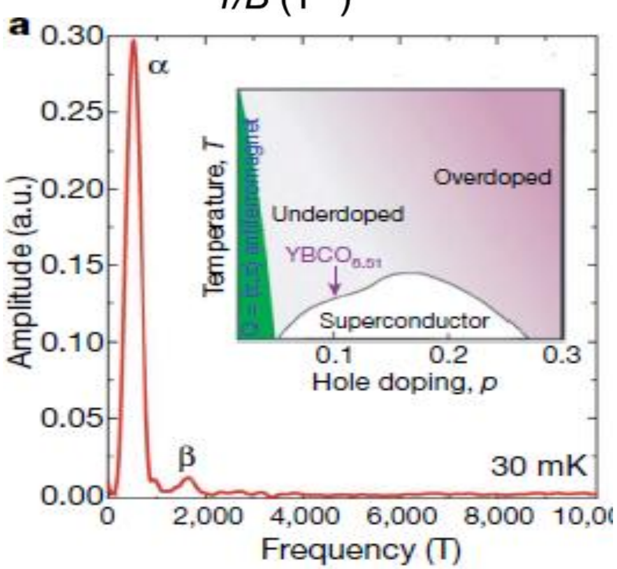
Can we use the idea of slow oscillations to explain the observed magnetic oscillations in YBCO?

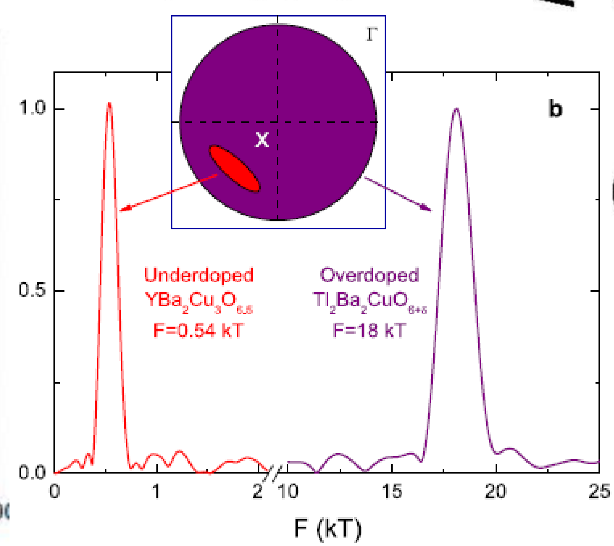
Observed MQO in YBCO







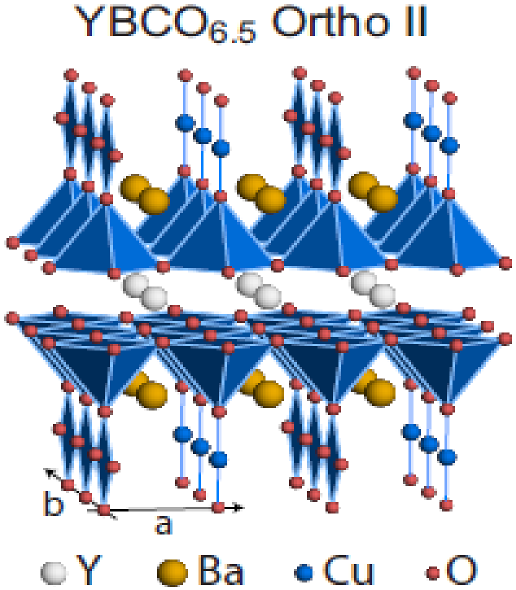


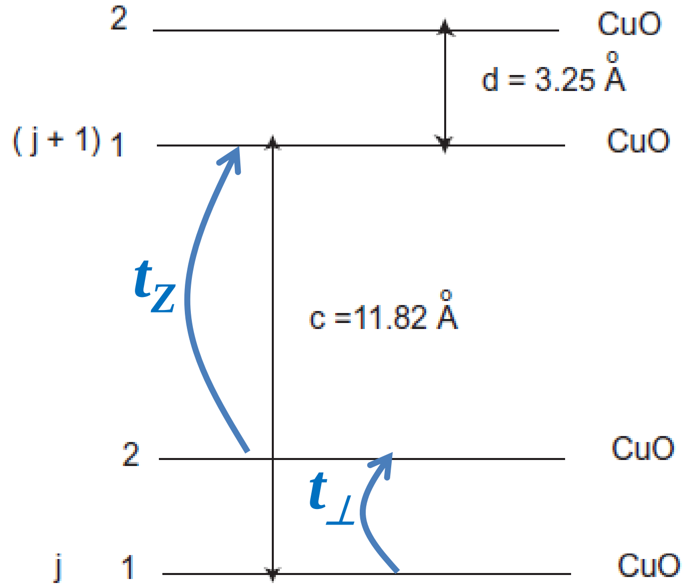


S.E. Sebastian et al., PRB 81, 214524 (2010)

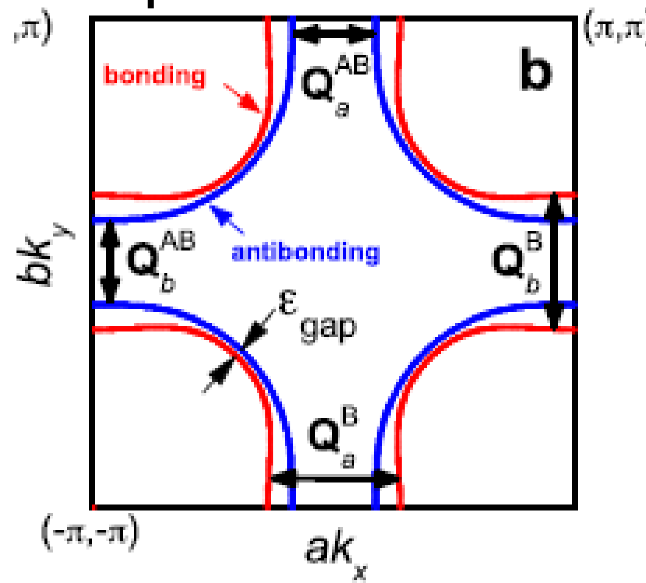
Bilayer crystal structure in YBCO

quasi-2D crystal structure with bilayers

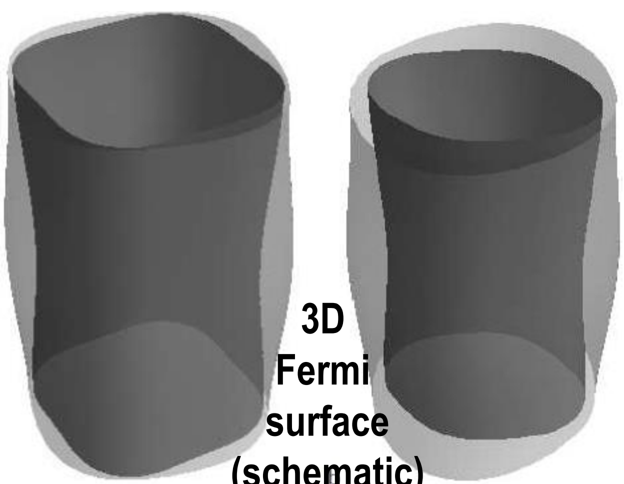




in-plane Fermi surface



The electron dispersion $\epsilon_\pm\left(k_z, \boldsymbol{k}_\parallel\right) = \epsilon_\parallel\left(\boldsymbol{k}_\parallel\right) \pm \sqrt{t_z^2 + t_\perp^2 + 2t_z t_\perp \cos\left[k_z\left(h+d\right)\right]}.$



At $t_\perp >> t_Z$ this simplifies to two quasi-2D subbands:

$$\epsilon_\pm\left(k_z, \boldsymbol{k}_\parallel\right) \approx \epsilon_\parallel\left(\boldsymbol{k}_\parallel\right) \pm t_\perp\left(\boldsymbol{k}_\parallel\right) \pm 2t_z\left(\boldsymbol{k}_\parallel\right)\cos\left[k_z\left(h+d\right)\right]$$

The corresponding density of states

$$\frac{g_{F\beta}}{g_{0\beta}} = 1 - 2J_0\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\sum_{l=\pm1}\cos\left(\frac{2\pi\left(\varepsilon + lt_\perp\right)}{\hbar\omega_c}\right)R_D$$

$$= 1 - 4J_0\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\cos\left(\frac{2\pi t_\perp}{\hbar\omega_c}\right)\cos\left(\frac{2\pi\varepsilon}{\hbar\omega_c}\right)R_D$$

MQO with bilayer splitting: analysis at arbitrary ratio $t_z / \hbar\omega_c$

At $t_\perp \gg t_Z$ the electron dispersion contains two quasi-2D subbands:

$$\epsilon_\pm(k_z, k_\parallel) \approx \epsilon_\parallel(k_\parallel) \pm t_\perp(k_\parallel) \pm 2t_z(k_\parallel)\cos[k_z(h+d)]$$

The corresponding density of states

$$\frac{g_{F\beta}}{g_{0\beta}} = 1 - \sum_{l=\pm 1} 2J_0\left(2\pi\frac{\Delta F_c}{B_z}\right)\cos\left(2\pi\frac{F_\beta - l\Delta F_\perp}{B_z}\right)R_D$$

where $\Delta F_c = 2t_z B/\hbar\omega_c \ll \Delta F_\perp = t_\perp B/\hbar\omega_c$

Diffusion coefficient

$$\frac{D_i}{D_{0i}} = 1 - \frac{2B_i}{A}\sum_{l=\pm 1} J_0\left(2\pi\frac{\Delta F_c}{B_z}\right)\cos\left(2\pi\frac{F_\beta - l\Delta F_\perp}{B_z}\right)R_D$$

Conductivity is a product of density of states (DoS) and diffusion coefficient:

$$\sigma_i(\varepsilon) = e^2 g(\varepsilon) D_i(\varepsilon)$$

we neglect second harmonics ~2F_β and use the identity:

$$\cos x \cos y = \frac{\cos(x-y) + \cos(x+y)}{2}$$

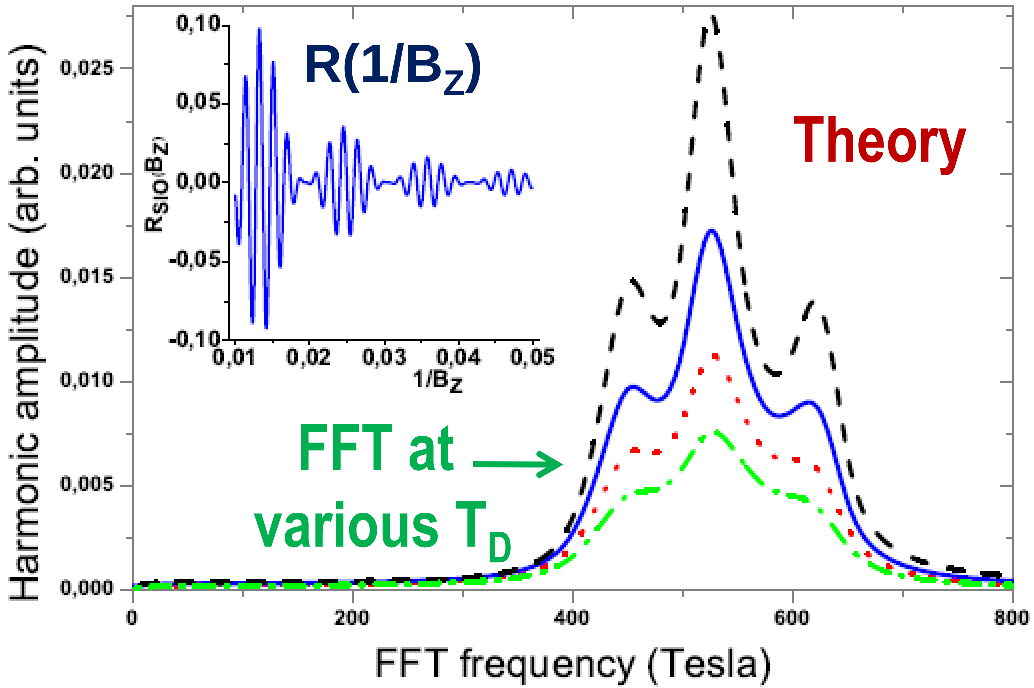
This gives slowly oscillating term in conductivity

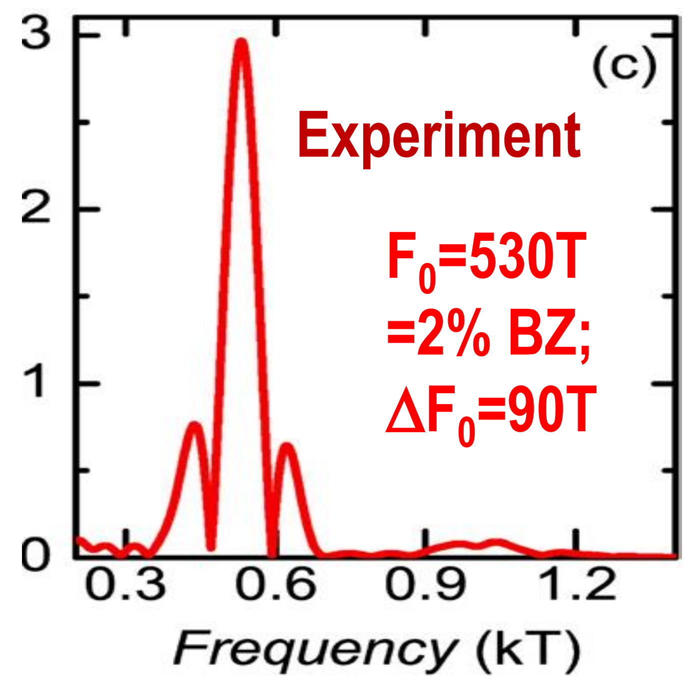
$$\sigma_{SlO}(B_z) \propto J_0^2\left(2\pi\frac{\Delta F_c}{B_z}\right)\cos\left(4\pi\frac{\Delta F_\perp}{B_z}\right)R_D^2$$

Results, comparison with experiment, and discussion

The slowly oscillating term in conductivity

$$\sigma_{SlO}(B_z) \propto J_0^2\left(2\pi\frac{\Delta F_c}{B_z}\right)\cos\left(4\pi\frac{\Delta F_\perp}{B_z}\right)R_D^2$$

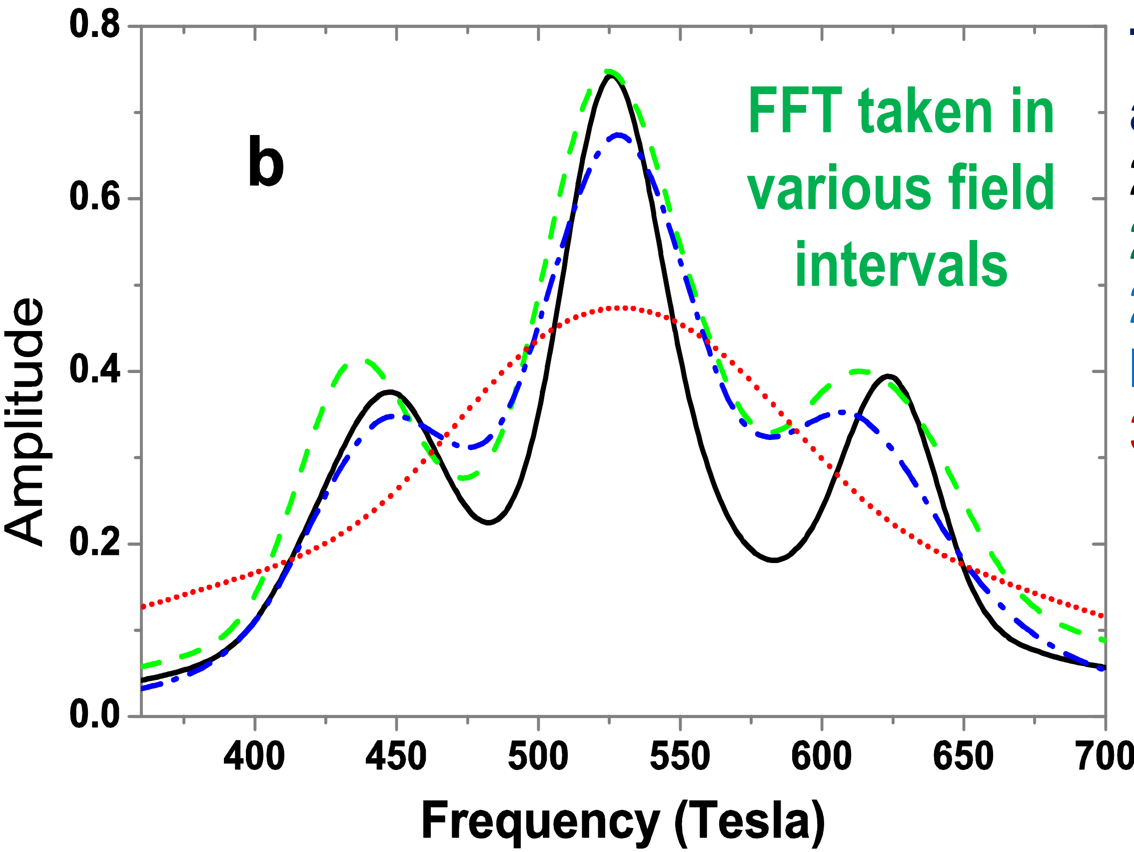




With increasing of Dingle temperature or with decreasing field range, two side peaks disappear, as they do in experiments in lower fields.

If the proposed interpretation is valid, and F_0 gives the bilayer splitting and one needs to look for fundamental frequency F_β and for very low frequency $2\Delta F_c$

Amplitude of side peaks of Fourier transform as function of the field interval of FFT

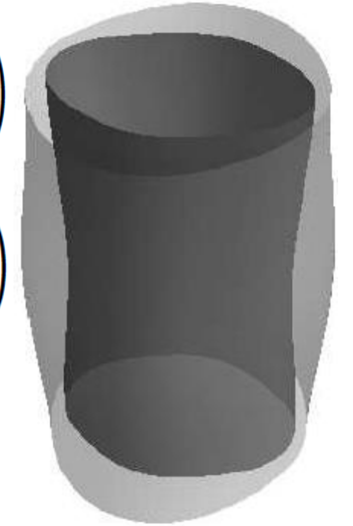


The conductivity Fourier transform at $T_D = 0$ in the finite field intervals:
20 T < *Bz* < 100 T (solid black line),
20T <*Bz* < 65 T (dashed green line),
25 T < B_z < 65 T (dot-dashed blue line), and
30 T < *Bz* < 65 T (dotted red line).

$$\sigma_{SlO}\left(B_z\right) \propto J_0^2\left(2\pi\frac{\Delta F_c}{B_z}\right)\cos\left(4\pi\frac{\Delta F_\perp}{B_z}\right)R_D^2$$

Combinatoric explanation of three MQO frequencies

Conductivity is a product of density of states (DoS) and diffusion coefficient: $\sigma_i(\varepsilon) = e^2 g(\varepsilon) D_i(\varepsilon)$



The oscillating DoS at the Fermi level is $$\frac{g_F}{g_0} = 1 + A \sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_0 + j\Delta F_\perp + l\Delta F_c}{B_z}\right)$$

and the diffusion coefficient is $$\frac{D_i}{D_{0i}} = 1 + B_i \sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_0 + j\Delta F_\perp + l\Delta F_c}{B_z}\right)$$

(where $\Delta F_c = 2t_z B/\hbar\omega_c$ **<<** $\Delta F_\perp = t_\perp B/\hbar\omega_c$**)**

The product $g(\varepsilon) D_{i,\beta}(\varepsilon)$ **contains**

$$P \equiv \left[1 + A \sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_0 + j\Delta F_\perp + l\Delta F_c}{B_z}\right)\right]\left[1 + B \sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_0 + j\Delta F_\perp + l\Delta F_c}{B_z}\right)\right]$$

$$= 1 + 2(A+B) \sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_0 + j\Delta F_\perp + l\Delta F_c}{B_z}\right) +$$

$$+AB \sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_\beta + j\Delta F_\perp + l\Delta F_c}{B_z}\right) \sum_{j',l'=\pm 1} \cos\left(2\pi \frac{F_\beta + j\,j'\Delta F_\perp + l\,l'\Delta F_c}{B_z}\right)$$

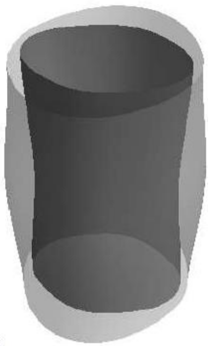
The last term gives frequency mixing and, neglecting second harmonics, *at j'=-1* it gives three close frequencies: $2\Delta F_\perp$ **and** $2\Delta F_\perp \pm 2\Delta F_c$

Combinatoric explanation of three MQO frequencies (2)

P.D. Grigoriev, T. Ziman, JETP Lett. 106, 361 (2017)

In the product

$$\sum_{j,l=\pm 1} \cos\left(2\pi \frac{F_\beta + j\Delta F_\perp + l\Delta F_c}{B_z}\right) \sum_{j',l'=\pm 1} \cos\left(2\pi \frac{F_\beta + j\, j'\Delta F_\perp + l\, l'\Delta F_c}{B_z}\right)$$



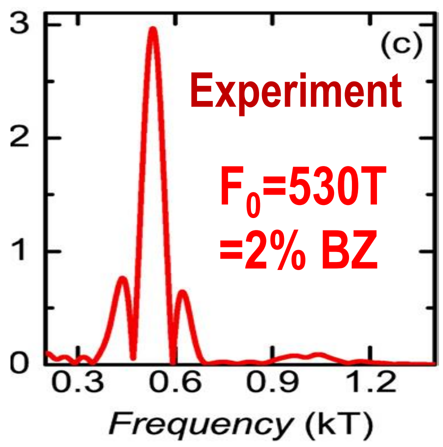
we neglect second harmonic ~$2F_\beta$ and use the identity

$$\cos x \cos y = \frac{\cos(x-y) + \cos(x+y)}{2}$$

Then at *j'=-1* the product contains only 3 close frequencies

$$\frac{1}{2} \sum_{j,l,l'=\pm 1} \cos\left(2\pi \frac{2j\Delta F_\perp + l(1-l')\Delta F_c}{B_z}\right) =$$

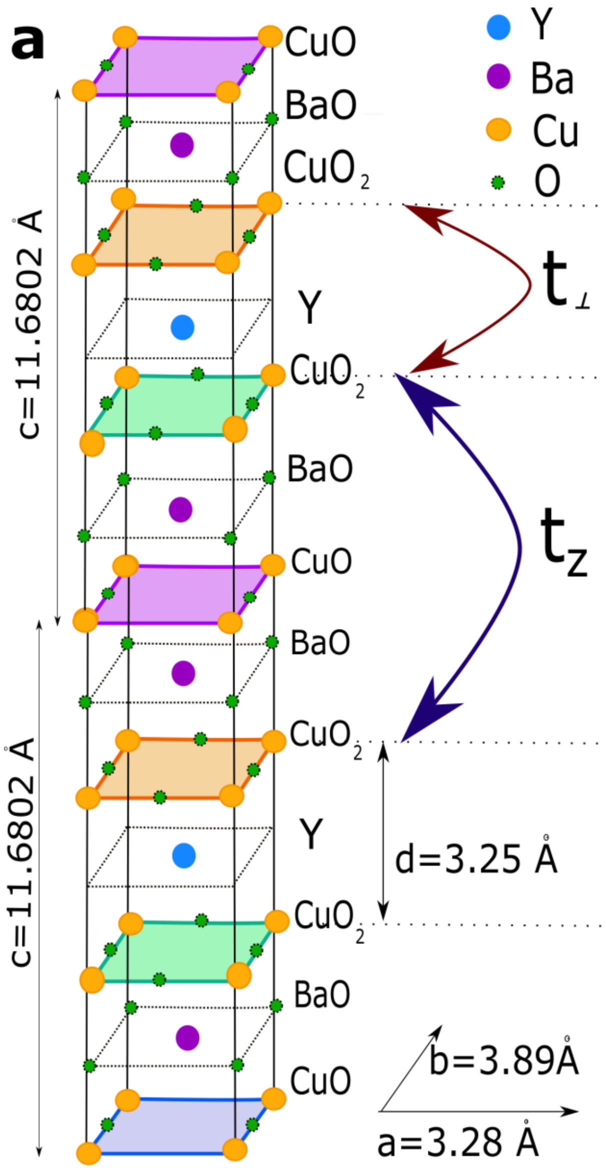
$$2\cos\left(4\pi \frac{\Delta F_\perp}{B_z}\right) + \sum_{l=\pm 1} \cos\left(4\pi \frac{\Delta F_\perp + l\Delta F_c}{B_z}\right)$$

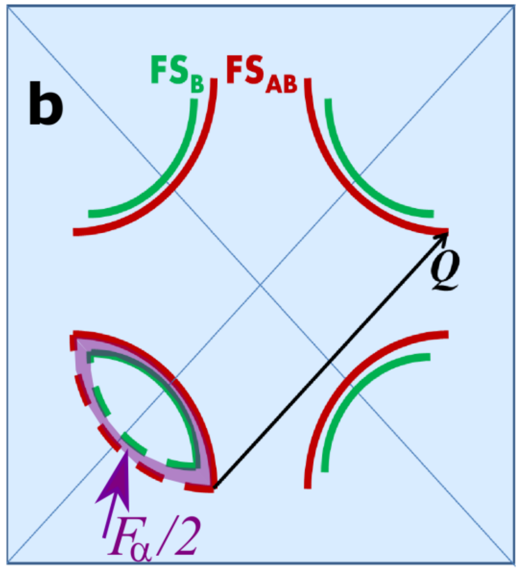


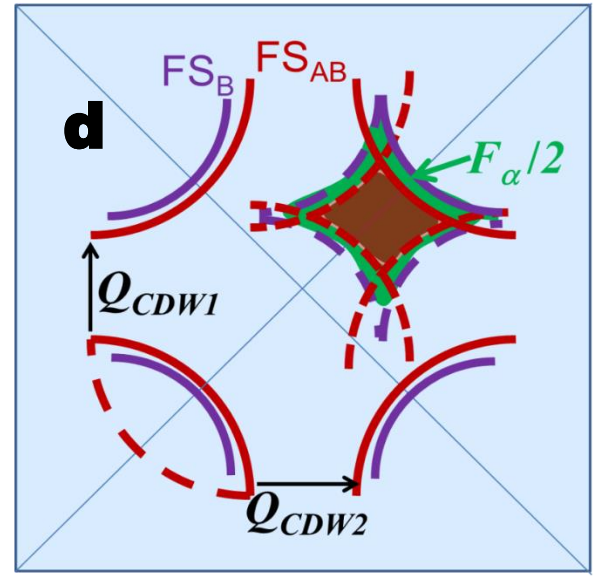
! The central frequency has twice larger amplitude than side frequencies

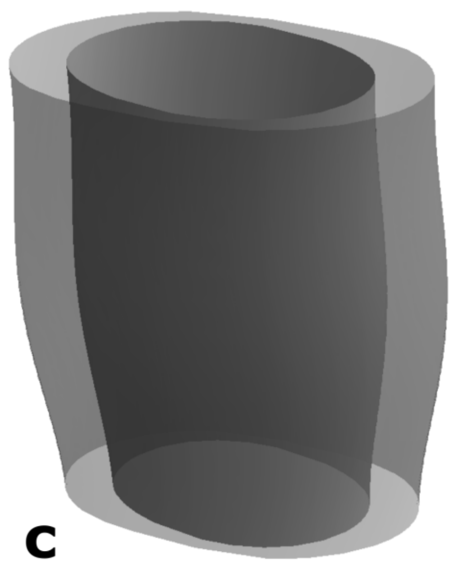
(Reminder: $\Delta F_c = 2t_z B/\hbar\omega_c$ << $\Delta F_\perp = t_\perp B/\hbar\omega_c$)

Geometrical interpretation of observed magnetic oscillation frequencies in YBCO







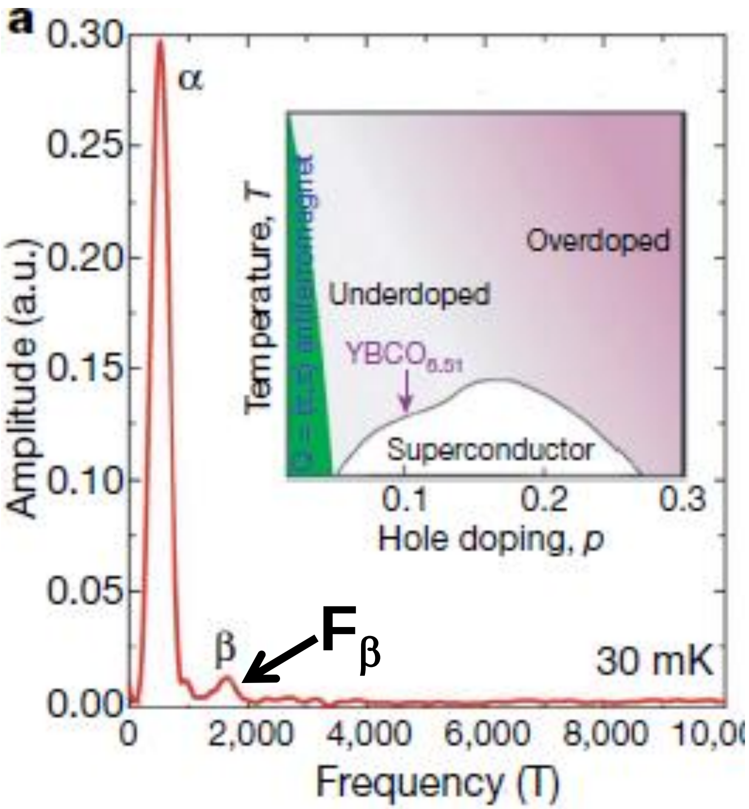


The observed MQO frequency correspond to the difference between antibonding (AB) and bonding (B) Fermi surfaces.

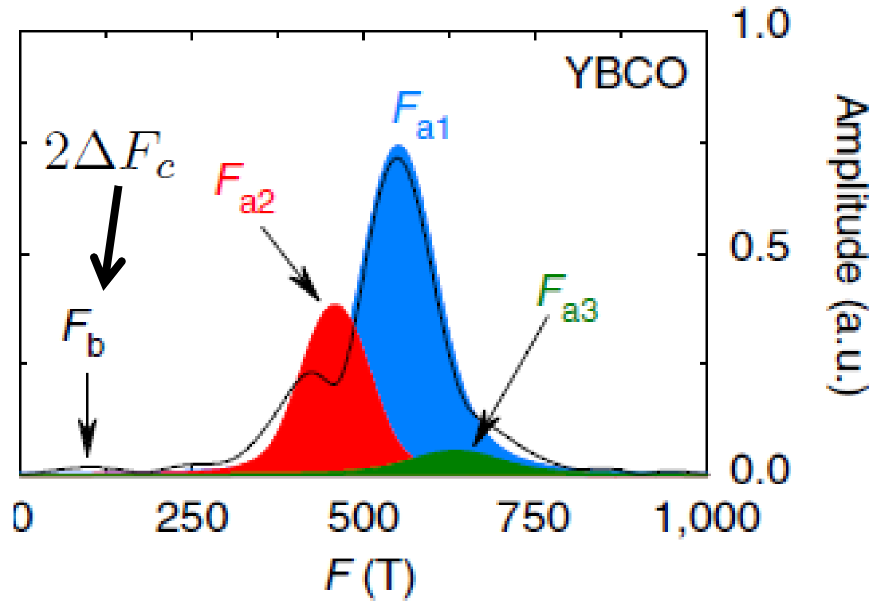
Both scenarios gives $F_\alpha \approx 2\%$ BZ, in agreement with our interpretation !

Other consequences: predicted frequencies

If the proposed interpretation is valid, and F_α gives the bilayer splitting rather than FS area, one needs to look for fundamental frequency F_β, especially in dHvA effect. Also for very low frequency $2\Delta F_c$



dHvA effect; S.E. Sebastian et al., Nature 454, 200 (2008).



N. Doiron-Leyraud et al., Nature Comm. 6, 6034 (2015).

$$\sigma_{SlO}\left(B_z\right) \propto J_0^2\left(2\pi\frac{\Delta F_c}{B_z}\right)$$

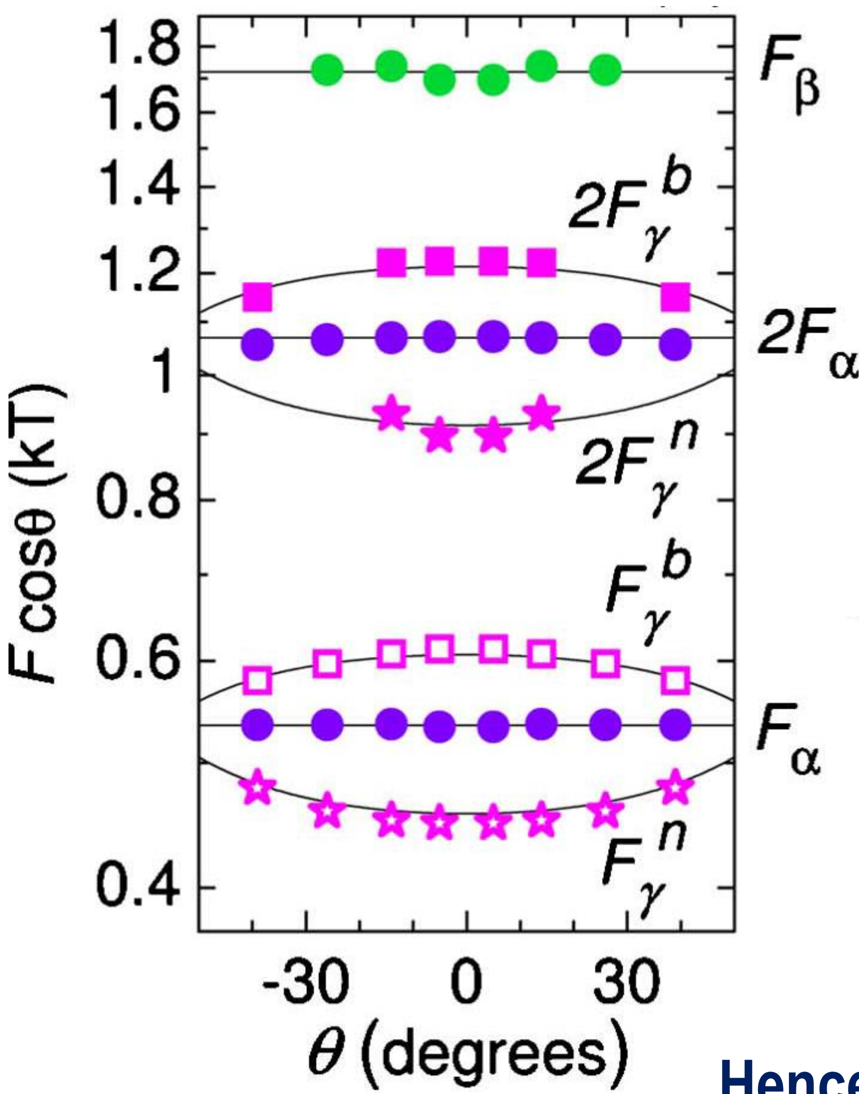
$$2\Delta F_c \approx 90T \sim 4t_z B/\hbar\omega_c$$

Main drawbacks of the FS reconstruction scenario

become arguments in favor of the proposed SIO scenario

1. ! FS reconstruction predicts many other MQO frequencies which are not observed in experiment, but all frequencies predicted by SIO
2. $F_\alpha \approx 530T$ and $F_\alpha \pm 90T$ frequencies weakly depend on doping level.
3. ! **The proposed scenario agrees with ARPES data**
4. How a weak fluctuating CDW ordering leads to FS reconstruction, i.e. creates a large gap, so that the magnetic breakdown at field B=100T cannot overcome it? For SIO no FS reconstruction is need.
5. The angular dependence of ΔF_α=90T frequency, described by $\Delta F_c \cos\theta \;\; \propto \;\; J_0(k_F c^\star \tan\theta)$, corresponds to the FS area ~πk_F^2 = 6% of BZ and to $F_\beta \approx 1.6kT$ rather than $F_\alpha \approx 530T$. In SIO F_α is not FS area.
6. **Spatial inhomogeneity in YBCO lead to variations of Fermi level along the sample, => strongly damps MQO but not SIO**
7. **In YBa2Cu4O8 no CDW was detected, but MQO are similar.**
8. **There are too many fitting parameters in FS reconstruction scenario, but not in slow-oscillations scenario!**

Angular dependence of three MQO frequencies



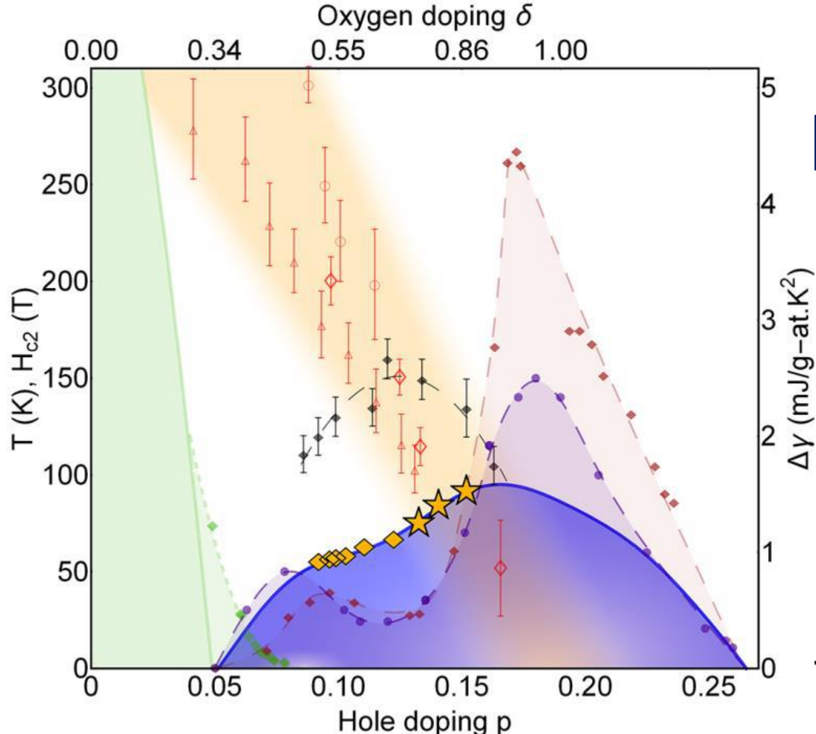
The split frequency fits the angular dependence, $\Delta F_c \cos\theta \propto J_0(k_F c^\star \tan\theta)$ suggesting that it originates from k_z dispersion, i.e. $\Delta F_c = 2t_z B/\hbar\omega_c \approx 90T$ Then $\Delta F_\perp = t_\perp B/\hbar\omega_c \approx 530T$ is reasonable for bilayer splitting.

The first Yamaji angle $\theta_{Yam} \approx 43^\circ$ corresponds to the FS pocket area $\sim\pi k_F^2$ = 6% of BZ and to $F_\beta \approx 1.6$kT rather than to stronger $F_\alpha \approx 530$T. => The most prominent frequency F_α does not correspond to FS pocket.

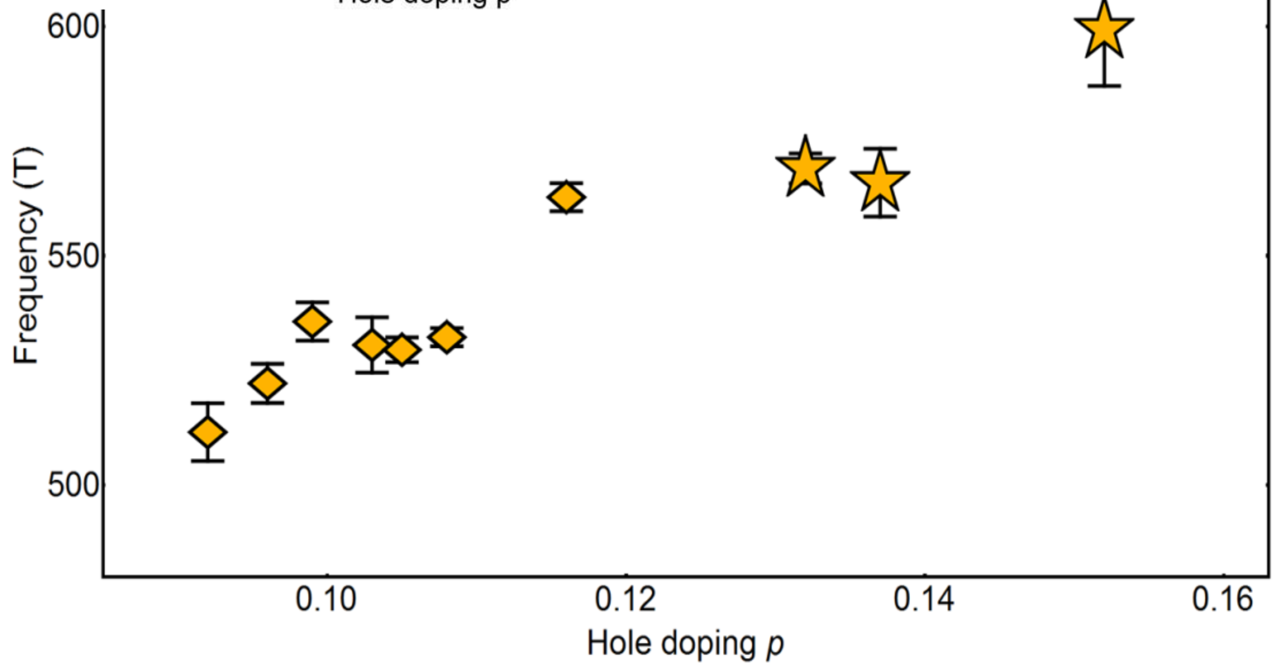
S.E. Sebastian et al., PRB 81, 214524 (2010)

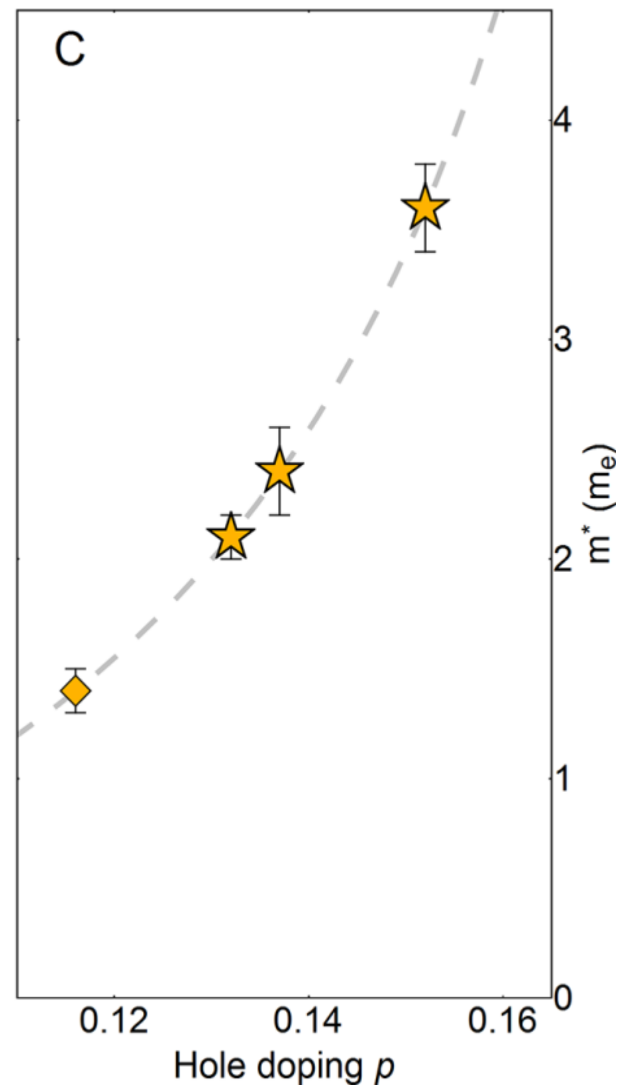
Hence, the angular dependence of three MQO frequencies confirms the proposed scenario.

Doping-dependence of MQO frequencies in YBCO is weak, contrary to m*

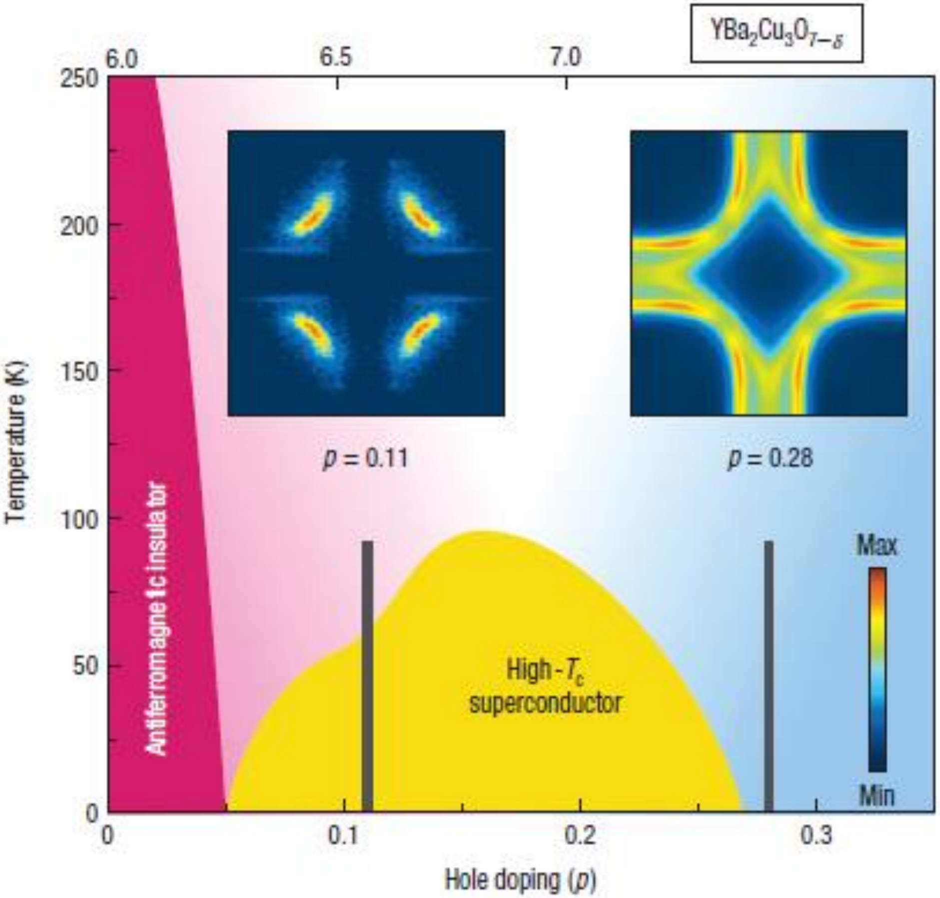


B. J. Ramshaw, S. E. Sebastian, et al., Science **348**, 317 (2015)

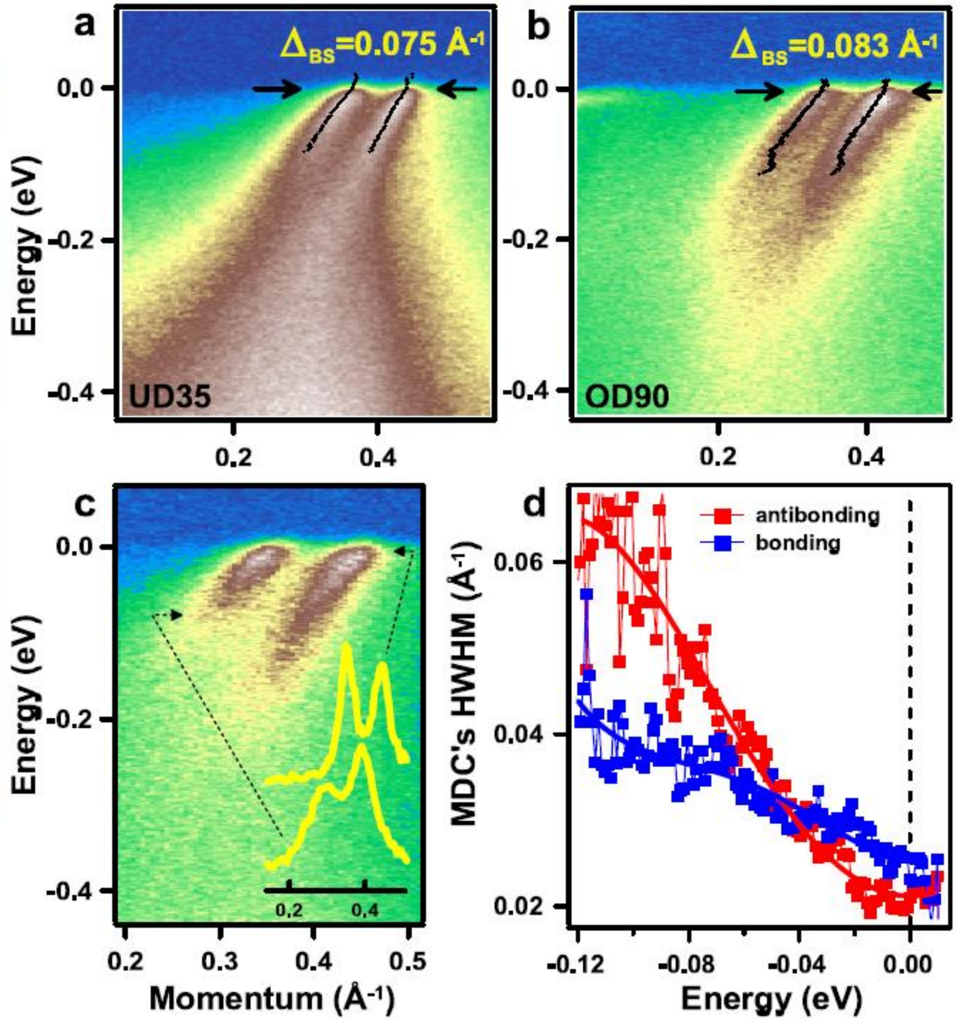




ARPES data (underdoped YBCO)



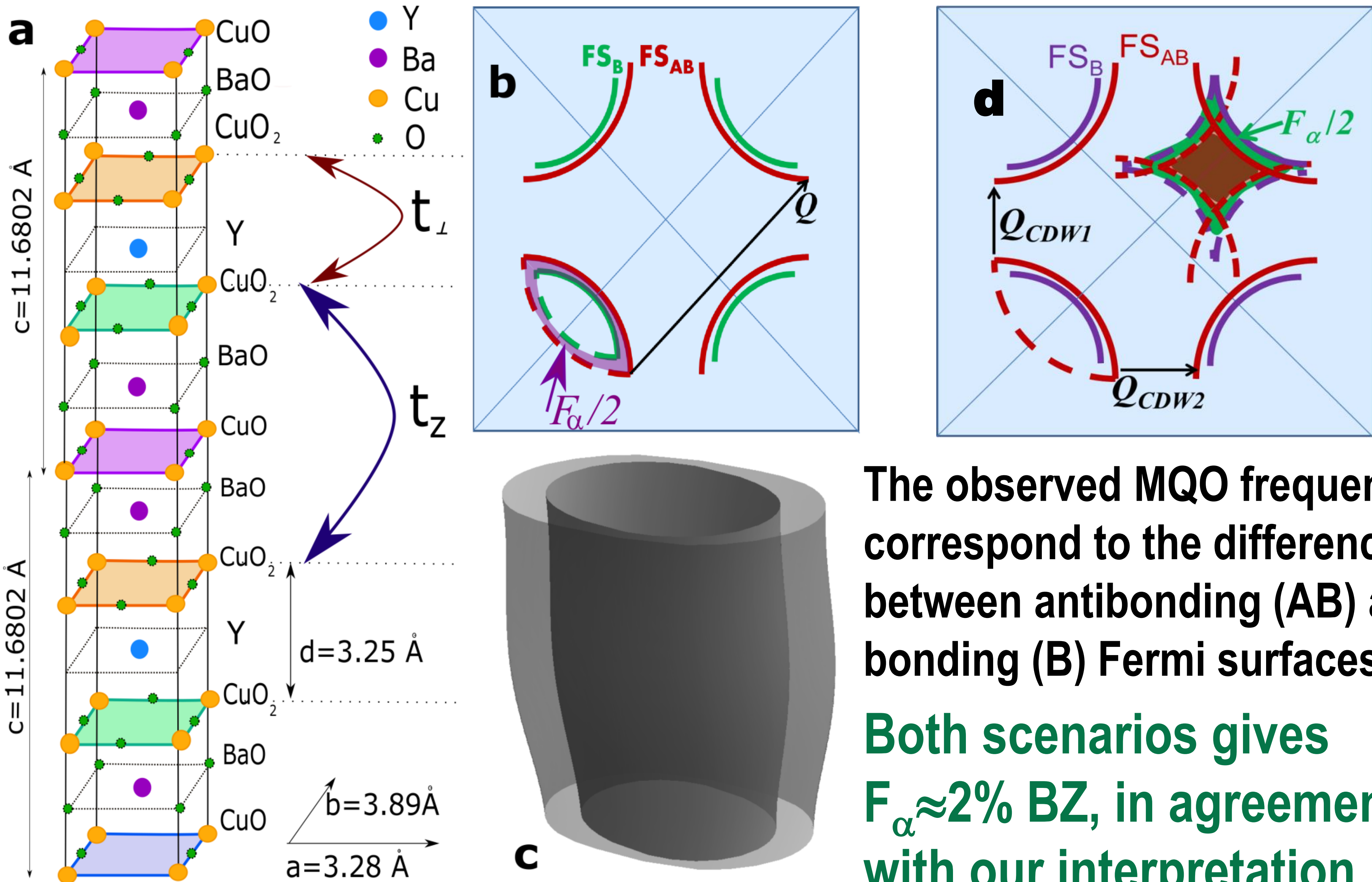
Phase diagram of YBCO by ARPES
M.A. Hossain et al., Nature Physics **4**, 527–531 (2008)



Bilayer splitting observed by ARPES
S.V. Borisenko et al., PRL **96,** 117004 (2006)

Our model indeed gives ~2% of the BZ !

Geometrical interpretation of observed magnetic oscillation frequencies in YBCO



The observed MQO frequency correspond to the difference between antibonding (AB) and bonding (B) Fermi surfaces.

Both scenarios gives $F_{\alpha} \approx 2\%$ BZ, in agreement with our interpretation !

Temperature dependence of slow oscillations

At finite temperature T the conductivity is

$$\sigma_{ij}(T) = \int d\varepsilon \left[-n_F'(\varepsilon)\right] \sigma_{ij}(\varepsilon), \quad (1)$$

where the derivative of Fermi distribution function

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

In the first order in small Dingle factor

$$\sigma_1(\varepsilon) \propto 1 - 2J_0\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\cos\left(2\pi\frac{\varepsilon \pm t_\perp}{\hbar\omega_c}\right)R_D$$

Integration over ε in Eq. (1) gives

$$\sigma_1(\mu) \propto 1 - 2J_0\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\cos\left(2\pi\frac{\mu \pm t_\perp}{\hbar\omega_c}\right)R_D R_T$$

with temperature damping factor

$$R_T = \left(2\pi^2 k_B T/\hbar\omega_c\right)/\sinh\left(2\pi^2 k_B T/\hbar\omega_c\right) \quad (2)$$

In the 2nd order in Dingle factor

$$\sigma_2(\varepsilon) \propto 4J_0^2\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\cos\left(2\pi\frac{\varepsilon - t_\perp}{\hbar\omega_c}\right)\cos\left(2\pi\frac{\varepsilon + t_\perp}{\hbar\omega_c}\right)R_D^2$$

$$= 2J_0^2\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\left[\cos\left(\frac{4\pi\varepsilon}{\hbar\omega_c}\right) + \cos\left(\frac{4\pi t_\perp}{\hbar\omega_c}\right)\right]R_D^2. \quad (14)$$

After integration over energy ε the ε-independent slow oscillating term does not acquire the temperature damping factor R_T as well as the main Dingle factor part from the sample inhomogeneities.

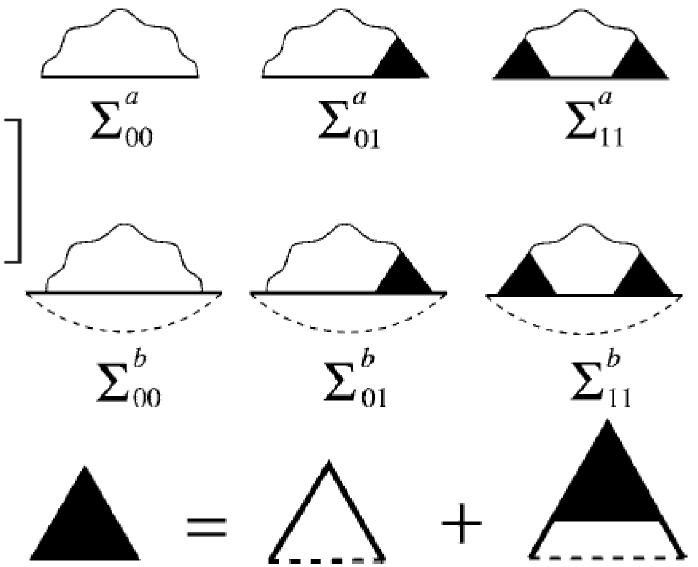
Possible origin of temperature damping of slow oscillations

The T-dependent correction to the MQO amplitude comes from the interplay of disorder and interaction:

$$A_1(T) \simeq A_1^{(0)}(T)\exp\left[-\frac{2\pi^2 T}{\omega_c}\frac{\delta m}{m}\right]\exp\left[\frac{\pi}{\omega_c \tau}\left(-\frac{\delta m}{m}+\frac{\delta\tau}{\tau}\right)\right]$$

where $$\frac{\delta m(T)}{m} = -\frac{\nu U_0}{2\pi E_F \tau}\ln\frac{E_F}{T}$$

and $$\frac{\delta\tau(T)}{\tau} = \nu U_0 \frac{T}{E_F} - \frac{\nu U_0}{2\pi E_F \tau}\ln\frac{E_F}{T}$$



Y. Adamov, I. V. Gornyi, and A. D. Mirlin, Phys. Rev. B 73, 045426 (2006).

The temperature damping of slow oscillations comes from the T-dependent Dingle factor $R_D(p) = \exp\left[-\pi / \tau(T)\,\omega_C\right]$

which is determined by e-e and e-ph interaction.

Damping by spatial inhomogeneity (2)

no effect for slow oscillations similar to the effect of temperature

The second-order terms (in Dingle factor) for conductivity give

$$\frac{\sigma_2}{\sigma_0} \propto \int d\mu\, D(\mu - \mu_0 - \Delta\mu) J_0^2\left(\frac{4\pi t_z}{\hbar\omega_c}\right) R_D^2$$

$$\times \left[\cos\left(\frac{4\pi\mu}{\hbar\omega_c}\right) R_T^2 + \cos\left(\frac{4\pi t_\perp}{\hbar\omega_c}\right)\right]$$

$$= \left[\cos\left(\frac{4\pi\mu_0}{\hbar\omega_c}\right) R_T^2 R_W^4 + \cos\left(\frac{4\pi t_\perp}{\hbar\omega_c}\right)\right] J_0^2\left(\frac{4\pi t_z}{\hbar\omega_c}\right) R_D^2.$$

SIO are not damped by spatial inhomogeneity and T

Temperature damping factor is $R_T = \left(2\pi^2 k_B T/\hbar\omega_c\right) / \sinh\left(2\pi^2 k_B T/\hbar\omega_c\right)$

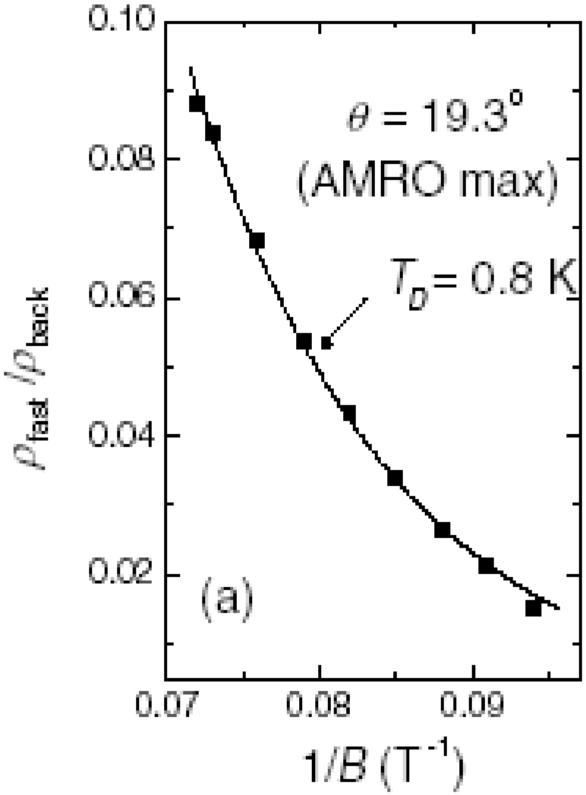
For Gaussian smearing of the Fermi energy μ $D(\Delta\mu) = (1/\sqrt{2\pi}W)\exp[-(\Delta\mu)^2/2W^2]$

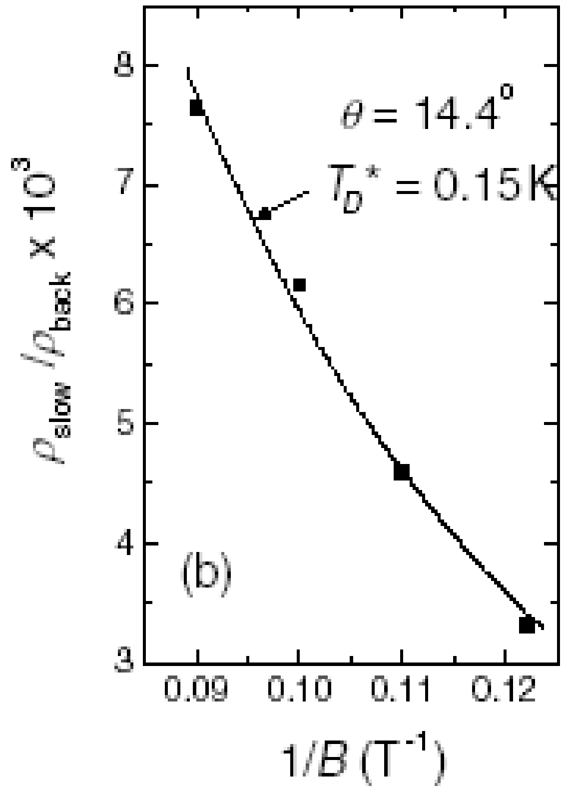
$R_W = \exp\left(-2\pi^2 W^2/\hbar^2\omega_c^2\right)$ is quadratic in B and harmonic number k

while the usual Dingle factor exponent is linear in k and 1/B: $R_D(k) = \exp\left(\frac{-\pi k}{\omega_c \tau}\right)$

Slow oscillations are damped much weaker by disorder

Phys. Rev. Lett. 89, 126802 (2002)



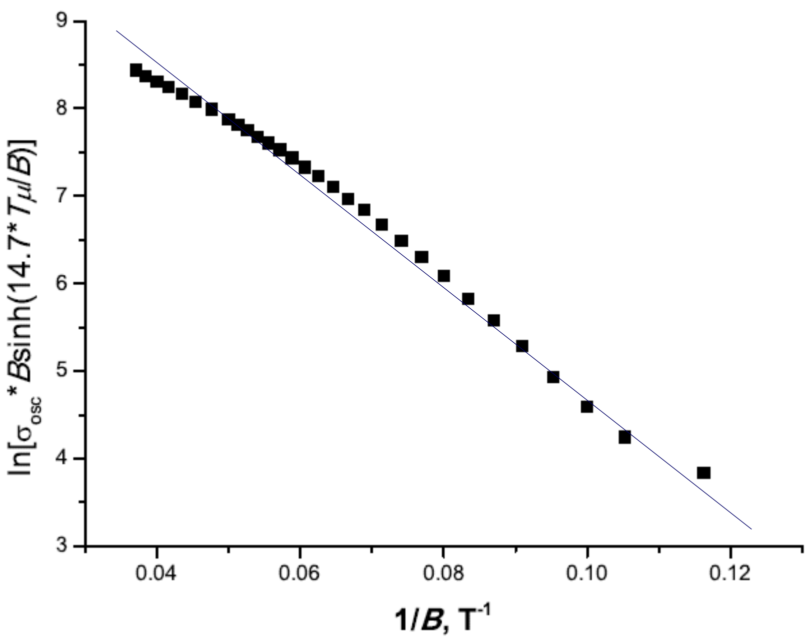


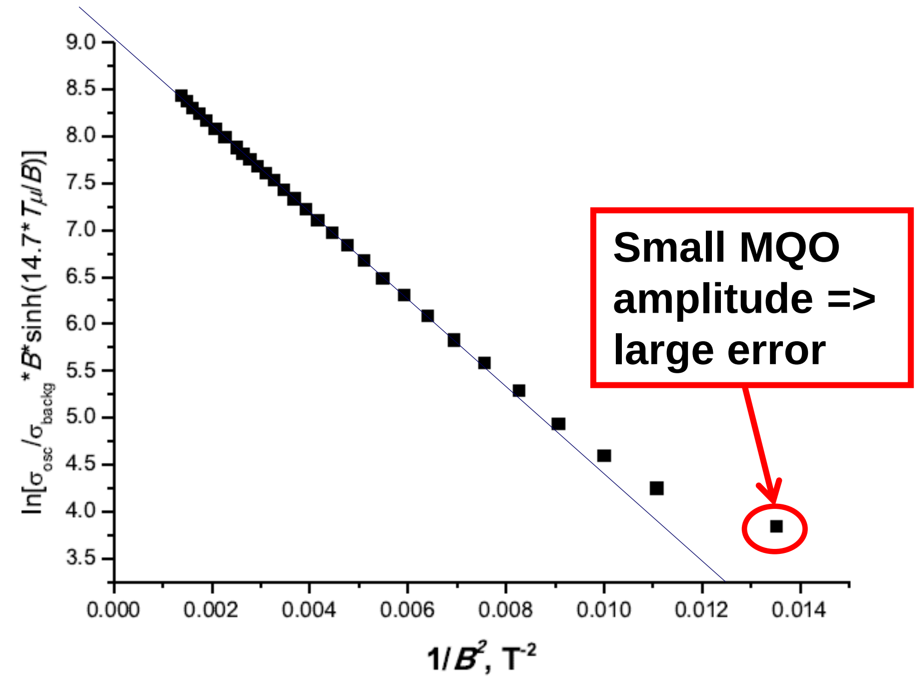
The Dingle temperatures of slow and fast oscillations strongly differ ! T_D^{Slow} does not contain long-range disorder, leading to macroscopic variations of the Fermi level. Hence one can separate the role of short-range and long-range crystal imperfections on the electron motion in a particular sample.

Therefore, the slow oscillations are damped much weaker by disorder, even though they appear in the second order in Dingle factor.

This is even more important in cuprate superconductors, e.g. YBCO, which are strongly inhomogeneous, and where SIO must be much stronger than usual MQO.

Field-dependence of MQO amplitude in layered organic metal α-$(BEDT\text{-}TTF)_2KHg(SCN)_4$



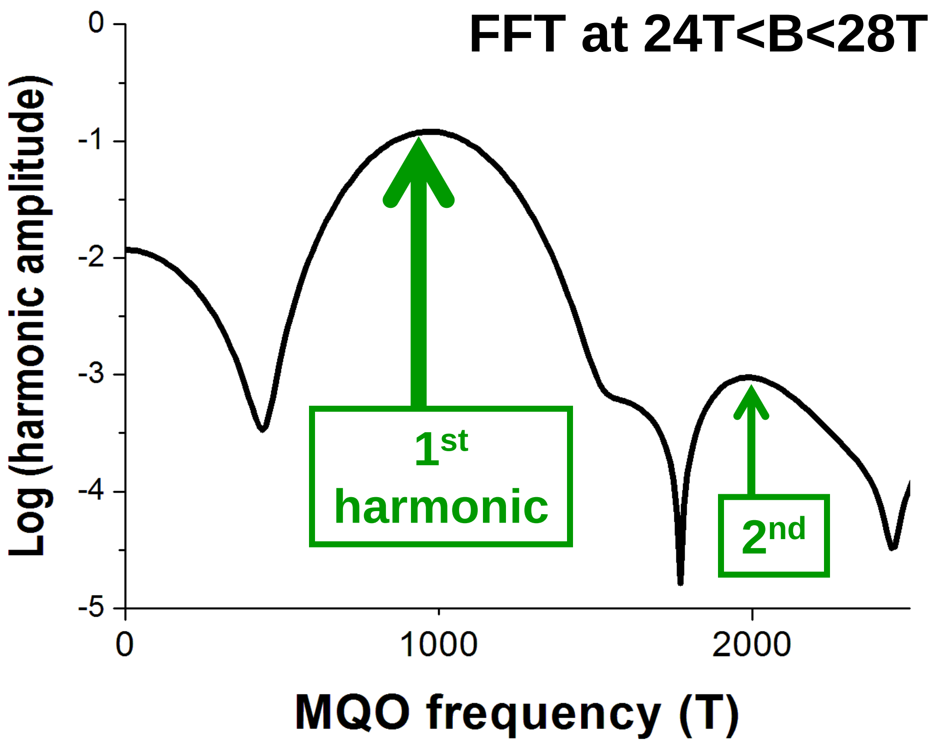


The Dingle plot, i.e. the logarithm of the amplitude of the first harmonic of MQO divided by the temperature damping factor R_T, plotted as function of the inverse magnetic field 1/*B*.

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

This corresponds to Gaussian LL shape => $R_{DG}(k) = \sqrt{\pi/2}\exp\left[-const \cdot k^2/B_z^2\right]$

Damping of higher harmonics of MQO in α-(BEDT-TTF)$_2$KHg(SCN)$_4$



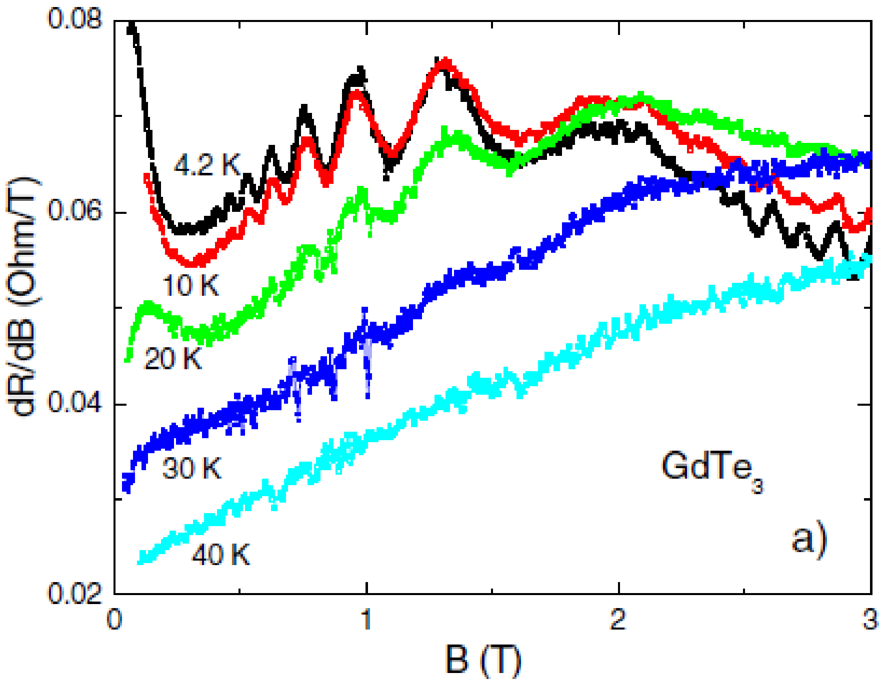
Calculation shows, that observed harmonic damping obeys that for Gaussian LL shape and Γ independent of *B* (long-range disorder in 2D)

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

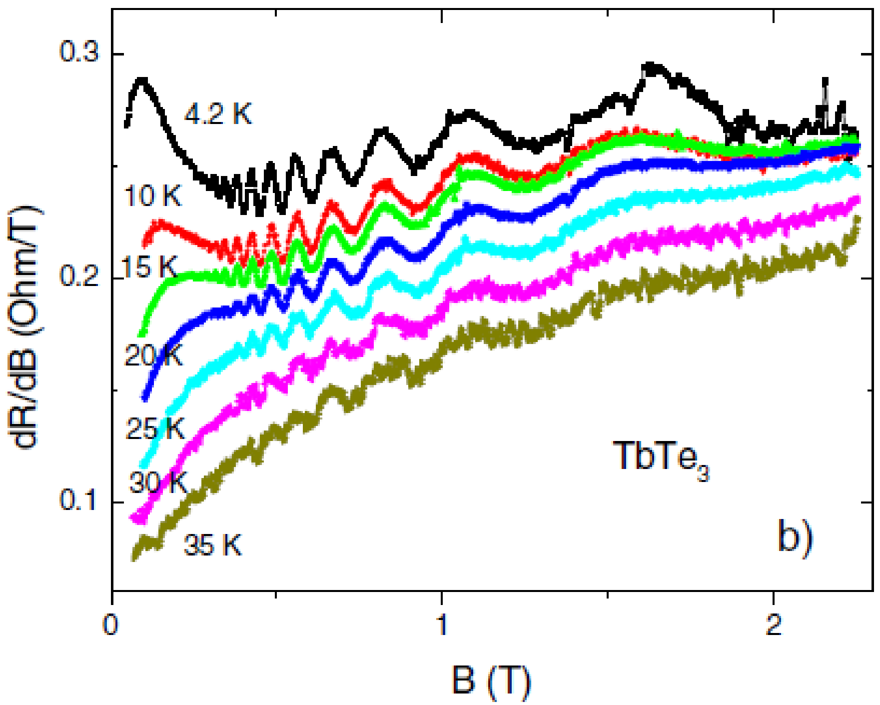
This is in strong contrast to 3D Dingle law but agrees with 2D DoS !

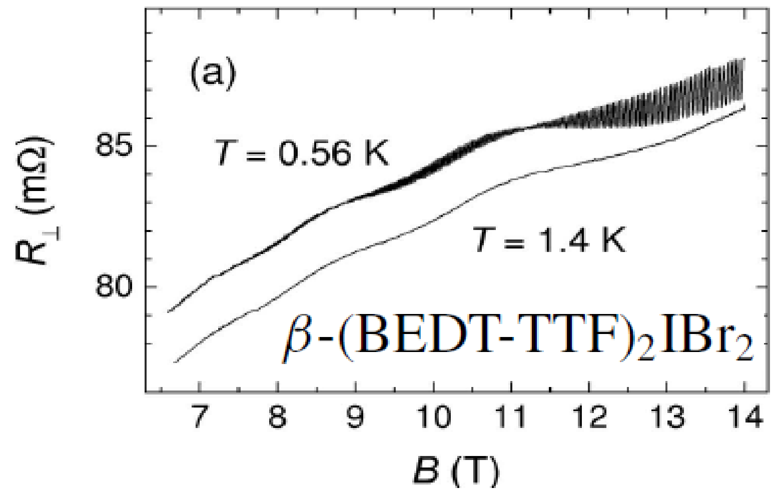
P. D. Grigoriev, M. V. Kartsovnik, W. Biberacher, PRB 86, 165125 (2012)

Slow oscillations from bilayer splitting in rare-earth tritellurides



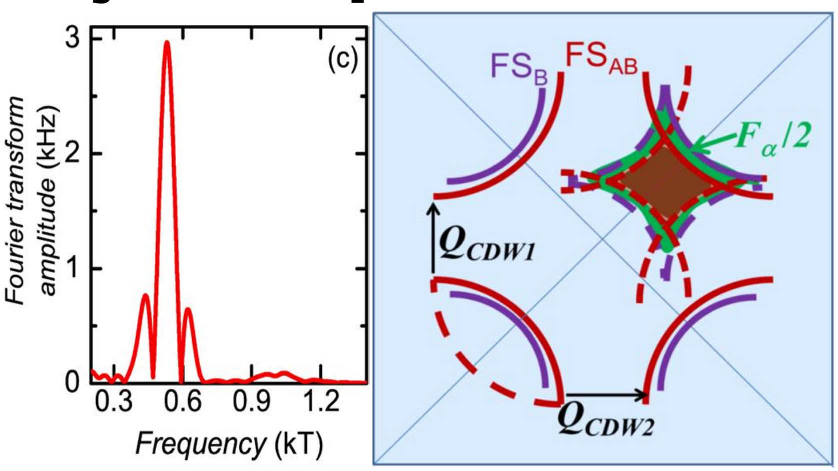
P.D. Grigoriev, A.A. Sinchenko et al., Eur. Phys. J. B 89, 151 (2016)



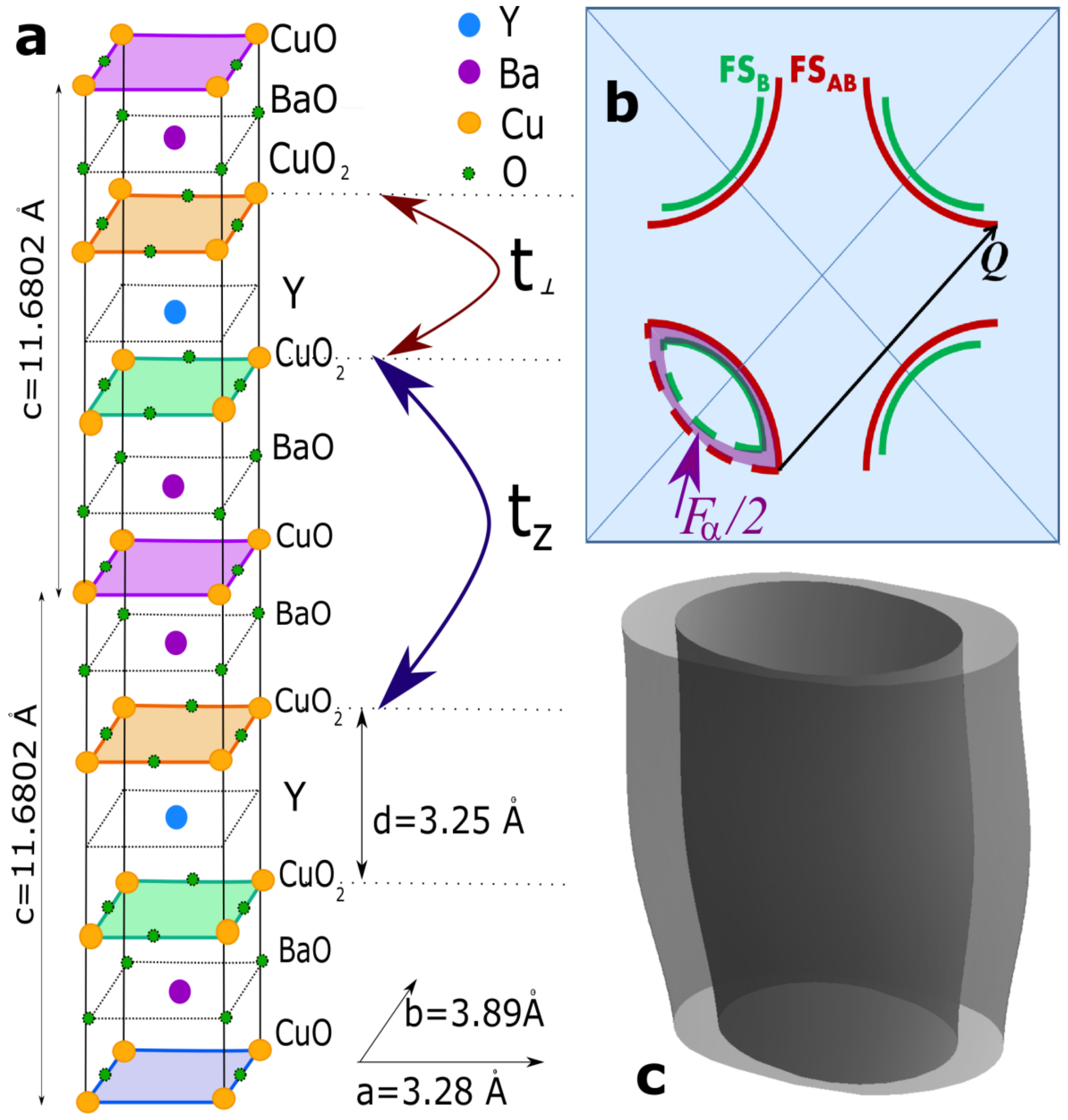


Conclusions

1. We propose that three observed (in YBCO) MQO frequencies $F_{\alpha}\approx 530T$ and $F_{\alpha}\pm 90T$ come from bilayer splitting $t_{\perp}$ and dispersion t_z, not from small (~2% BZ) Fermi-surface pocket.
2. This model naturally gives 3-peak spectrum of MQO and agrees with experiments without many adjustable parameters.

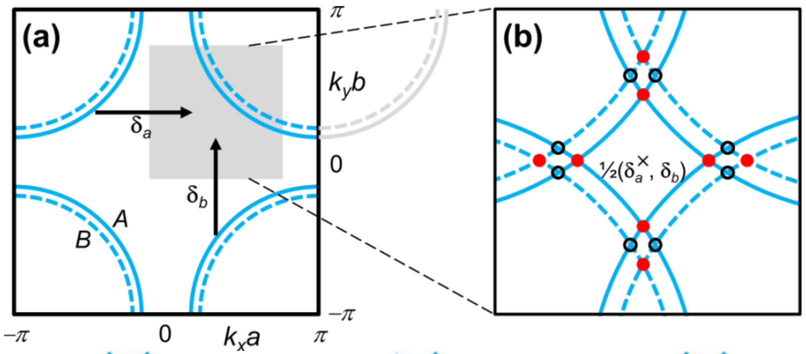


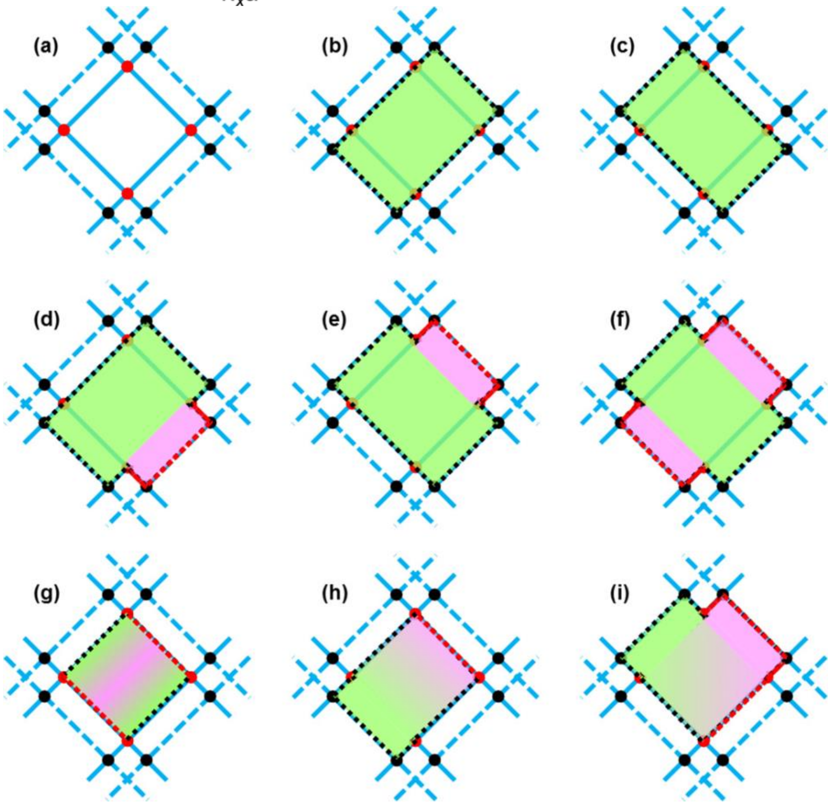
Geometrical interpretation of observed magnetic oscillation frequencies in YBCO

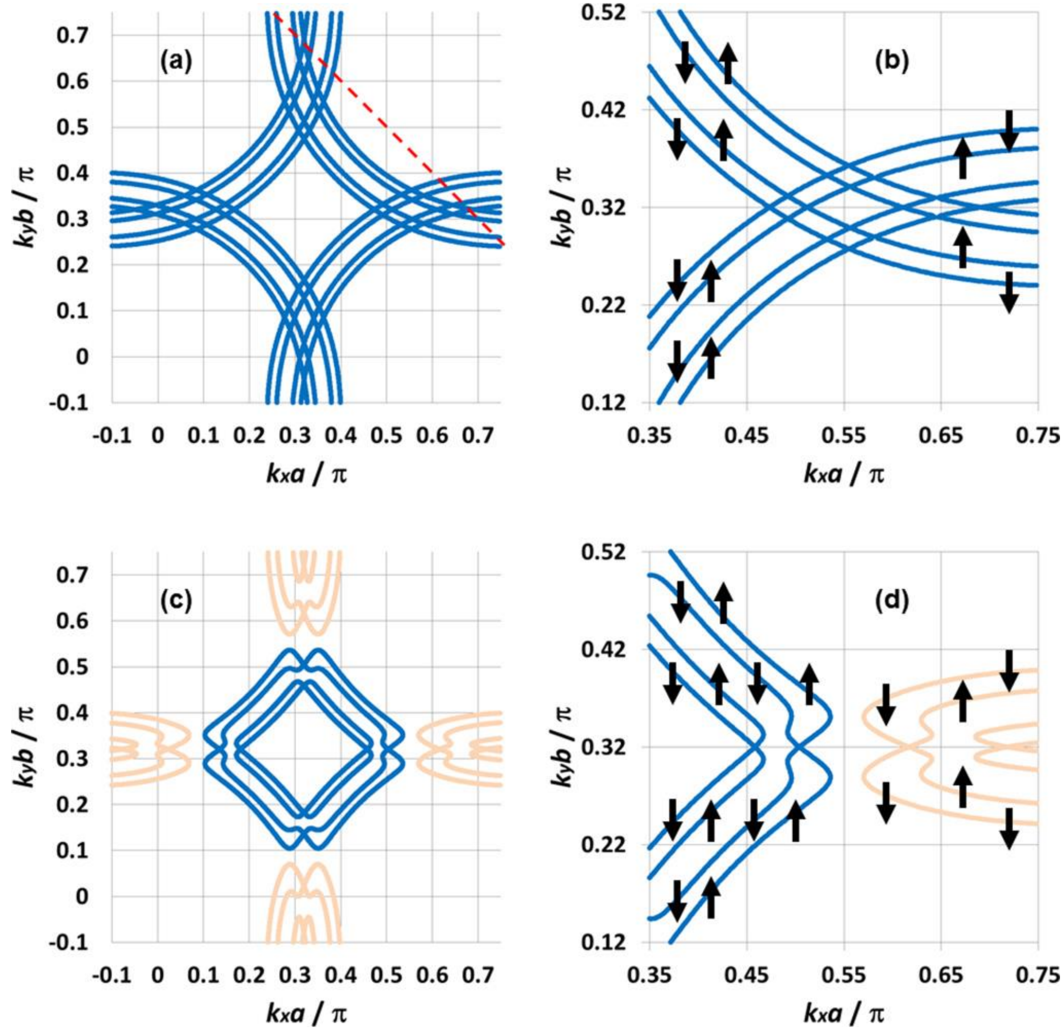


Appendices

FS reconstruction with spin-orbit







A.K.R.Briffa et al., Phys. Rev. B 93, 094502 (2016)

Model involves (1) FS reconstructtion by CDW; (2) bilayer and spin-orbit splitting; (3) magnetic breakdown between some subbands.

Damping by long-range spatial inhomogeneity is similar to the effect of temperature

Take the Gaussian distribution of the spatially fluctuating shift of Fermi energy *μ*(*r*), given by the normalized weight

$$D(\Delta\mu) = (1/\sqrt{2\pi}W)\exp[-(\Delta\mu)^2/2W^2]$$

Then conductivity acquires the coordinate averaging:

$$\sigma = \int d\mu\, \sigma(\mu) D(\mu - \mu_0 - \Delta\mu),$$

The first-order terms give MQO, where the last damping factor

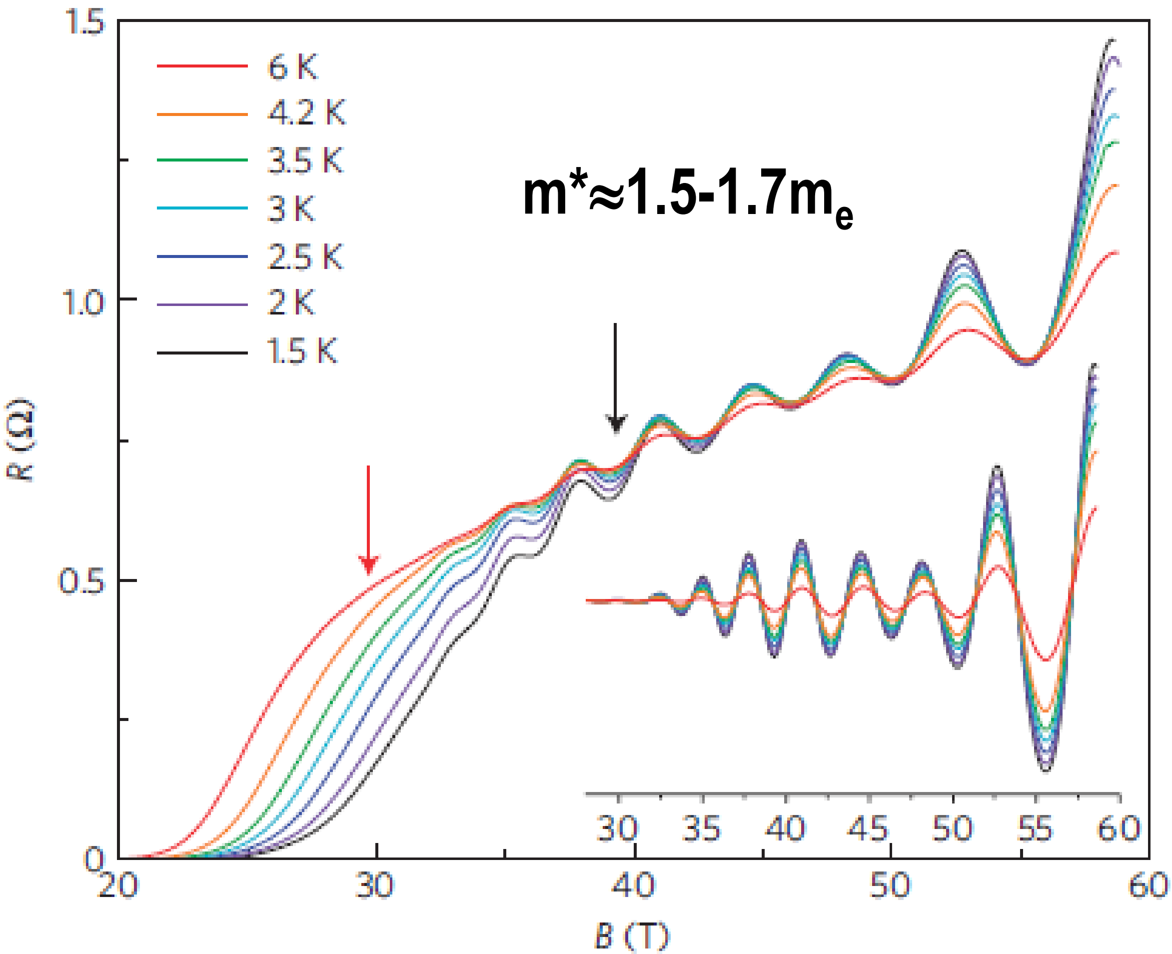
$$R_W = \exp\left(-2\pi^2 W^2/\hbar^2\omega_c^2\right)$$

comes from long-range spatial inhomogeneities

$$\frac{\sigma_1}{\sigma_0} \propto \int d\mu\, D(\mu - \mu_0 - \Delta\mu) 2J_0\left(\frac{4\pi t_z}{\hbar\omega_c}\right) \times \cos\left(2\pi \frac{\mu \pm t_\perp}{\hbar\omega_c}\right) R_D R_T$$

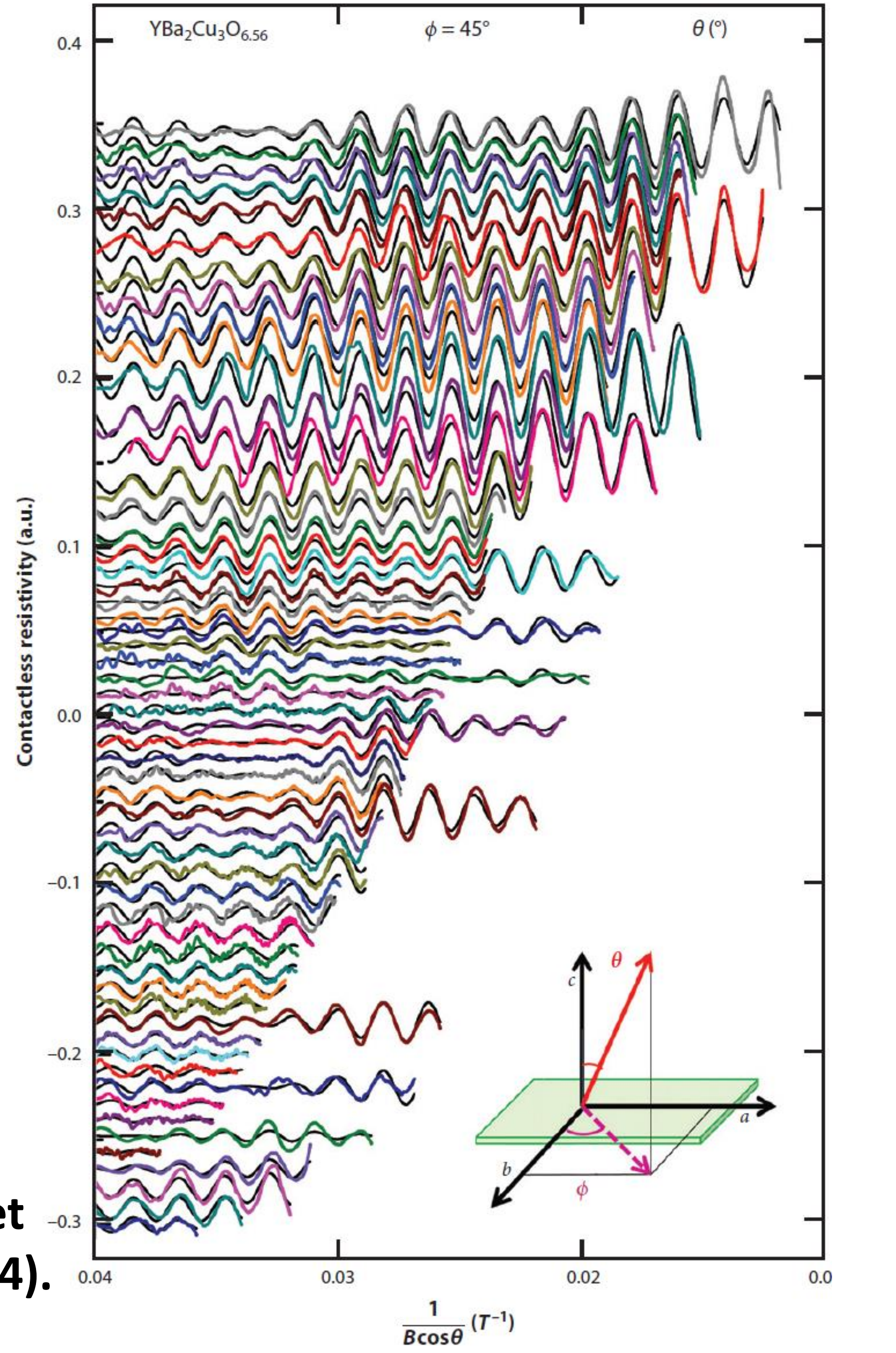
$$= 2J_0\left(\frac{4\pi t_z}{\hbar\omega_c}\right)\cos\left(2\pi\frac{\mu_0 \pm t_\perp}{\hbar\omega_c}\right) R_D R_T R_W$$

Temperature dependence of the amplitude of magnetic oscillations in YBCO



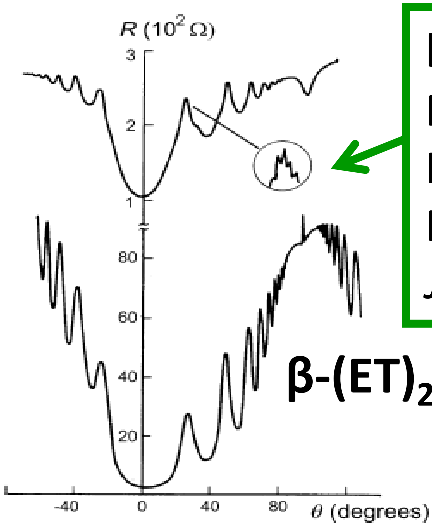
B.J. Ramshaw et al., *Nature Physics* **7**, 234 (2011)

Spin-zeros on MQO in YBCO?



Sebastian SE, Harrison N, et al. Nature 511, 61–64 (2014).

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

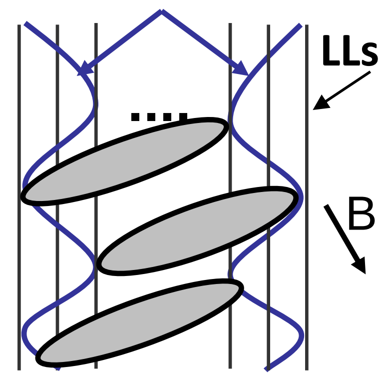


β-$(ET)_2IBr_2$

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

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

Fermi surface



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

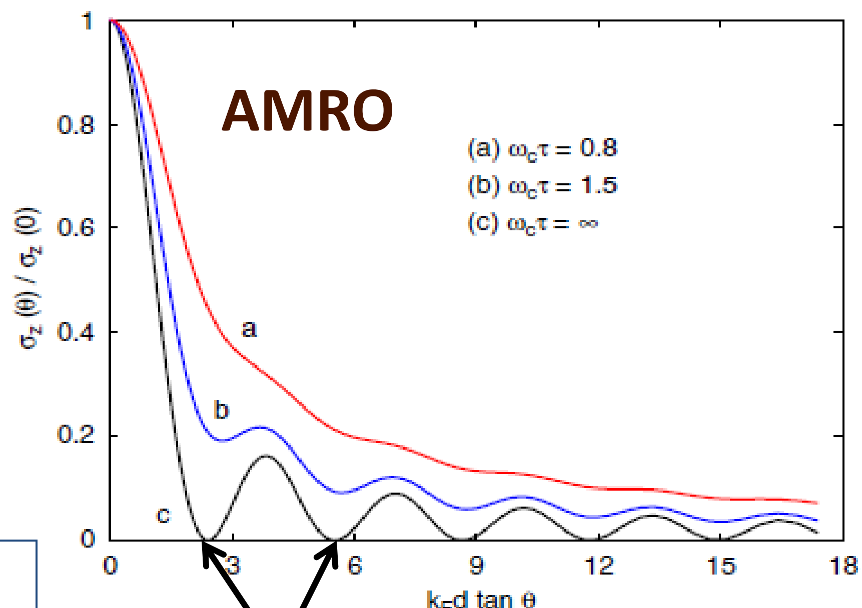
$\varepsilon(p)=\varepsilon_{||}(p_{||})+2t_z\cos(p_z d/\hbar)$,

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

Fourier transform of DoS in quasi-2D metals

Electron dispersion in Q2D metals $\epsilon_{n,k_z} = \hbar\omega_c(n+1/2) - 2t\cos(k_z d)$

The density of states (DoS) is given by $g(\epsilon) = \sum_{n=0}^{\infty} \frac{N_{LL}}{\sqrt{4t^2 - [\epsilon - \hbar\omega_c(n+1/2)]^2}}$

Applying the Poisson summation formula

$$\sum_{n=n_0}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_a^{\infty} e^{2\pi i k n} f(n)\, dn,$$

one obtains

$$g(\epsilon) \propto 1 + 2\sum_{k=1}^{\infty} (-1)^k \cos\left(\frac{2\pi k\epsilon}{\hbar\omega_c}\right) J_0\left(\frac{4\pi k t}{\hbar\omega_c}\right)$$

T. Champel and V. P. Mineev, Philos. Mag. B **81**, 55 (2001).