Tasks

(1) Read chapter 9:

(2) Solve exercise sheets

(3) Who is summarizing next week?

16th Lecture	13h00 – 15h00 Chapter 9: tight-binding	
18th Lecture	10h00 – 12h00 Chapter 9: Quantum Oscillation	
23th Lecture	13h00 – 15h00 Chapter 9: Quantum Oscillation	**(Hand-in exercise)**
25th Lecture	10h00 – 12h00 Wrap-up	
30th Exercise	13h00 – 15h00	**(Hand-in exercise)**
01st Lecture	10h00 -- 12h00 Exam focus	

Last – Exercise Sheet 11

Exercise 3 *Tight binding model*
In the lecture, we derived the tight-binding expression for a two-dimensional square lattice:

$$\epsilon_k = -\epsilon_0 - 2t[\cos(k_x a) + \cos(k_y a)] \tag{1}$$

(a) Plot, using your favourite computer program, (1) the full three-dimensional band structure ϵ_k versus k_x and k_y as a surface plot, (2) the band structure along the zone diagonal $k_x = k_y$, and (3) the Fermi surface ($\epsilon_k = \epsilon_{\mathrm{F}}$) for systems with $\mu = \epsilon_{\mathrm{F}}$ (metals), having the values $\epsilon_{\mathrm{F}} = -\epsilon_0$ and $\epsilon_{\mathrm{F}} = -\epsilon_0 \pm 2t$. [Hint: Set $t = 1$ meaning that ϵ_k is plotted in units of t, set $\epsilon_0 = 0$, plot k_x, k_y in units of π/a]

(b) In the lecture, we developed the tight binding only to first order. Let's include second order terms. We define t' as the integral over next-nearest neighbours that are given by $\vec{\rho}_m = (\pm a, \pm a)$ and $(\pm a, \mp a)$. Show that the tight-binding dispersion becomes:

$$\epsilon_k = -\epsilon_0 - 2t[\cos(k_x a) + \cos(k_y a)] - 4t'[\cos(k_x a)\cos(k_y a)] \tag{2}$$

(c) Let's say that $\mu = -\epsilon_0 - 0.87t$. Compare the Fermi surfaces for $t' = 0$ and $t' = -0.2t$.

(d) Figure 2 displays a Fermi surface of a two-dimensional electron gas (2DEG) produced by depositing potassium on an insulating substrate (Ca_2RuO_4). Extract the Fermi momentum k_{F}.

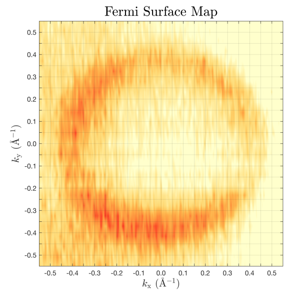


Figure 2: Fermi surface of a 2DEG on Ca_2RuO_4. Dark colours correspond to high intensities.

(e) Show that in two dimensions, the electron density is given by $n = k_{\mathrm{F}}^2/(2\pi)$. Compare this with the results for three-dimensions.

(f) The lattice constant is 3.89 Å. What is the area of the Fermi surface? What is the Brillouin zone area and what is the ratio between the two? How does it relate to the electron density?

(g) Calculate the electronic density of states in two-dimensions. Show that it is independent of ϵ_k. Compare with the three-dimensional result.

Exercise 1 *Quantum oscillations on quasi two-dimensional systems*
In $Tl_2Ba_2CuO_{6+\delta}$, quantum oscillations with a frequency of $F = 18.1$ kT are observed (B. Vignolle et al., Nature **455**, 952-955 (2008)).

(a) Use the Onsager relation ($S = 2\pi\frac{eF}{\hbar}$) to calculate the Fermi surface area.

(b) If we assume a circular Fermi surface shape, what is the Fermi momentum?

Exercise 2 *Quantum oscillations in gold*
Estimate the Fermi energy of gold (in eV) based on the oscillations of the spin susceptibility in a magnetic field, see figure 1. Which of the two superimposed oscillations corresponds to the largest orbit on the Fermi-sphere? Compare the result with the literature value $\epsilon_{\mathrm{F}} = 5.51$ eV. Where is the other oscillation originating from?

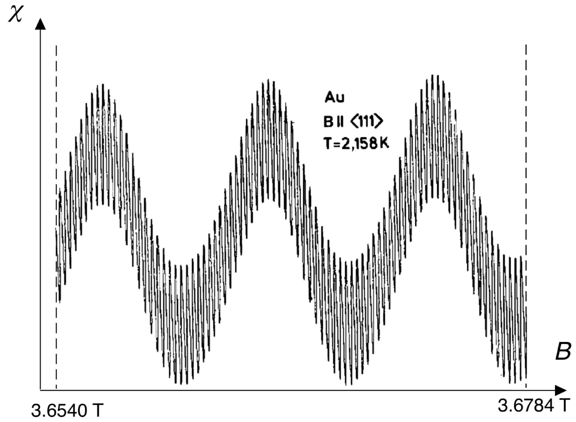


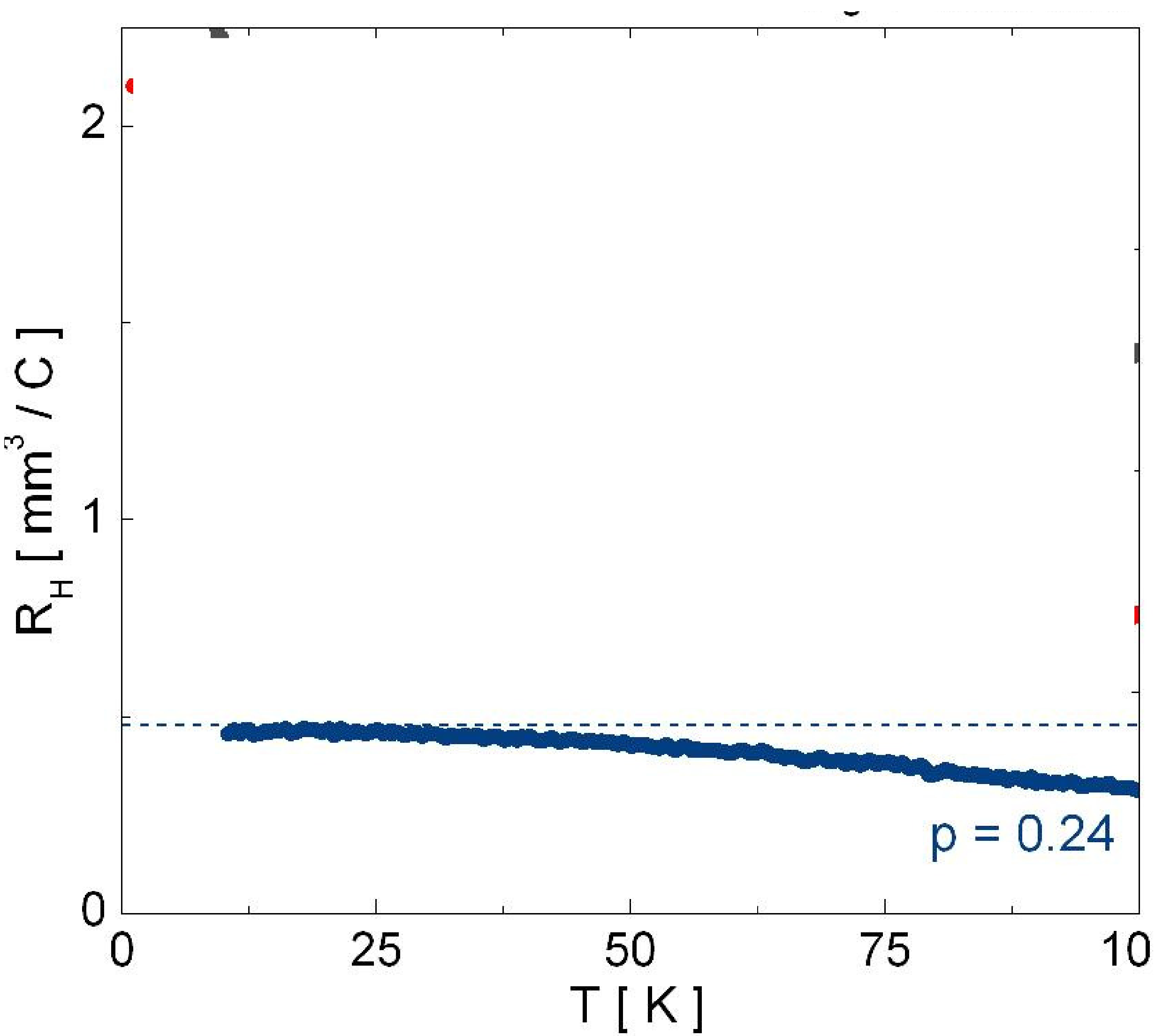
Figure 1: The spin susceptibility of gold in a magnetic field.

Luttinger’s Theorem

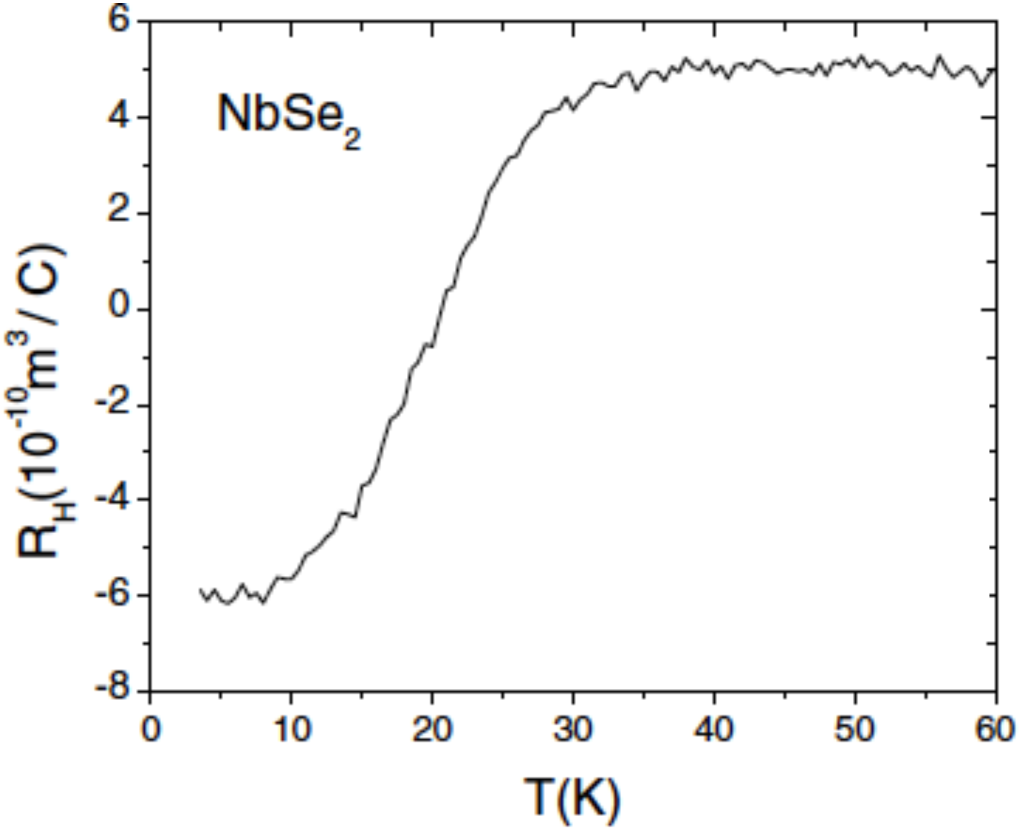
Luttinger's theorem states that **the volume enclosed by a material's Fermi surface is directly proportional to the particle density**.

$$n = \frac{N}{V} = (3\pi^2)^{-1} {k_F}^3$$

Hall effect: Carrier density

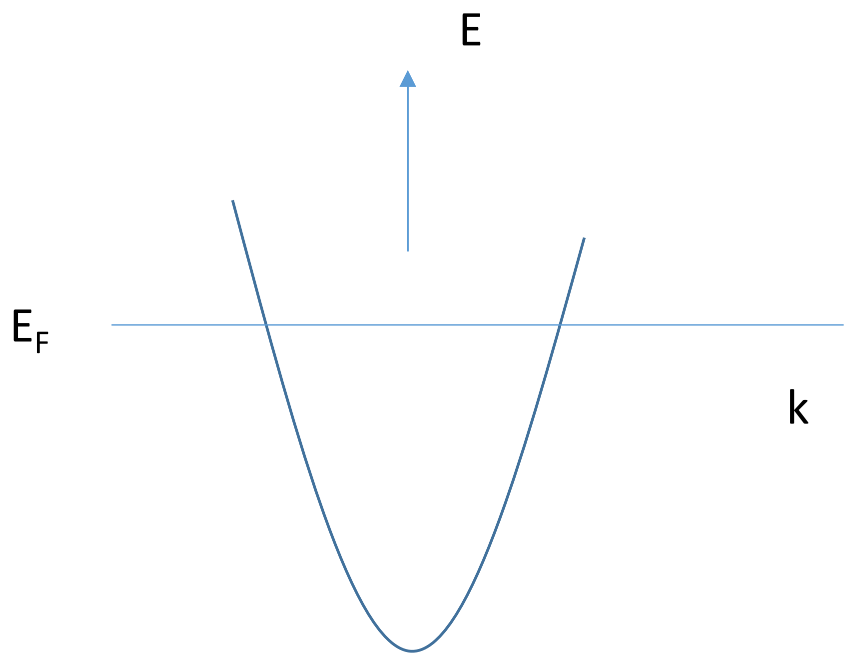


Fermi surface reconstruction

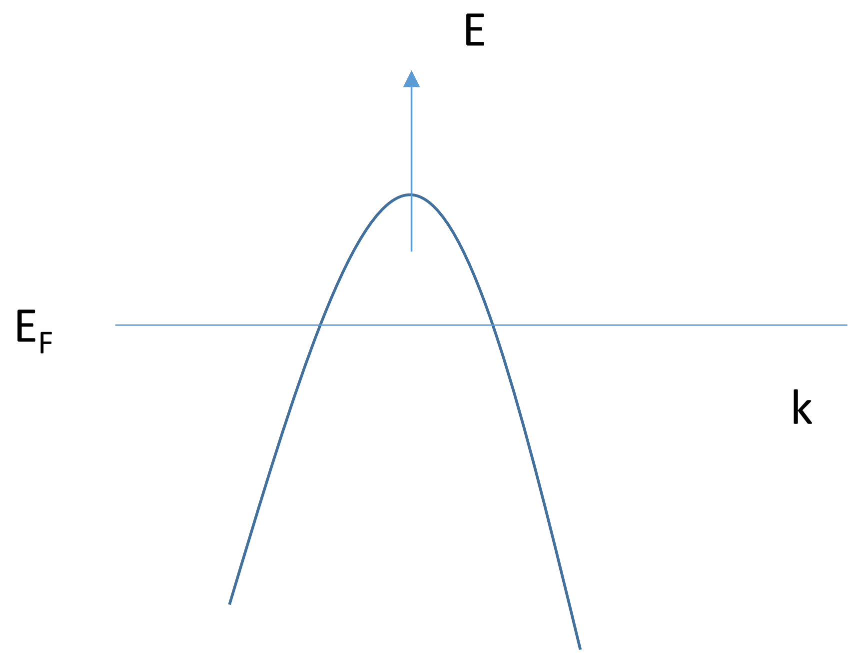


PRL 91, 066602 (2003)

Electron versus Hole like bands

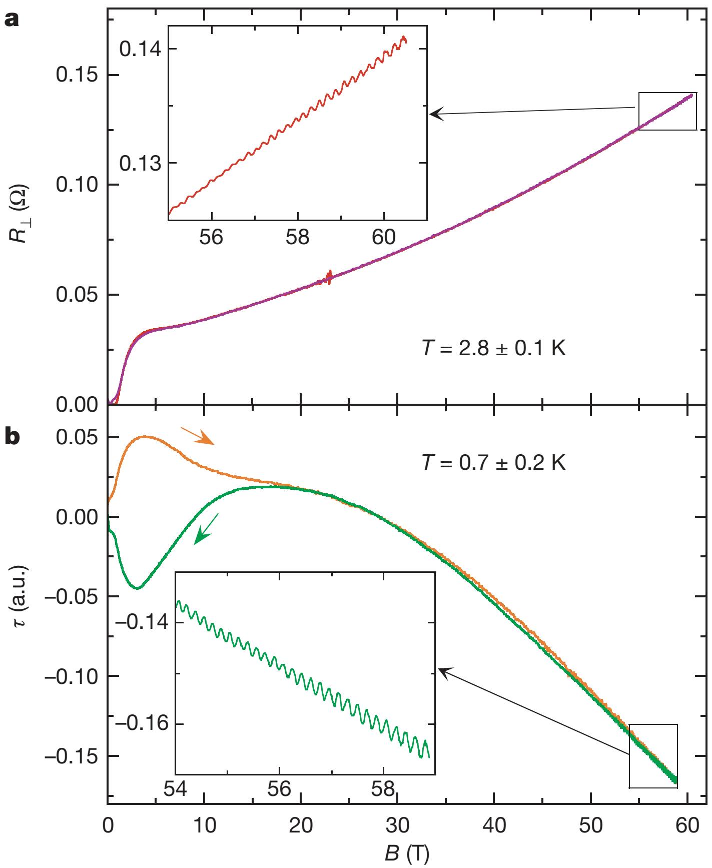


Electron-Like Band



Hole-Like Band

QUANTUM OSCILLATIONS:



Nature **455**, 952 (2008)

$Tl_2Ba_2CuO_{6+x}$

Shubnikov-de Haas effect =

Quantum oscillations with resistivity

De Haas–van Alphen effect =

Quantum oscillations with magnetic susceptibility

Outline:

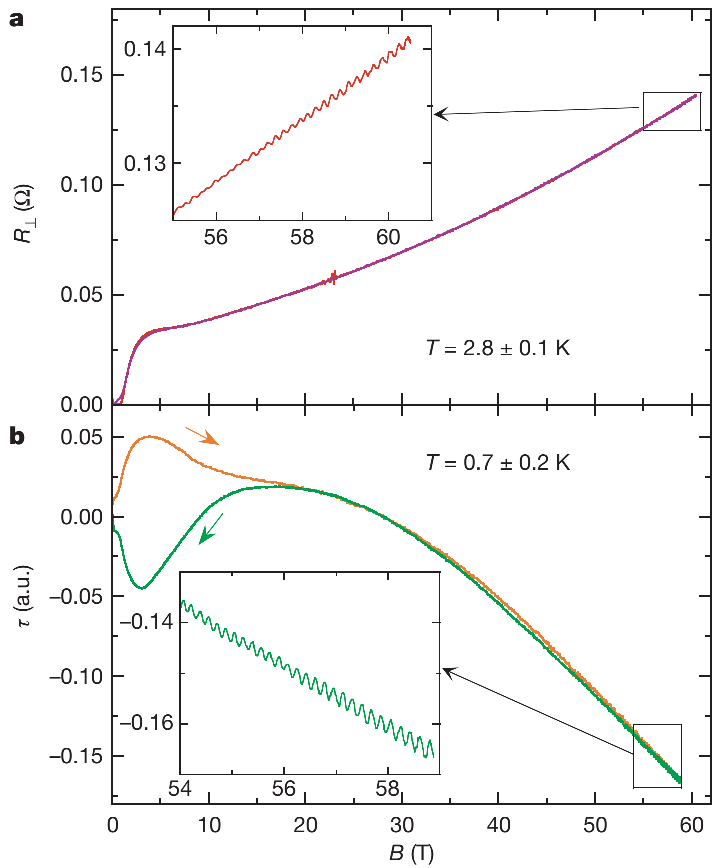
(1) Landau quantization / Landau levels:

Gives an understanding of why quantum oscillations exist.

(2) Onsager relation:

Gives a quantitative relation between the oscillations
and the Fermi surface area

QUANTUM OSCILLATIONS:



Nature **455**, 952 (2008)

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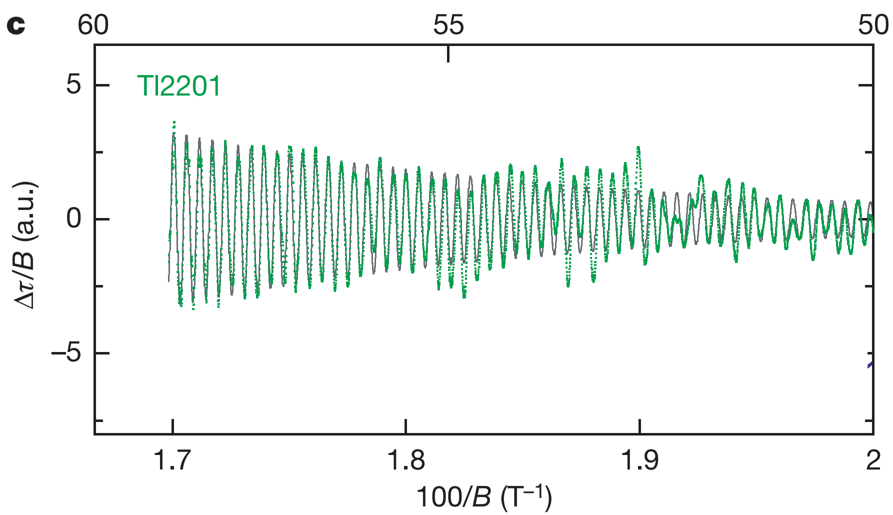
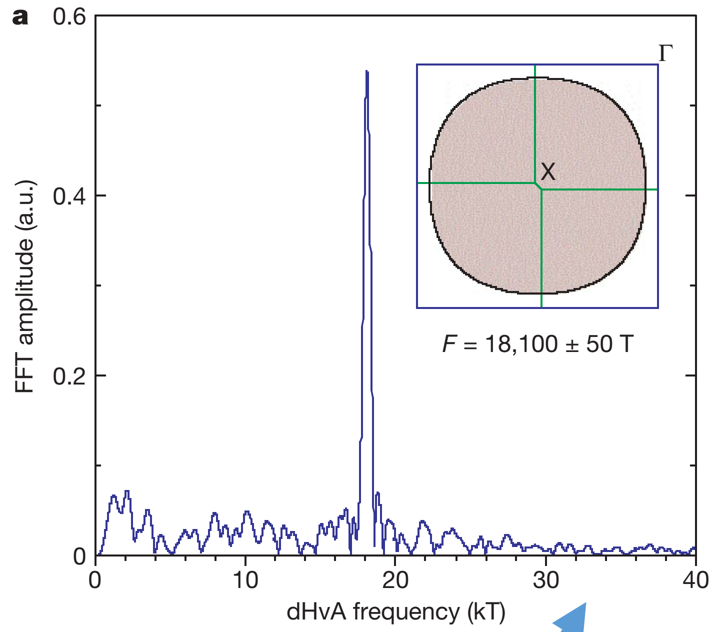
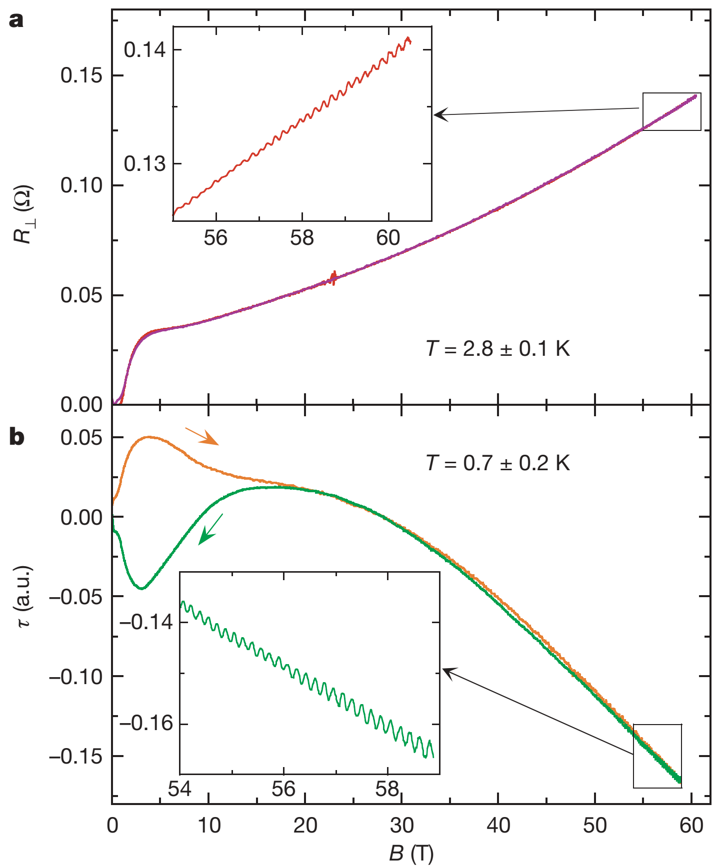


QUANTUM OSCILLATIONS:

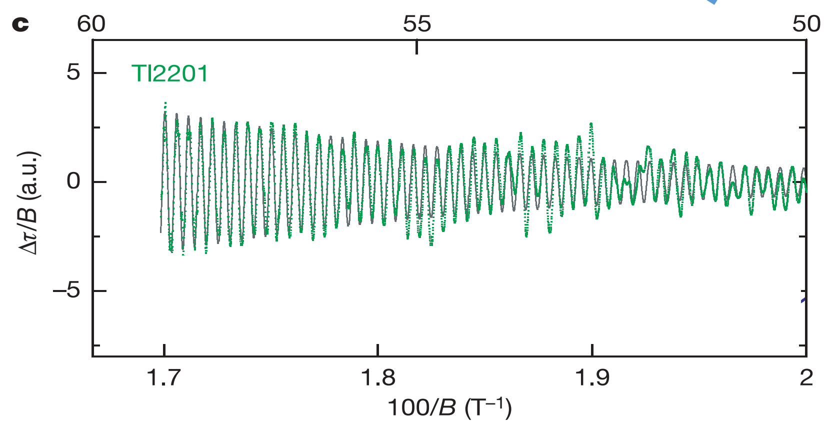
(c) Fourier Transform



(a) RAW DATA



(b) OSCILLATIONS VERSUS 1/B

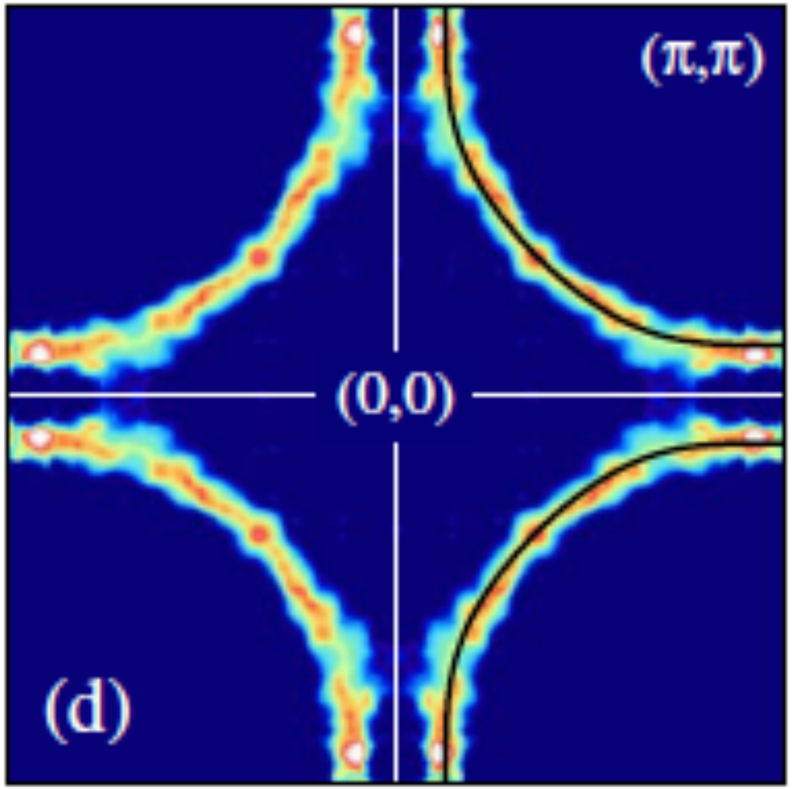


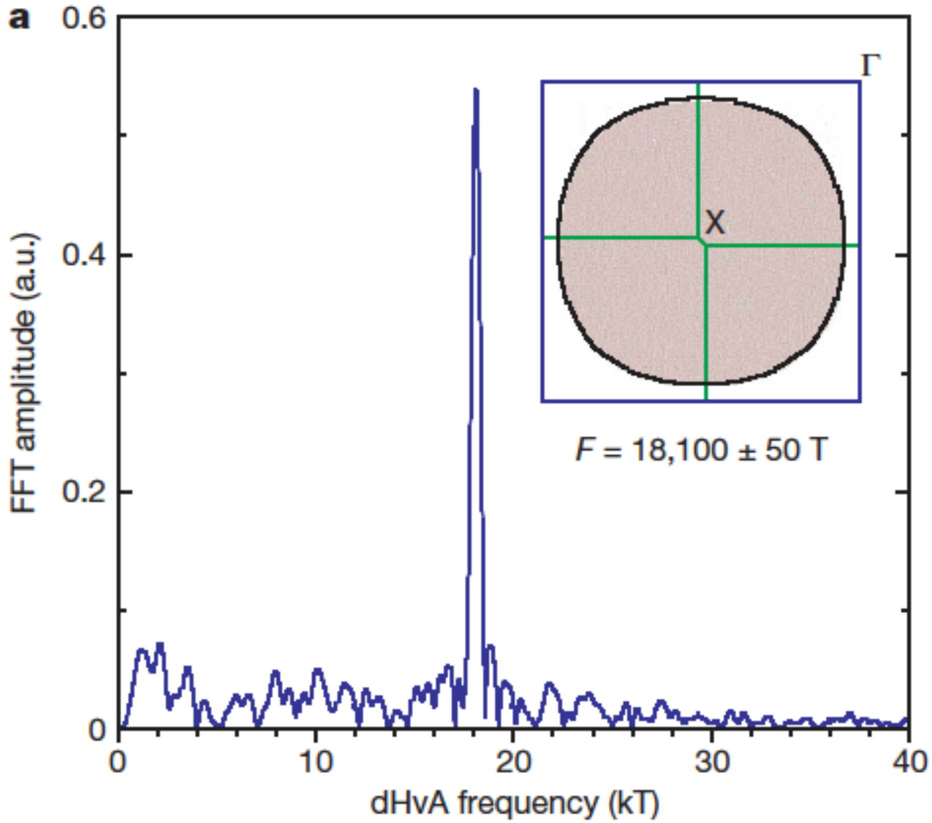
Nature **455**, 952 (2008)

$Tl_2Ba_2CuO_{6+x}$

Fermi surface:

ARPES vs Quantum Oscillations

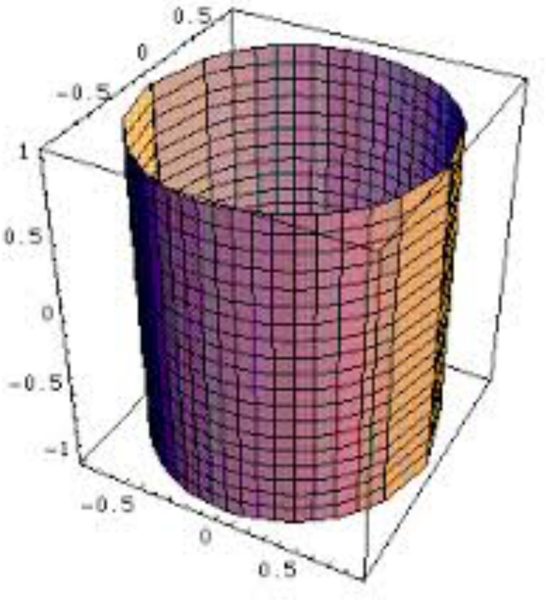


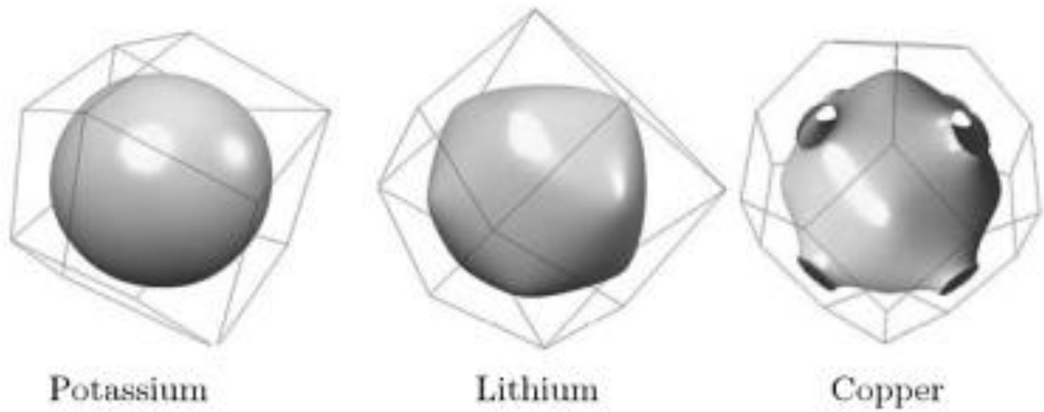


PRL **95**, 077001 (2005)
Data taken @ Swiss Light Source

Nature 455, 952 (2008)
$Tl_2Ba_2CuO_{6+y}$ (Tl2201)

2D and 3D Fermi surfaces





QUANTUM OSCILLATIONS: Gold

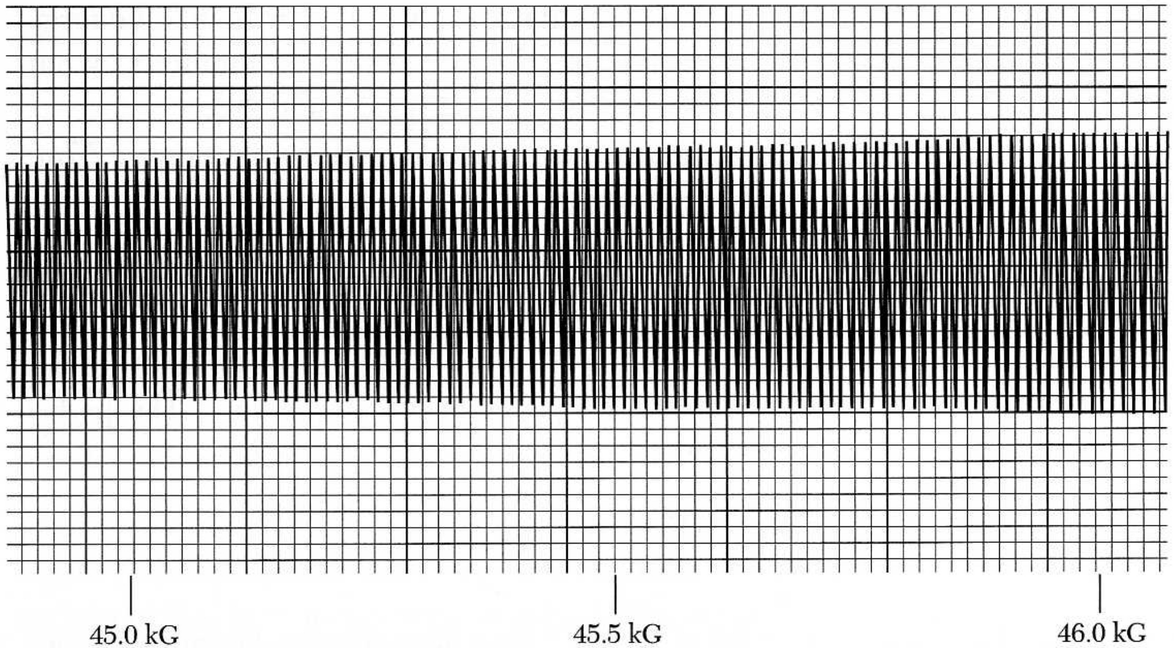


Figure 31 De Haas-van Alphen effect in gold with **B** || [110]. The oscillation is from the dog's bone orbit of Fig. 30. The signal is related to the second derivative of the magnetic moment with respect to field. The results were obtained by a field modulation technique in a high-homogeneity superconducting solenoid at about 1.2 K. (Courtesy of I. M. Templeton.)

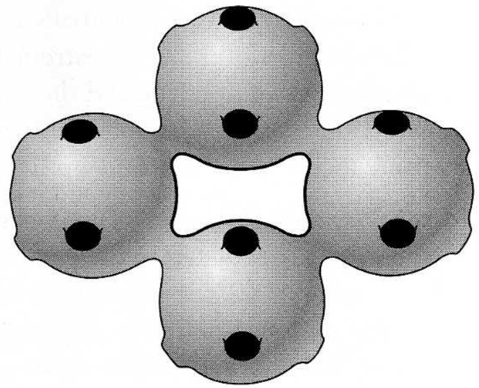
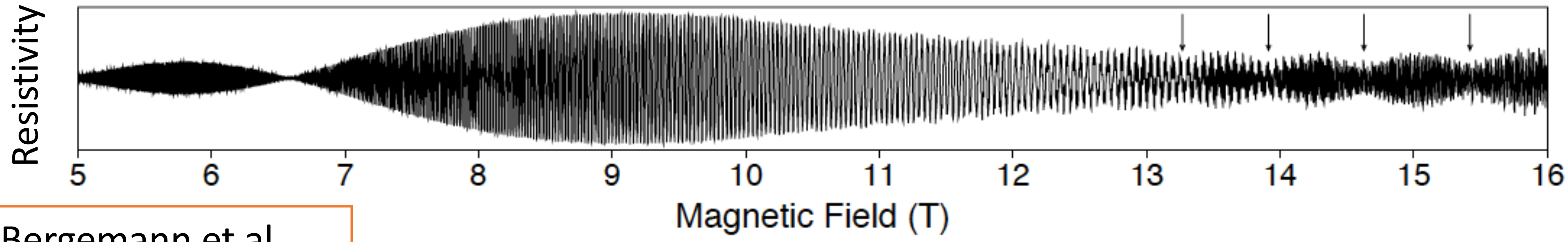
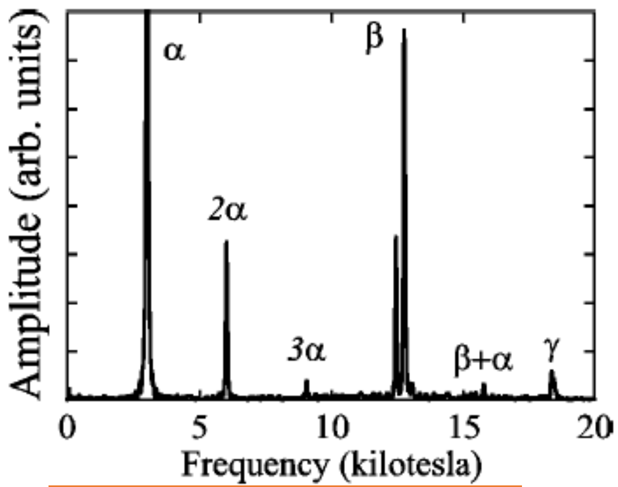


Figure 30 Dog's bone orbit of an electron on the Fermi surface of copper or gold in a magnetic field. This orbit is classified as holelike because the energy increases toward the interior of the orbit.

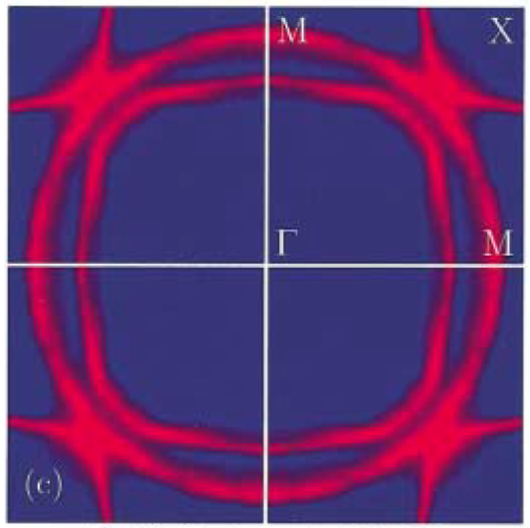
Multi – band metals



Bergemann et al,
PRL 84, 2662 (2000)

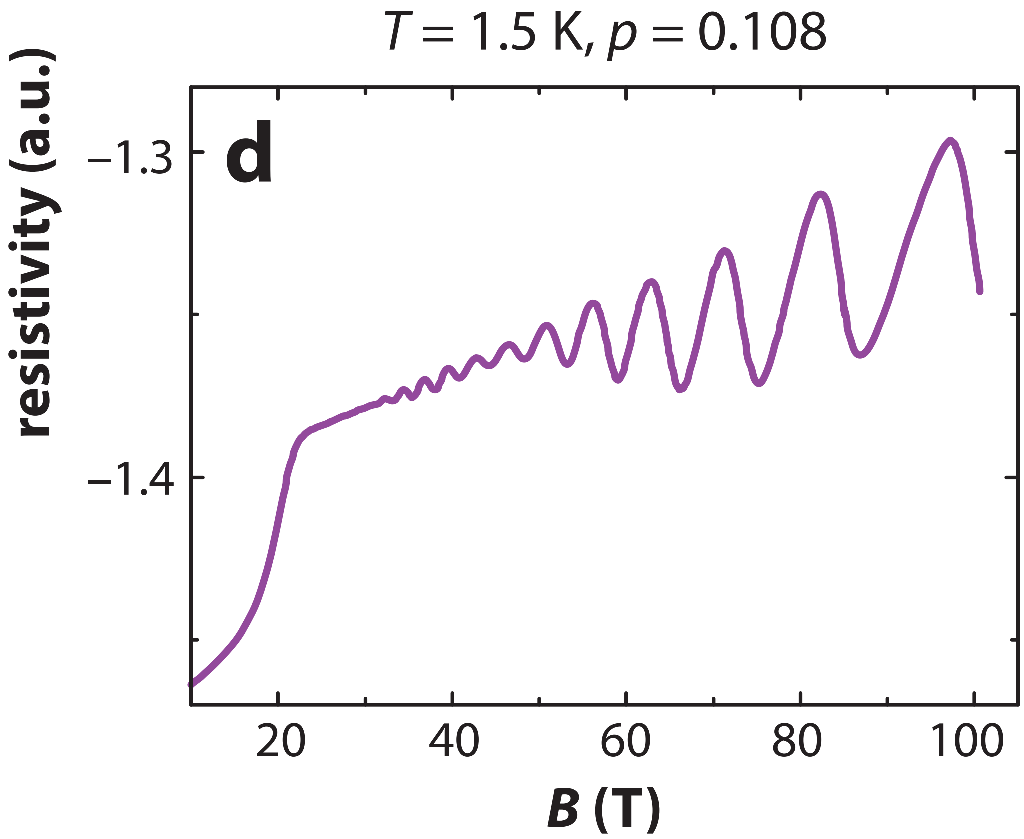


A.P. Mackenzie et al,
JPSJ 67, 385 (2003)



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

QUANTUM OSCILLATIONS:



OSCILLATION AMPLITUDE

$$\propto \; e^{\left(\frac{-\pi\hbar k_F}{eB\ell}\right)}$$

Where ℓ = mean free path

Resistivity measurement of a high-temperature superconductor: $YBa_2Cu_3O_{6.51}$ (YBCO)

http://www.annualreviews.org/doi/pdf/10.1146/annurev-conmatphys-030212-184305

QUANTUM OSCILLATIONS:

Temperature dependence

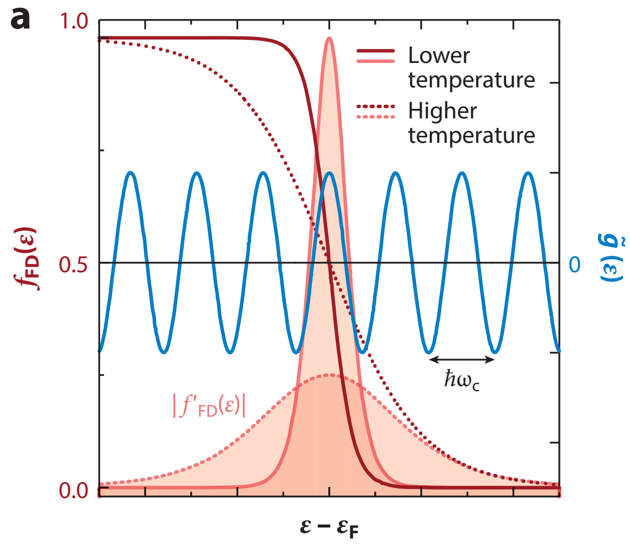
Thermal Condition:

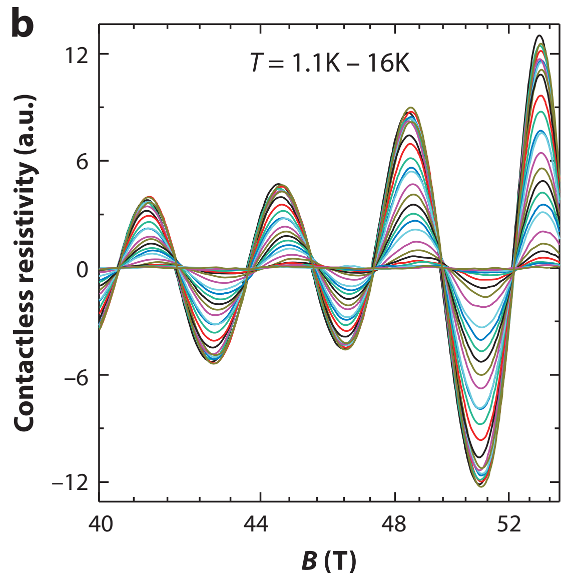
$$\hbar\omega_c > k_B T$$

Landau level splitting > thermal energy

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

Temperature dependence of the oscillatory amplitude yield information about the electronic mass.



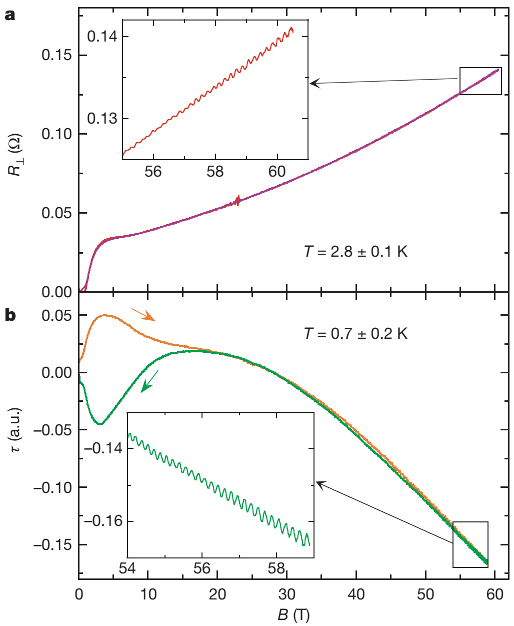


annurev-conmatphys-030212-184305

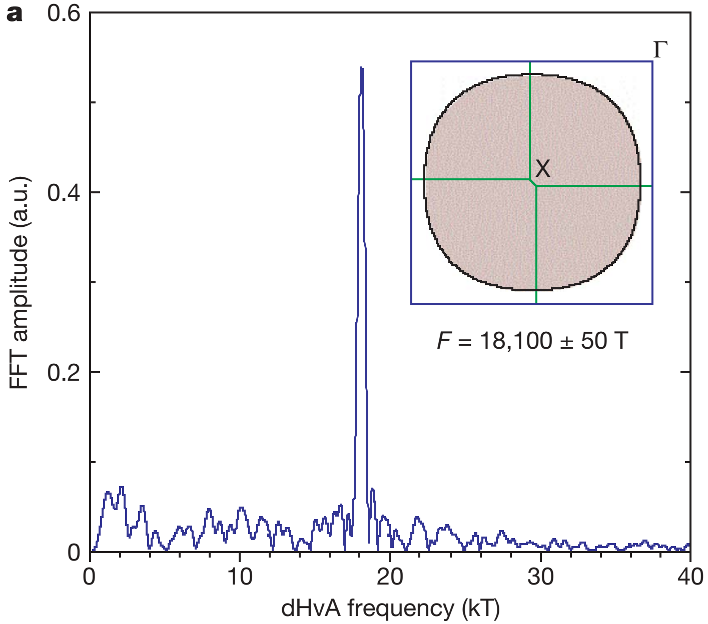
Electronic Mass

(1) Quantum Oscillation experiments:

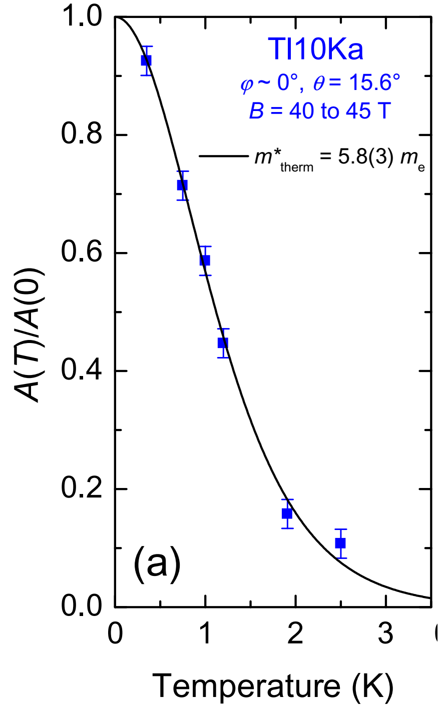
(a) RAW DATA



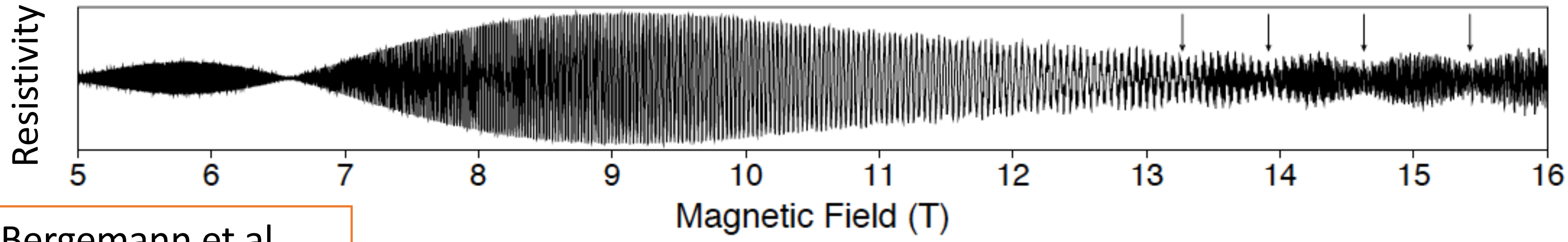
(b) Fourier Transform



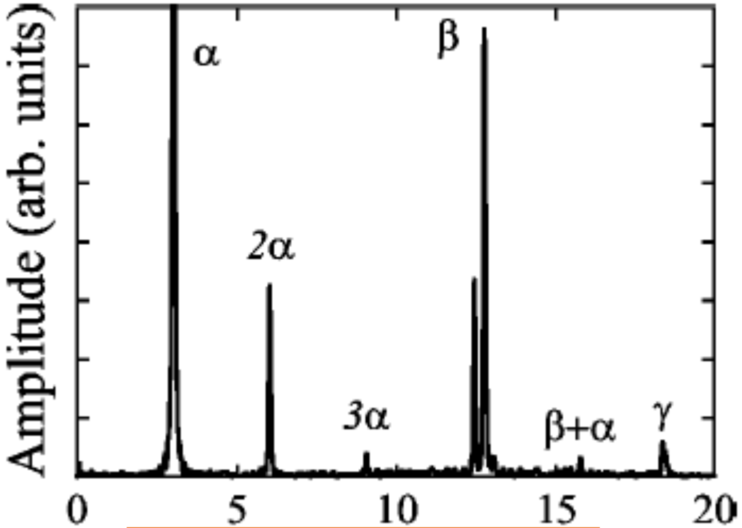
(c) T-dependence



Multi – band metals: Sr_2RuO_4



Bergemann et al, PRL 84, 2662 (2000)



A.P. Mackenzie et al, JPSJ 67, 385 (2003)

TABLE II. Summary of quasiparticle parameters of Sr_2RuO_4.

Fermi-surface sheet	α	β	γ
Character	Holelike	Electronlike	Electronlike
k_F ($Å^{-1}$)[a]	0.304	0.622	0.753
m^* (m_e)[b]	3.3	7.0	16.0

A.P. Mackenzie et al, RMP 75, 657 (2003)

Quantum Oscillation (QO) experiments