Second semester Grading: homework: 60% term report: 40%

Part IV: ELECTRON TRANSPORT

Chapter 16: Dynamics of Bloch Electrons

Chapter 17: Transport Phenomena and Fermi Liquid Theory

Chapter 18: Microscopic Theories of Conduction

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Chapter 23: Optical Properties of Metals and Inelastic Scattering Part VI: MAGNETISM

Chapter 24: Classical Theories of Magnetism and Ordering

Chapter 25: Magnetism of Ions and Electrons

Chapter 26: Quantum Mechanics of Interacting Magnetic Moments

Chapter 27: Superconductivity

Chap 16 Dynamics of Bloch electrons

- Classical electron dynamics: Drude model
- Semiclassical electron dynamics
 - Effective mass, Bloch oscillation, Zener tunneling
- Quantizing semiclassical dynamics
 - Wannier-Stark ladders, de Haas-van Alphen effect



Drude theory of electrical transport (1900)

Classical theory (\rightarrow)

$$m\frac{d\langle \vec{v} \rangle}{dt} = -e\vec{E} - m\frac{\langle \vec{v} \rangle}{\tau}$$
$$\rightarrow \langle \vec{v} \rangle = -\frac{e\tau}{m}\vec{E} \quad \text{at steady state}$$

- The source of resistance comes from electron scattering with defects and phonons.
- If these two types of scatterings are not related, then

$$\frac{1}{\tau} = \frac{1}{\tau_i} + \frac{1}{\tau_{ph}(T)}$$
 (Matthiessen's rule)

• Current density $\vec{j} = (-e)n\langle \vec{v} \rangle = \frac{ne^2\tau}{m}\vec{E} = \sigma\vec{E}$ conductivity or $\vec{E} = \rho\vec{j}$ resistivity

Determine the scattering time from measured resistivity ρ

- At room temp $\rho_{Cu} = 1.7 \times 10^{-8} \Omega m$ the electron density $n = 8.5 \times 10^{28} m^{-3}$ $\rightarrow \tau = m/\rho ne^2 = 2.5 \times 10^{-14} s$
- Fermi velocity of copper $1.6 \times 10^6 ms^{-1}$ mean free path $\ell = v_F \tau = 40$ nm
- For a very pure Cu crystal at 4K, the resistivity reduces by a factor of 100000, which means ℓ increases by the same amount ($\ell = 0.4$ cm). This cannot be explained using the classical theory.

$$\rho = \rho_i + \rho_{ph}(T) = \frac{m}{ne^2} \frac{1}{\tau_i} + \frac{m}{ne^2} \frac{1}{\tau_{ph}(T)}$$

• For a crystal without any defect, the only resistance comes from phonon. Therefore, at very low T, the electron mean free path theoretically can be infinite



Thermal conduction in metal

Both electron and phonon can carry thermal energy In a metal, electrons are dominant

heat current density (classical theory)



Lorentz number

L=2.45×10⁻⁸ watt-ohm/deg²

$L imes 10^8$ watt-ohm/deg ²			$L imes 10^8 ext{ watt-ohm/deg}^2$		
Metal	0°C	100°C	Metal	0°C	100°C
Ag	2.31	2.37	Pb	2.47	2.56
Au	2.35	2.40	Pt	2.51	2.60
Cd	2.42	2.43	Sn	2.52	2.49
Cu	2.23	2.33	W	3.04	3.20
Mo	2.61	2.79	Zn	2.31	2.33

Table 5 Experimental Lorenz numbers

Semiclassical electron dynamics

Consider a wave packet with average location r and wave vector k, then

$$\begin{cases} \dot{\vec{r}}(\vec{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}} \\ \hbar \dot{\vec{k}} = q \left(\vec{E} + \frac{\dot{\vec{r}}(\vec{k})}{c} \times \vec{B} \right) \end{cases}$$

Derivation neglected here

• Notice that *E* is the external field, which does not include the lattice field. The effect of lattice is hidden in $\varepsilon_n(k)$!

Range of validity

• This looks like the usual Lorentz force eq. But It is valid only when Interband transitions can be neglected. (One band approximation)

$$eEa << \varepsilon_g \sqrt{\frac{\varepsilon_g}{\varepsilon_F}} \qquad \qquad \text{May not be valid in small gap or heavily} \\ \text{doped semiconductors, but} \\ \text{``never close to being violated in a metal''} \\ \hbar \omega_c << \varepsilon_g \sqrt{\frac{\varepsilon_g}{\varepsilon_F}}, \quad \hbar \omega_c \cong 1.16 \cdot 10^{-4} \left[B / T \right] \text{ eV}$$

- E and B can be non-uniform in space, but they have to be much smoother than the lattice potential.
- E and B can be oscillating in time, but with the condition $\hbar\omega \ll \varepsilon_g$

Effective mass of a Bloch electron

The electron near band bottom is like a free electron

$$\varepsilon(\vec{k}) = \varepsilon_0 + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \varepsilon(\vec{k})}{\partial k_i \partial k_j} k_i k_j + O(k^3) \approx \varepsilon_0 + \frac{1}{2} \sum_{i,j} \left(\frac{1}{m^*}\right)_{ij} p_i p_j$$

effective mass matrix (symmetric) $\left(\frac{1}{m^*}\right)_{ij} \equiv \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(\vec{k})}{\partial k_i \partial k_j}$

- For a spherical FS, $m_{ij}^*=m^* \delta_{ij}$, only one m^* is enough.
- In general, electron in a flatter band has a larger m^*

•
$$a_i = \frac{d}{dt} \upsilon_i = \frac{d}{dt} \frac{d\varepsilon}{\hbar dk_i} = \sum_j \frac{d^2 \varepsilon}{\hbar dk_i dk_j} \dot{k}_j = \sum_i (m^{*-1})_{ij} \hbar \dot{k}_j$$

or $m^* \vec{a} = \hbar \dot{\vec{k}}$

• If ε (k) is \bigwedge (e.g. at the top of a valence band) then $m^*<0$

For an ellipsoidal FS, there can be at most three different m^* s Eg. the FS of Si is made of six identical ellipsoidal pockets



For Si, $\varepsilon_g = 1.1 \text{ eV}$, $m_L = 0.9 \text{ m}$, $m_T = 0.2 \text{ m}$

Bloch electron in an uniform electric field

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{E} \to \hbar \vec{k}(t) = -e\vec{E}t$$

Energy dispersion (periodic zone scheme, 1D)



- In a DC electric field, the electrons decelerate and reverse its motion at the BZ boundary.
- A DC bias produces an AC current ! (called Bloch oscillation)

• Why the oscillation is not observed in ordinary crystals?

To complete a cycle (*a* is the lattice constant),

 $eET/\hbar = 2 \pi /a \rightarrow T=h/eEa$

For $E=10^4$ V/cm, and a=1 A, $T=10^{-10}$ sec

But electron collisions take only about 10⁻¹⁴ sec.

. a Bloch electron cannot get to the zone boundary without de-phasing.

To observe it, one needs

• a stronger E field \rightarrow but only up to about 10⁶ V/cm (for semicond)

• a larger $a \rightarrow$ use superlattice (eg. a = 100 A)

• reduce collision time \rightarrow use crystals with high quality (Mendez et al, PRL, 1988)

• Bloch oscillators generate THz microwave: frequency $\sim 10^{12-13}$, wave length $\lambda \sim 0.01$ mm - 0.1mm (Waschke et al, PRL, 1993)

Quantization of Bloch oscillations: Wannier-stark ladders



Mendez and Bastard, Phys Today 1993

+3

1.70

Zener tunneling

• One band approximation

$$\psi_{n\vec{k}} \to \psi_{n\vec{k}(t)}, \quad \vec{k}(t) = \vec{k}_0 - \frac{e}{\hbar}\vec{E}t$$
$$H\psi_{n\vec{k}(t)} = \varepsilon_{n\vec{k}(t)}\psi_{n\vec{k}(t)}$$

• Beyond 1-band approx.

$$\begin{split} \left| \psi(t) \right\rangle &= \sum_{n} C_{n}(t) \left| \psi_{nk(t)} \right\rangle \\ H \left| \psi(t) \right\rangle &= i\hbar \frac{\partial}{\partial t} \left| \psi(t) \right\rangle \\ \rightarrow \varepsilon_{nk(t)} C_{n} &= i\hbar \frac{dC_{n}}{dt} - ie\vec{E} \cdot \sum_{n'} C_{n'} \left\langle \psi_{nk(t)} \right| \frac{\partial \psi_{n'k(t)}}{\partial \vec{k}} \right\rangle \end{split}$$

• To simplify, consider only 2 bands, with $C_1(0)=1$, $C_2(0)=0$, then

$$\begin{cases} \varepsilon_1 C_1 = i\hbar \dot{C}_1 - ieC_1 \vec{E} \cdot \langle \psi_1 | \frac{\partial \psi_1}{\partial \vec{k}} \rangle - ieC_2 \vec{E} \cdot \langle \psi_1 | \frac{\partial \psi_2}{\partial \vec{k}} \rangle \\ \varepsilon_2 C_2 = i\hbar \dot{C}_2 - ieC_1 \vec{E} \cdot \langle \psi_2 | \frac{\partial \psi_1}{\partial \vec{k}} \rangle - ieC_2 \vec{E} \cdot \langle \psi_2 | \frac{\partial \psi_2}{\partial \vec{k}} \rangle \\ \sim O(E^2), \text{ neglect.} \end{cases}$$



• To 0th order

$$C_1^0(t) = \exp\left(-\frac{i}{\hbar}\int_0^t dt \, \varepsilon_{1k(t')}\right)$$

Let

$$C_2(t) = \alpha(t) \exp\left(-\frac{i}{\hbar} \int_0^t dt' \varepsilon_{2k(t')}\right)$$

then

$$\frac{d\alpha}{dt} \approx \frac{e}{\hbar} \vec{E} \cdot \left\langle \psi_2 \right| \frac{\partial \psi_1}{\partial \vec{k}} \right\rangle \exp\left[-\frac{i}{\hbar} \int_0^t dt \left(\varepsilon_{1k(t)} - \varepsilon_{2k(t)}\right)\right]$$

• Assume
$$\frac{e}{\hbar}\vec{E} \cdot \langle \psi_2 | \frac{\partial \psi_1}{\partial \vec{k}} \rangle \equiv \Delta_{21}$$
 is roughly independent of t
(compared to the exponential)
$$\begin{cases} \varepsilon_1 = \varepsilon_v^0 - \frac{\hbar^2 k^2}{2m_v^3} \\ \varepsilon_2 = \varepsilon_c^0 + \frac{\hbar^2 k^2}{2m_c^3} \end{cases} \rightarrow \varepsilon_2 - \varepsilon_1 = \varepsilon_g + \frac{\hbar^2 k^2}{2\mu}, \quad \frac{1}{\mu} \equiv \frac{1}{m_v^3} + \frac{1}{m_c^3} \end{cases}$$
$$\rightarrow \alpha(T) \cong \Delta_{21} \int_0^T dt \exp\left[\frac{i}{\hbar} \int_0^t dt' \left(\varepsilon_g + \frac{\hbar^2 k(t')^2}{2\mu}\right)\right] \end{cases}$$

• Extrema of $F(t)$ is at $= F(t)$
 $\frac{d}{dt} \int_0^t dt' \cdots = 0$
 $\rightarrow \varepsilon_g + \frac{\hbar^2 k(\tau)^2}{2\mu} = 0$
 $\alpha \cong \Delta_{21} \exp\left[\frac{i}{\hbar} \int_0^\tau dt' \left(\varepsilon_g + \frac{\hbar^2 k(t')^2}{2\mu}\right)\right]$
 $q \equiv k(\tau)$
 $\cdots = \Delta_{21} \exp\left[-\frac{2i}{3eE} \varepsilon_g q\right] = \Delta_{21} \exp\left[-\frac{2}{3} \frac{\varepsilon_g^{3/2}}{2E} \frac{\sqrt{2\mu}}{\hbar}\right] \sim \exp(-10^3)$
 \therefore one-hand approx is never close to being violated in metals

... one-band approx. is never close to being violated in metals





Bloch electron in an uniform magnetic field

$$\hbar \frac{d\vec{k}}{dt} = -e \frac{\vec{v}}{c} \times \vec{B}, \quad \vec{v}_k = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$$
$$\rightarrow \vec{k} \cdot \vec{B} = 0, \quad \vec{k} \cdot \vec{v}_k = \frac{1}{\hbar} \frac{d \varepsilon(\vec{k})}{dt} = 0$$

Therefore, 1. Change of *k* is perpendicular to the *B* field, k_{\parallel} does not change and 2. ε (*k*) is a constant of motion

This determines uniquely the electron orbit on the FS



• For a spherical FS, it just gives the usual cyclotron orbit

• For a connected FS, there might be open orbits

Cyclotron orbit in real space

The above analysis gives us the orbit in k-space. What about the orbit in r-space?

$$\hbar \vec{k} = -\frac{e}{c} \vec{r} \times \vec{B} \rightarrow \vec{r} = -\frac{\hbar c}{eB^2} \vec{B} \times \vec{k} + \vec{r}_{\parallel}$$
$$\rightarrow \vec{r}_{\perp}(t) - \vec{r}_{\perp}(0) = -\frac{\hbar c}{eB} \hat{B} \times [\vec{k}(t) - \vec{k}(0)]$$



- r-orbit is rotated by 90 degrees from the k-orbit and scaled by $\hbar c/eB \equiv \lambda_B^2$
- magnetic length $\lambda_B = 256 \text{ A at } B = 1 \text{ Tesla}$

De Haas-van Alphen effect (1930)

In a high magnetic field, the magnetization of a crystal oscillates as the magnetic field increases

Similar oscillations are observed in other physical quantities, such as

- magnetoresistivity (Shubnikov-de Haas effect, 1930)
- specific heat
- sound attenuation
- ... etc





Basically, they are all due to the quantization of electron energy levels in a magnetic field (Landau levels, 1930)

Quantization of the cyclotron orbits

• In the discussion earlier, the radius of the cyclotron orbit can be varied continuously, but due to their wave nature, the orbits are in fact quantized.

• Bohr-Sommerfeld quantization rule (Onsager, 1952)

for a closed cyclotron orbit,

$$\oint d\vec{r} \cdot \vec{p} = \left(n + \frac{1}{2}\right)h$$
Why (q/c)A is momentum
of field? See Kittel App. G.
where $\vec{p} = \vec{p}_{kin} + \vec{p}_{field} = \hbar \vec{k} + \frac{q}{c} \vec{A}, q = -e$

$$\oint d\vec{r} \cdot \hbar \vec{k} = -\frac{e}{c} \oint d\vec{r} \cdot \vec{r} \times \vec{B} = 2\frac{e}{c} \Phi$$
Gauge dependence prob?
Not worse than the gauge
dependence in qV.

$$\frac{e}{c} \oint d\vec{r} \cdot \vec{A} = \frac{e}{c} \Phi$$

$$\Rightarrow \Phi_n = \left(n + \frac{1}{2}\right) \frac{hc}{e}$$

• the *r*-orbit is quantized in units of

flux quantum: $hc/e \equiv \Phi_0 = 4.14 \cdot 10^{-7} \text{ gauss} \cdot \text{cm}^2$

• Since a *k*-orbit (circling an area *S*) is closely related to a *r*-orbit (circling an area *A*), the orbits in *k*-space are also quantized

$$S_n = \frac{A_n}{\lambda_B^4} = \left(n + \frac{1}{2}\right) \frac{2\pi e}{\hbar c} B \qquad \text{(Onsager, 1952)}$$

• Energy of the orbit (for a spherical FS)

$$\varepsilon_n = \frac{\left(\hbar k_n\right)^2}{2m} = \left(n + \frac{1}{2}\right)\hbar\omega_c$$
 Landau levels

• Degeneracy of the Landau level (assuming spin degeneracy)

$$D = 2\frac{2\pi eB / \hbar c}{(2\pi / L)^2}$$
$$= \frac{2BL^2}{hc / e} = 2\frac{\Phi_{\text{sample}}}{\Phi_0}$$

 \bullet Notice that the k_z direction is not quantized

$$\varepsilon_{n,k_z} = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m}$$



In the presence of *B*, the Fermi sphere becomes a stack of cylinders.

Note:

- Fermi energy \sim 1 eV, cyclotron energy \sim 0.1 meV (for B = 1 T)
 - . . the number of cylinders usually \sim 10000

need low T and high B to observe the fine structure

• Radius of cylinders $\propto \sqrt{B}$, so they expand as we increase *B*. The orbits are pushed out of the FS one by one.



• Successive B's that produce orbits with the same area:

 $S_n = (n+1/2) 2 \pi e/\hbar c B$ $S_n' = (n-1/2) 2 \pi e/\hbar c B' (B' > B)$

$$\Rightarrow S\left(\frac{1}{B} - \frac{1}{B'}\right) = \frac{2\pi e}{\hbar c}$$

equal increment of 1/B reproduces similar orbits

Oscillation of the DOS at the Fermi energy



- The number of states at E_F are highly enhanced when there are extremal orbits on the FS
- There are extremal orbits at regular interval of 1/*B*
- This oscillation in 1/B can be detected in any physical quantity that depends on the DOS

• Number of states are proportional to areas of cylinders in energy shell



Determination of FS



• In the dHvA experiment of silver, the two different periods of oscillation are due two different extremal orbits

Recall that
$$S_e\left(\frac{1}{B} - \frac{1}{B'}\right) = \frac{2\pi e}{\hbar c}$$

• Therefore, from the two periods we can determine the ratio between the sizes of the "neck" and the "belly"



A₁₁₁(belly)/A₁₁₁(neck)=51



Bloch electron in crossed E and H fields (both uniform)

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{E} - e\frac{\dot{\vec{r}}}{c} \times \vec{B}$$
$$= -\frac{e}{c\hbar} \frac{\partial \tilde{\varepsilon}}{\partial \vec{k}} \times \vec{B}$$
where $\tilde{\varepsilon}(\vec{k}) = \varepsilon(\vec{k}) - \hbar \vec{k} \cdot \vec{w}, \vec{w} \equiv c \frac{E}{B} \hat{E} \times \hat{B}$



The 2nd term is usually very small compared to ε (k) So the effect is to tilt the band structure slightly (max along **w**, min \perp **w**), and earlier analysis about the cyclotron orbit still applies (not restricted to closed orbits).

Real space orbit

Current density $\vec{j}_{\perp} = -en\langle \dot{\vec{r}}_{\perp} \rangle$

If "all" orbits on the FS are closed, then

$$\dot{\vec{r}}_{\perp}
angle = e \frac{E}{B} \hat{E} \times \hat{B} \longrightarrow \vec{j}_{\perp} = -\frac{nec}{B} \hat{E} \times \hat{B}$$

This result is valid for different band structures!

ExB drift

(independent of the sign of charge)

Derivation of the semiclassical dynamics

(generalized version, only an outline. See Marder Sec. 16.4 for more)

1. Construct a wavepacket from one Bloch band that is localized in both the *r* and the *k* spaces.



2. Using the time-dependent variational principle to get the effective Lagrangian

$$\begin{split} L_{eff}\left(\vec{r}_{c},\vec{k}_{c};\vec{r}_{c},\vec{k}_{c}\right) &= \left\langle W\left|i\hbar\frac{\partial}{\partial t}-H\left|W\right\rangle\right.\\ &= &\hbar\vec{k}_{c}\cdot\vec{R}+\hbar\vec{k}_{c}\cdot\dot{\vec{r}}_{c}-\frac{e}{c}\vec{A}\cdot\dot{\vec{r}}_{c}-\varepsilon(\vec{r}_{c},\vec{k}_{c})\right. \end{split}$$



Berry connection

$$\vec{R}(\vec{k}) \equiv i \left\langle u_n \right| \frac{\partial}{\partial \vec{k}} \left| u_n \right\rangle$$

Wavepacket energy

$$\varepsilon(\vec{r},\vec{k}) = \varepsilon_0(\vec{k}) - e\phi(\vec{r}) + \frac{e}{2mc}\vec{L}(\vec{k})\cdot\vec{B}$$

Self-rotating angular momentum

$$\vec{L}(\vec{k}) = m \langle W | (\vec{r} - \vec{r}_c) \times \vec{v} | W \rangle$$

3. Using the L_{eff} to get the equations of motion

$$\begin{cases} \hbar \frac{d\vec{k}}{dt} = -e\vec{E} - \frac{e}{c}\vec{r} \times \vec{B} \\ \frac{d\vec{r}}{dt} = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}} - \vec{k} \times \vec{\Omega}(\vec{k}) \\ \varepsilon(\vec{k}) = \varepsilon_0(\vec{k}) - e\phi(\vec{r}) + \frac{e}{2mc}\vec{L}(\vec{k}) \cdot \vec{B} \end{cases}$$

Berry curvature

 $\vec{\Omega}(\vec{k}) = \nabla \times \vec{R}(\vec{k})$

Three basic quantities of a Bloch electron:

- Bloch energy $\mathcal{E}_0(\vec{k})$
- Berry curvature,
 (~an effective B field in k-space)

 $\vec{\Omega}(\vec{k}) = i \left\langle \frac{\partial u}{\partial \vec{k}} \right| \times \left| \frac{\partial u}{\partial \vec{k}} \right\rangle$

• Angular momentum (in Rammal-Wilkinson form)

$$\vec{L}(\vec{k}) = \frac{m}{i\hbar} \left\langle \frac{\partial u}{\partial \vec{k}} \right| \times \left(E_0 - H \right) \left| \frac{\partial u}{\partial \vec{k}} \right\rangle$$

Two "kinetic" momenta $m\vec{v}$ and $\hbar\vec{k}$

Chang and Niu, PRB 1996 Sundaram and Niu, PRB 1999