Fermi Surface
part II: measurements

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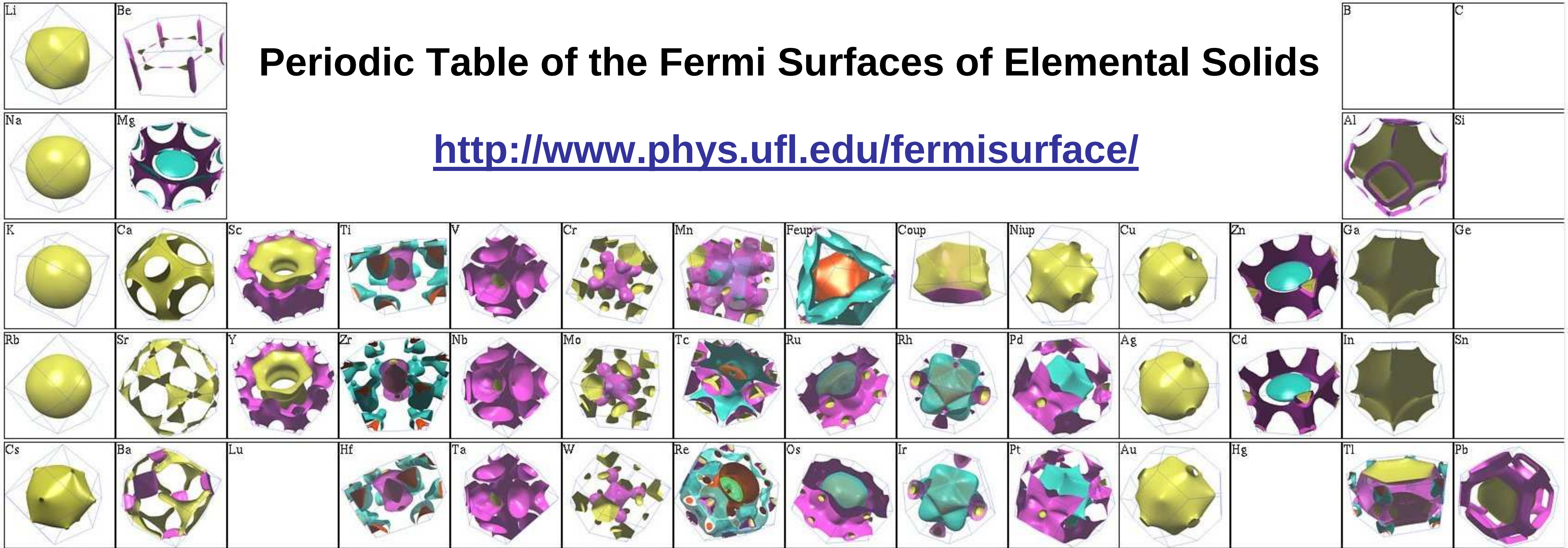


Periodic Table of the Fermi Surfaces of Elemental Solids

http://www.phys.ufl.edu/fermisurface/

Outline

I. Why and how to measure a Fermi surface ?

II. Angular Resolved Photoemission Electron Spectroscopy (ARPES)

III. Quantum oscillations (QO)
   1) History
   2) Theory
      a) Semiclassical theory
      a) Landau levels quantification
      b) Lifshitz-Kosevich theory
      c) High magnetic field phenomena
   3) High magnetic fields facilities
   4) Fermiology

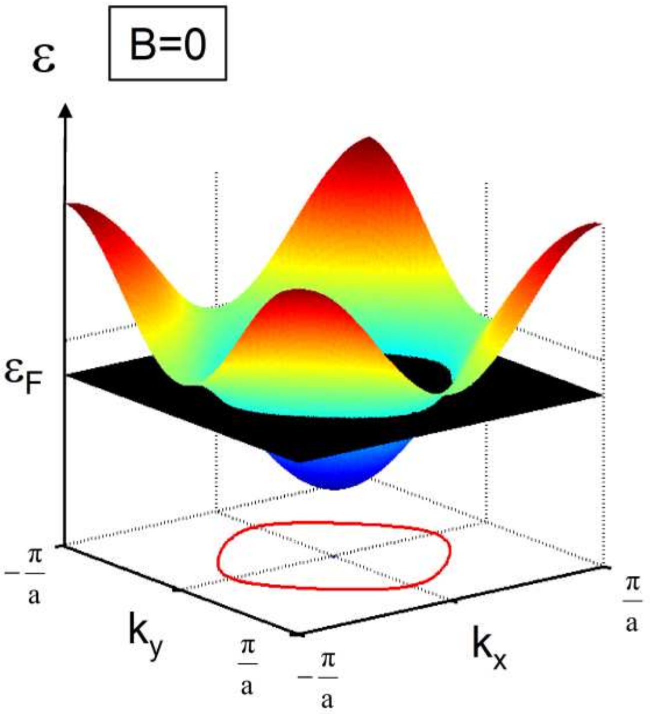
IV. Hot topics
   1) Phase transition
   2) High T_c superconductors

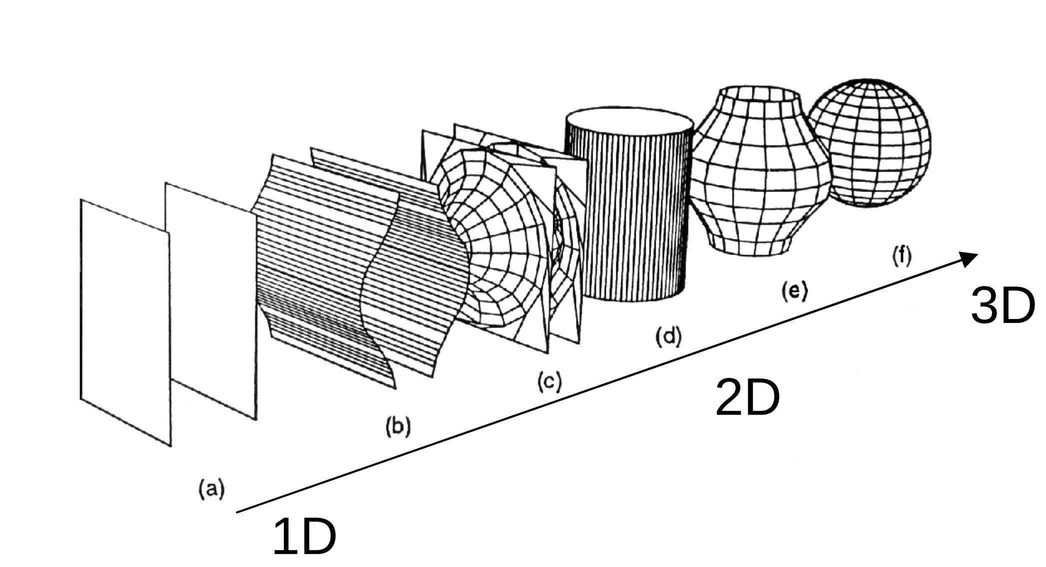
I. Why and how to measure a Fermi surface

2D: $E(\vec{k}) = -2t\left(\cos(k_x a) + \cos(k_y b)\right)$

E_F ~ 1-10 eV

Typical excitations (ΔV, ΔT) ~meV





Comparison with band structure calculations, effect of interactions, phase transitions…

FS measurements

- Global properties: C_v, χ_{Pauli}, R_H, $\Delta\rho/\rho$...
- Topographic properties: ARPES, AMRO, QO

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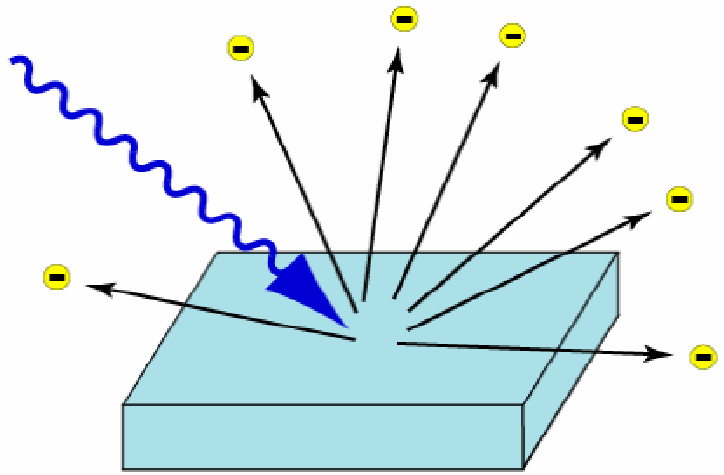
II. ARPES



Photoelectric effect:

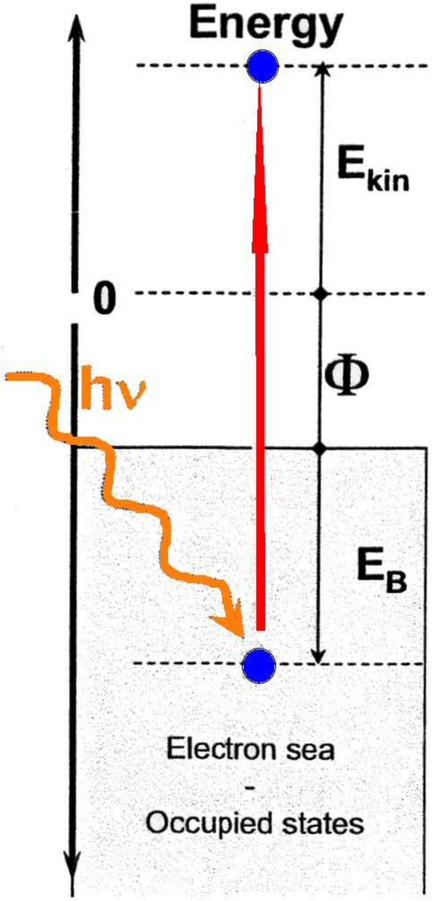
1886: 1st experimenal work by Hertz

1905: Theory by Einstein

Work function of the surface (Potential barrier)

$$\boxed{E_{kin} = h\upsilon - E_B - \phi}$$

Binding energy of the electron in the solid



II. ARPES

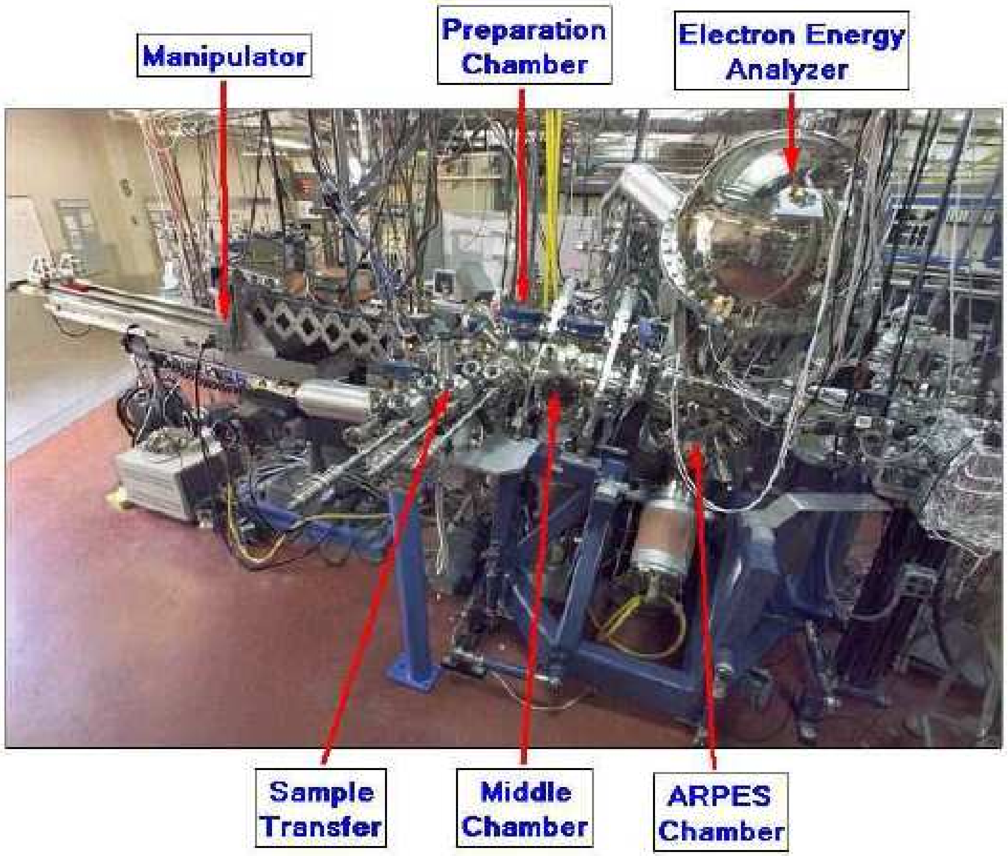
Angular Resolved PhotoEmission Spectroscopy

Angular ↔ Momentum resolved

- **High resolution**

ΔE (meV)	$\Delta\theta$
2-10	0.2°

- Ultra-high vacuum (~ 10^{-11} torr)
- High angular precision (+/- 0.1°)
- Low base temperature (< 10 K)
- Wide temperature range (10-350 K)
- Variable photon energies (12-30 eV)
- Multiple light sources (He lamp)
- Control of light polarization
- Single crystal cleaving tools
- Sample surface preparation & cleaning



Vacuum

$\boxed{E_{kin}}$

$\boxed{K}$

Conservation laws

$$E_{kin} = h\upsilon - E_B - \phi$$

$$\vec{k}_f - \vec{k}_i = \cancel{\vec{k}_{h\nu}}$$

Solid

$\boxed{E_B}$

$\boxed{k}$

X. J. Zhou et al, Treatise of HTSC

II. ARPES

Synchroton SOLEIL

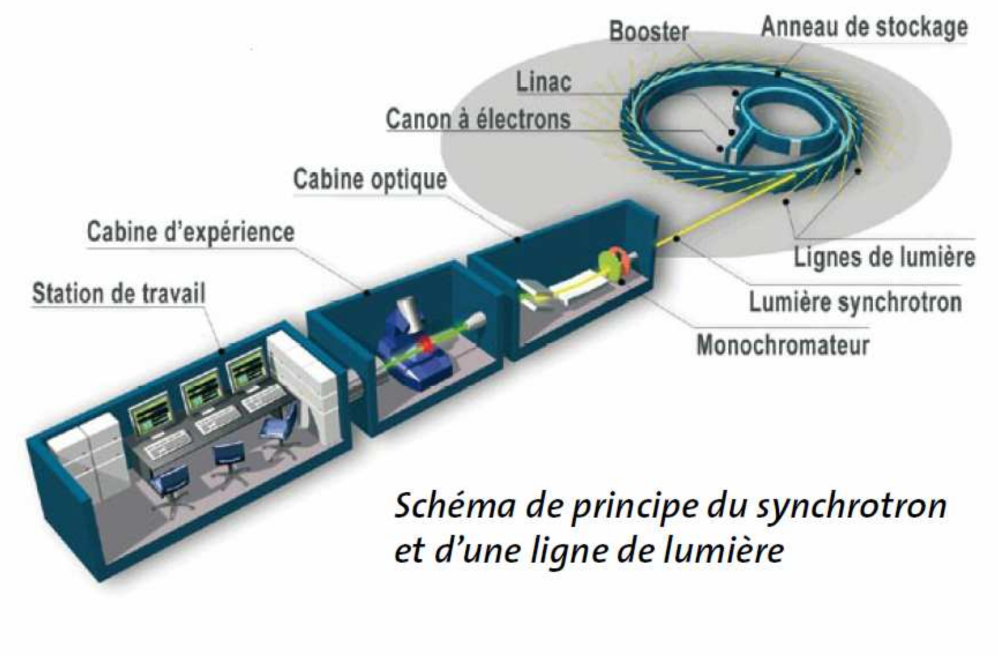
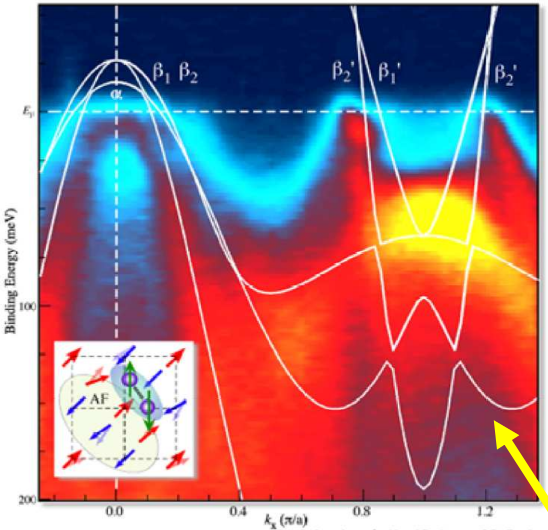


Schéma de principe du synchrotron et d'une ligne de lumière

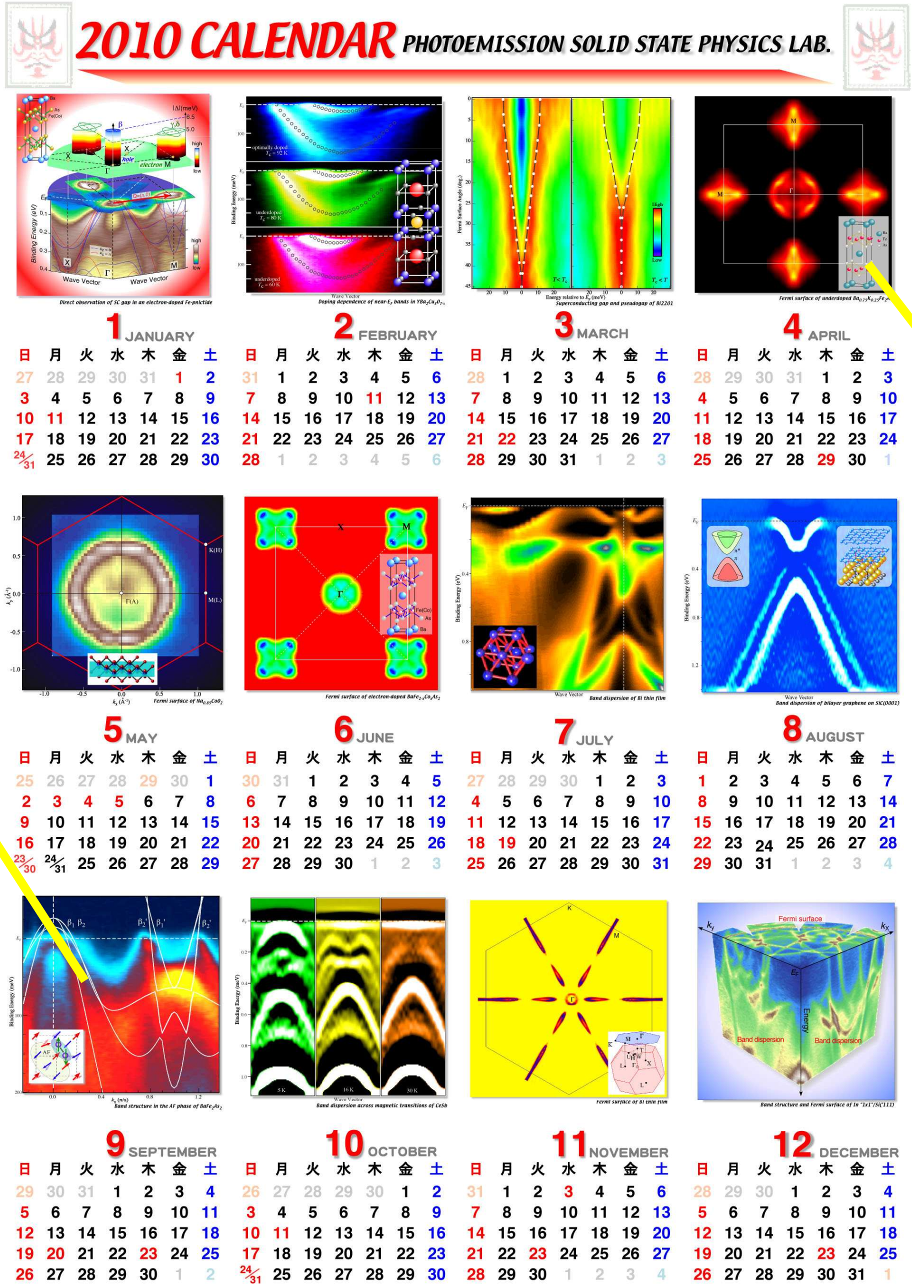
From IR to RX

http://www.synchrotron-soleil.fr/

II. ARPES



Band structure in the AF phase of $BaFe_2As_2$



2010 CALENDAR PHOTOEMISSION SOLID STATE PHYSICS LAB.

Direct observation of SC gap in an electron-doped Fe-pnictide

1 JANUARY

日	月	火	水	木	金	土
27	28	29	30	31	1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24/31	25	26	27	28	29	30

Doping dependence of near-E_F bands in $YBa_2Cu_3O_{7-\delta}$

2 FEBRUARY

日	月	火	水	木	金	土
31	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	1	2	3	4	5	6

Superconducting gap and pseudogap of Bi2201

3 MARCH

日	月	火	水	木	金	土
28	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	31	1	2	3

Fermi surface of underdoped $Ba_{0.75}K_{0.25}Fe_2As_2$

4 APRIL

日	月	火	水	木	金	土
28	29	30	31	1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	1

Fermi surface of $Na_{0.85}CoO_2$

5 MAY

日	月	火	水	木	金	土
25	26	27	28	29	30	1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23/30	24/31	25	26	27	28	29

Fermi surface of electron-doped $BaFe_{2-x}Co_xAs_2$

6 JUNE

日	月	火	水	木	金	土
30	31	1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	1	2	3

Band dispersion of Bi thin film

7 JULY

日	月	火	水	木	金	土
27	28	29	30	1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

Band dispersion of bilayer graphene on SiC(0001)

8 AUGUST

日	月	火	水	木	金	土
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	31	1	2	3	4

Band structure in the AF phase of $BaFe_2As_2$

9 SEPTEMBER

日	月	火	水	木	金	土
29	30	31	1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28	29	30	1	2

Band dispersion across magnetic transitions of CeSb

10 OCTOBER

日	月	火	水	木	金	土
26	27	28	29	30	1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24/31	25	26	27	28	29	30

Fermi surface of Bi thin film

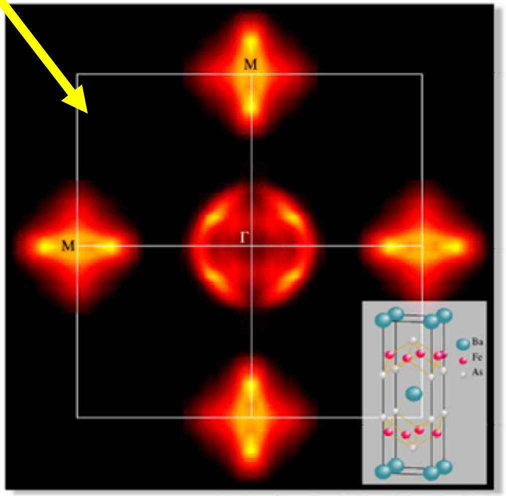
11 NOVEMBER

日	月	火	水	木	金	土
31	1	2	3	4	5	6
7	8	9	10	11	12	13
14	15	16	17	18	19	20
21	22	23	24	25	26	27
28	29	30	1	2	3	4

Band structure and Fermi surface of In "1x1"/Si(111)

12 DECEMBER

日	月	火	水	木	金	土
28	29	30	1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28	29	30	31	1



Fermi surface of underdoped $Ba_{0.75}K_{0.25}Fe_2As_2$

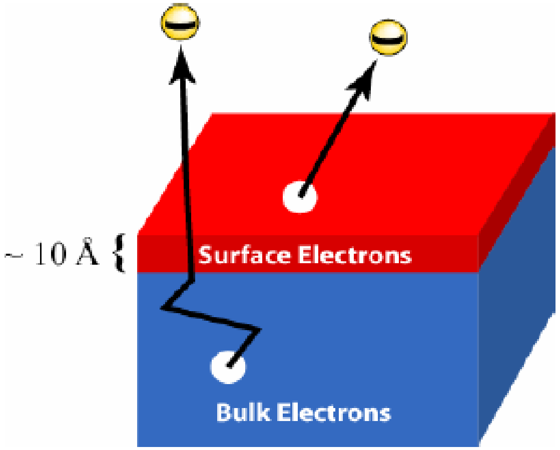
http://arpes.phys.tohoku.ac.jp/contents/calendar-e.html

II. ARPES

Advantages

- **Direct information about the electronic states!**
- Straightforward comparison with theory - little or no modeling.
- High-resolution information about **BOTH energy** and **momentum**
- **Surface-sensitive probe**
- Sensitive to "**many-body**" effects
- Can be applied to small samples (100 μm x 100 μm x 10 nm)

Limitations

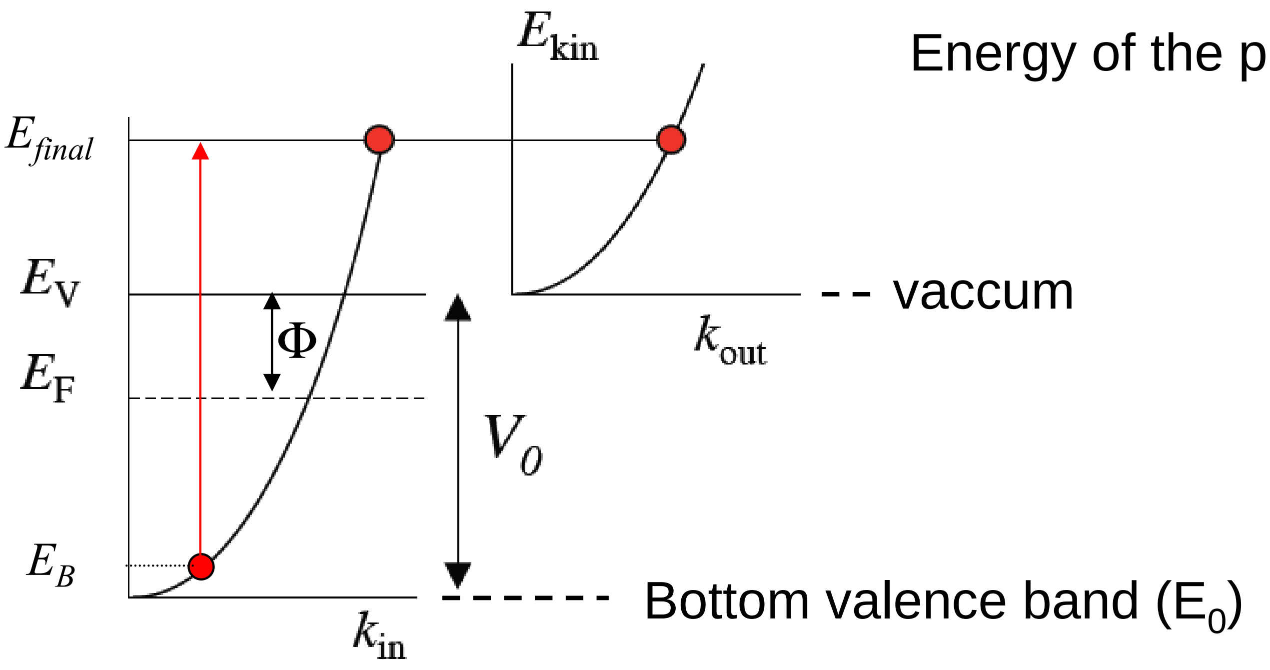


- **Not bulk sensitive**
- Requires clean, atomically flat surfaces in **ultra-high vacuum**
- Cannot be studied as a function of pressure or magnetic field

A. Damascelli, http://www.physics.ubc.ca/~quantmat/ARPES/PRESENTATIONS/Talks/ARPES_Intro.pdf

II. ARPES

Conservation laws



Energy of the photoelectron outside the solid

$$E_{kin} = \frac{\hbar^2 K^2}{2m}$$

One match the free-electron parabolas inside and outside the solid to obtain **k** inside the solid

$$\boxed{E_{kin} = h\upsilon - E_B - \phi}$$

E_B, E_0 and E_{final} are referenced to E_F

E_{kin} is referenced to E_{vaccum}

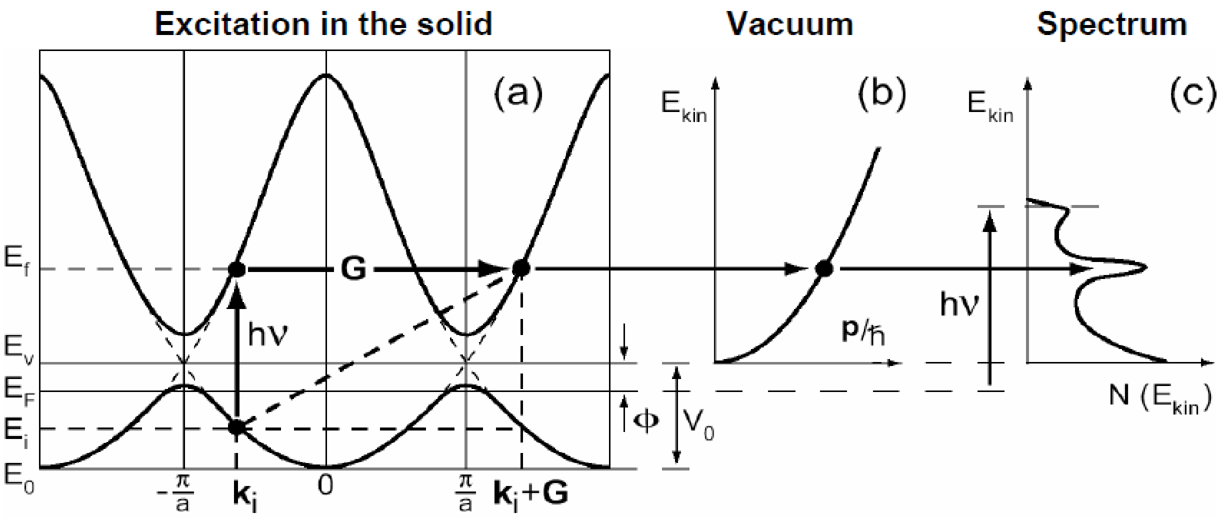
II. ARPES

Conservation laws

$$\vec{k}_f - \vec{k}_i = \cancel{\vec{k}_{h\nu}}$$

Ultraviolet ($h\nu < 100$ eV) $\Rightarrow$ $k_{h\nu} = 2\pi/\lambda = 0.05$ Å^{-1}

$2\pi/a = 1.5$ Å^{-1} ($a = 4$ Å)



$$\vec{k}_f - \vec{k}_i = 0$$

or

$$\vec{k}_f - \vec{k}_i = \vec{G}$$

Umklapp $\Rightarrow$ Shadow bands or superstructures

1) The surface does not perturb the translational symmetry in the x-y plane:

$\vec{k}_{//}$ is conserved (within $\vec{G}_{//}$)

$$\boxed{k_{//} = K_{//} = \frac{1}{\hbar}\sqrt{2mE_{kin}}\,\sin\theta}$$

A. Damascelli et al, RMP’03

II. ARPES

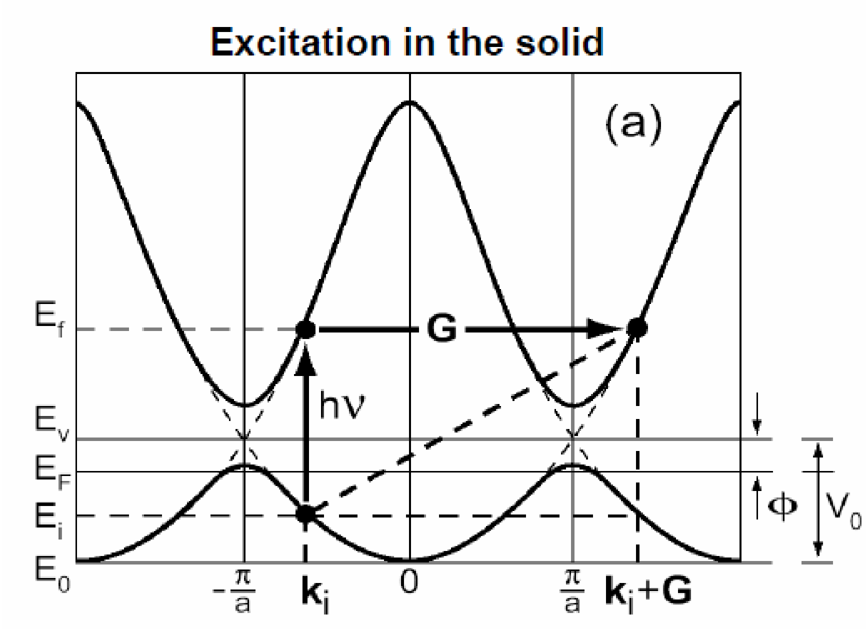
Conservation laws

2) Abrupt potential change along z $\Rightarrow \vec{k}_\perp$ is not conserved across the surface

But determination of $\vec{k}_\perp$ needed for 3D system to map E(k)

Hyp: Nearly free electron description for the final bulk Bloch states

Excitation in the solid



$$E_f(\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} - |E_0| = \frac{\hbar^2\left(\vec{k}_{//}^2 + \vec{k}_\perp^2\right)}{2m} - |E_0|$$

$$E_f = E_{kin} + \phi \quad \text{and} \quad \frac{\hbar^2 \vec{k}_{//}^2}{2m} = E_{kin} \sin^2\theta$$

$$\boxed{k_\perp = \frac{1}{\hbar}\sqrt{2m\left(E_{kin}\cos^2\theta + V_0\right)}}$$

$$V_0 = |E_0| + \phi$$

A. Damascelli et al, RMP'03

II. ARPES

2D case

FWHM of an ARPES peak $\Bigg\}$ $$\Gamma = \frac{\dfrac{\Gamma_i}{|v_{i\perp}|} + \dfrac{\Gamma_f}{|v_{f\perp}|}}{\left| \dfrac{1}{v_{i\perp}} \left[1 - \dfrac{m v_{i\|} \sin^2 \vartheta}{\hbar k_{\|}} \right] - \dfrac{1}{v_{f\perp}} \left[1 - \dfrac{m v_{f\|} \sin^2 \vartheta}{\hbar k_{\|}} \right] \right|}$$

Γ_i, Γ_f → inverse lifetime of photoelectron and photohole
v_i, v_f → group velocities ($\hbar v_{i\perp} = \partial E_i / \partial k_\perp$)

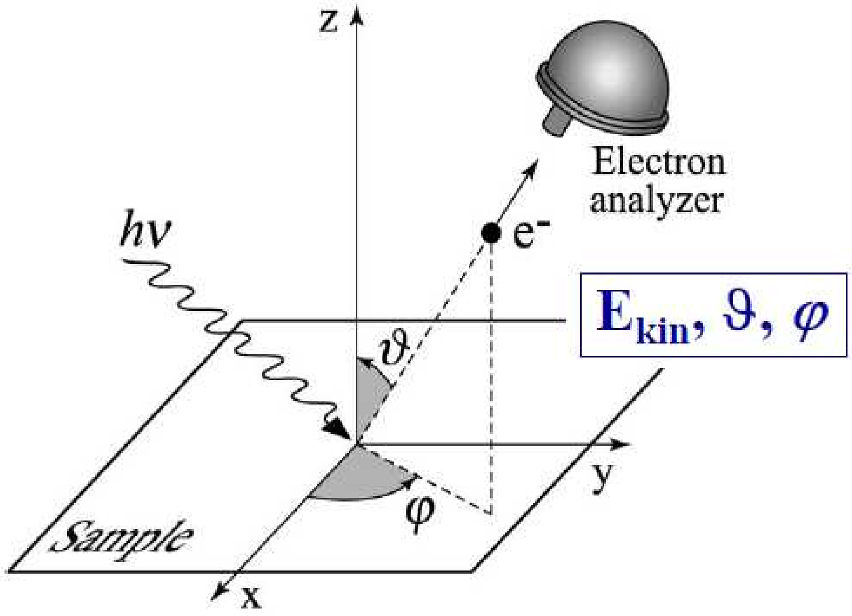
If $|v_{i\perp}| \approx 0$ $\Rightarrow$ $$\Gamma = \frac{\Gamma_i}{\left| 1 - \dfrac{m v_{i\|} \sin^2 \vartheta}{\hbar k_{\|}} \right|} \equiv C\,\Gamma_i$$

When $k_{//}$ is completely determined (2D), ARPES lineshape can be directly interpreted as lifetime

A. Damascelli et al, RMP’03

II. ARPES

Non-interacting case



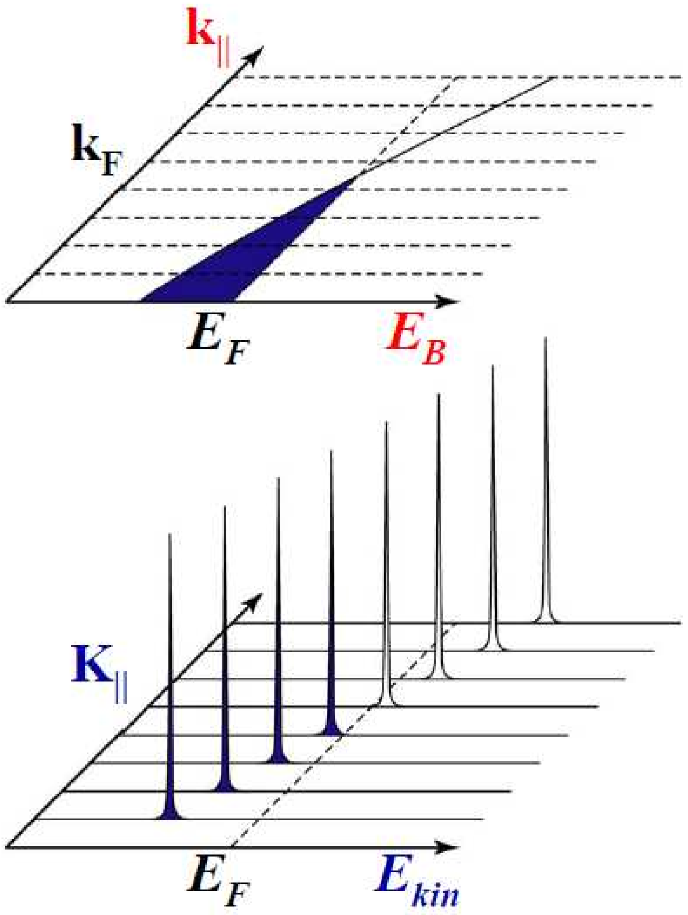
Energy Conservation

$$E_{kin} = h\nu - \phi - |E_B|$$

Momentum Conservation

$$\hbar \mathbf{k}_{||} = \hbar \mathbf{K}_{||} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$

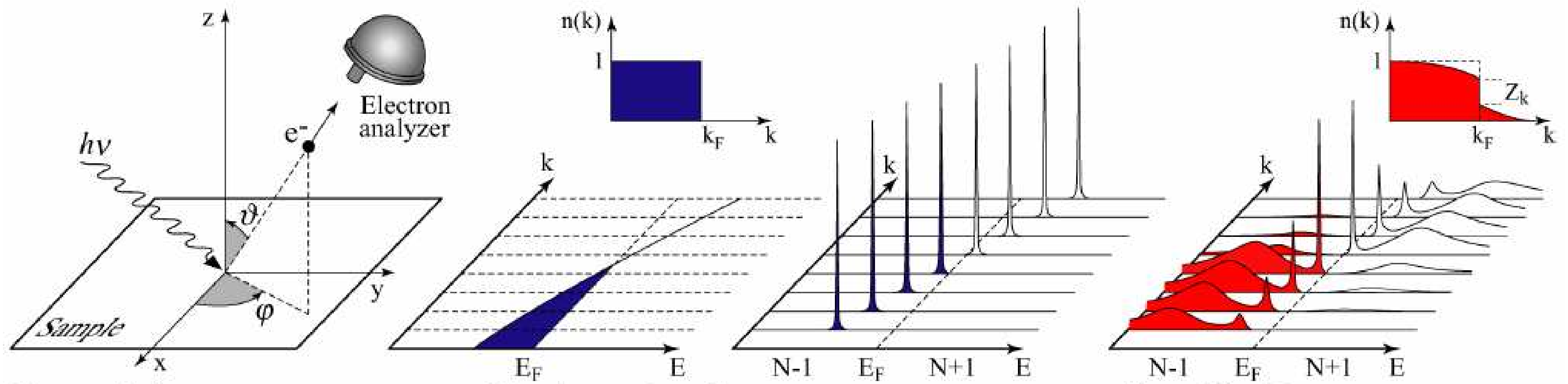
Electrons in Reciprocal Space



A. Damascelli et al, RMP'03

II. ARPES

Interacting systems



Photoemission geometry

Non-interacting electron system

Fermi liquid system

Photoemission intensity: $I(k,\omega)=I_0\,|M(k,\omega)|^2 f(\omega)\,A(k,\omega)$

Single-particle spectral function

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

$\Sigma(k,\omega)$: the "self-energy" captures the effects of interactions

Non-interacting

$$A(\mathbf{k},\omega)=\delta(\omega-\epsilon_k)$$

No Renormalization

Infinite lifetime

Fermi Liquid

$$A(\mathbf{k},\omega)=Z_{\mathbf{k}}\frac{\Gamma_{\mathbf{k}}/\pi}{(\omega-\varepsilon_{\mathbf{k}})^2+\Gamma_{\mathbf{k}}^2}+A_{inc}$$

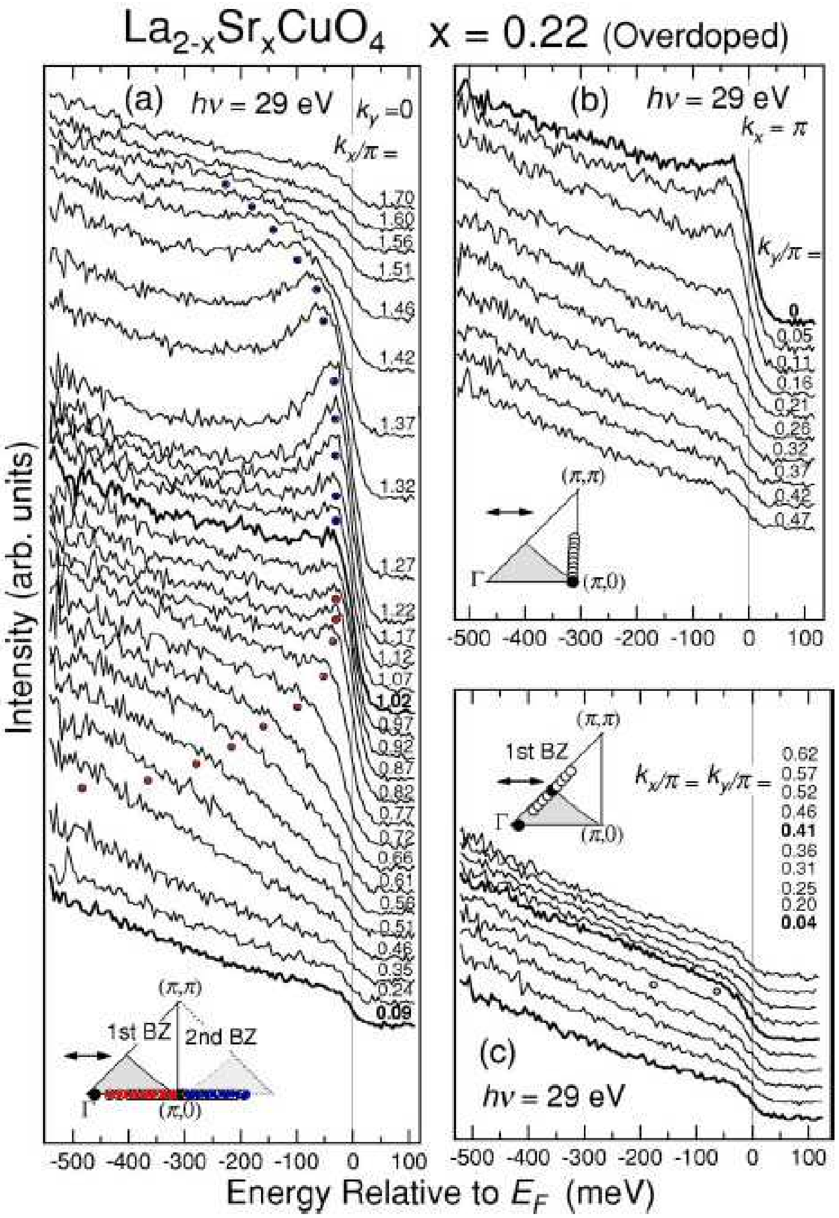
$$m^*>m \qquad |\varepsilon_{\mathbf{k}}|<|\epsilon_{\mathbf{k}}|$$

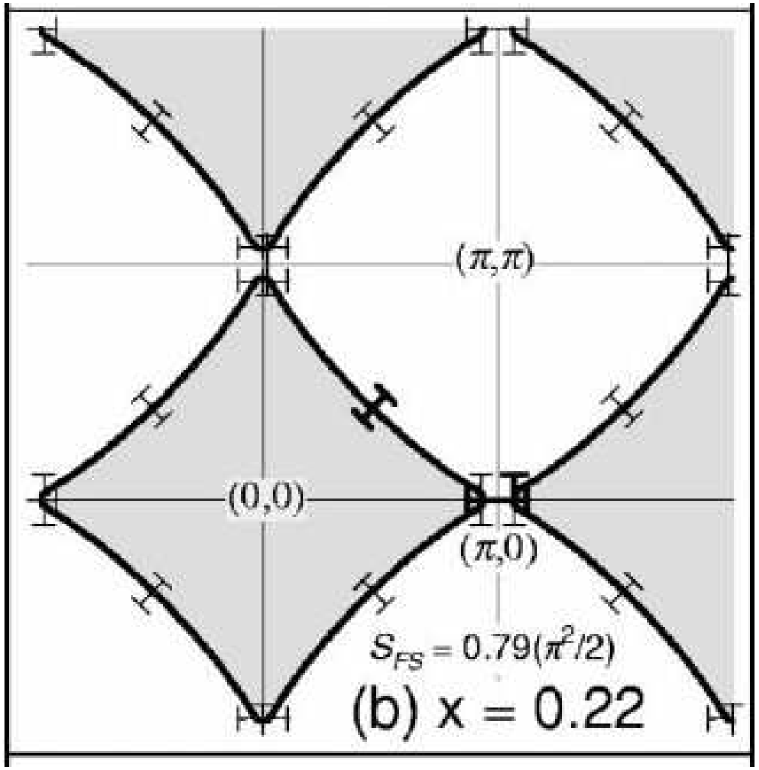
$$\tau_{\mathbf{k}}=1/\Gamma_{\mathbf{k}}$$

A. Damascelli et al, RMP'03

II. ARPES

Example: Quasi-2D overdoped cuprate





A. Ino et al, PRB'02

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III.1 History

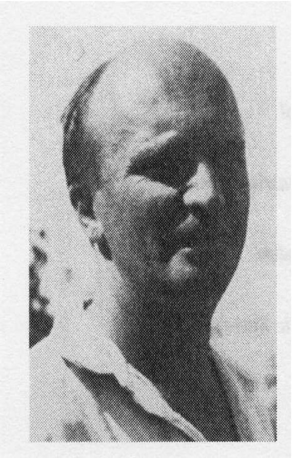
1930 de Haas-van Alphen / Shubnikov-de Haas effects

W.J. de Haas

(1878-1960)

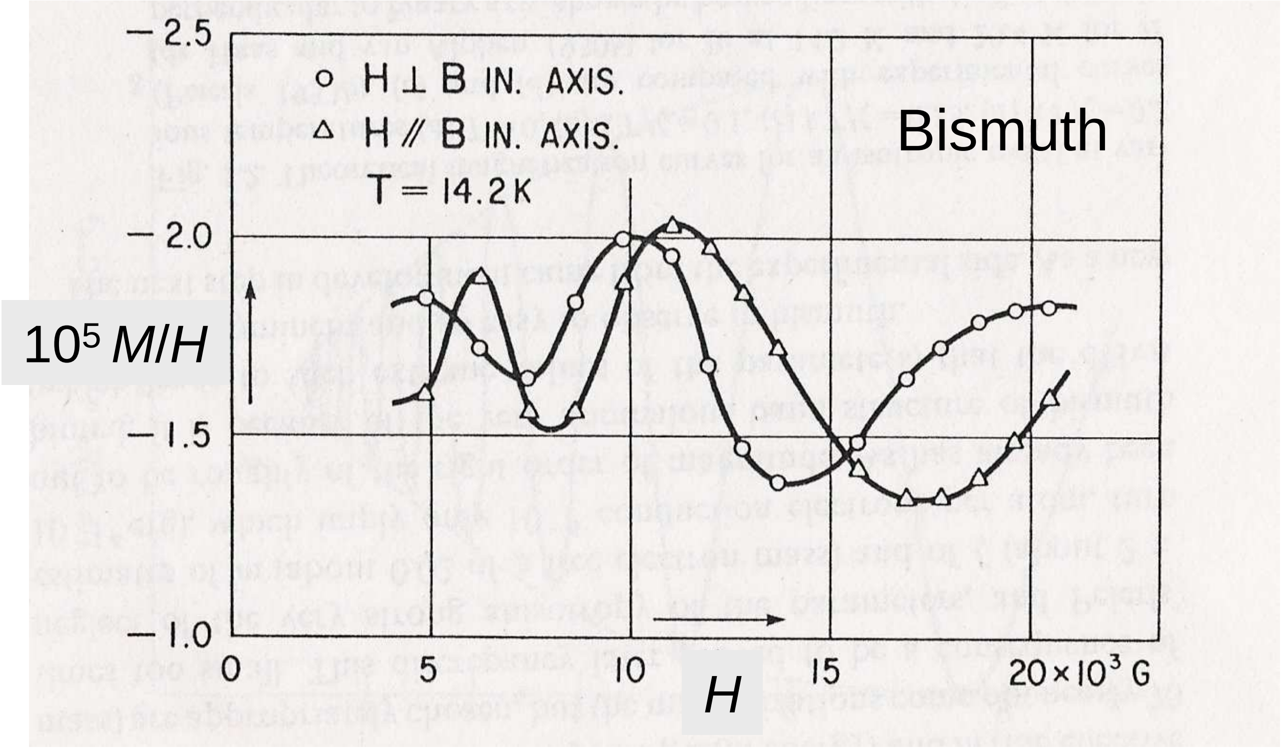
P.M. van Alphen

(1906-1967)



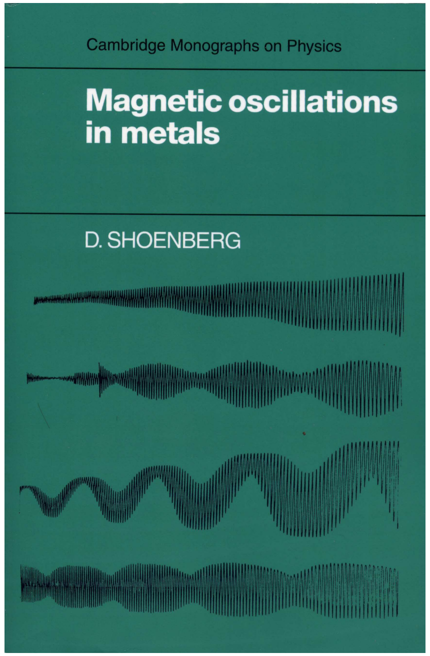
L.V. Shubnikov

(1901-1937)



III.1 History

The experimental pioneer …



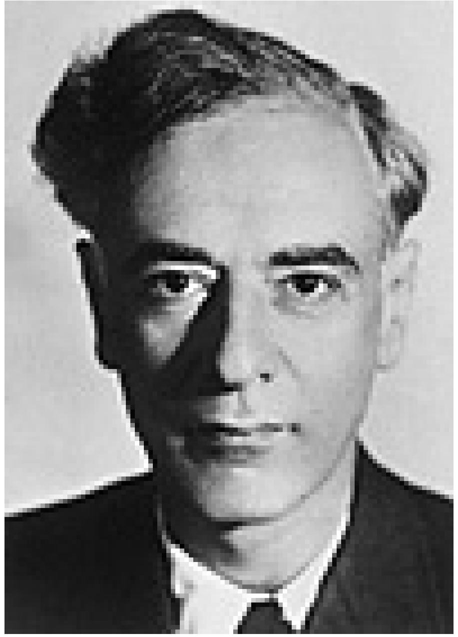
Cambridge Monographs on Physics

Magnetic oscillations in metals

D. SHOENBERG

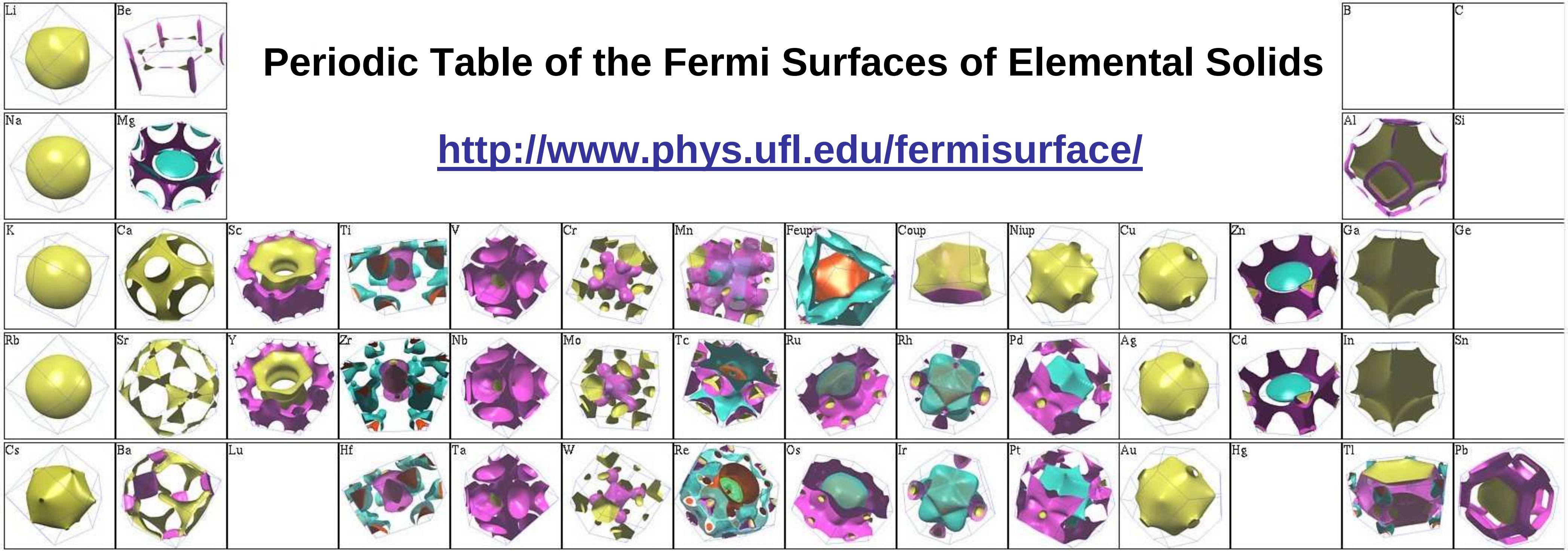
David Shoenberg (1911 - 2004)

and his friend the other post-doc



L.D. Landau (1908 – 1968)

III.1 History



Periodic Table of the Fermi Surfaces of Elemental Solids

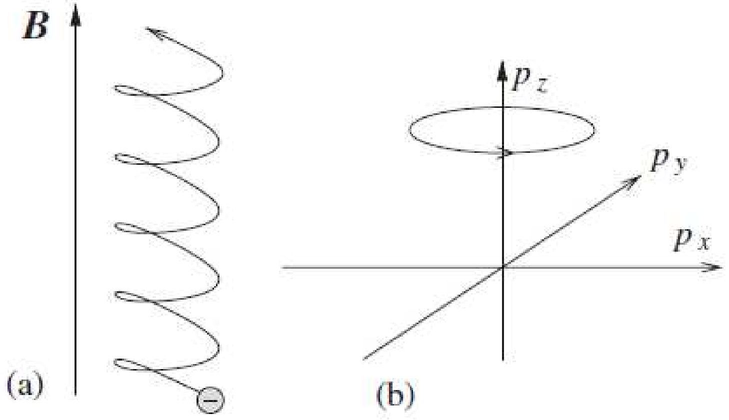
http://www.phys.ufl.edu/fermisurface/

1950 – 70: Two decades of mapping 3D Fermi surfaces of 'simple' metals.

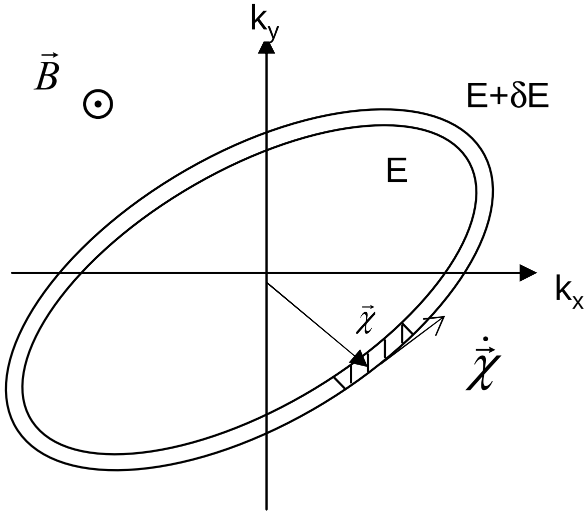
III.2 Theory

Semiclassical theory

$$\begin{cases} \frac{d\vec{k}}{dt} = \frac{1}{\hbar}\vec{F} \\ \vec{v} = \frac{1}{\hbar}\nabla_k \varepsilon(\vec{k}) \end{cases} \Rightarrow \quad \hbar\frac{d\vec{k}}{dt} = q\left(\vec{V}\times\vec{B}+\vec{E}_{el}\right)$$



Real space Momentum space



χ and ρ are the projection of **k** and **r** in the plane ⊥ to **B**

$$d^2\mathrm{A} = d\chi.\dot{\chi}.dt$$

$dE = \vec{\nabla}_\chi E.d\chi$ with $\vec{\nabla}_\chi E = \hbar\dot{\vec{\rho}}$

$d\dot{\mathrm{A}} = \frac{qB}{\hbar^2}dE \Rightarrow d\mathrm{A} = \frac{qB}{\hbar^2}dE.T$ with $T = 2\pi/\omega_c$

$$\boxed{\omega_c = \frac{2\pi|q|B}{\hbar^2}.\frac{dE}{dA}}$$

$$\omega_c = \frac{qB}{m_c} \Rightarrow \boxed{m_c = \frac{\hbar^2}{2\pi}\left(\frac{dA}{dE}\right)_{\dot{k}_z}}$$

III.2 Theory

Onsager relation

Bohr-Sommerfeld condition: $\oint \vec{p}.d\vec{r} = (n+\gamma)h$

$$\vec{p} = h\vec{k} + q\vec{A}$$

$$\oint \vec{p}_{\perp}.d\vec{\rho} = q\oint \vec{\rho}\times\vec{B}.d\vec{\rho} + q\oint \vec{\mathrm{A}}.d\vec{\rho}$$

$$\oint \vec{p}_{\perp}.d\vec{\rho} = -q\vec{B}\oint \vec{\rho}\times d\vec{\rho} + q\iint \vec{B}.\vec{n}.dS$$

$$\oint \vec{p}_{\perp}.d\vec{\rho} = -2q\Phi + q\Phi = -q\Phi$$

$\phi_n = \frac{h}{e}(n+\gamma)$ with $A_n = \frac{\Phi_n}{B}\left(\frac{eB}{\hbar}\right)^2$

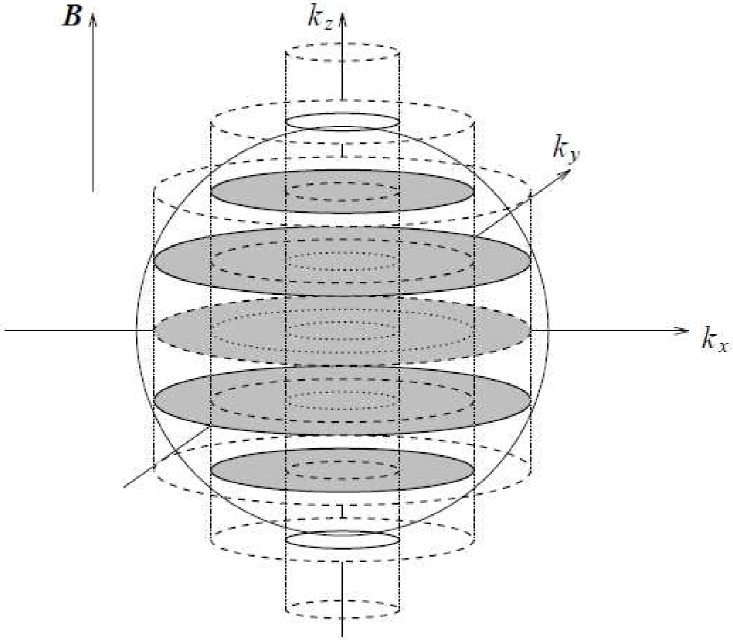
$$\boxed{A_n = \frac{2\pi eB}{\hbar}\left(n+\gamma\right)}$$ Onsager relation

γ=0.5 for free electrons

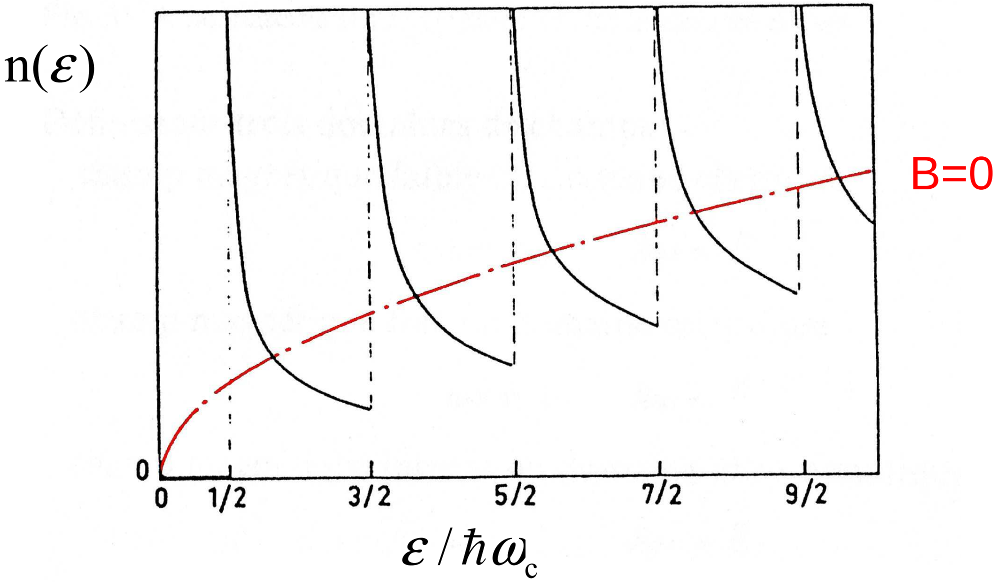
III.2 Theory

Onsager relation $\boxed{A_n = \frac{2\pi eB}{\hbar}(n+0.5)}$ $\Leftrightarrow$ $\pi\left(k_x^2+k_y^2\right)=\frac{2\pi eB}{\hbar}(n+0.5)$

Landau tubes



Density of states



Oscillation when $A_n=A_F(k_z)$ $\Leftrightarrow$ $A_F = \frac{2\pi eB}{\hbar}(n+0.5)$

$\boxed{(n+0.5)=\frac{\hbar A_F}{2\pi e}\frac{1}{B}}$ Oscillation periodic in 1/B with $\boxed{F=\frac{\hbar A_F}{2\pi e}}$

III.2 Theory

Quantum theory

3D

- Free electrons in high magnetic fields ⇒ Landau levels (LL)

$$H=\frac{1}{2m}\left(p-q\vec{A}\right)^2 \quad\Rightarrow\quad \left(E-\frac{\hbar^2k_z^2}{2m}\right)\varphi(x)=\left[\frac{p_x^2}{2m}+\frac{1}{2}m\omega_c^2\left(x-x_0\right)^2\right]\varphi(x)$$

(jauge de Landau)

$$\vec{A}=(0;Bx;0)$$

Equation of a harmonic oscillator with pulsation ω_c and orbits centred at $x_0=\frac{\hbar k_y}{qB}$

Solutions:

$$\boxed{E=E_z+E_\perp=\frac{\hbar^2k_z^2}{2m}+\hbar\omega_c\left(n+\frac{1}{2}\right)}$$

- Degeneracy of each Landau level g_L: $0<x_0<L_x \quad\Rightarrow\quad 0<k_y<\frac{qBL_x}{\hbar}$

$$g_L=\frac{qBL_x}{\hbar}/\frac{2\pi}{L_y} \quad\Rightarrow\quad \boxed{g_L=L_xL_y\frac{q}{\hbar}B}$$

- Density of states (1 LL): $n(E_z)=2*g_L*n_{1D}(E_{zn})$ where $n_{1D}(E_z)=L_z\left(\frac{2m}{\hbar^2}\right)^{0.5}\frac{1}{\sqrt{E_z}}$

For a given E

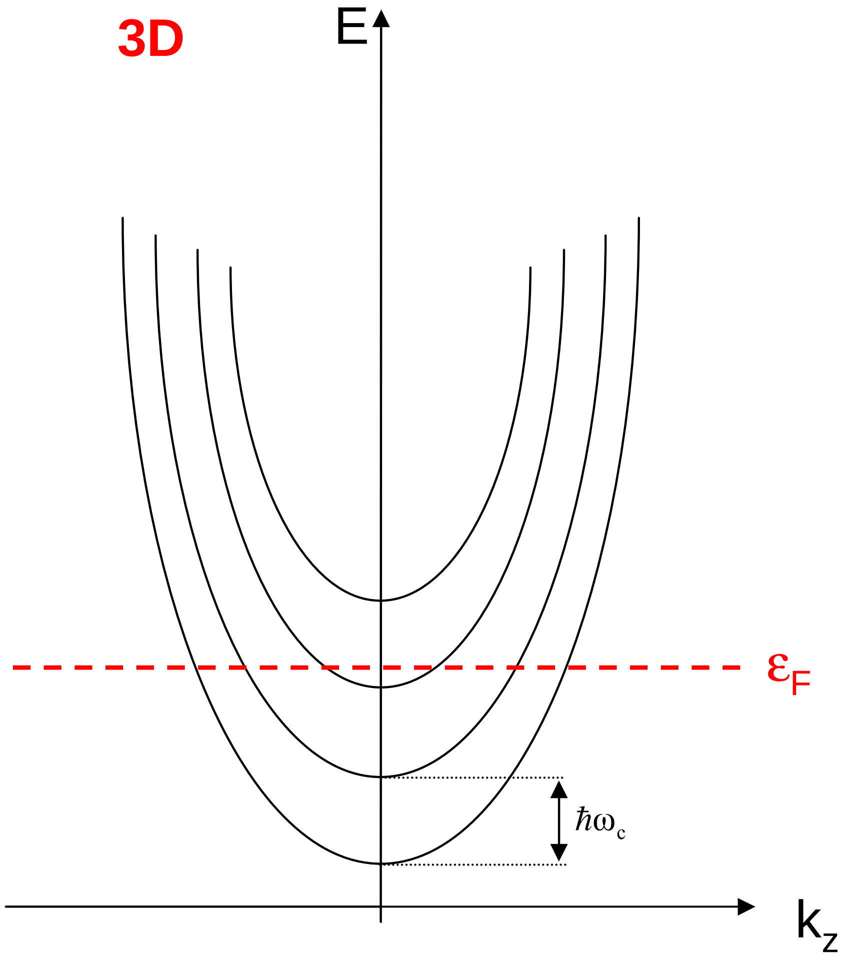
$$\boxed{n(E)=2\pi V\left(\frac{2m}{\hbar^2}\right)^{3/2}\hbar\omega_c\sum_{n=0}^{\infty}\frac{1}{\sqrt{E-\hbar\omega_c(n+0.5)}}}$$

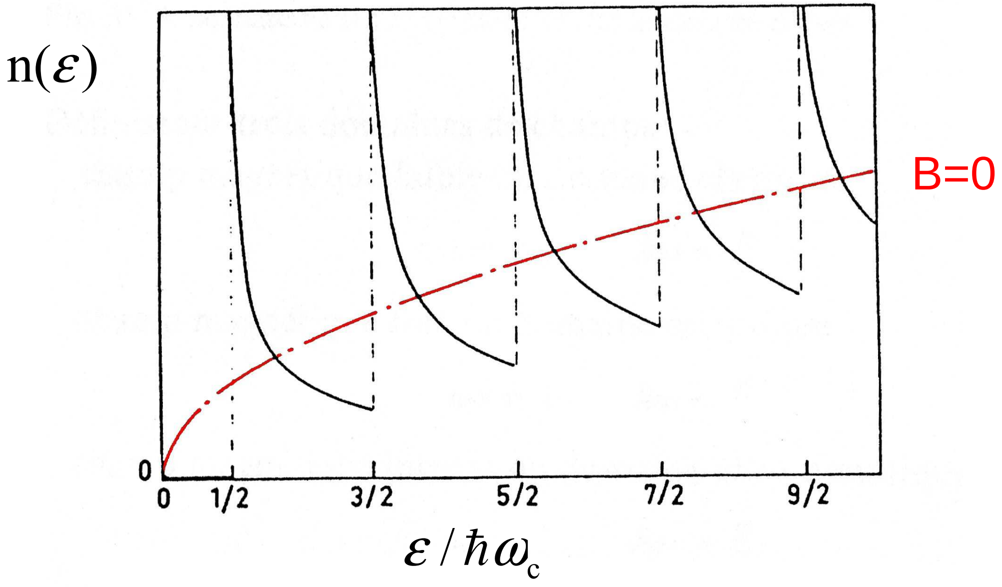
III.2 Theory

$$E = E_z + E_\perp = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c\left(n+\frac{1}{2}\right) \qquad \omega_c = \frac{qB}{m_c}$$

$$n(E) = 2\pi V\left(\frac{2m}{\hbar^2}\right)^{3/2}\hbar\omega_c\sum_{n=0}^{\infty}\frac{1}{\sqrt{E-\hbar\omega_c(n+0.5)}}$$

Density of states





$\Downarrow$

Oscillation of most electronic properties

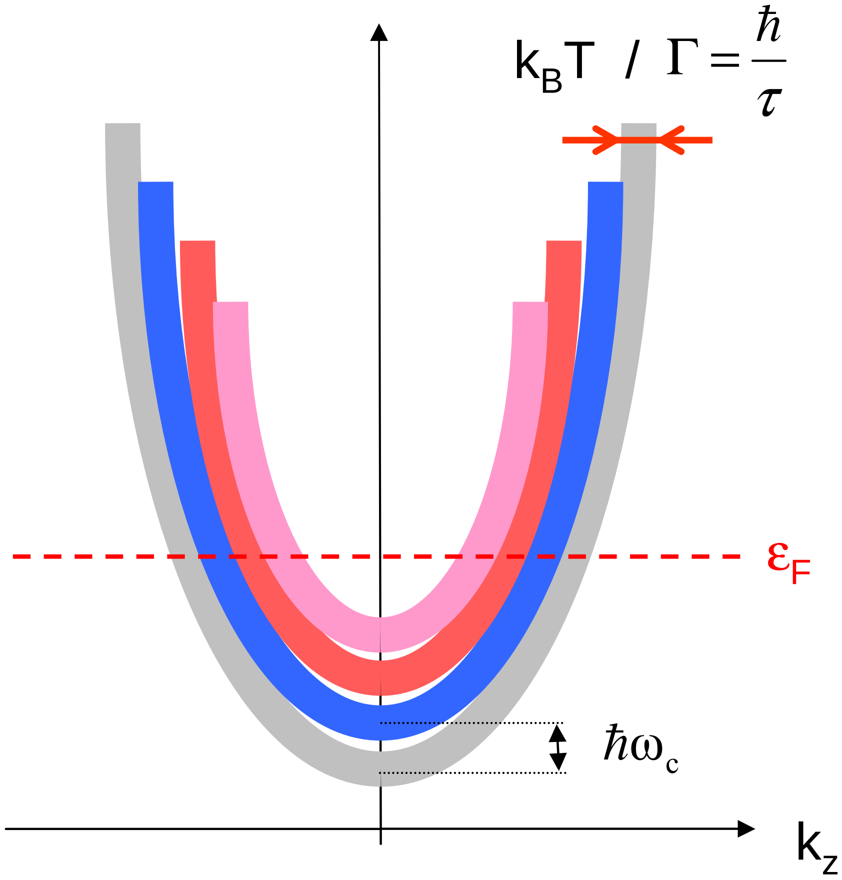
Magnetization: de Haas-van Alphen (dHvA)

Resistivity: Shubnikov-de Haas (SdH)

III.2 Theory

Temperature / Disorder effects on quantum oscillations

$$\omega_c = \frac{eB}{m^*}$$



- **Low T measurements**

$$\hbar\omega_c > k_B T$$

- **Need high quality single crystals**

$$\hbar\omega_c > \frac{\hbar}{\tau} \quad \Rightarrow \quad \omega_c\tau > 1$$

III.2 Theory

Lifshitz-Kosevich theory (1956)

T≠0

p=1

$$\Delta R, \Delta M \propto R_T\, R_D\, R_S \sin\left[2\pi\left(\frac{F}{B}-\gamma\right)\right]$$

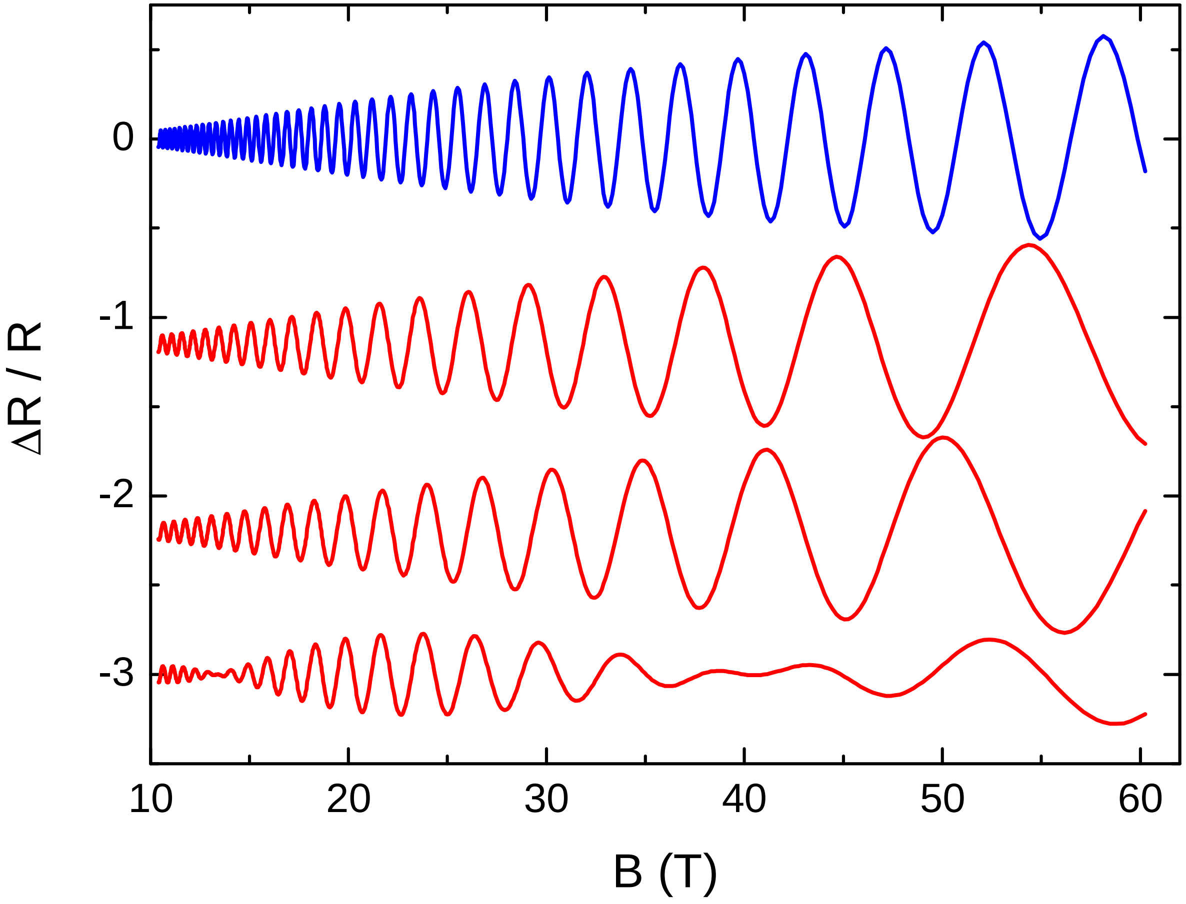
$\frac{F}{B}=\frac{\hbar}{2\pi q}\frac{A_F}{B}$	Onsager relation	⇒ A_F	Extremal area
$R_T=\frac{X}{sh(X)}$	where $X=14.694\times Tm_c/B$	⇒ m^*	Cyclotron mass
$R_D=\exp\left(-\frac{14.694\times T_D m_c}{B}\right)=\exp\left(-\frac{\pi}{\mu B}\right)$		⇒ $T_D=\frac{\hbar}{2\pi k_B\tau}$	Dingle temperature (mean free path)
$R_S=\cos\left(\frac{\pi}{2}m_b^* g\right)$		⇒ $m_b^* g$	

Direct measure of the Fermi surface extremal area

(but number of orbits ? location in k-space ?)

III.2 Theory

Extremal Area

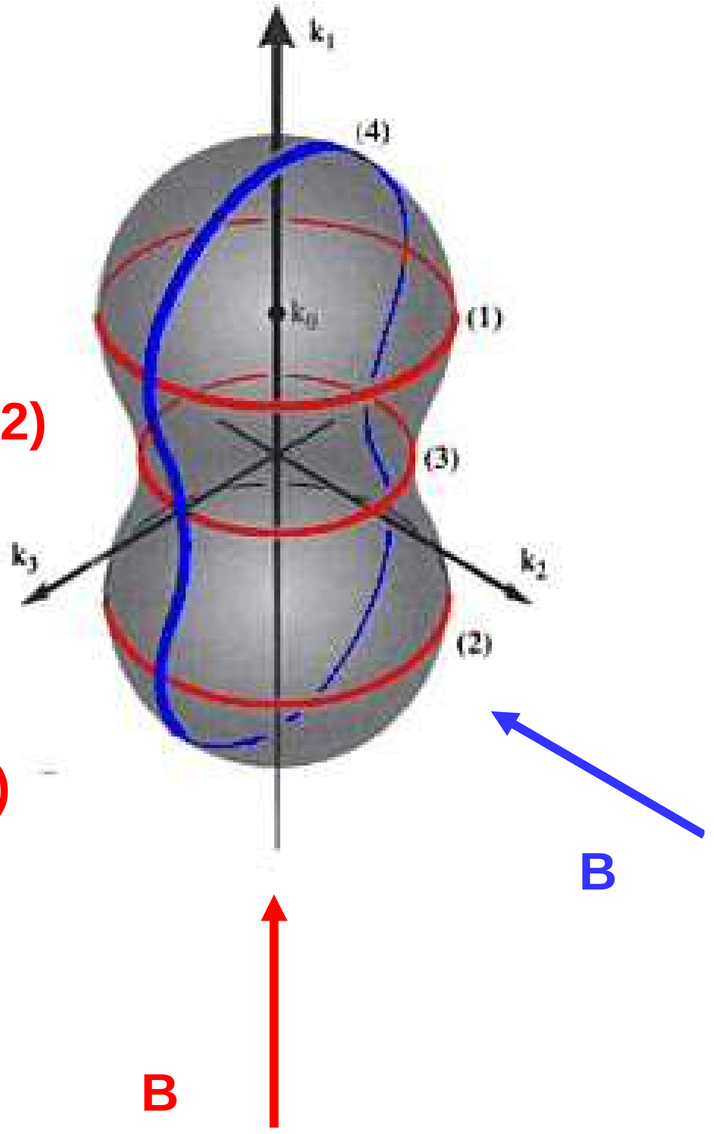


(4)

(1) or (2)

(3)

(1)+(3)



(4)	F=500 T
(1)	F=250 T
(3)	F=230 T

III.2 Theory

Energy scales

- $k_B T$=0.09 meV/K ⇒ 1 meV=11.6 K
- $\hbar\omega_c = \hbar\frac{eB}{m} = 0.12\times B\ \ meV/T$

$$\hbar\omega_c = 4.6\,meV\ \ @\ 40\,T$$

- $g\mu_B B$=0.12 x B meV / T

$g\mu_B B$=4.6 meV @ 40 T

- cyclotron orbits $r_c = \frac{\hbar k_F}{eB}$

k_F=7 nm^{-1} ⇒ r_c=100 nm @ 40 T

k_F=1.3 nm^{-1} ⇒ r_c=14 nm @ 40 T

Dingle term

(the evil term!)

$$R_D = \exp\left(-\frac{\pi}{\omega_c\tau}\right) = \exp\left(-\frac{\pi\hbar\langle k_F\rangle}{eB\langle\ell\rangle}\right) = \exp\left(-\frac{\pi r_c}{\ell}\right)$$

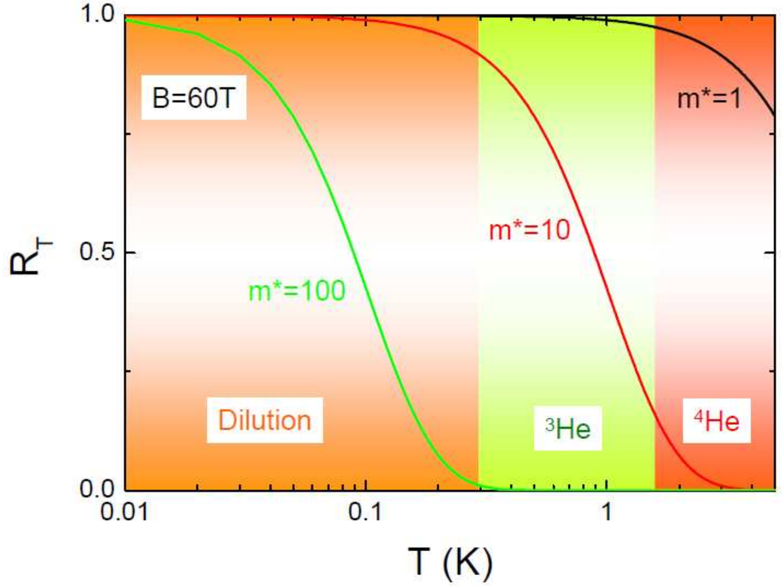
For $k_F \approx$ 7 nm-1 (large FS)

$\ell = 100\text{Å},\quad \mathrm{R_D} = 10^{-16}\quad @\quad \mathrm{B} = 40\mathrm{T}$

$\ell = 500\text{Å},\quad \mathrm{R_D} = 10^{-4}\quad @\quad \mathrm{B} = 40\mathrm{T}$

Temperature damping term

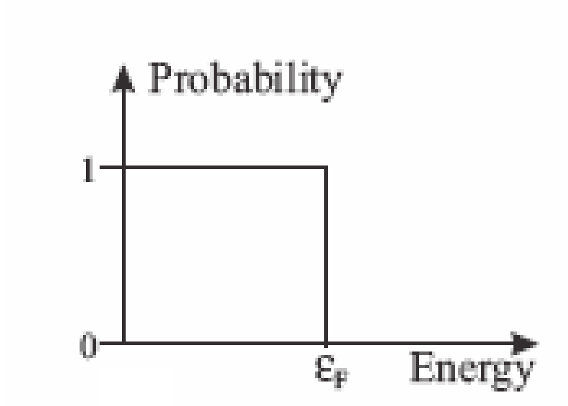
$$R_T = \frac{u_0 T m_c / B}{\sinh(u_0 T m_c / B)}$$

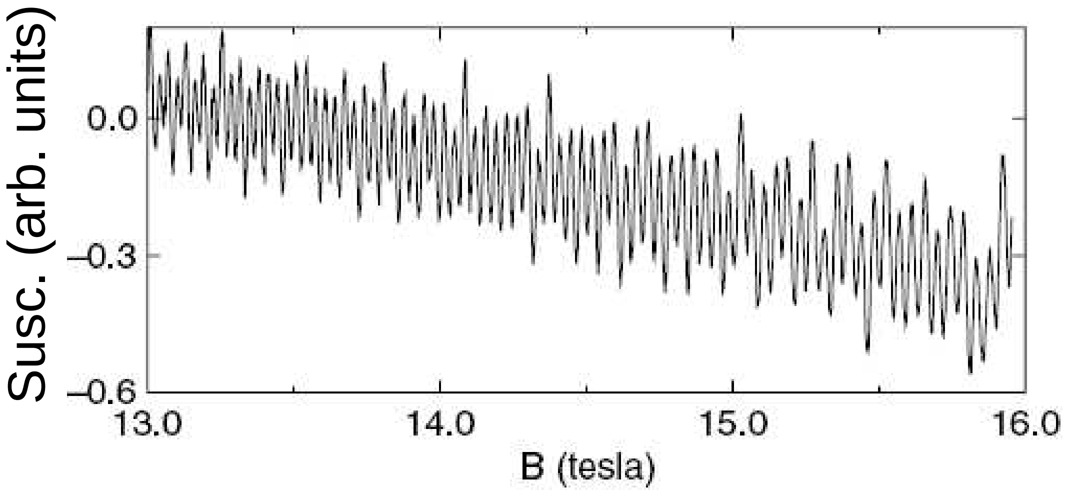


III.2 Theory

Effect of interactions

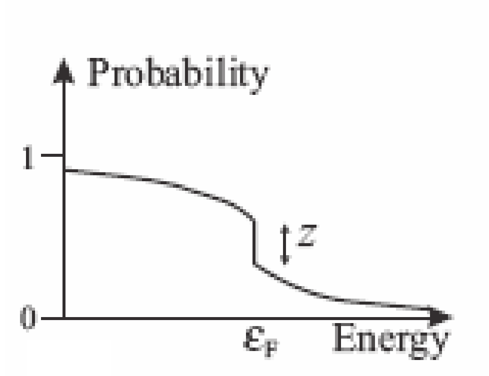
Electrons in Fermi gas at *T*=0

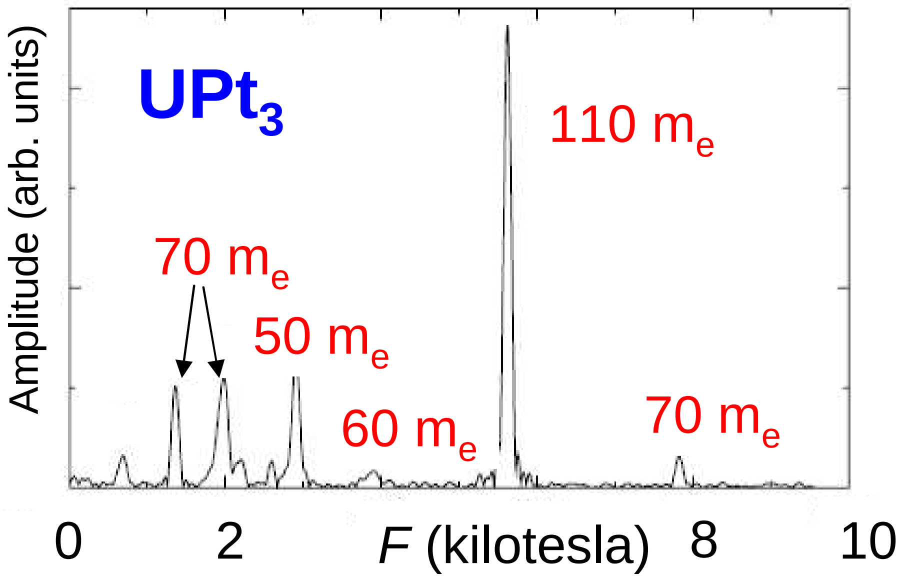




13

Electrons in Fermi liquid at *T*=0

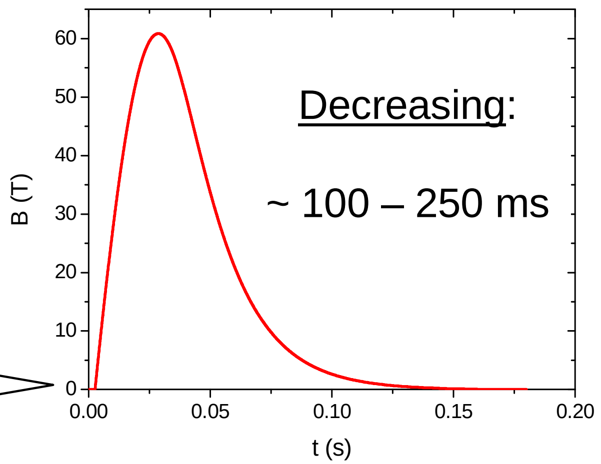




L. Taillefer et al, J. Magn. Magn. Mater’87

III.3 High magnetic fields lab.

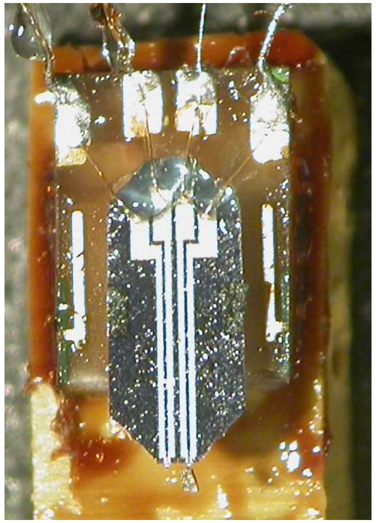
High speed digitizer — *Numerical lock-in* ⇨ **R**



<u>Decreasing</u>:

~ 100 – 250 ms

$$\boxed{\tau = \left|\vec{M} \times \vec{B}\right|}$$



Piezoresistif cantilever

http://www.toulouse.lncmi.cnrs.fr/

III.3 High magnetic fields lab.

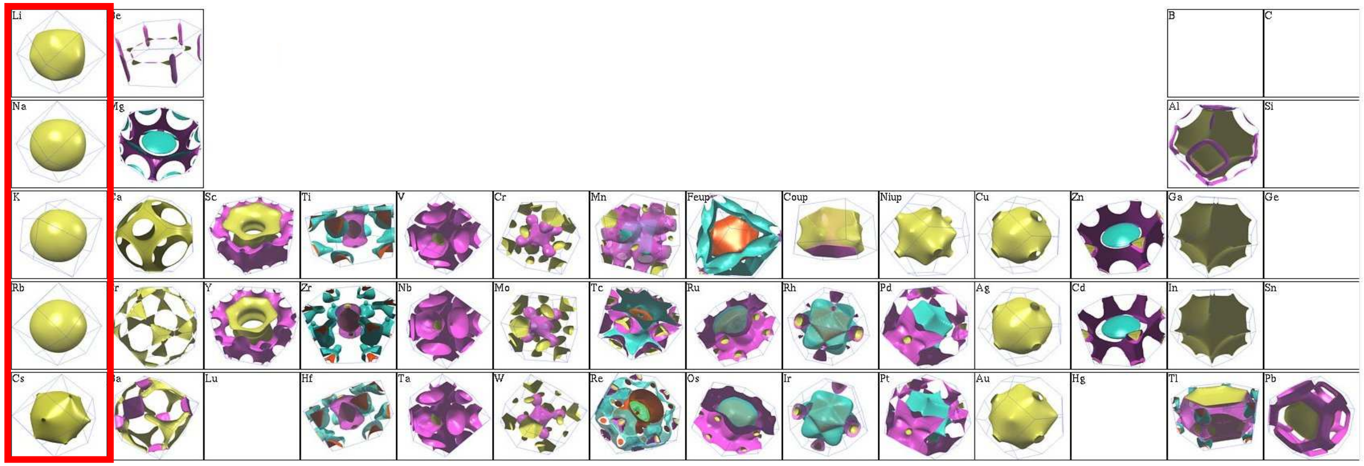
DC field installation LNCMI Grenoble

24 MW

300 l/s

III.4 Fermiology

Potassium



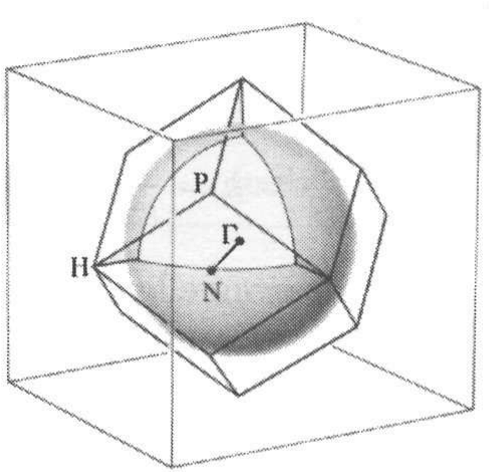
1 conduction electron
(body-centered cubic)

$$n = \frac{k_F^3}{3\pi^2} = \frac{2}{a^3}$$

$$\boxed{k_F = 0.620 \frac{2\pi}{a}}$$

Alkali metals:

Li: $1s^2s^1$
Na: $[Ne]3s^1$
K: $[Ar]4s^1$
Rb: $[Kr]5s^1$
Cs: $[Xe]6s^1$



$$\boxed{\Gamma N = 0.707 \frac{2\pi}{a}}$$

$\Rightarrow$ The sphere is inside of the first Brillouin zone

III.4 Fermiology

Potassium

Volume 6, Number 11 PHYSICAL REVIEW LETTERS June 1, 1961

DE HAAS–VAN ALPHEN EFFECT IN POTASSIUM*

A. C. Thorsen and T. G. Berlincourt

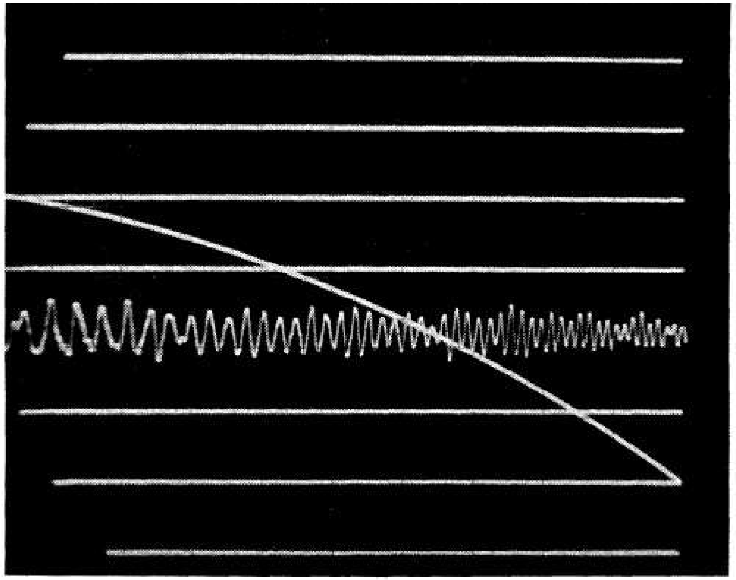


FIG. 1. de Haas–van Alphen effect in potassium at 1.77°K. The oscillating trace (≈ 0.1-mv amplitude) shows the output from a pickup coil containing the sample. The curved trace shows the field increasing from 151.7 to 158.5 kilogauss during a sweep time of about 1.0 millisecond (time increasing from right to left).

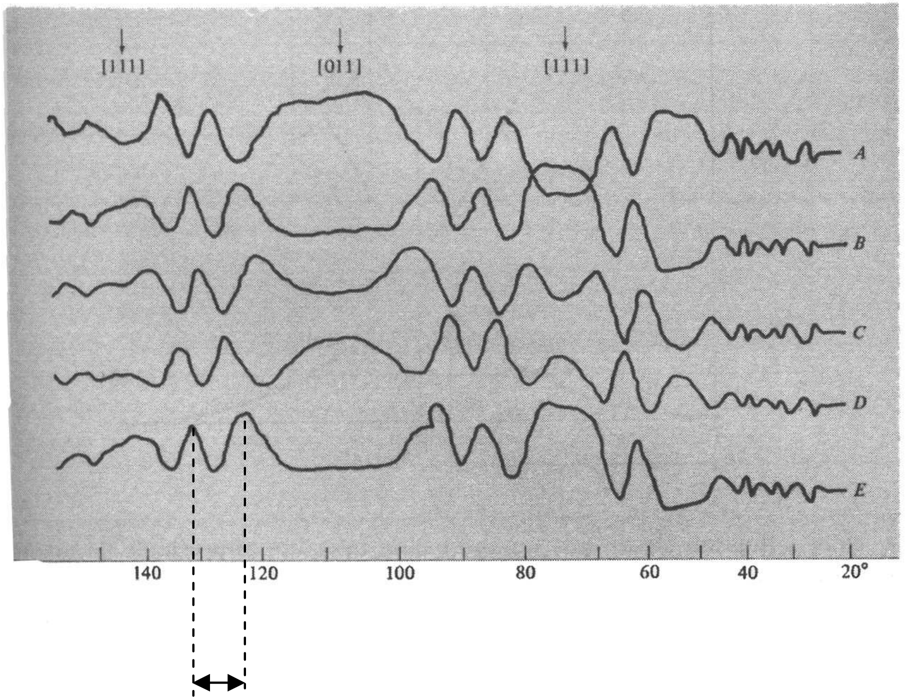
$$F = \frac{\hbar A_F}{2\pi e}$$

A_{exp}=(1.74 ±0.02) 10^{16} cm^{-2}

A_{theo}=1.748 10^{16} cm^{-2} (free electron)

Deviation from the sphere

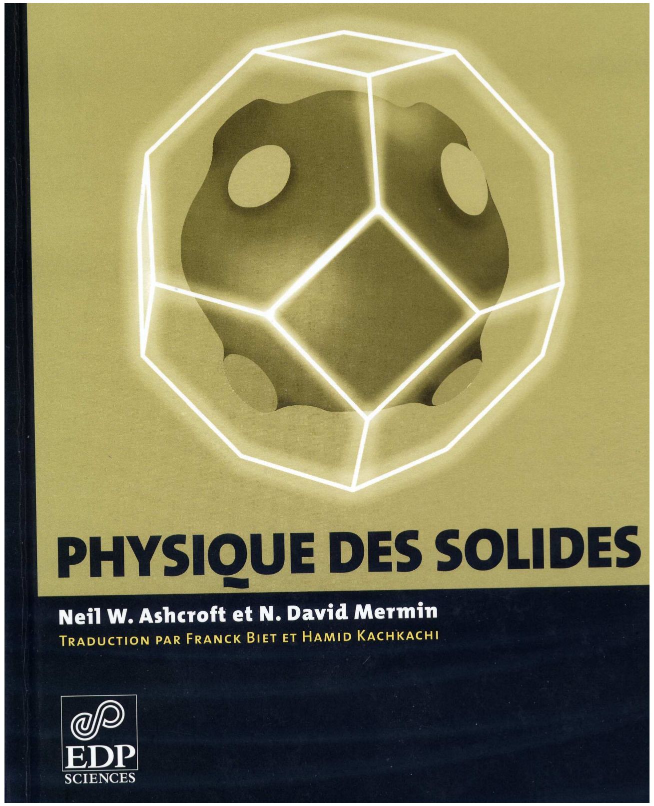
Fixed magnetic field and rotation



$\Delta A \sim 10^{-4}$ A

III.4 Fermiology

Noble Metals: Cu, Ag, Au (f.c.c.)

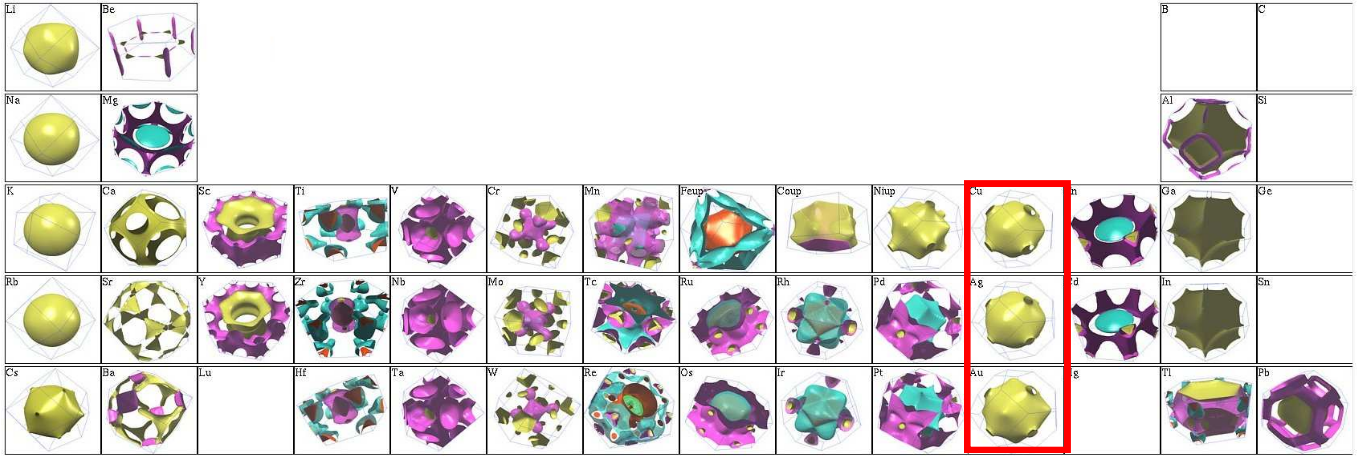


PHYSIQUE DES SOLIDES

Neil W. Ashcroft et N. David Mermin

Traduction par Franck Biet et Hamid Kachkachi

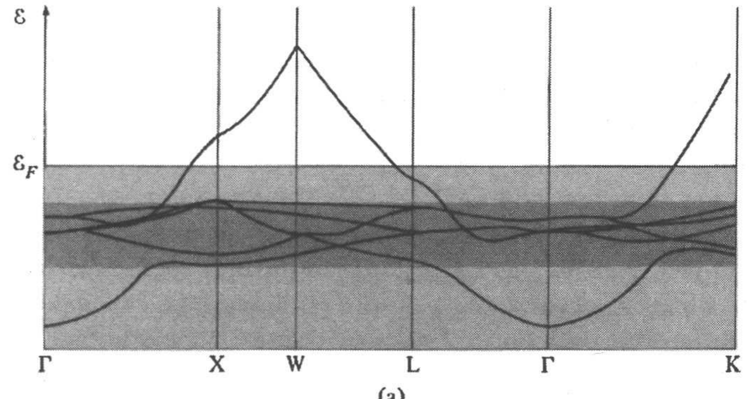
EDP SCIENCES



Li:	$1s^2s^1$	-
Na:	$[Ne]3s^1$	-
K:	$[Ar]4s^1$	Cu: $[Ar]3d^{10}4s^1$
Rb:	$[Kr]5s^1$	Ag: $[Kr]4d^{10}5s^1$
Cs:	$[Xe]6s^1$	Au: $[Xe]4f^{14}5d^{10}6s^1$

Free electron models:

FS=sphere inside the FBZ



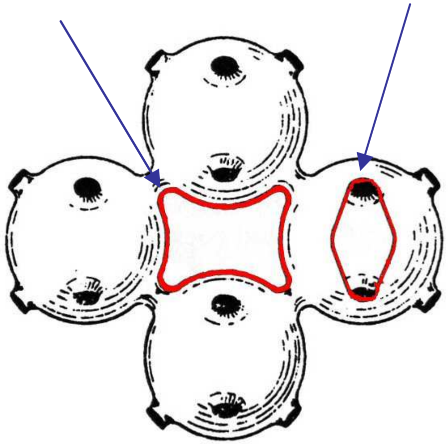
} *d*-bands

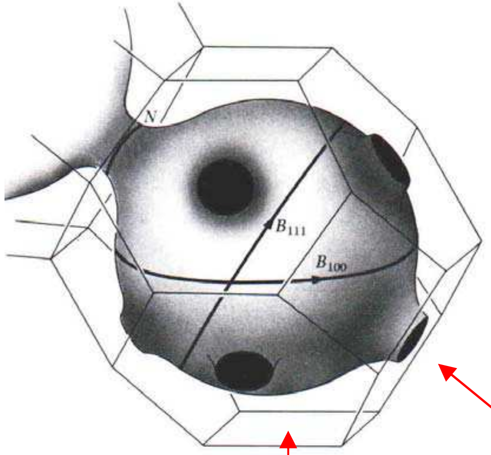
III.4 Fermiology

<110>

Dog's bone

Lemon





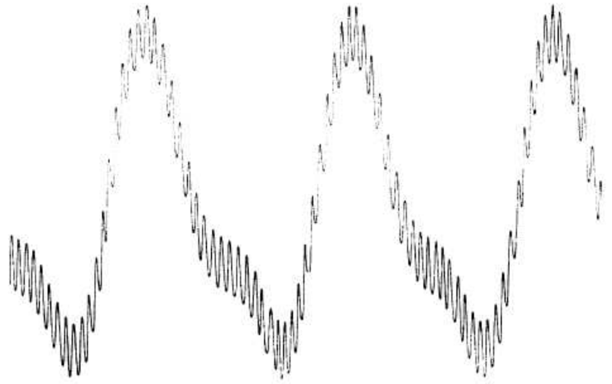
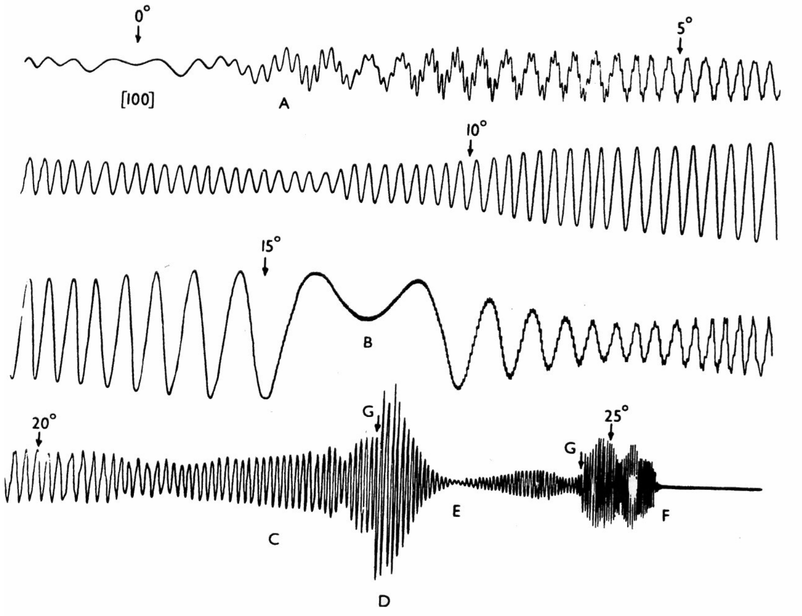


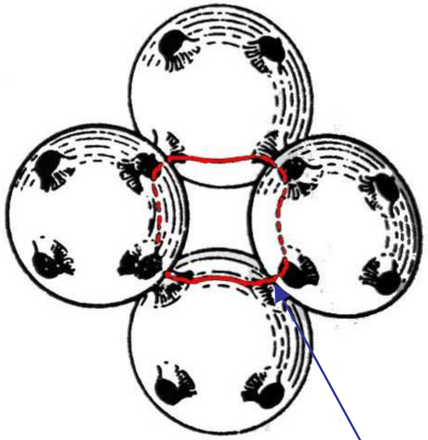
FIG. 1. A typical recording of torque versus H near the ⟨111⟩ axis. The low frequencies are F_N and its second harmonic and the high frequency is F_{B1}.

A.S. Joseph et al, Phys. Rev'66

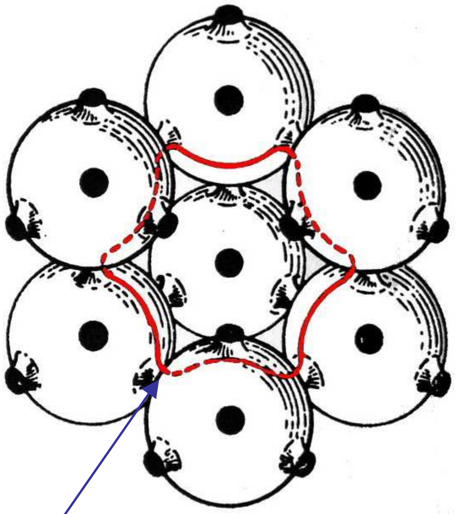
<100>

<111>





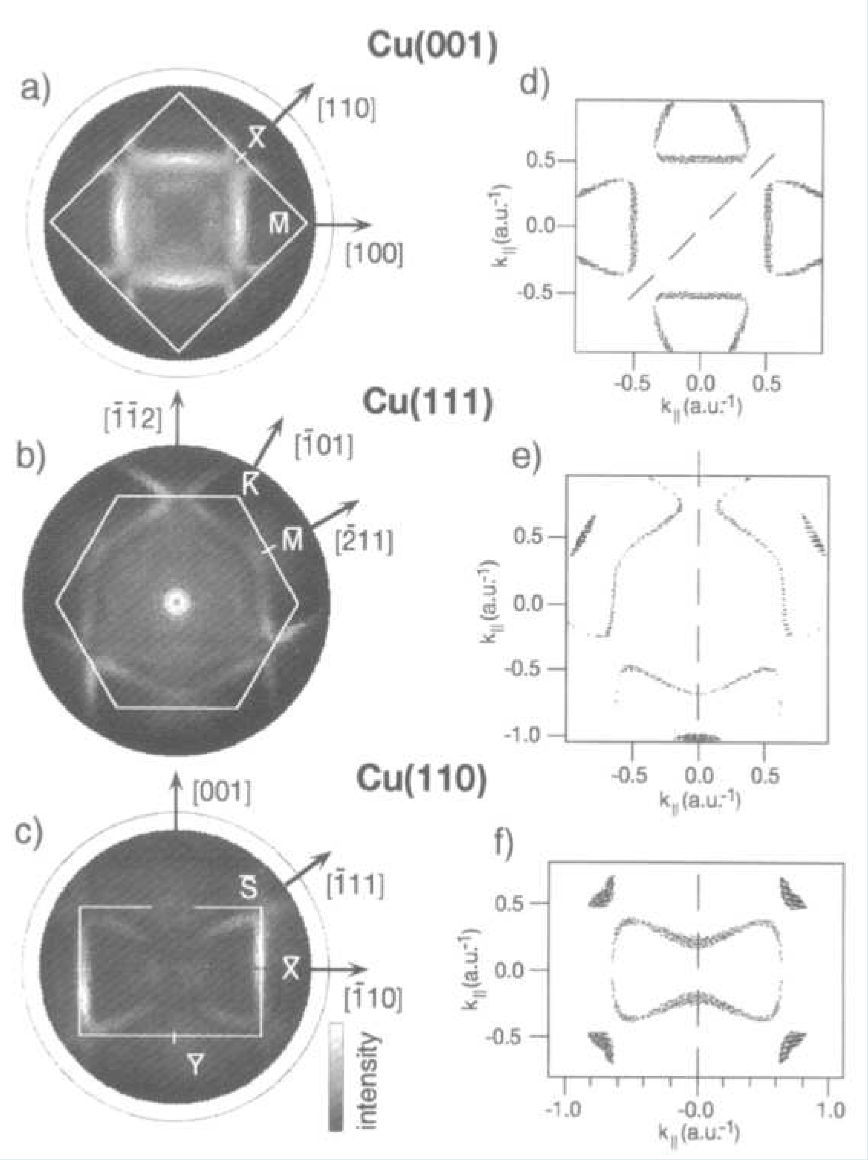
4-corner Rosetta

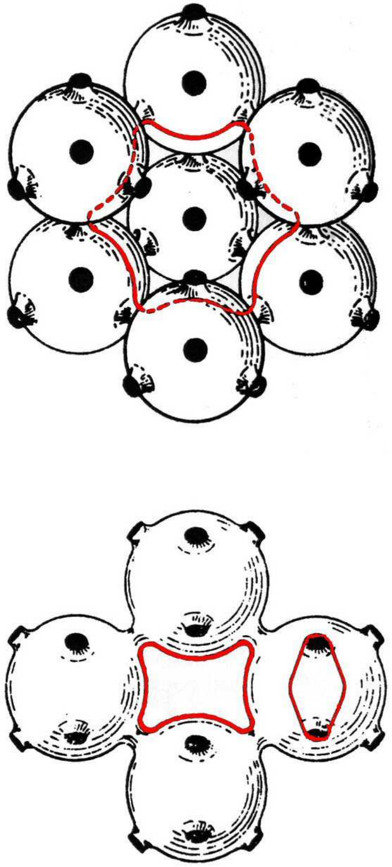


6-corner Rosetta

III.4 Fermiology

ARPES in Cu



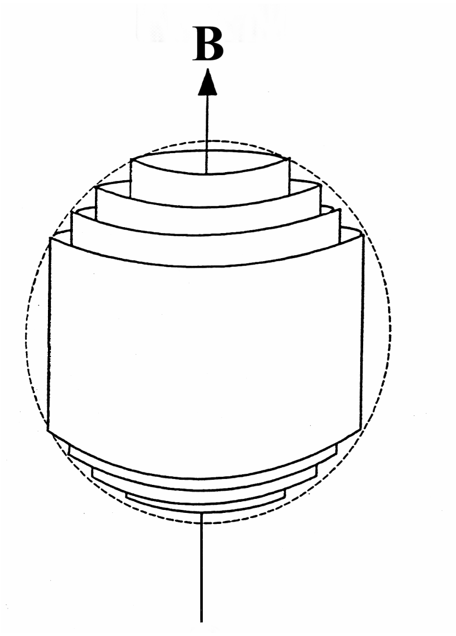


P. Aebi et al, Surface Science'94

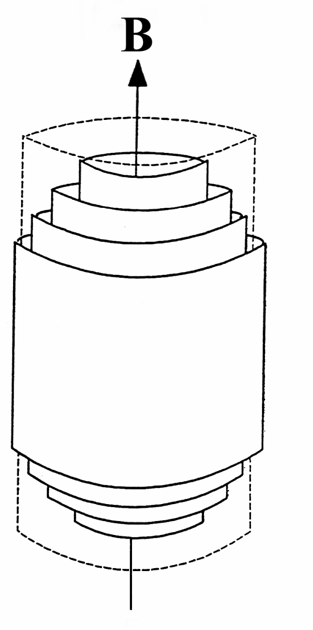
III.4 Fermiology

Quasi 2D case

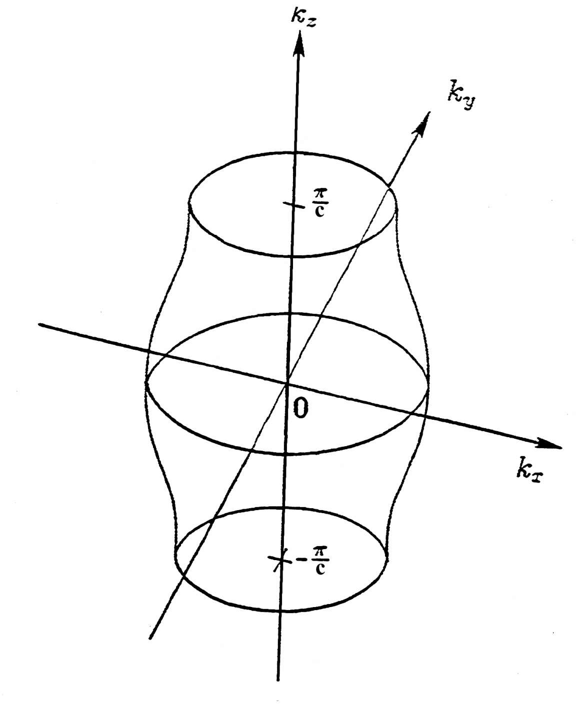
3D



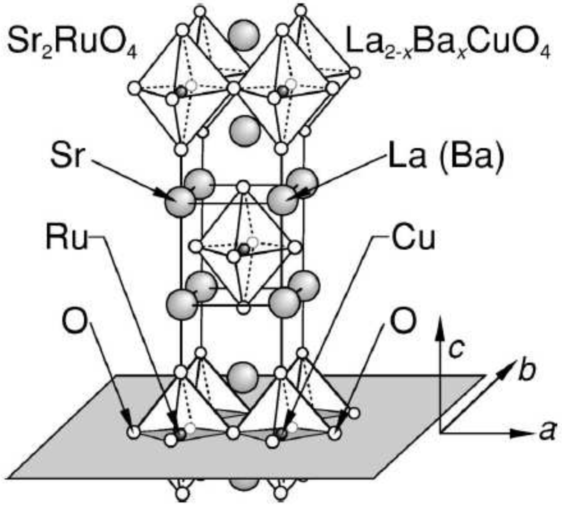
2D



Q2D



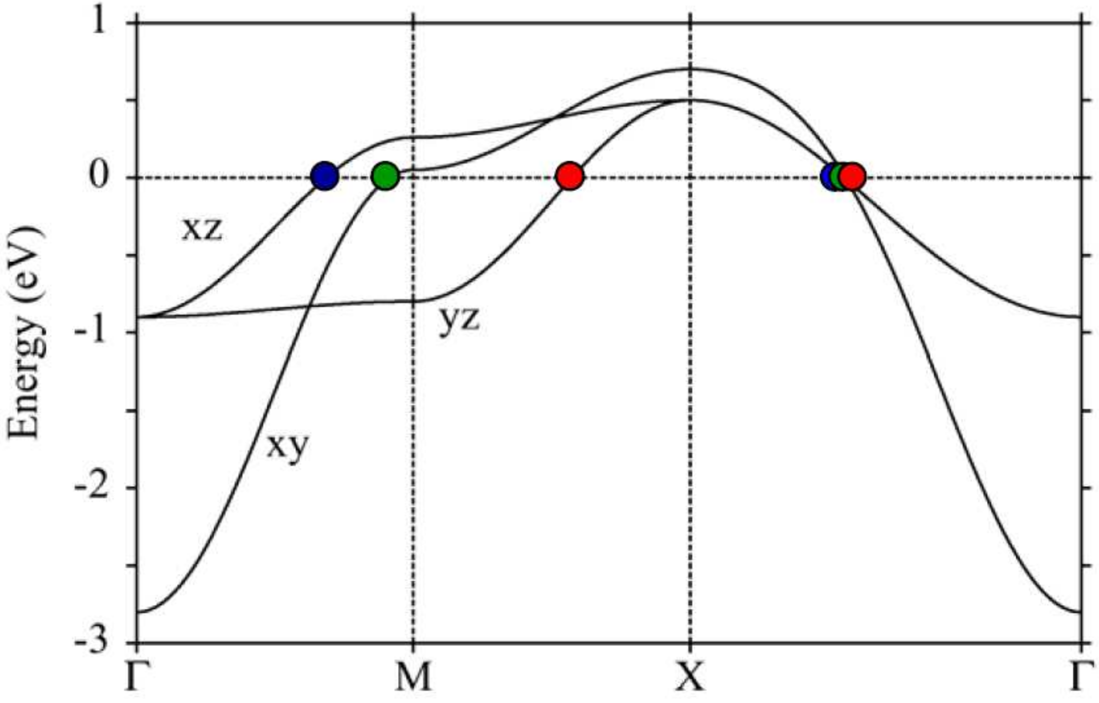
III.4 Fermiology



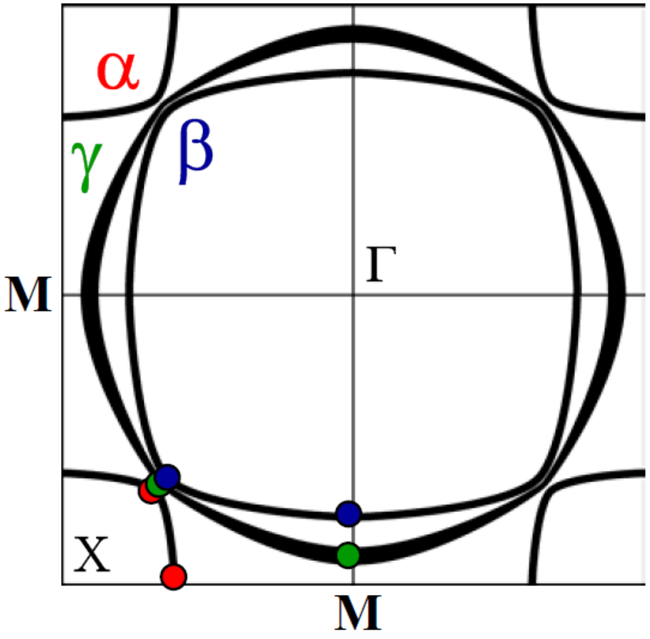
Sr_2RuO_4: a Quasi-2D Fermi liquid (school case…)

Band structure calculations

3 sheets of FS
- α hole like
- β, γ electron like



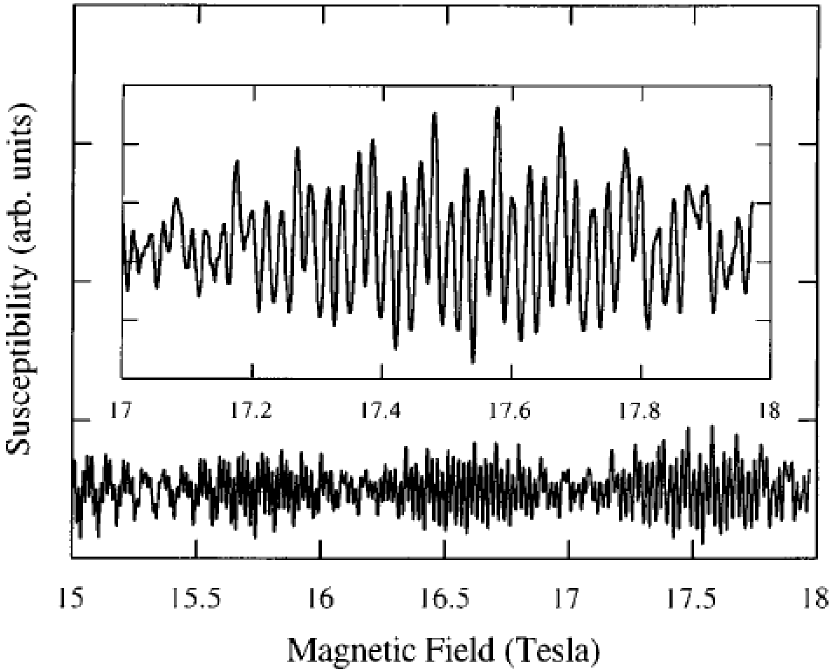
A. Liebsch *et al*, PRL **84**, 1591 (2000)

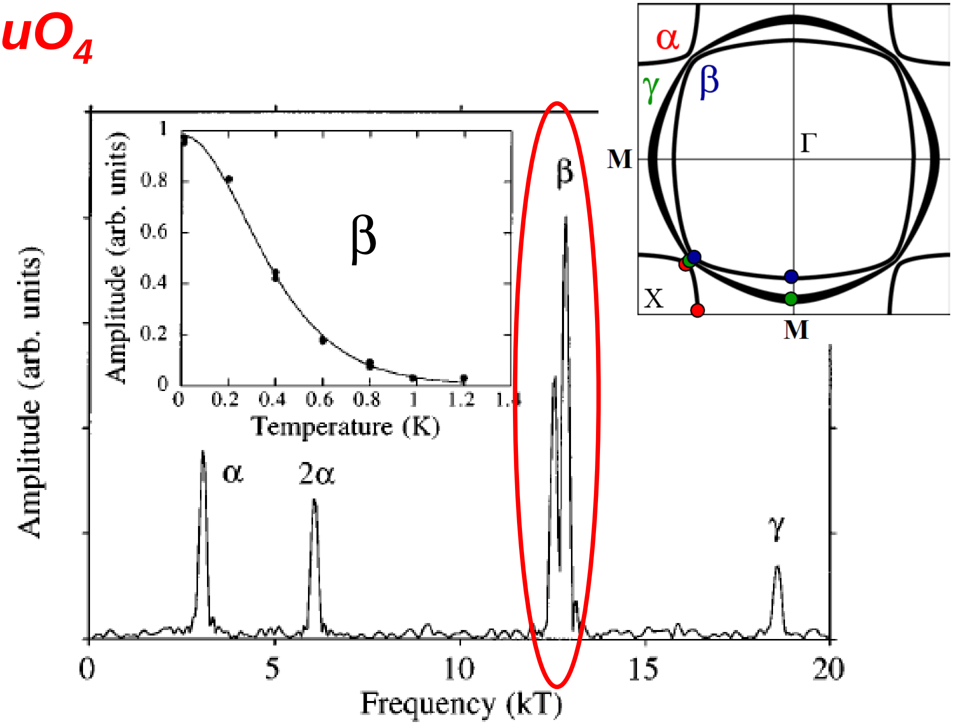


I.I. Mazin *et al*, PRL **79**, 733 (1997)

III.4 Fermiology

Sr_2RuO_4

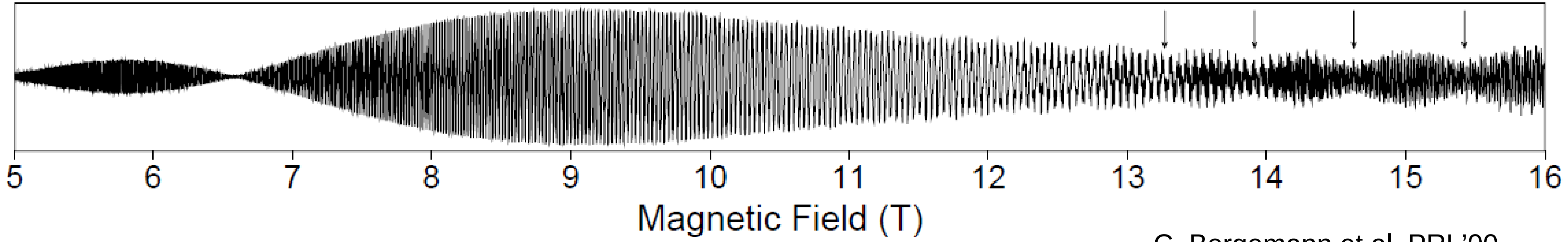




A. P. Mackenzie et al, PRL'96

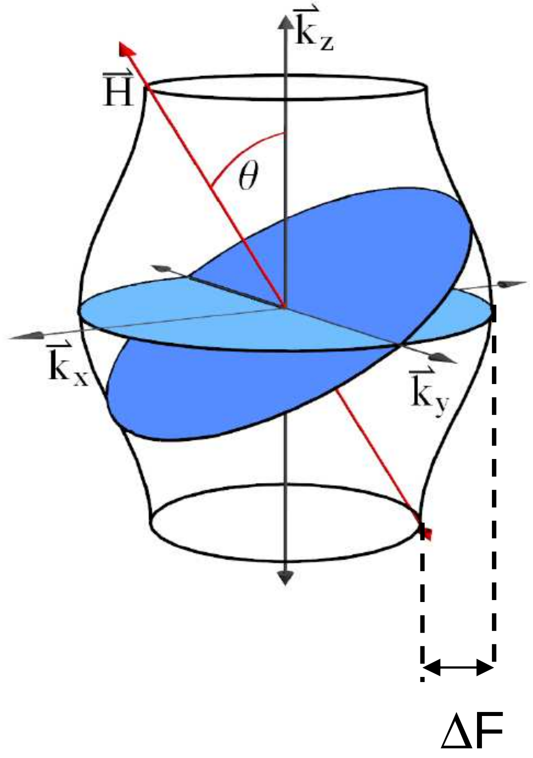
	α	β	γ
Frequency F (kT)	3.05	12.7	18.5
Average k_F (Å^{-1})	0.302	0.621	0.750
$\Delta k_F/k_F$ (%)	0.21	1.3	$<$0.9
Cyclotron mass (m_e)	3.4	6.6	12.0
Band calc. F (kT)	3.4	13.4	17.6
Band calc. $\Delta k_F/k_F$ (%)	1.3	1.1	0.34
Band mass (m_e)	1.1	2.0	2.9

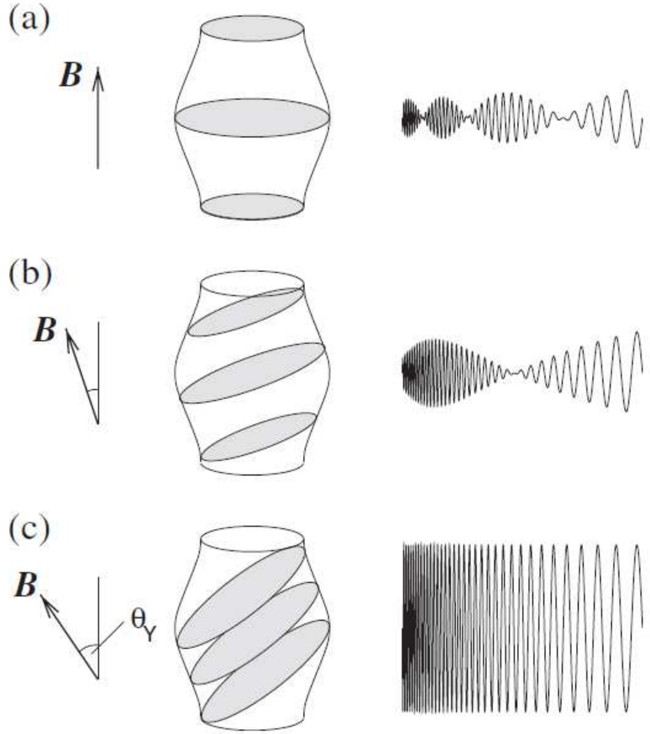
III.4 Fermiology



C. Bergemann et al, PRL’00

$$\boxed{\Delta R, \Delta M \propto R_T\, R_D\, R_S \sin\left[2\pi\left(\frac{F}{B\cos\theta}-\gamma\right)\right] J_0\left[2\pi\frac{\Delta F}{B\cos\theta}J_0(k_F c\tan\theta)\right]}$$

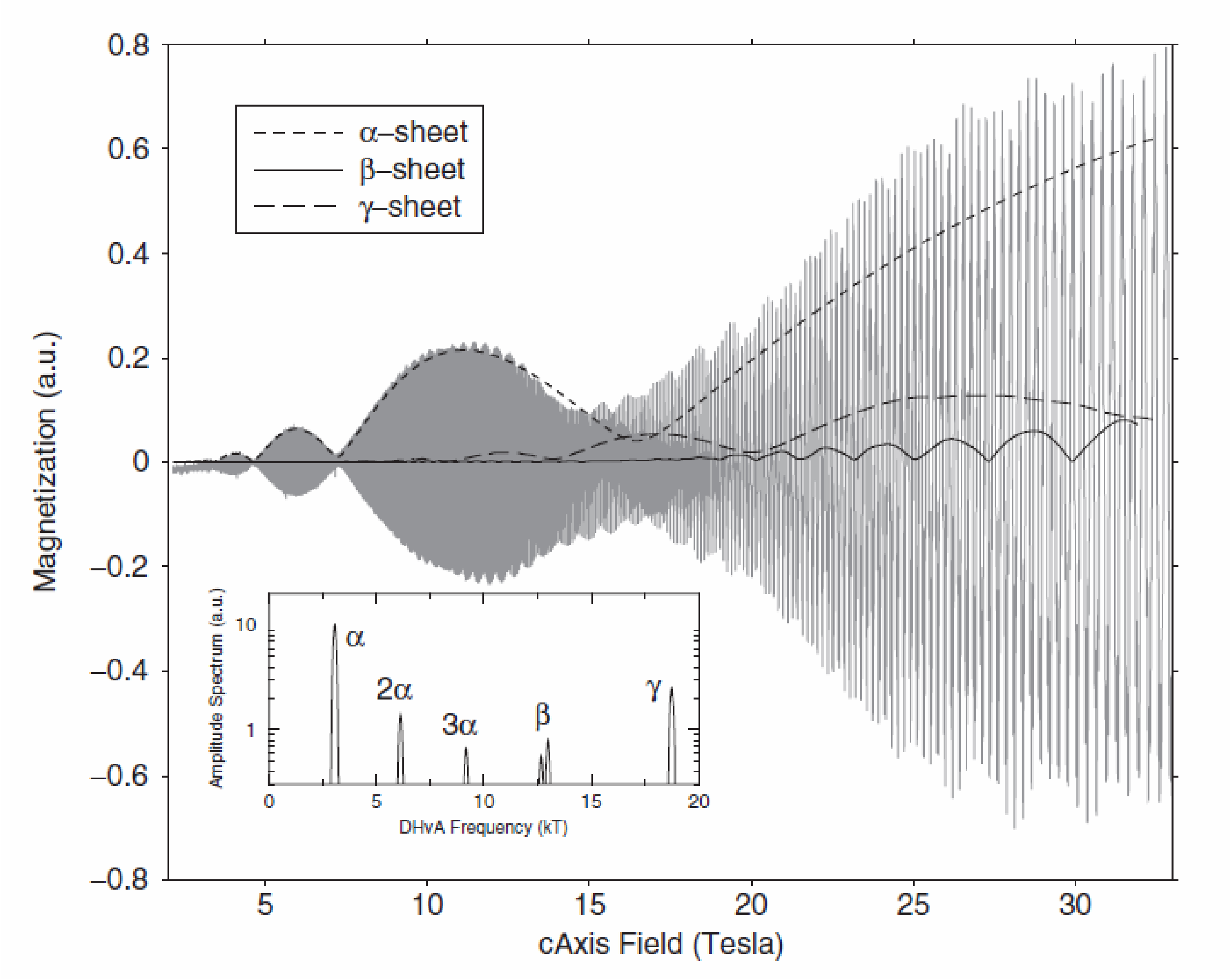




C. Bergemann et al,
Advances in Physics’03

III.4 Fermiology

Sr_2RuO_4

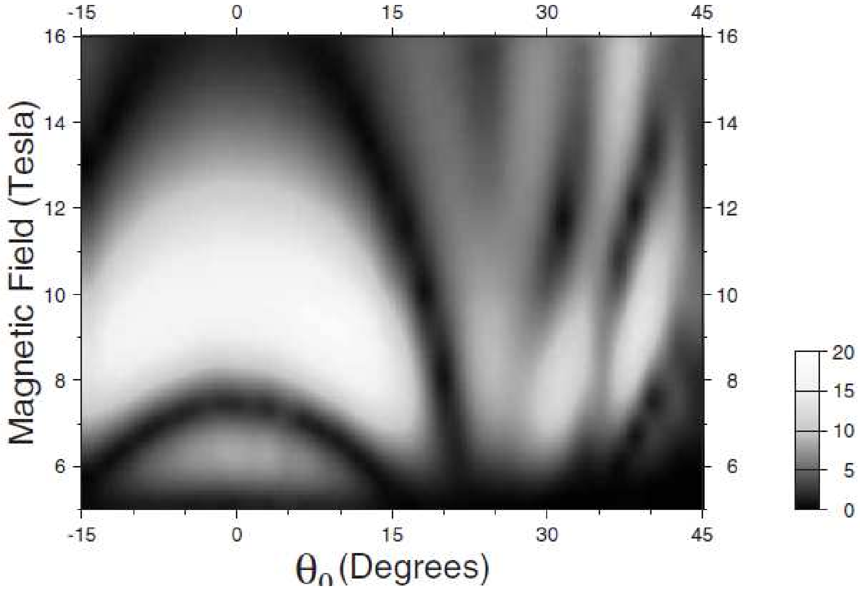


C. Bergemann et al, Advances in Physics'03

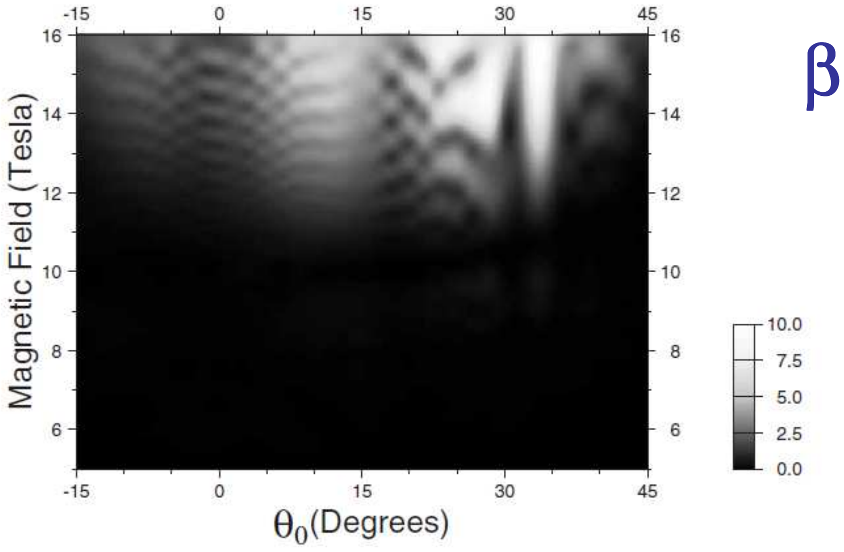
III.4 Fermiology

Sr_2RuO_4: Angular dependence of the amplitude of QO

α

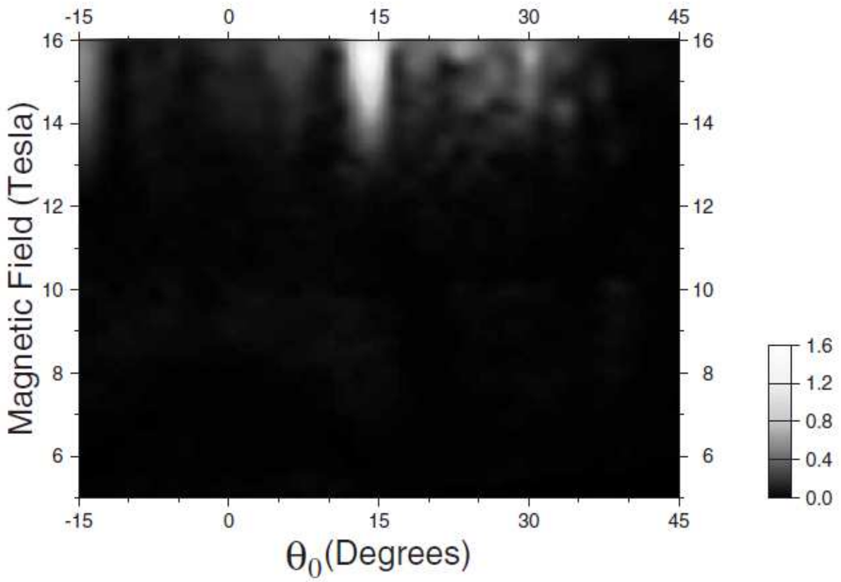


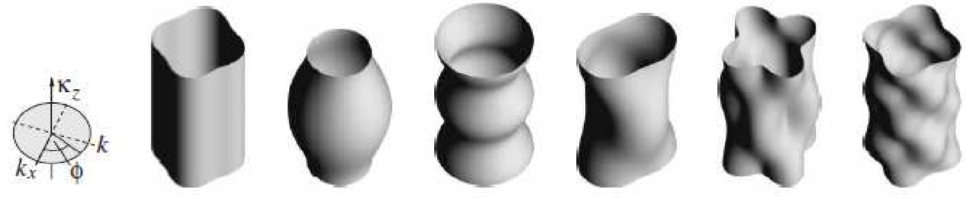
β



$$k_F(\phi,\kappa)=\sum_{\substack{\mu,\nu\ge 0\\ \mu\ \text{even}}} k_{\mu\nu}\cos\nu\kappa\begin{cases}\cos\mu\phi & (\mu \bmod 4 \equiv 0)\\ \sin\mu\phi & (\mu \bmod 4 \equiv 2)\end{cases} \qquad (1)$$

γ



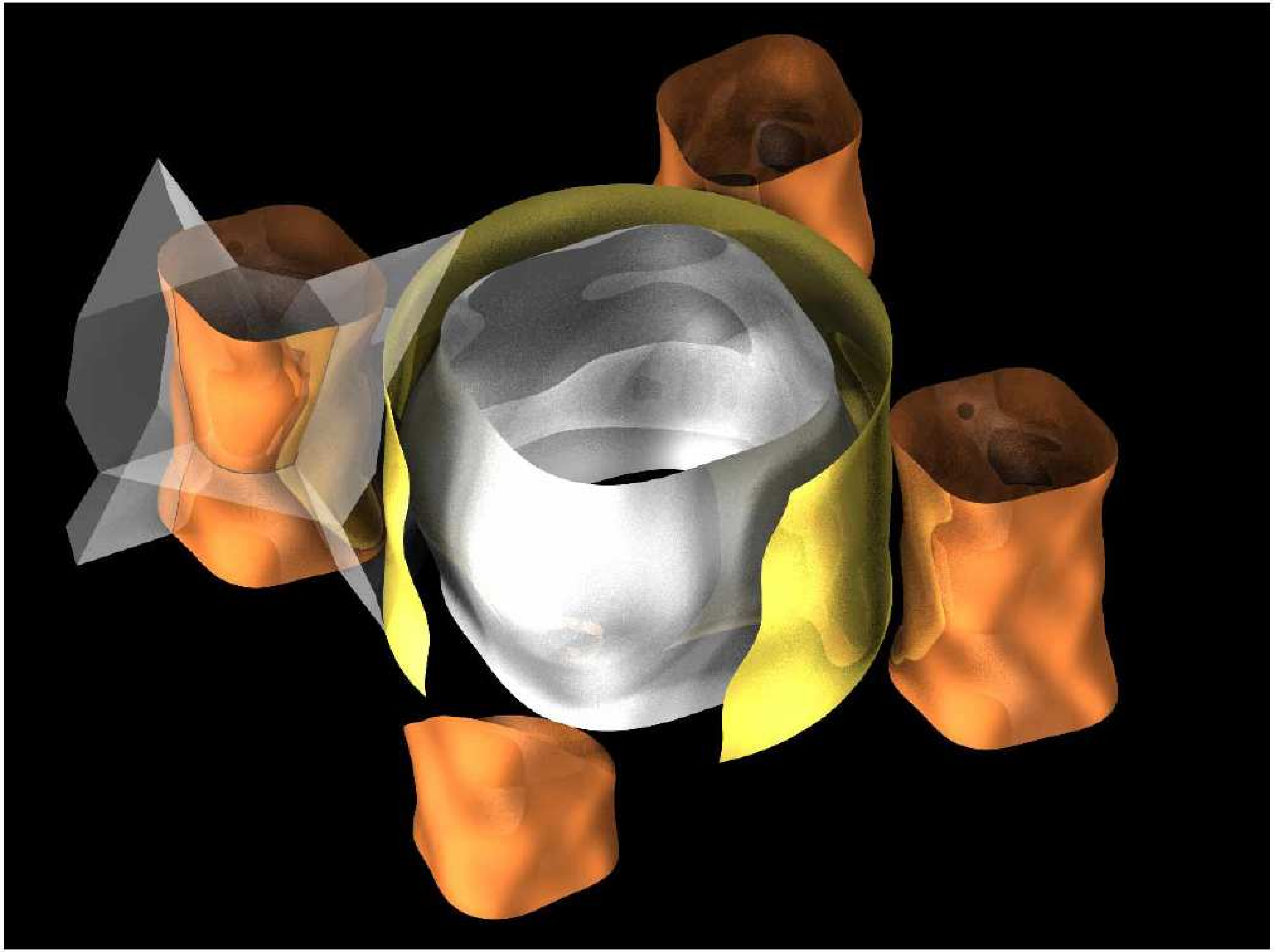


	k_{00}	k_{40}	k_{01}	k_{02}	k_{21}	k_{41}	k_{42}
α	304	−10	—	0.31	1.3	—	−1.0
β	622	−45	3.8	small	—	−0.6	small
γ	753	small	small	0.53	—	small	0.5

C. Bergemann et al, Advances in Physics'03

III.4 Fermiology

Sr_2RuO_4



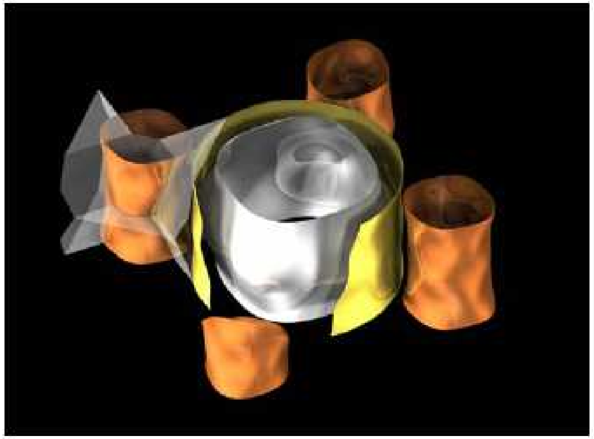
C. Bergemann et al, Advances in Physics'03

III.4 Fermiology

ARPES in Sr_2RuO_4

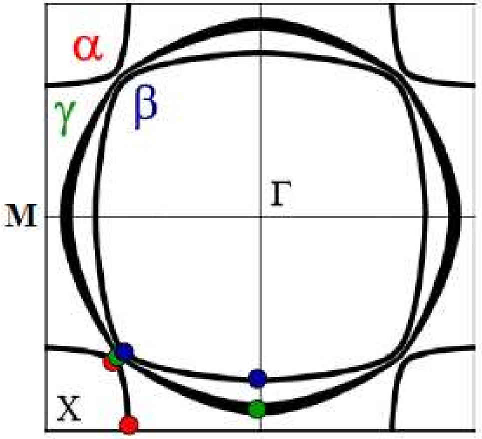
First measurements give results different from band structure calculations!

de Haas-van Alphen



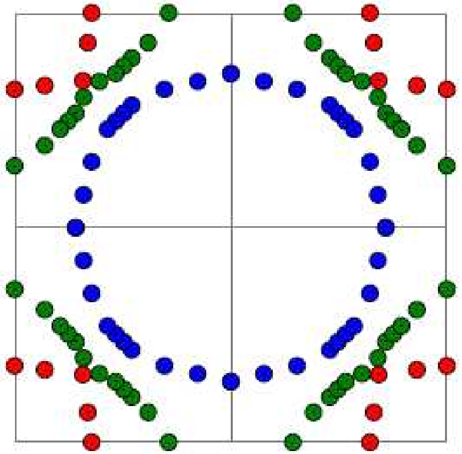
A.P. Mackenzie *et al.*, PRL **76**, 3786 (1996)
C. Bergemann *et al.*, PRL **84**, 2662 (2000)

LDA



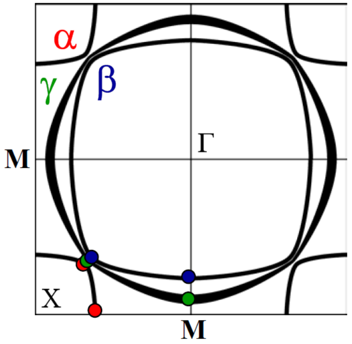
I.I. Mazin *et al.*, PRL **79**, 733 (1997)

ARPES



T.Yokoya *et al.*, PRB **54**, 13311 (1996)
D.H. Lu *et al.*, PRL **76**, 4845 (1996)

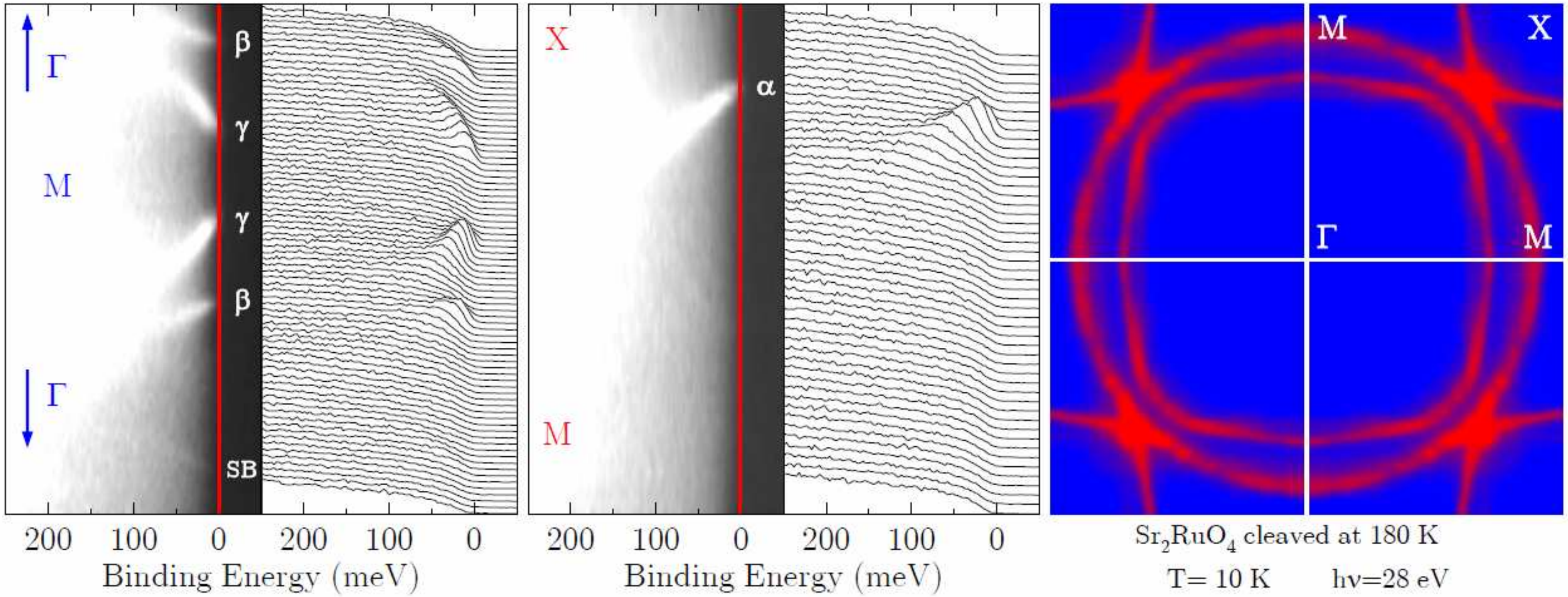
III.4 Fermiology



ARPES in Sr_2RuO_4

BUT surface atomic reconstruction seen by STM (Matzdorf et al. Science'00)

Solution: Sample cleaved at 180 K ⇒ surface-related features are suppressed !



A. Damascelli *et al.*, PRL **85**, 5194 (2000)

Outline

I. Why and how to measure a Fermi surface ?

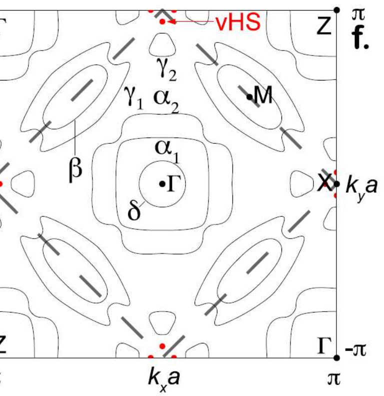
II. Angular Resolved Photoemission Electron Spectroscopy (ARPES)

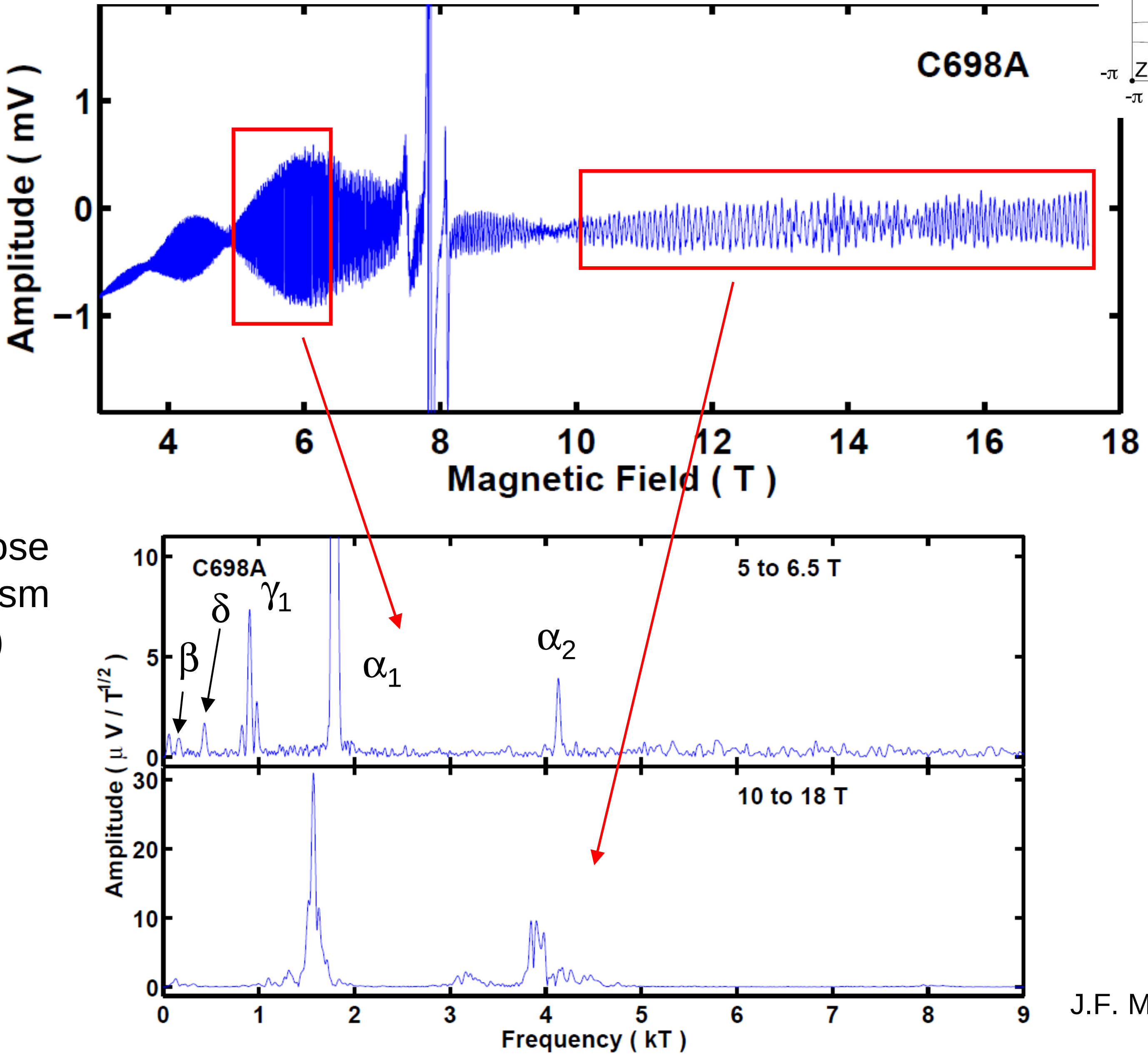
III. Quantum oscillations (QO)
  1) History
  2) Theory
    a) Semiclassical theory
    a) Landau levels quantification
    b) Lifshitz-Kosevich theory
    c) High magnetic field phenomena
  3) High magnetic fields facilities
  4) Fermiology

IV. Hot topics
  1) Phase transition
  2) High T_c superconductors

IV. Hot topics

QO across the metagnetic transition in $Sr_3Ru_2O_7$



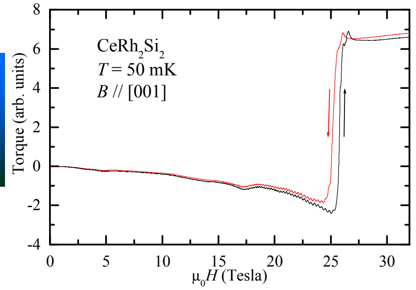


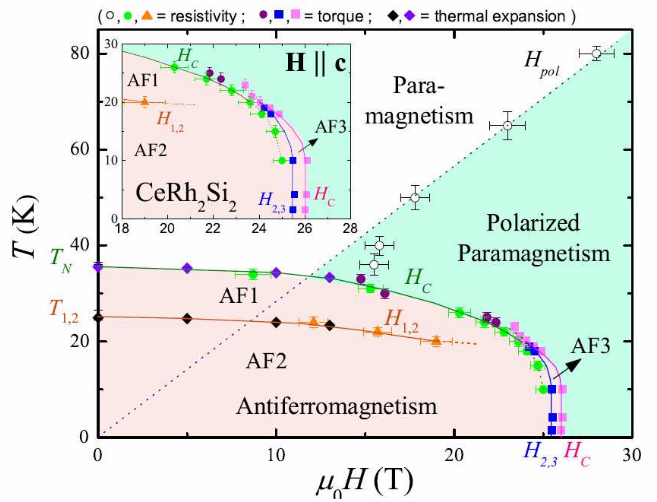
Paramagnet close
to ferromagnetism
(small moment)

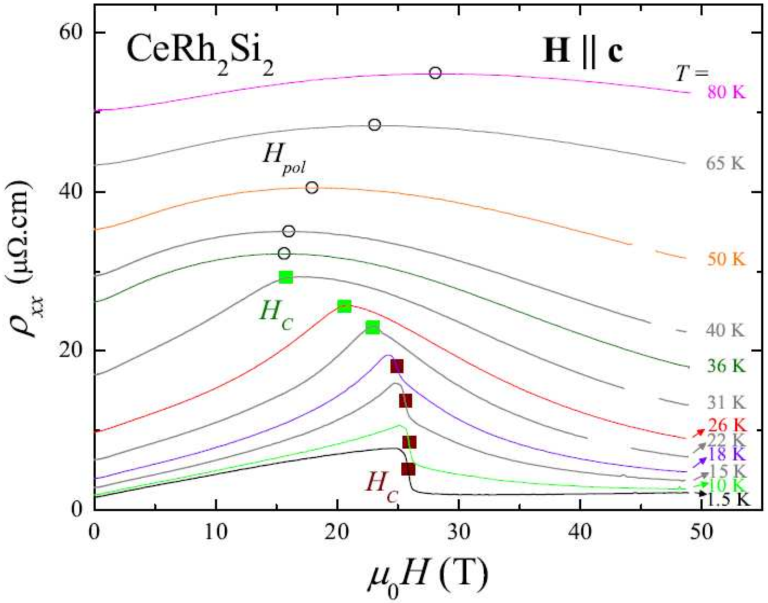
J.F. Mercure et al, PRB10

IV. Hot topics

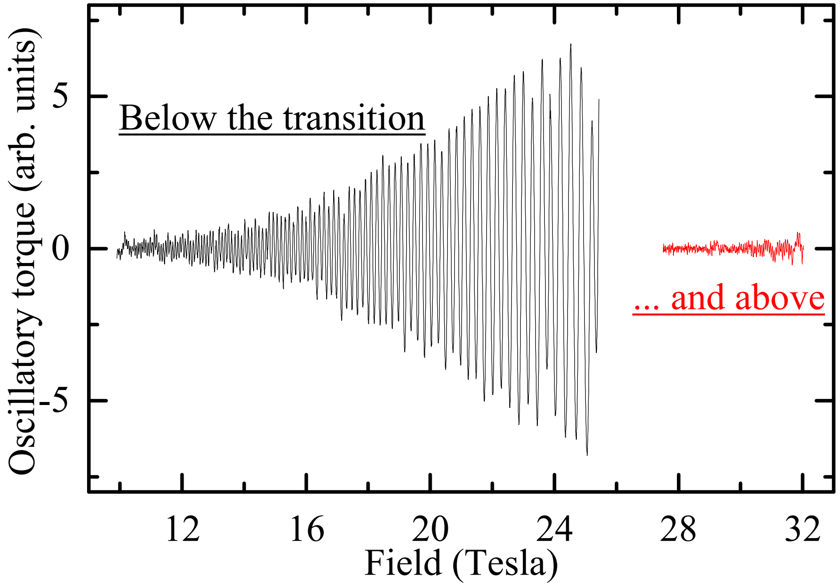
QO across the metagnetic transition in $CeRh_2Si_2$

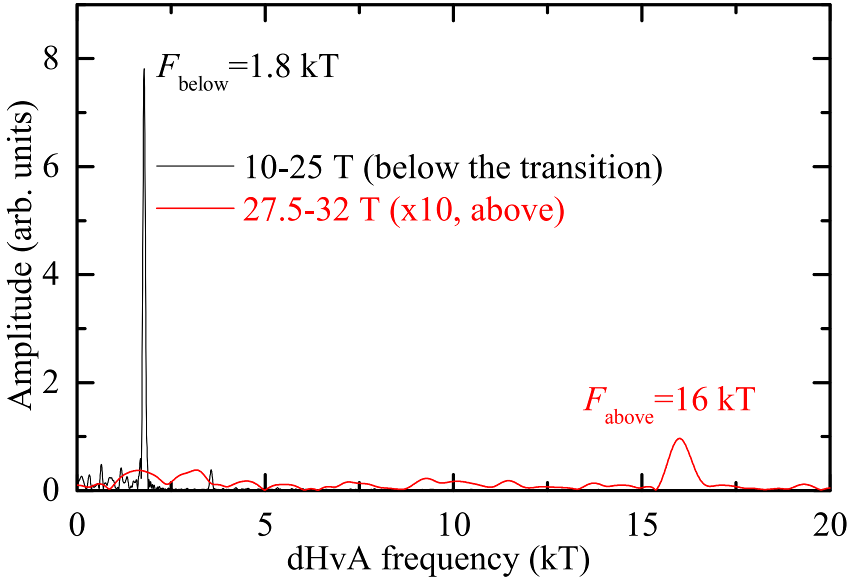






W. Knafo et al, PRB10



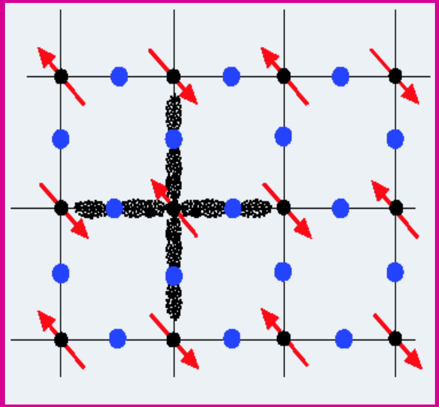


I. Sheikin et al, unpublished

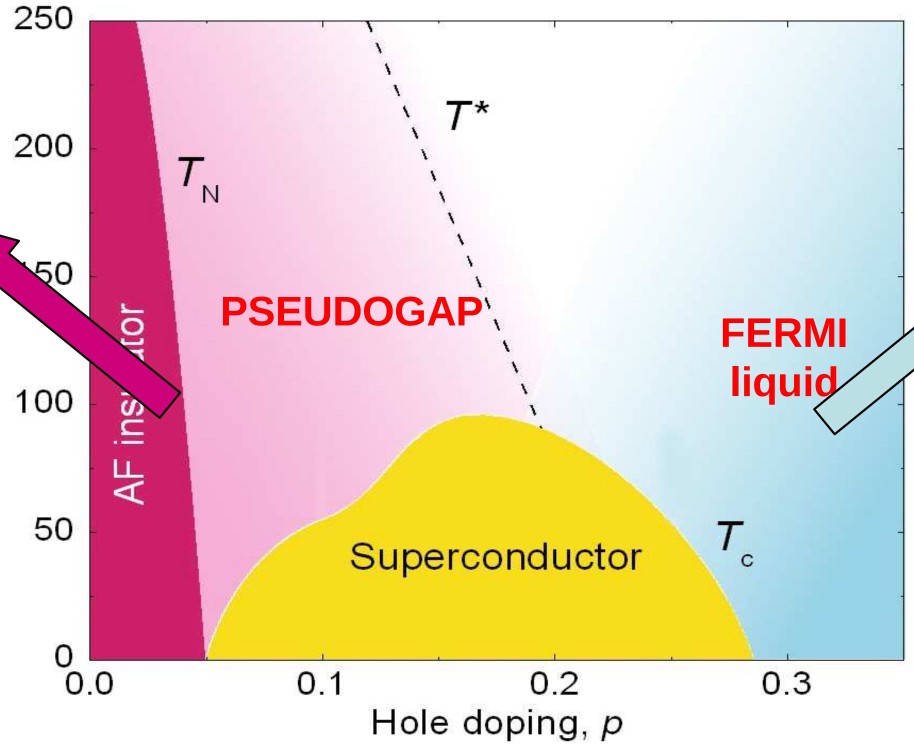
IV. Hot topics

QO in high T_c superconductors

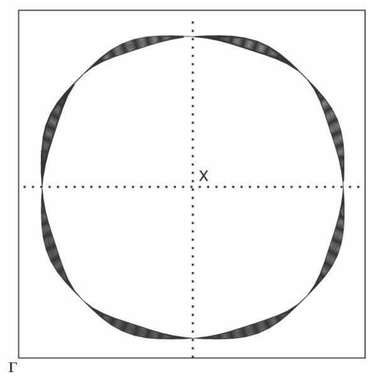
Mott insulator



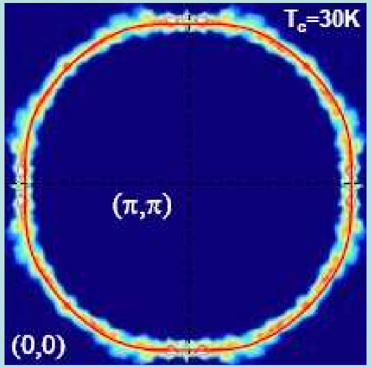
½ filling
strong e-e repulsion
AF ground state



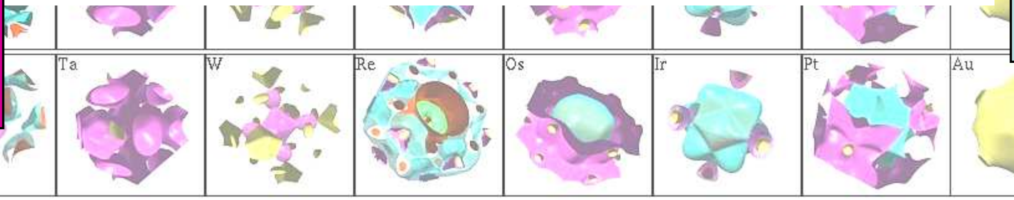
$Tl_2Ba_2CuO_{6+\delta}$
p~0.25



Hussey *et al*, *Nature*'03

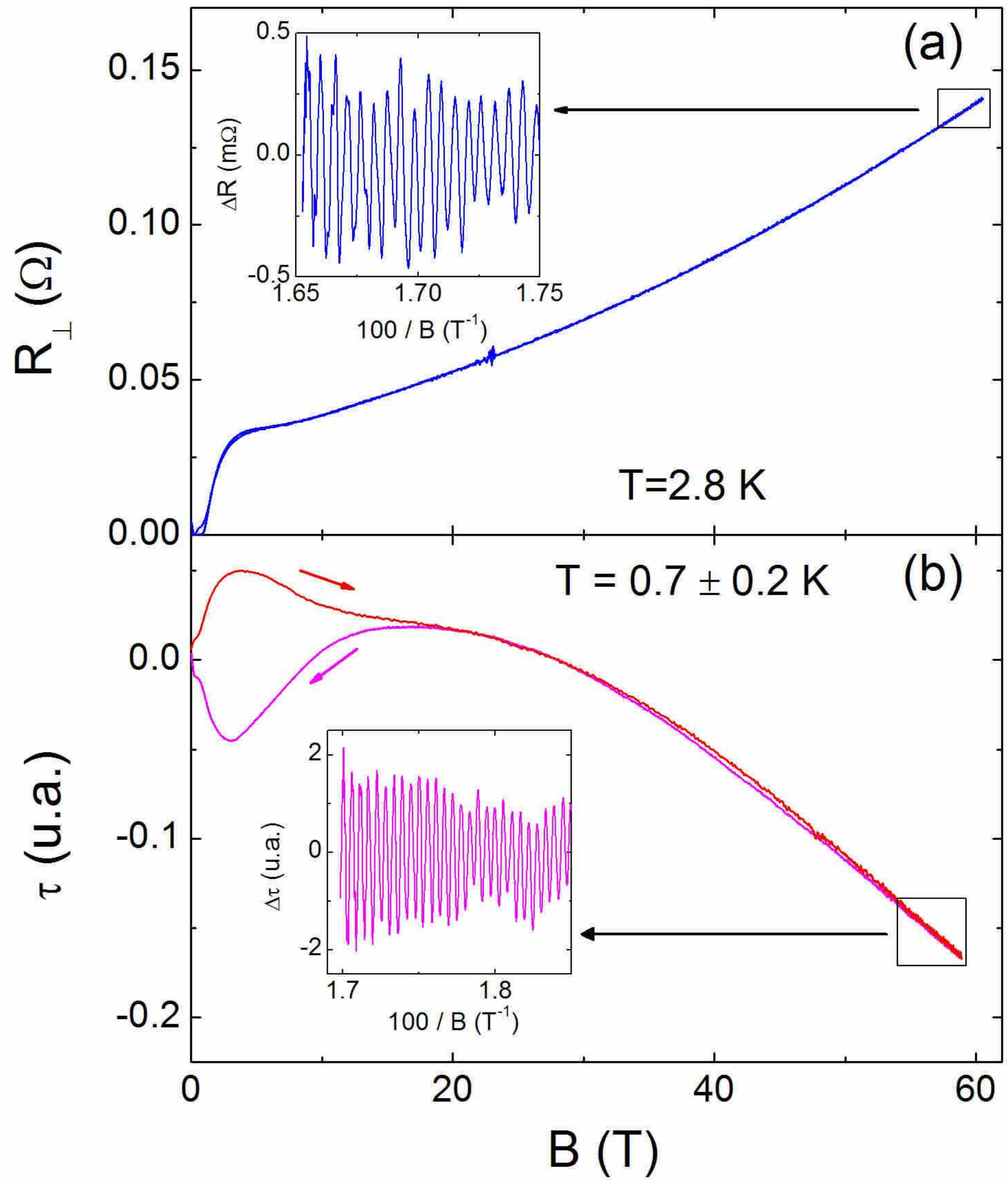


Platé *et al*, PRB'05



IV. Hot topics

Overdoped $Tl_2Ba_2CuO_{6+\delta}$



$$F = \frac{\phi_0}{2\pi^2} A_k$$

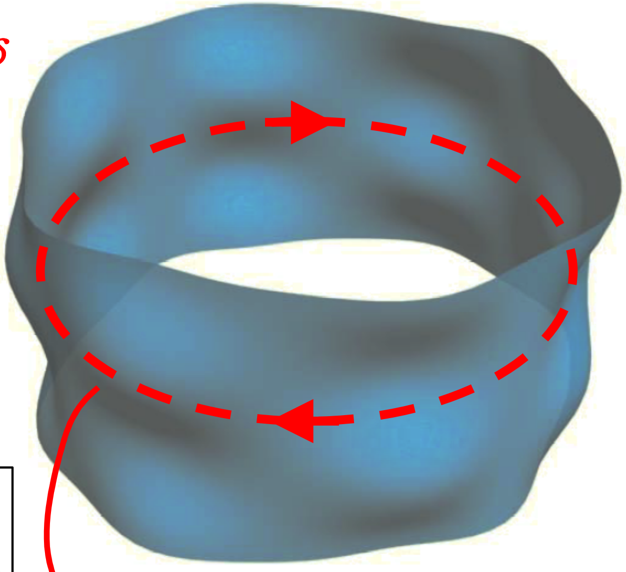
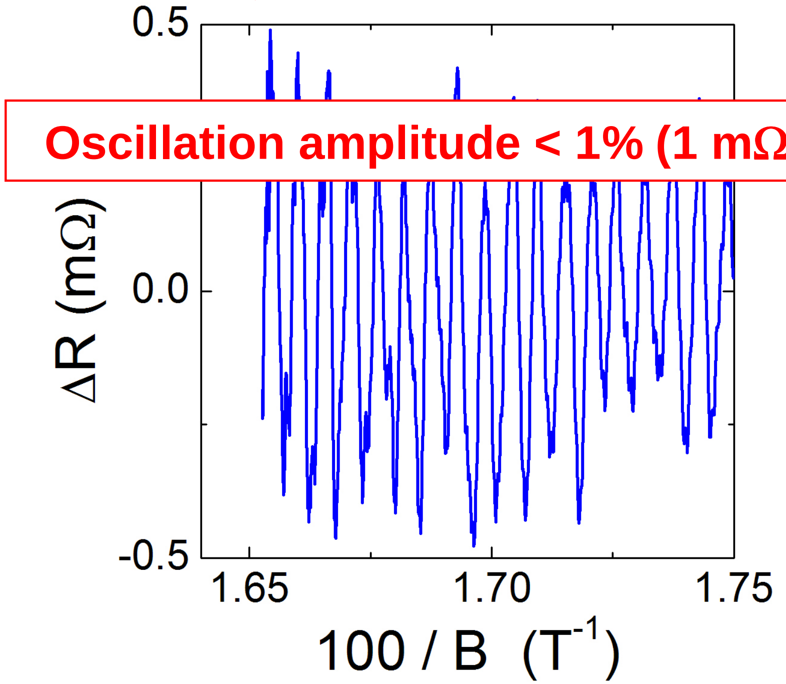


Photo credit: N. Hussey



Oscillation amplitude < 1% (1 mΩ) !

B. Vignolle et al, Nature'08

IV. Hot topics

Overdoped $Tl_2Ba_2CuO_{6+\delta}$

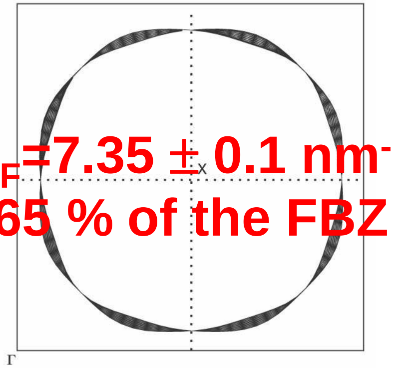
F=18100 ± 50 T

Onsager relation :

$$F = \frac{\phi_0}{2\pi^2} A_k$$

$A_k = \pi k_F^2$ ⇒ k_F=7.42 ± 0.05 nm^{-1}

AMRO



k_F=7.35 ± 0.1 nm^{-1}

65 % of the FBZ

Hussey *et al*, *Nature*'03

Luttinger theorem :

$$n = \frac{2A_k}{(2\pi)^2} = \frac{F}{\phi_0}$$

⇒ Carrier density: n=1.3 carrier /Cu atom (n=1+p with p=0.3)

Effective mass : $R_T = \frac{X}{sh(X)}$ $X = 14.694 \times T m_c / B$ ⇒ *m^*= (4.1 ± 1) m_0*

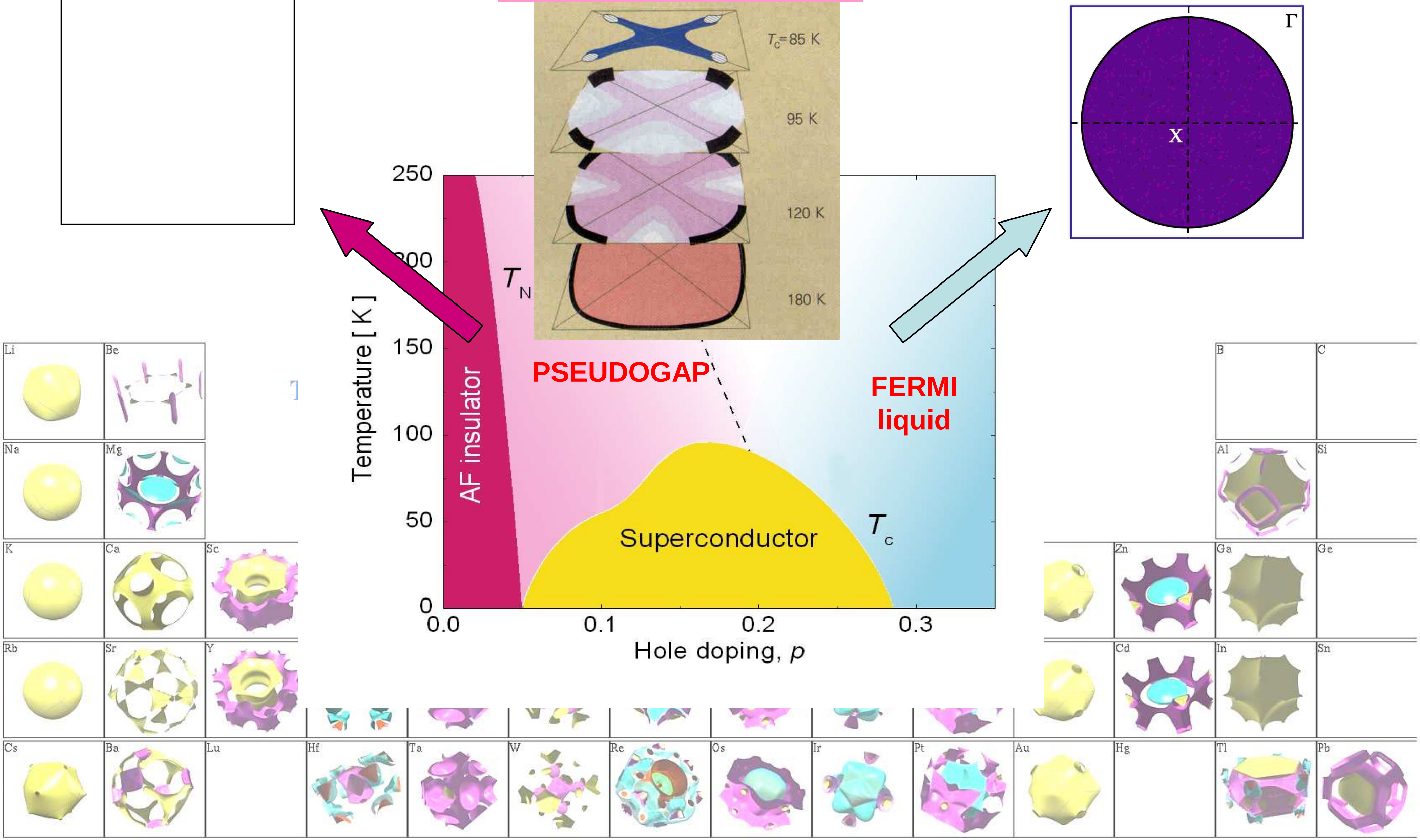
Electronic specific heat: $\gamma_{el} = \frac{\pi N_A k_B^2 a^2}{3\hbar^2} m^*$ ⇒ $\gamma_{el} = 6 \pm 1 \,\mathrm{mJ/mol.K^2}$

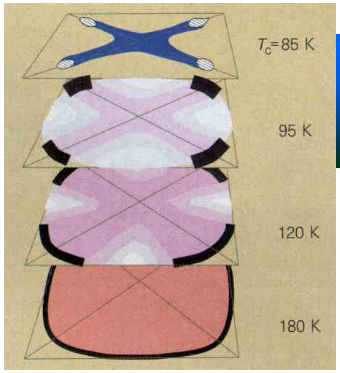
For overdoped polycristalline Tl-2201: $\gamma_{el} = 7 \pm 2 \,\mathrm{mJ/mol.K^2}$ (Loram et al, Physica C'94)

Mean free path : $R_T = \exp\left(- \frac{\pi \hbar k_F}{e B \ell} \right)$ ⇒ ℓ_{dHvA}≈320 Å (ℓ_{transp}≈670 Å)

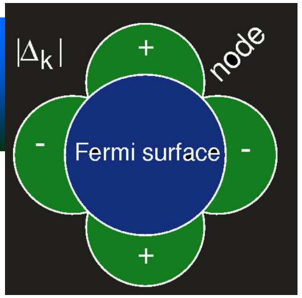
IV. Hot topics

ARPES⇒ Fermi arcs





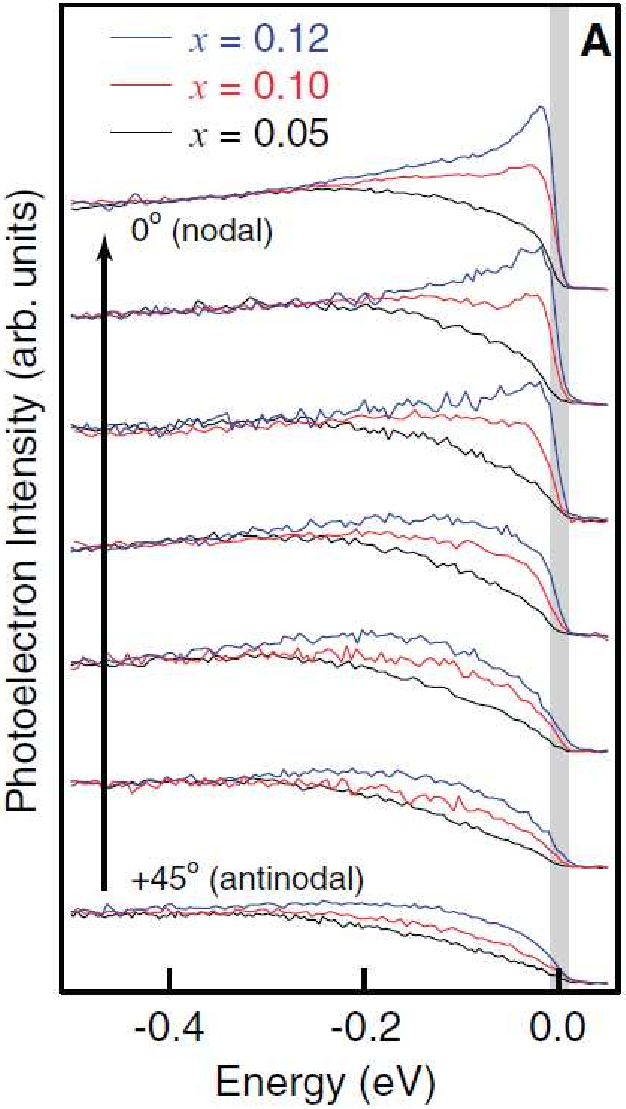
IV. Hot topics

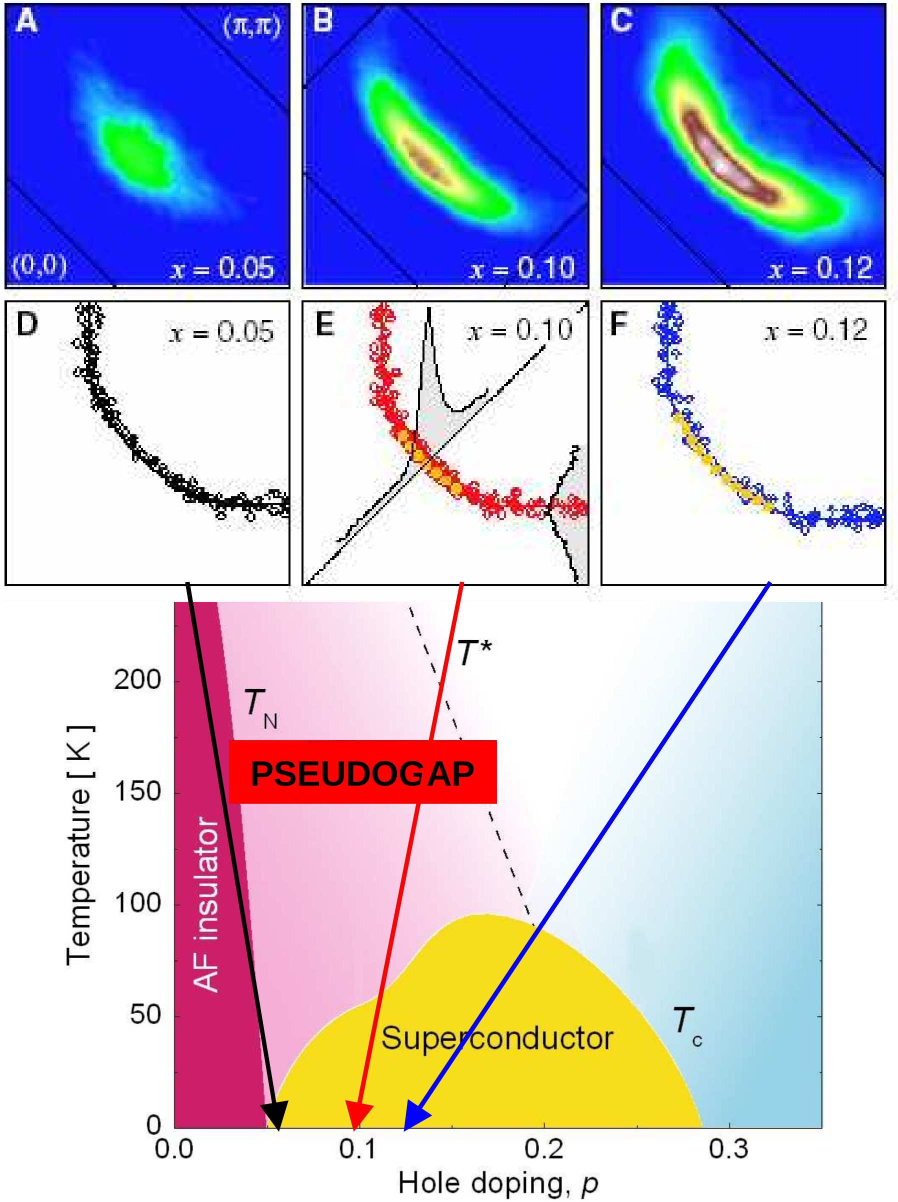


ARPES in underdoped HTSC

$Ca_{2-x}Na_xCuO_2Cl_2$

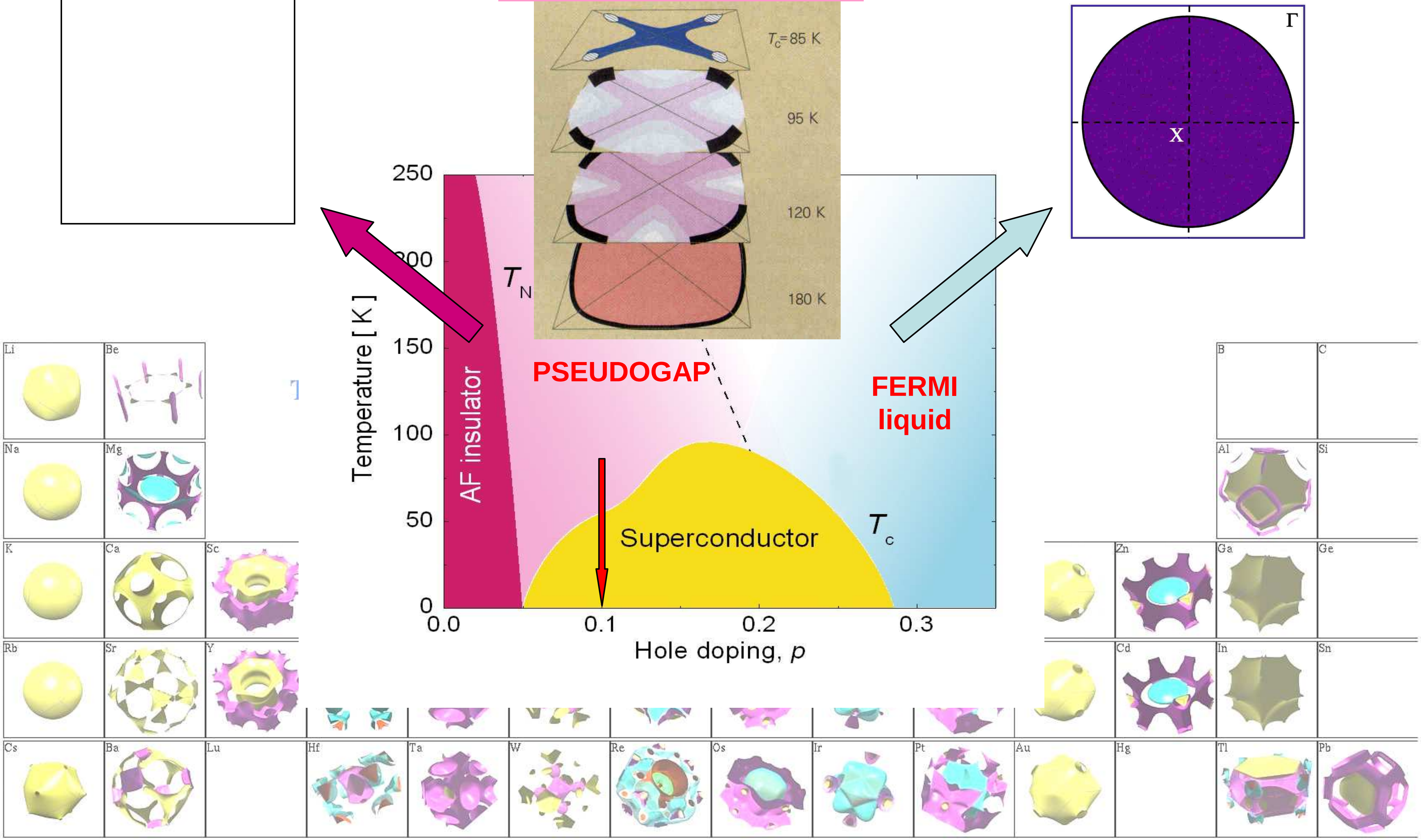
K. Shen *et al.*, Science'05





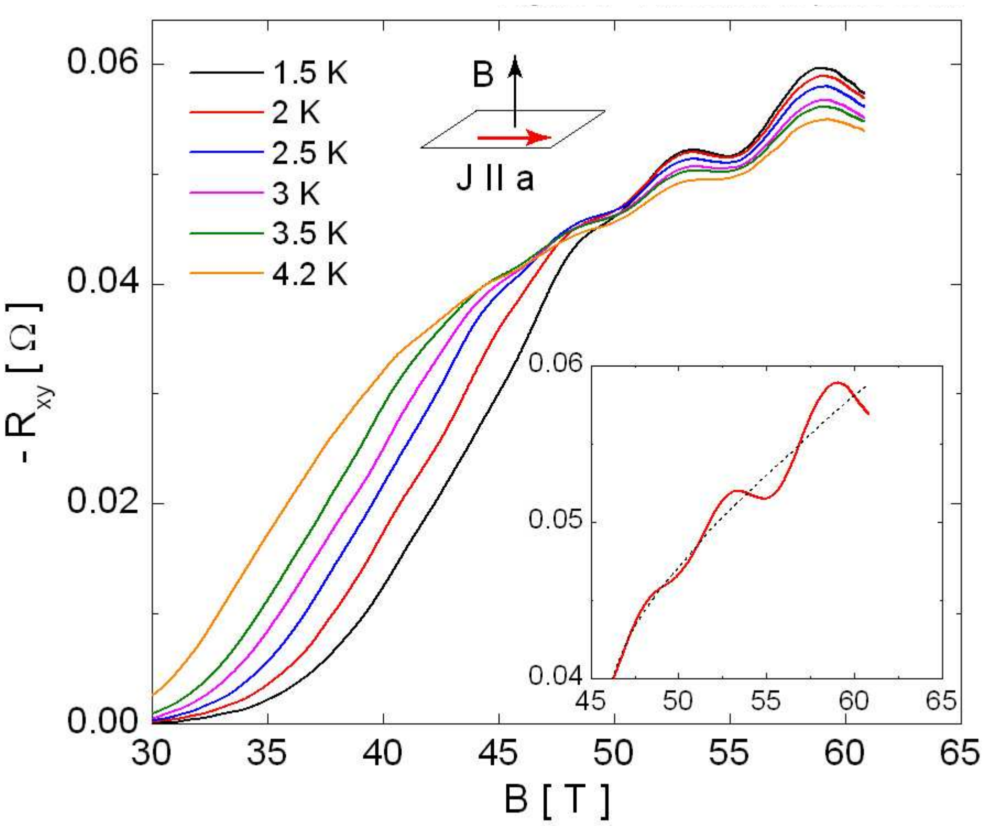
IV. Hot topics

ARPES⇒ Fermi arcs



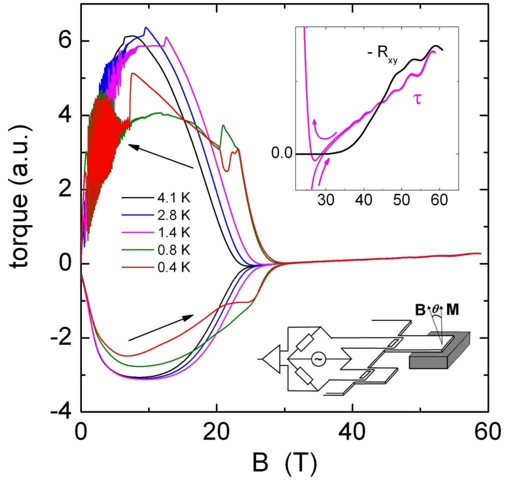
IV. Hot topics

Shubnikov - de Haas

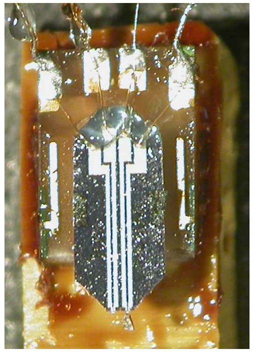


N. Doiron-Leyraud et al, Nature'07

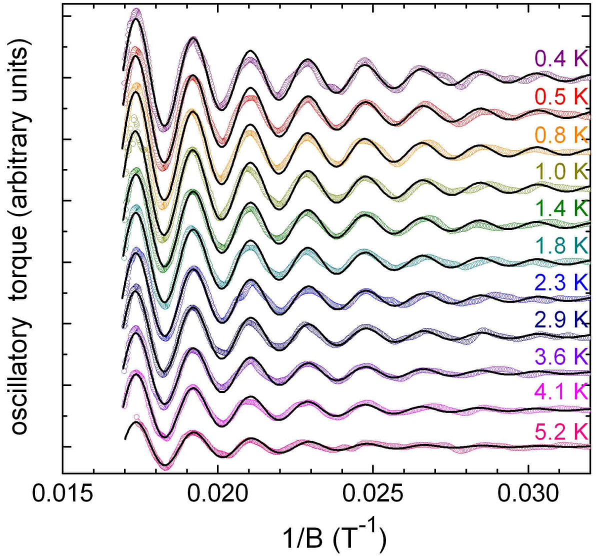
de Haas – van Alphen



D. Vignolles



Piezoresistif cantilever

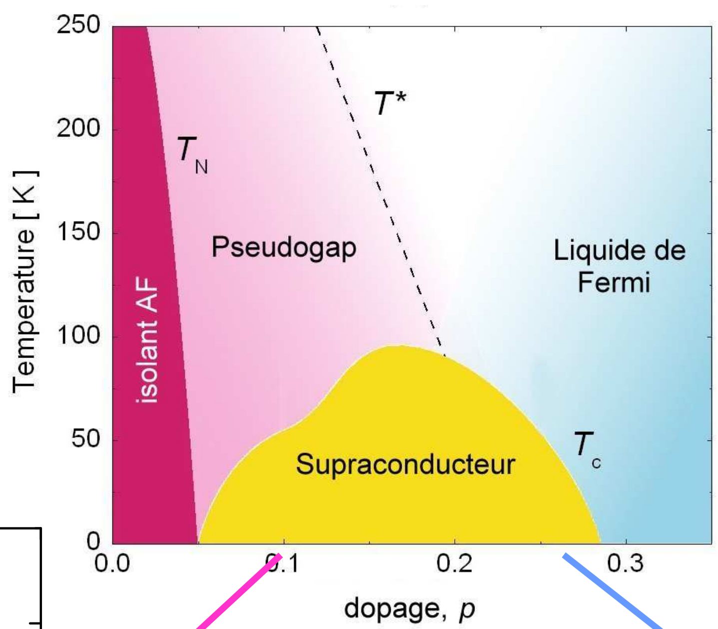


C. Jaudet et al, PRL'08

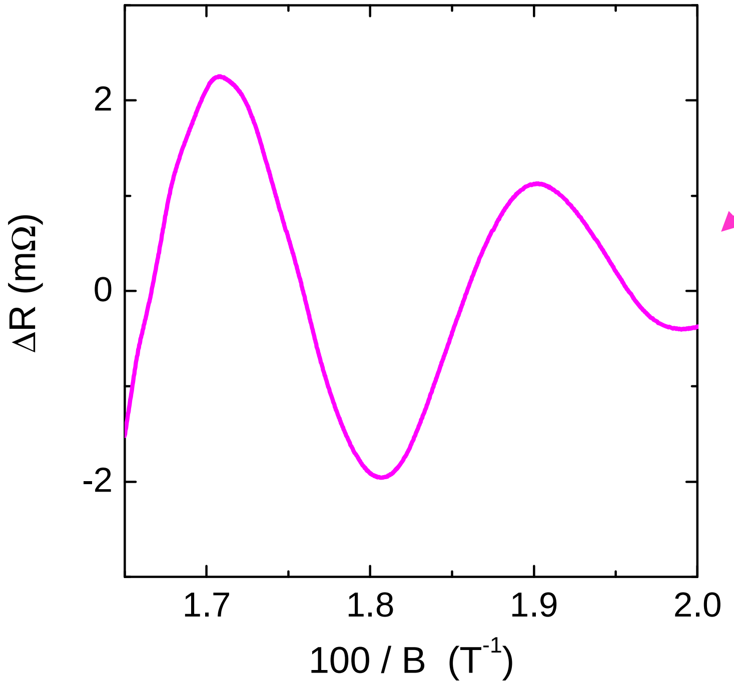
underdoped
$YBa_2Cu_3O_y$

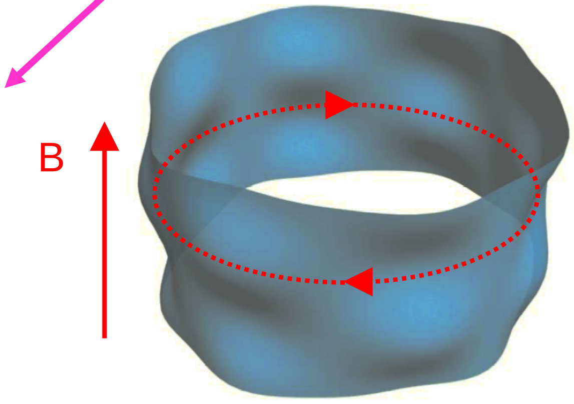
IV. Hot topics

underdoped
$YBa_2Cu_3O_{6.5}$

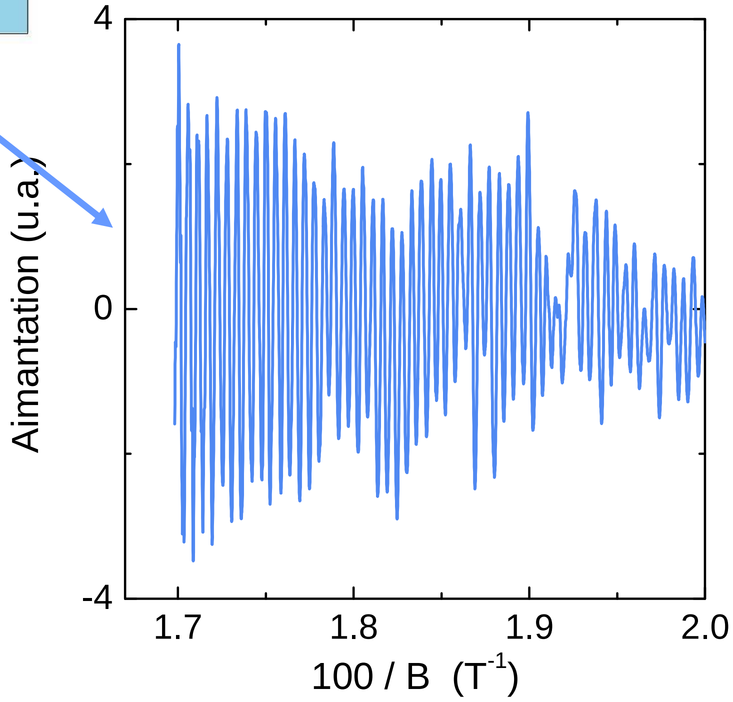


overdoped
$Tl_2Ba_2CuO_{6+\delta}$





$$F = \frac{\phi_0}{2\pi^2} A_k$$



N. Doiron-Leyraud et al, Nature'07

B. Vignolle et al, Nature'08

IV. Hot topics

$YBa_2Cu_3O_{6.5}$

Frequency : F = (530 ± 20) T

$A_k = 5.1\ nm^{-2}$

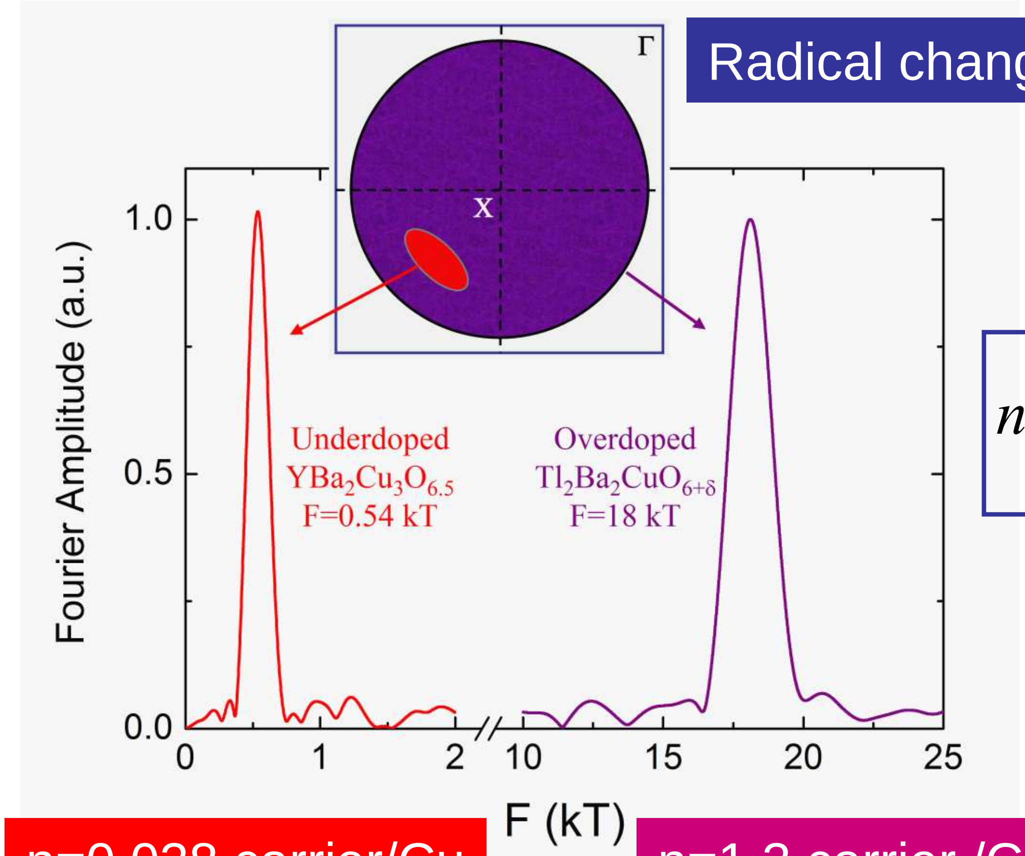
= 1.9 % of 1st Brillouin zone

$Tl_2Ba_2CuO_{6+\delta}$

Frequency : F = (18100 ± 50) T

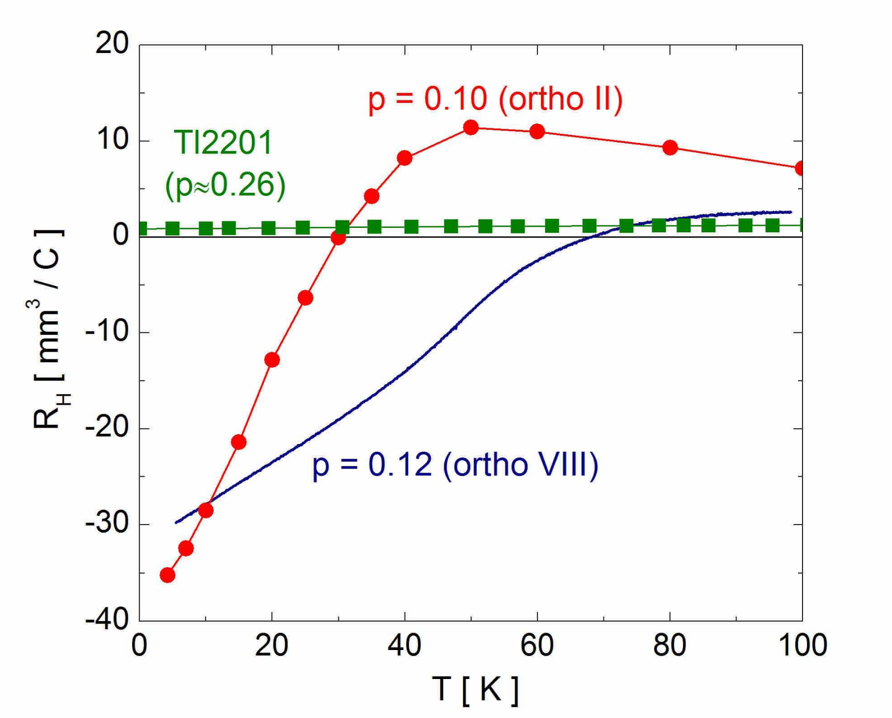
$A_k = 173.0\ nm^{-2}$

= 65 % of 1st Brillouin zone



Radical change of the carrier density

$$n = \frac{F}{\phi_0}$$



n=0.038 carrier/Cu

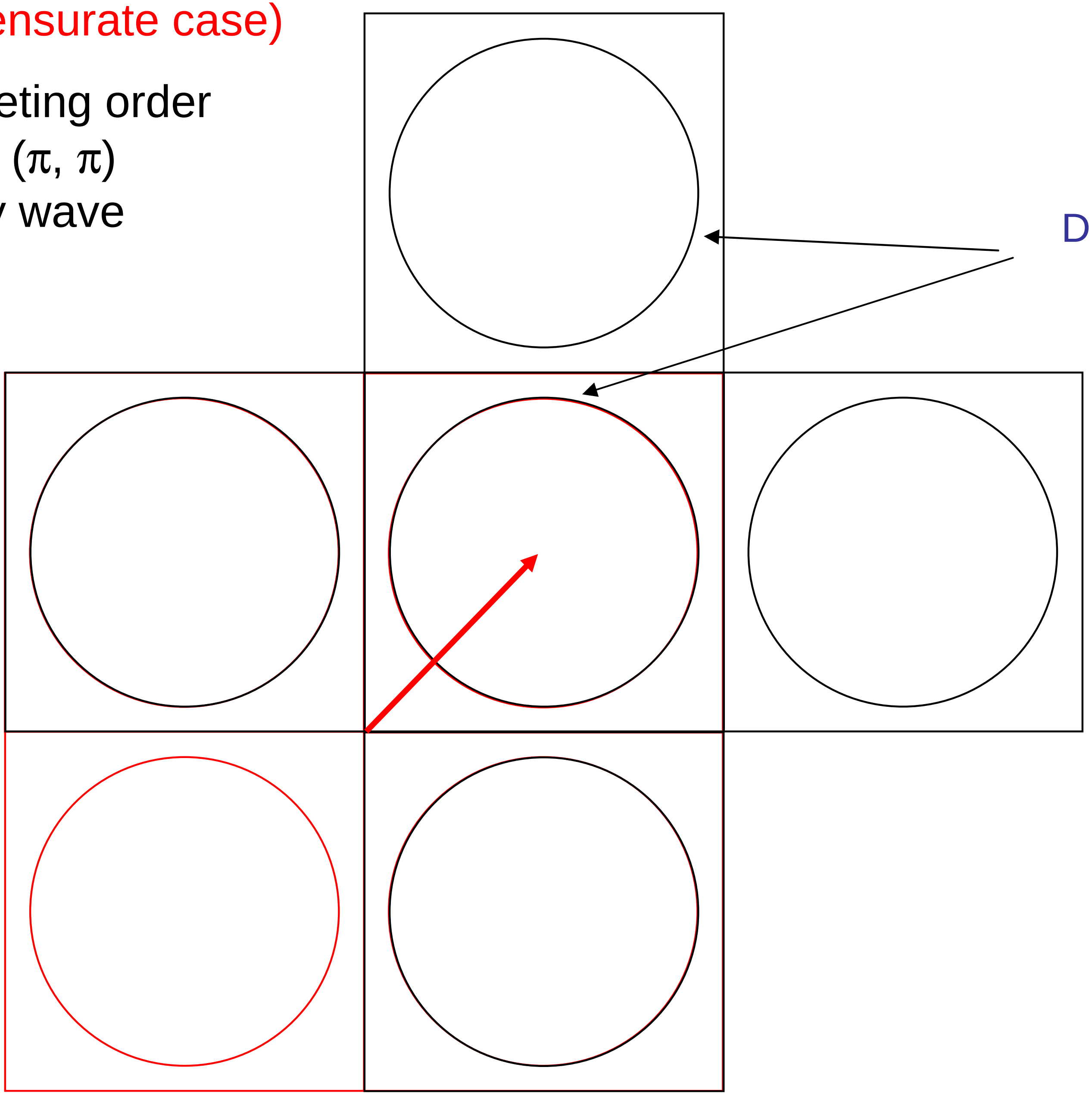
n=1.3 carrier /Cu

IV. Hot topics

Example of Fermi surface reconstruction

(commensurate case)

e.g. competing order
- AF order (π, π)
- *d*-density wave



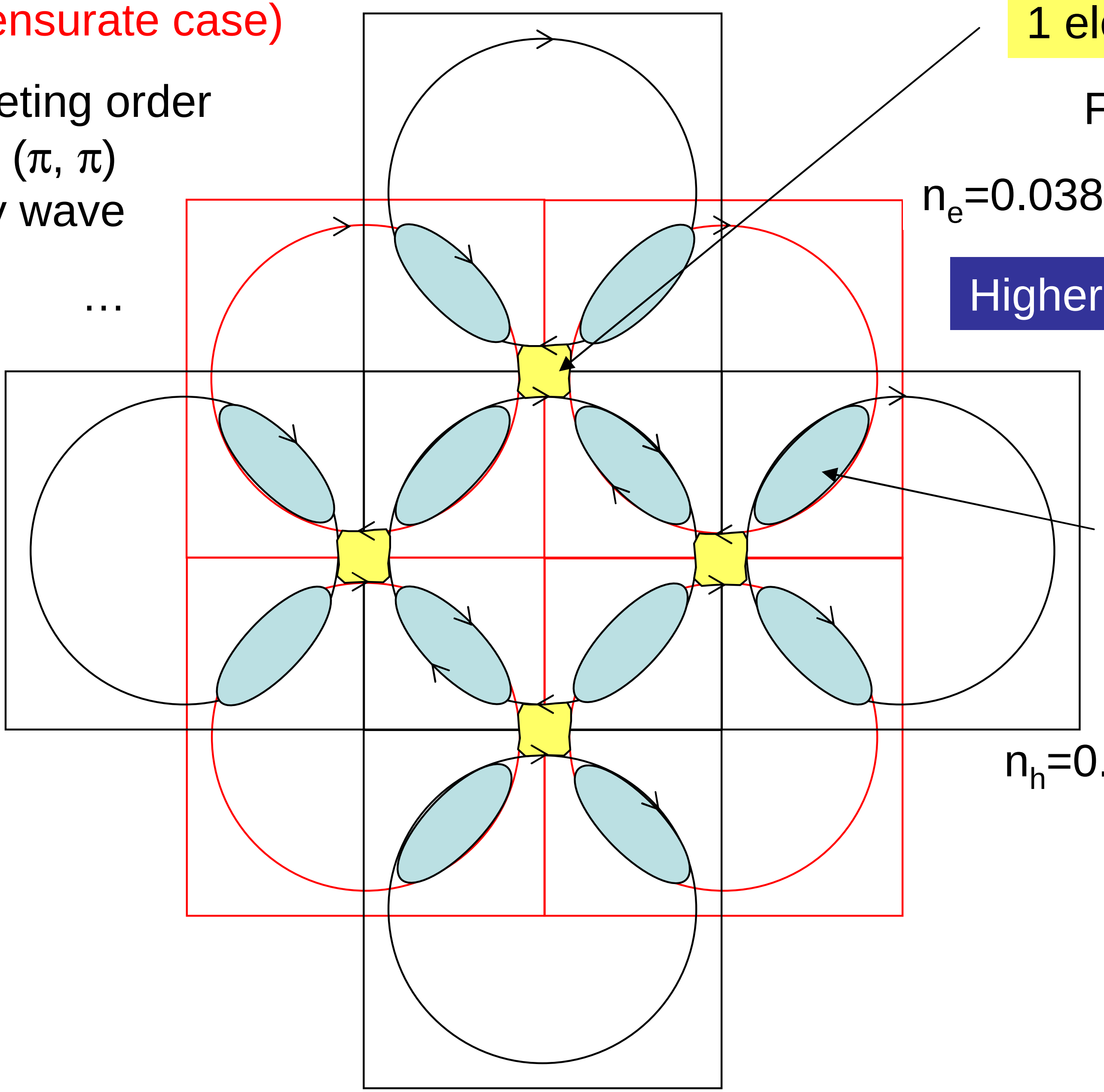
IV. Hot topics

Fermi surface reconstruction

(commensurate case)

e.g. competing order
- AF order (π, π)
- *d*-density wave

…



1 electron pocket

F_{SdH}=530 T

n_e=0.038 electron/Cu atom

Higher mobility at low T

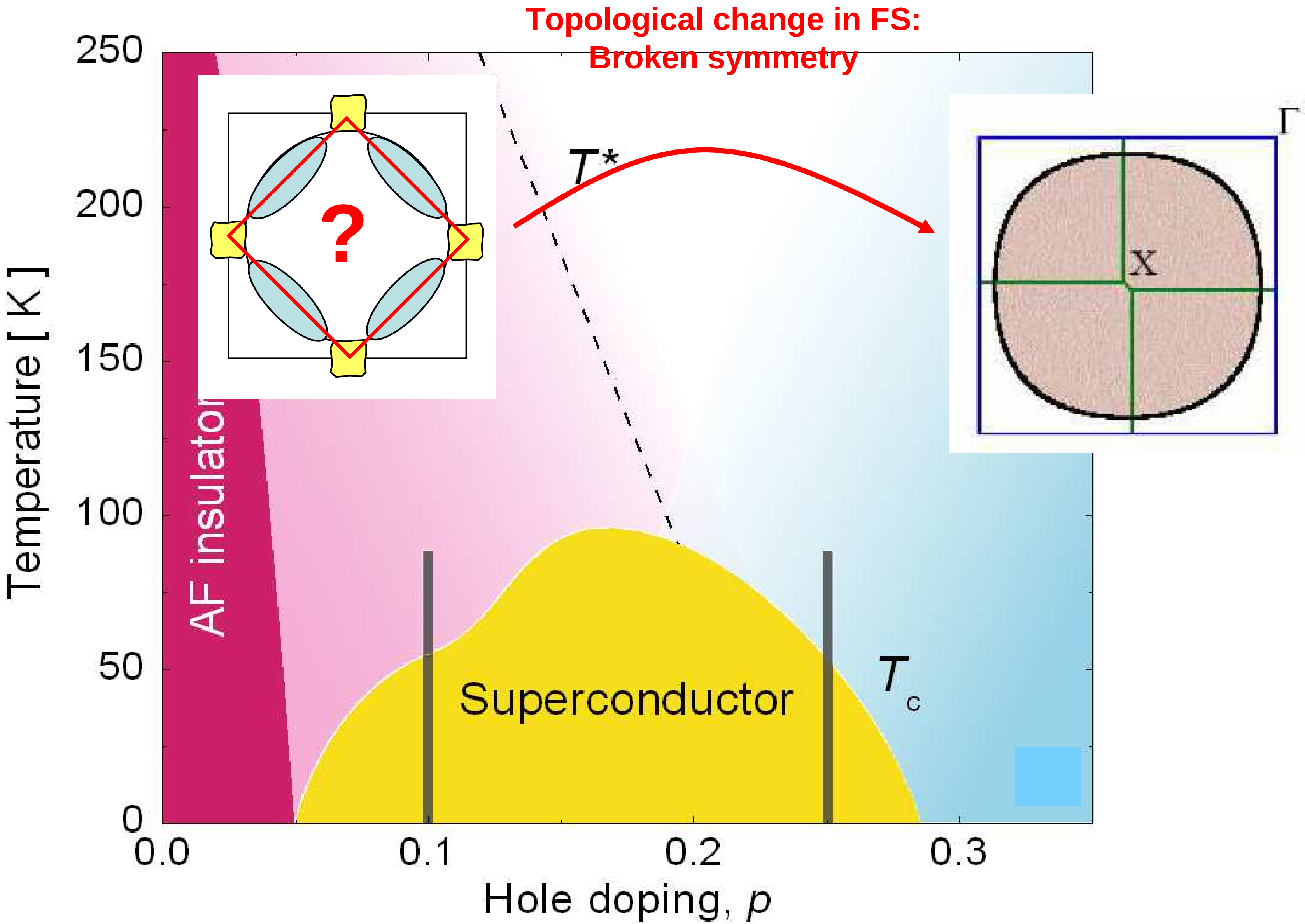
2 hole pockets

F_{SdH}=990 T

n_h=0.138 hole/Cu atom

$n=n_h-n_e=p=0.1$

IV. Hot topics



underdoped

overdoped

References

ARPES:

- A. Damascelli, Z-X Shen and Z. Hussain, " Angle-resolved photoemission spectroscopy of the cuprate superconductors", *Rev. Mod. Phys.* **75**, 473 (2003)

- A. Damascelli, Z-X Shen and Z. Hussain, " Probing the Electronic Structure of Complex Systems by ARPES", *Physica Scripta.* **109**, 61 (2004)

- S. Hüfner, ‘‘Photoelectron Spectroscopy,’’ (Springer-Verlag, Berlin, 1995)

- http://www.physics.ubc.ca/~quantmat/ARPES/PRESENTATIONS/talks.html

- http://www-bl7.lbl.gov/BL7/who/eli/SRSchoolER.pdf

Quantum oscillations:

- D. Shoenberg, "Magnetic oscillations in metals" (Ed. Cambridge Monographs on Physics)

- W. Mercouroff, "La surface de Fermi des métaux" (Ed. Masson)

- C. Bergemann, A. Mackenzie, S. Julian, D. Forsythe and E. Ohmichi, " Quasi-two-dimensional Fermi liquid properties of the unconventional superconductor Sr_2RuO_4", *Advances in Physics* **52**, 639 (2003)

I. Why and how to measure a Fermi surface

Global properties

- **Specific heat** $$\boxed{C_v = \frac{\partial U}{\partial T} = \frac{\pi^2}{3} k_B g(E_F) \times T}$$ where $U = \int_0^{E_F} E\, n(E) f(E) dE$

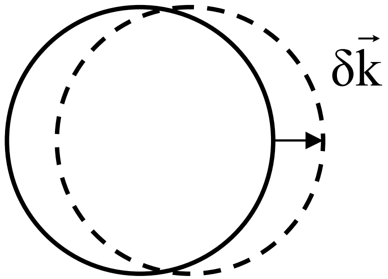
$$g(E_F) = \frac{m^* k_F}{\hbar^2 \pi^2}$$

- **Pauli susceptibility** $$\boxed{\chi_{Pauli} = \frac{g\mu_B^2}{2} g(E_F)}$$

- **Hall effect** $$\boxed{R_H = \frac{\rho_{xy}}{B} = \frac{1}{nq}}$$

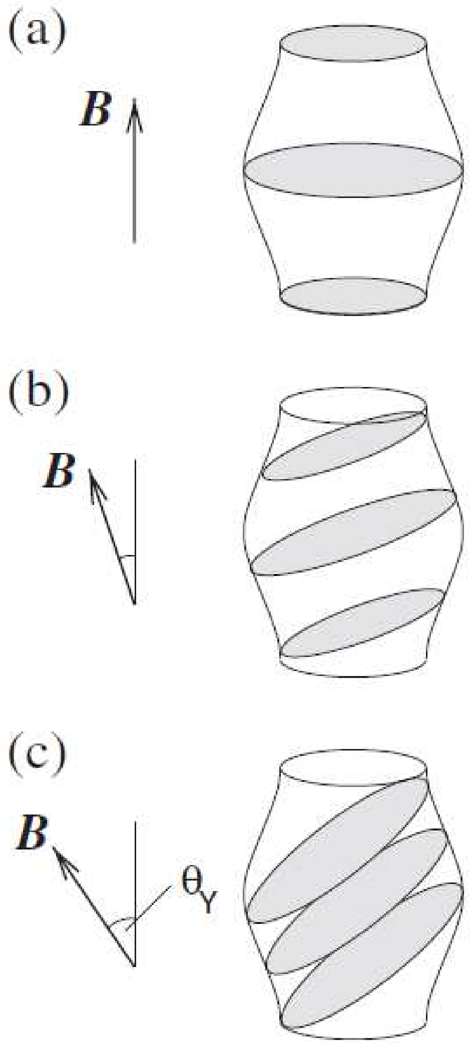
- **Magnetoresistance** $\vec{J} = ne\vec{v} = e\int_{SF} \vec{v} \frac{\delta\vec{k}.d\vec{S}}{4\pi^2}$ where $\delta\vec{k} = \frac{e\tau}{\hbar}\vec{E}$

$$\boxed{\vec{J} = \frac{e^2\tau}{4\pi^3\hbar} \int_{SF} \vec{v}.d\vec{S}\ \vec{E}}$$

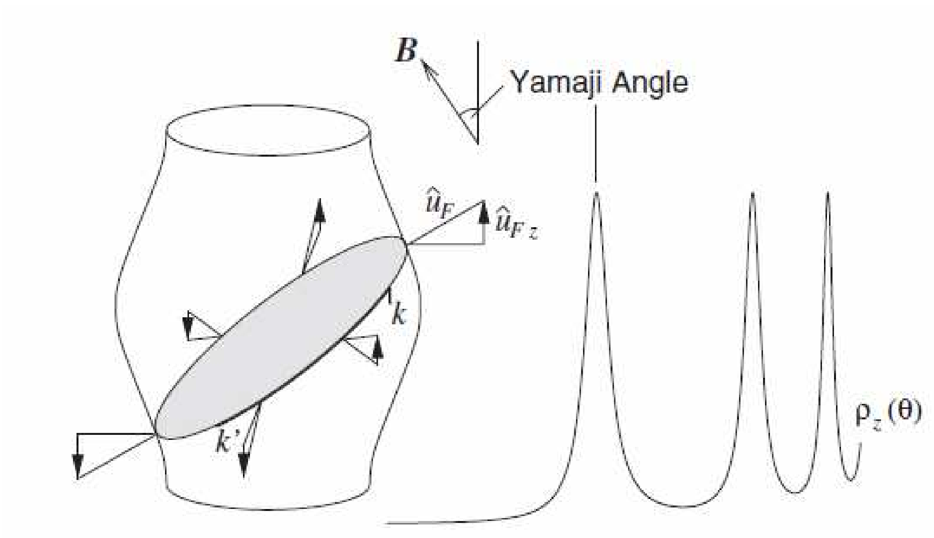


AMRO

Angular dependence of the MagnetoResistance Oscillations



Work at 2D and for simple Fermi surface



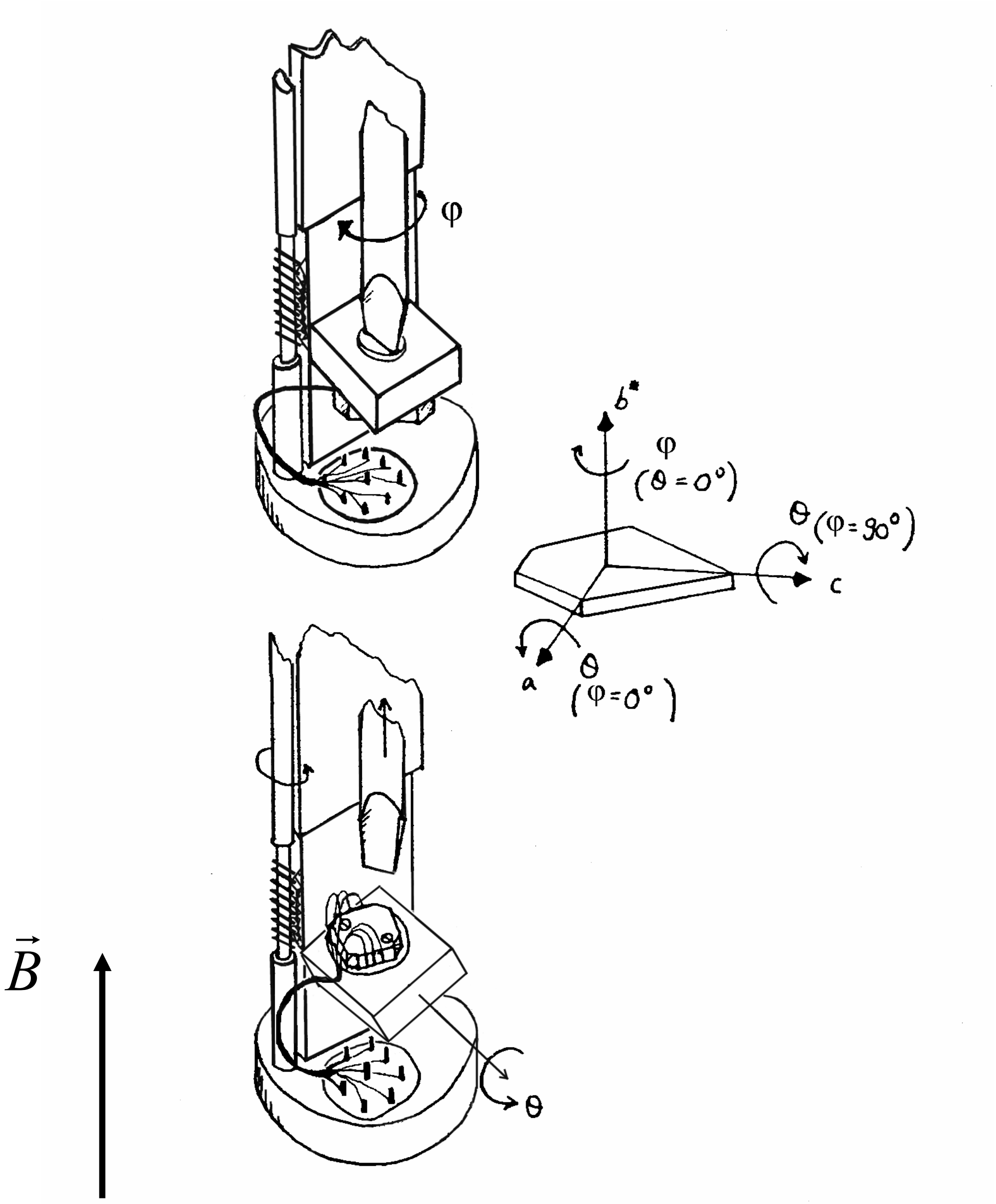
At particular angles (‘Yamaji angles’)

$$\boxed{v_z = \frac{1}{\hbar}\frac{\partial E}{\partial k_z} = 0}$$

Semi-classical effect

C. Bergemann et al,
Advances in Physics’03

AMRO



- Two-axis rotation probe

  Θ → Polar angle

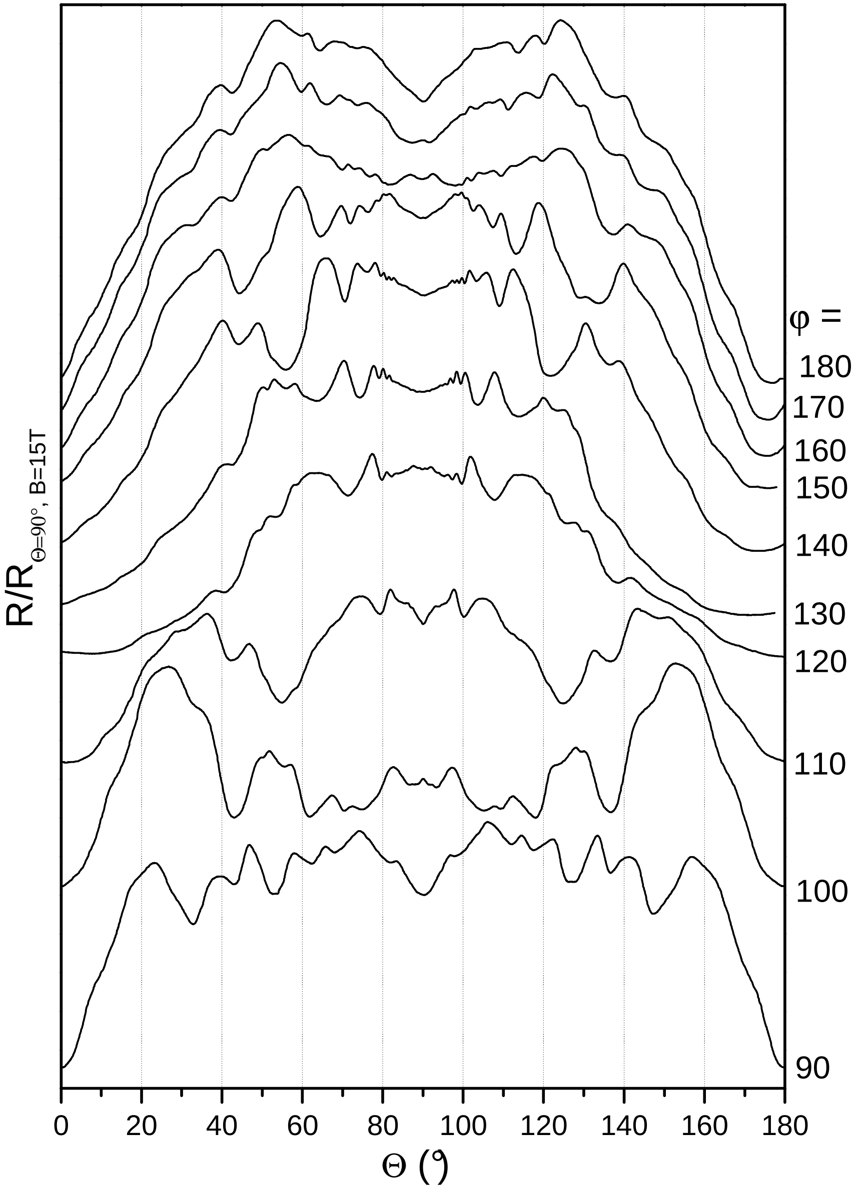
  φ → Azimutal angle

- Steady magnetic fields

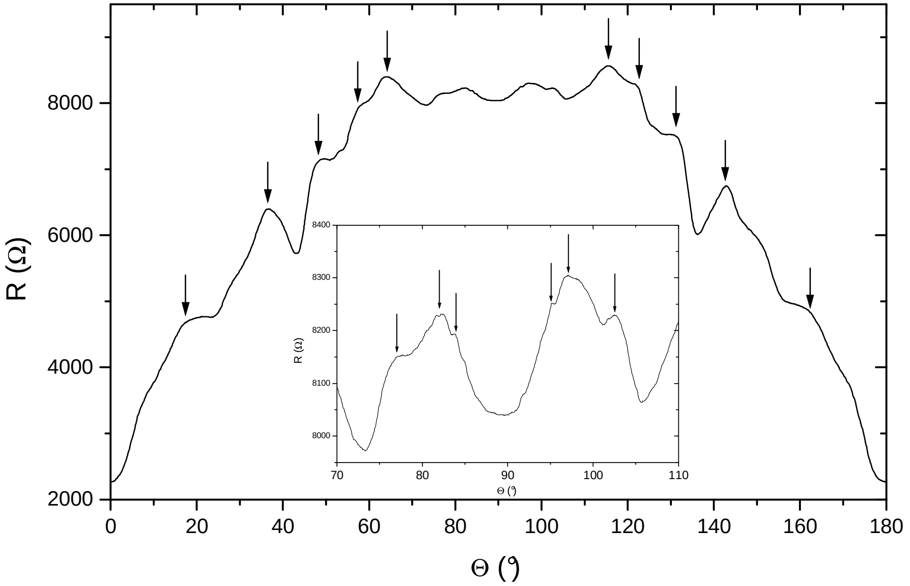
AMRO

Max. of the magnetoresistance when $$c\,k_{//}\tan(\Theta_i)=\pi(i\pm 1/4)$$

Projection of k_F in the plane ⊥ to **B**



Quasi-2D organic metal:
$(\mathrm{BED0\text{-}TTF})_2\mathrm{ReO_4H_2O}$

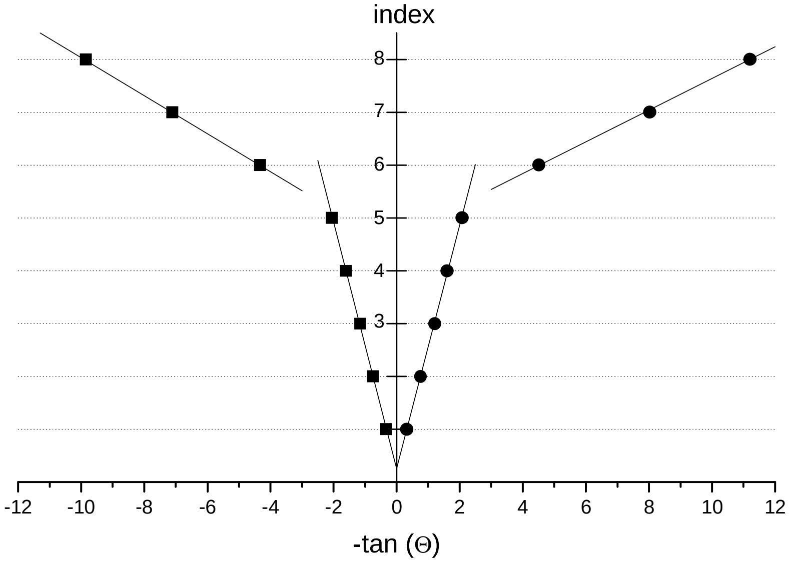


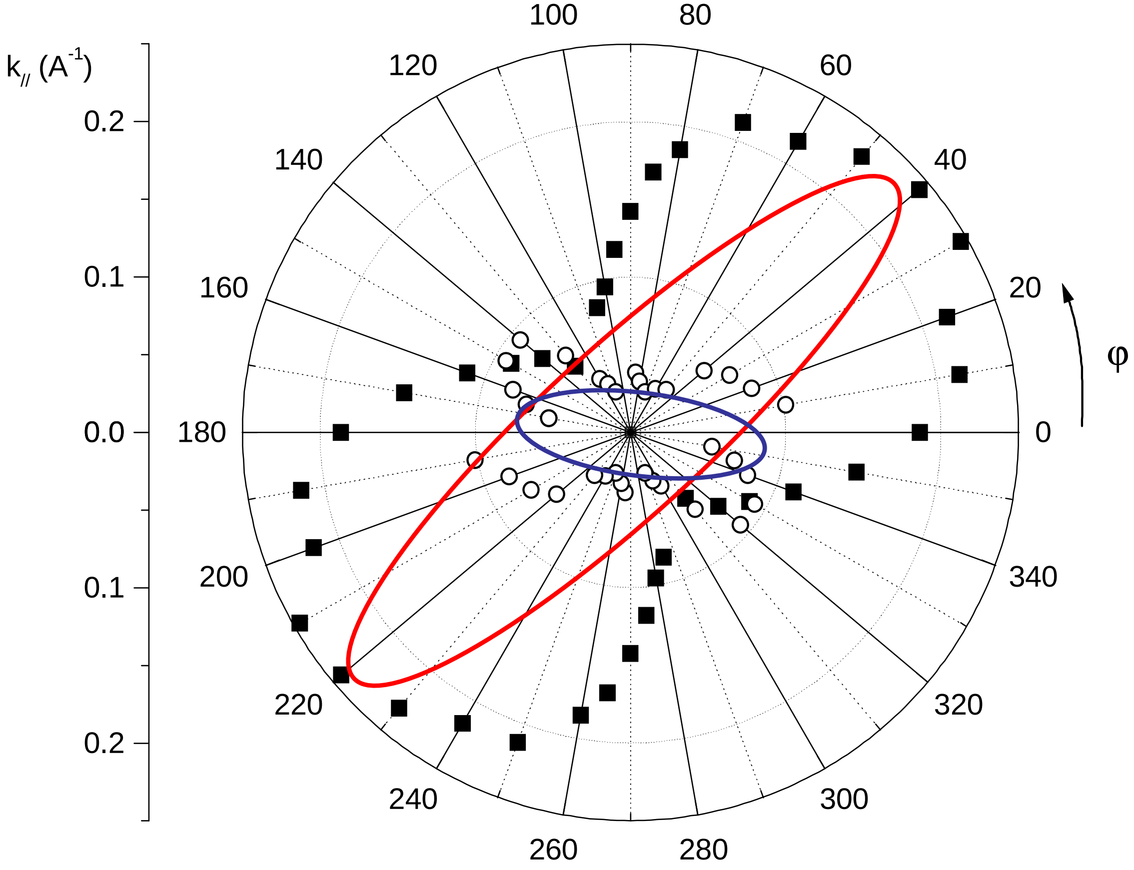
C. Proust et al, *Synthetic Metals*'99

AMRO

Quasi-2D organic metal: (BED0-TTF)$_2$ReO$_4$H$_2$O

$$c\,k_{//}\tan(\Theta_i)=\pi(i\pm 1/4)$$

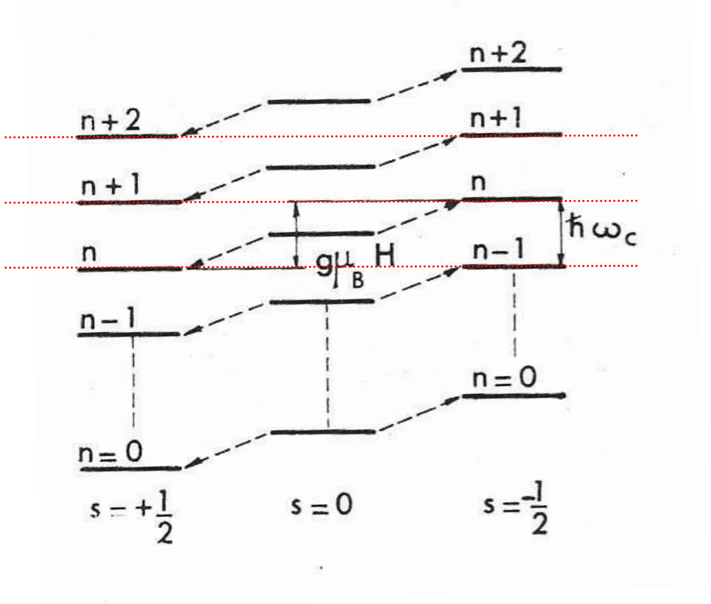




C. Proust et al, *Synthetic Metals*'99

III.2 Theory

Spin splitting in Quantum oscillations

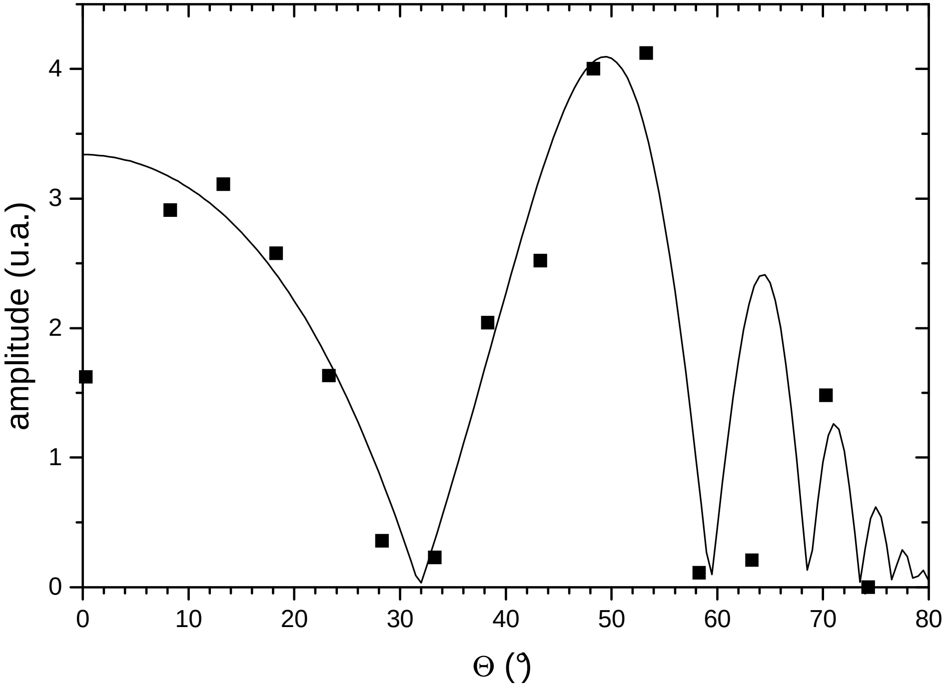


Spin splitting: $\Delta E = g\mu_B B$

Free electron: $\Delta E = 2 * \frac{e\hbar}{2m_0} B = \hbar \frac{eB}{m_0} = \hbar\omega_c$

No change of the frequency
but additional damping factor due to phase shift

$$\boxed{R_S = \cos\left(2\pi\frac{\Delta E}{\hbar\omega_c}\right) = \cos\left(\frac{\pi}{2}m_0 g\right)}$$



<u>Particular case</u>: spin zero phenomena

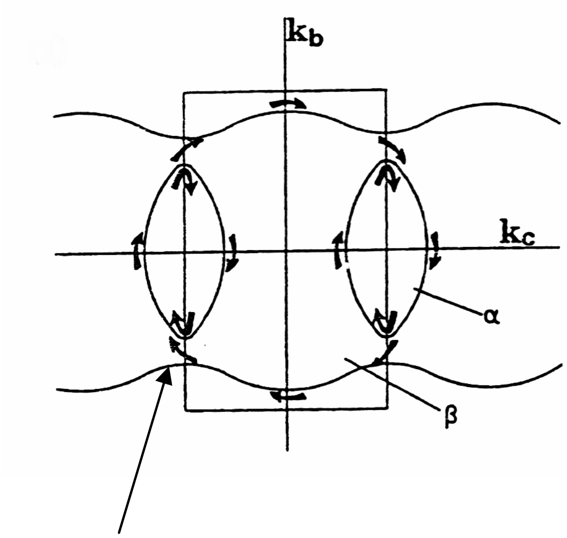
Assume $m_0(\theta) = \frac{m_0}{\cos(\theta)}$

$$R_S = \cos\left(\frac{\pi m_0 g}{2\cos(\theta)}\right) = 0$$

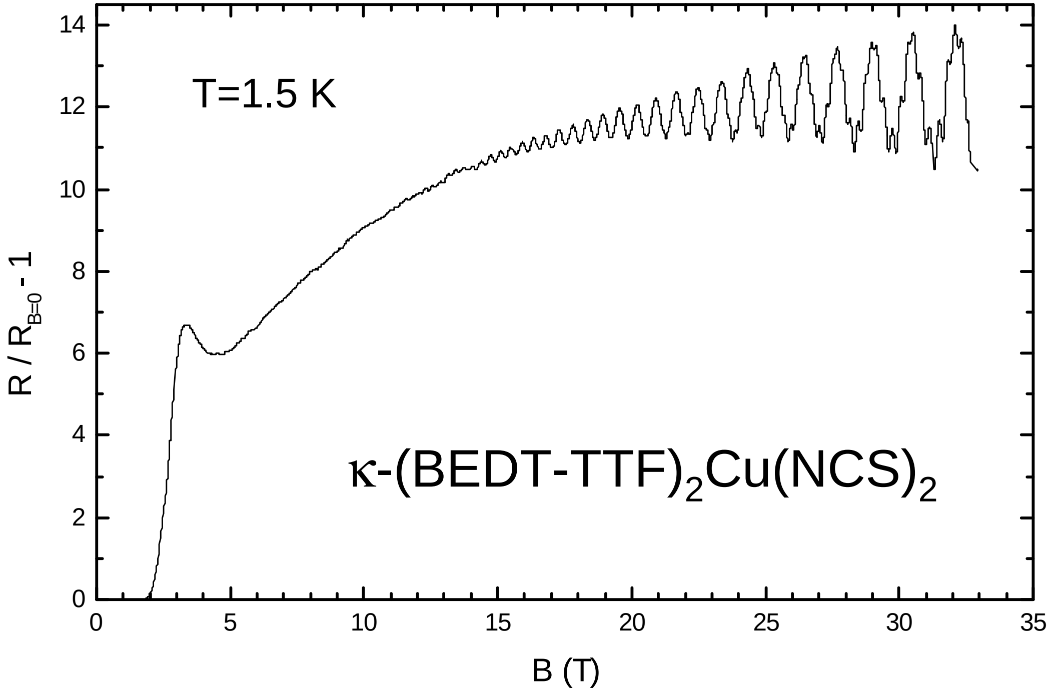
when $\boxed{\cos(\theta_k) = \frac{g m_0}{2k+1}}$

III.2 Theory

Magnetic breakdown (Cohen&Falicov 1961)



Probability *p* of MB



In strong magnetic fields, electron can tunnel from one orbit to another

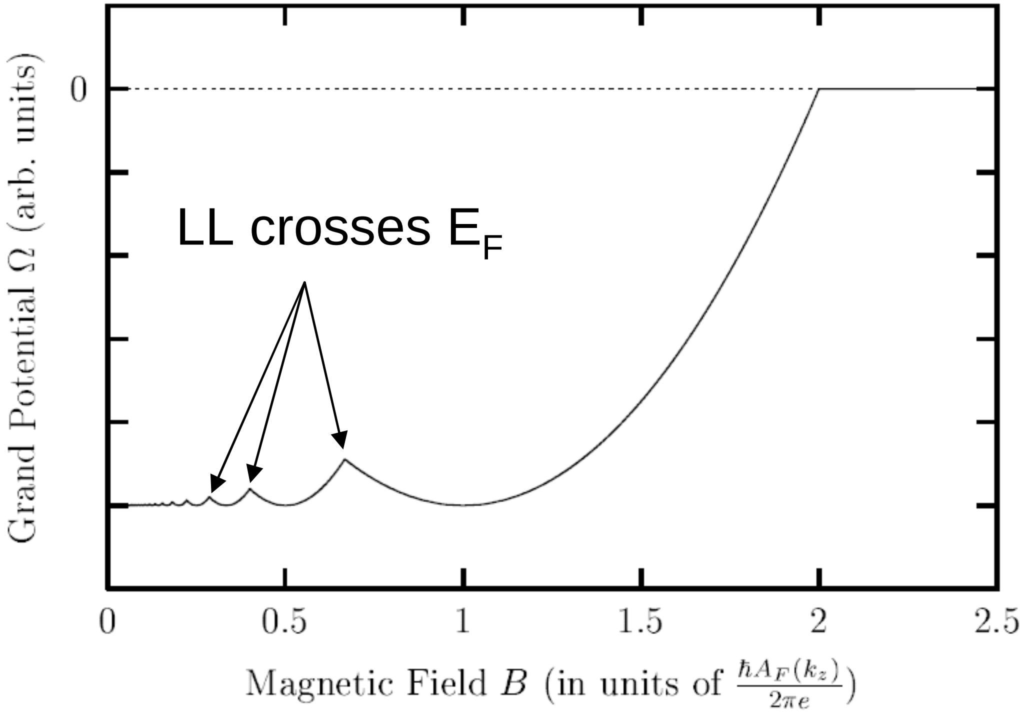
$$p^2 = \exp\left(-\frac{B_0}{B}\right) \qquad \text{where} \qquad B_0 \propto \frac{\Delta^2 m_c}{e\hbar E_F}$$

$\Delta \rightarrow$ ‘Energy gap’ (forbidden band) between the two orbits

III.2 Theory

Lifshitz-Kosevich theory (1956)

T=0 $M = -\left(\frac{\partial \Omega}{\partial B}\right)_{\mu,T}$ where $\Omega = \sum_{all\, electrons}(E - E_F)$ Thermodynamic grand potential



$$\Omega = \frac{qB}{\pi^2\hbar}\int_0^{\kappa_0}\sum_{n=0}^{n_m}\left(\frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c(n+0.5) - E_F\right)dk_z$$

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$$\boxed{\tilde{M} \propto \sum_{\text{extremal } A_F} \frac{F B^{\frac{1}{2}}}{m^* \left|\frac{\partial^2 A_F}{\partial k_z^2}\right|^{\frac{1}{2}}} \sum_{p=1}^{\infty} p^{-\frac{3}{2}} \sin\left(2\pi p\left(\frac{F}{B} - \gamma\right) \pm \frac{\pi}{4}\right)}$$

$$F = \frac{\hbar A_F}{2\pi e}$$

III.3 High magnetic fields lab.

III.3 High magnetic fields lab.

State of the art technical performances

Superconducting: USA: 33,8 T (NHMFL)
(Commercial: 23 T Bruker)

Resistif : USA: 45,5 T (NHMFL, hybride)
Japan: 38,9 T (TML, hybride)
Europe: 35 T (LNCMI)

Pulsed : USA: 89,8 T (NHMFL)
Japan: 82 T (Osaka)
Europe: 87 T (HLD)