Fermi surfaces and metals

• Higher BZ, Fermi surface
• Semiclassical electron dynamics (see Chap 8)
• de Haas-van Alphen effect

(the Sec on “Calculation of energy bands” will be skipped)
• Beyond 1\textsuperscript{st} Brillouin zone (for square lattice)

• Reduced zone scheme

\begin{align*}
\text{Every Brillouin zone has the same area} \\
\text{At zone boundary, } \mathbf{k} \text{ satisfies the Laue condition } \mathbf{k} \cdot \mathbf{G} = \frac{\mathbf{G}}{2} \\
\text{Bragg reflection at zone boundaries produce energy gaps}
\end{align*}
Beyond the 1\textsuperscript{st} Brillouin zone

BCC crystal (e.g. Alkali metal)

FCC crystal (e.g. noble metal)
Fermi surface for 2D *empty* square lattice

- For a *monovalent* element, the Fermi wave vector
  \[ k_F = \sqrt{2\pi/a} \]

- For a *divalent* element
  \[ k_F = \sqrt{4\pi/a} \]

- For a *trivalent* element
  \[ k_F = \sqrt{6\pi/a} \]

- Distortion due to lattice potential

\[ r_2^2 - r_1^2 \propto |U_G| \]

Chap 9 of A+M, Prob.1
A larger Fermi sphere (empty lattice)

- Extended zone scheme
- Reduced zone scheme
- Periodic zone scheme

Again if we turn on the lattice potential, then the corners become rounded.
• The first BZ of bcc lattice (its reciprocal lattice is fcc lattice)

• The first BZ of fcc lattice (its reciprocal lattice is bcc lattice)
Fermi surface of alkali metal (monovalent, BCC)

\[ k_F = (3\pi^2 n)^{1/3} \]
\[ n = \frac{2}{a^3} \]
\[ \rightarrow k_F = (3/4\pi)^{1/3}(2\pi/a) \]
\[ \Gamma_N = (2\pi/a)[1/2]^{1/2} \]
\[ \therefore k_F = 0.877 \Gamma_N \]

Percent deviation of \( k \) from the free electron value < 1% (mostly)
Fermi surface of **noble metal** (monovalent, FCC)

\[
k_F = (3\pi^2 n)^{1/3}, \\
n = \frac{4}{a^3} \\
\rightarrow k_F = (3/2\pi)^{1/3}(2\pi/a) \\
\Gamma L = ___ \\
k_F = ___ \Gamma L
\]
Fermi surface of Al (trivalent, FCC)

$1^{\text{st}}$ BZ

$2^{\text{nd}}$ BZ

$3^{\text{rd}}$ BZ

- Empty lattice approximation

- Actual Fermi surface

Ref: Fermi surface database
The Fermi Surface Database
(click icons)
• Higher BZ, Fermi surface
• Semiclassical electron dynamics
• de Haas-van Alphen effect

In what follows, CGS is used. To convert to SI, just set $c=1$. 
Classical picture
(Drude, Lorentz)
• Particle (localized)

Electron scattering

Quantum picture
(Sommerfeld, Bloch)
• Bloch wave (extended)

Semiclassical picture
• Wavepacket

(Superposition of Bloch states)
Semiclassical electron dynamics (Kittel, Chap 8, p.192)

Equation of motion for a wave packet in band-\( n \) with average location \( r \) and wave vector \( k \):

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

Derivation neglected

- \( E \) is the external field, not including the lattice field.
  The effect of lattice is hidden in \( \varepsilon_n(\vec{k}) \)!

Range of validity (App. J of A+M)
- It is valid only when inter-band transition can be neglected.

That is, the electron moves in one band only.
(One band approximation)

- \( E(\vec{r},t) \) and \( B(\vec{r},t) \) can vary in space-time, as long as characteristic length \( \lambda \gg a \), and \( \hbar \omega \ll \varepsilon_g \).
Bloch electron in an uniform electric field (Kittel, p.197)

\[ \hbar \frac{dk}{dt} = -e\vec{E} \rightarrow \hbar \vec{k}(t) = -e\vec{E}t \]

- Energy dispersion (1D, periodic zone scheme)

- 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)
• Partially filled band without scattering

\[ \sum_{\text{filled states}} -\frac{eE}{\hbar} \]

\[ \varepsilon(k) \]

• Partially filled band with scattering time \( \tau \)

\[ \varepsilon(k) \]

\[ -\frac{eE\tau}{\hbar} \]

• Current density

\[ j = (-e) \frac{1}{V} \sum_{k \in \text{filled states}} v_k \]
• Why the oscillation is not observed in ordinary crystal?
The electron has to maintain phase coherence.
To complete a cycle \((a\) is the lattice constant),
\[
e\frac{ET}{\hbar} = \frac{2\pi}{a} \rightarrow T = \frac{\hbar}{eEa}
\]
For \(E=10^4\) V/cm, and \(a=1\) A, \(T=10^{-10}\) s.
But electron collisions take only about \(10^{-14}\) s.
\(\therefore\) a Bloch electron cannot reach zone boundary without de-phasing.
To observe it, one needs
• a stronger \(E\) field \(\rightarrow\) but only up to about \(10^6\) 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 \(\text{THz microwave:}\)
  frequency \(\sim 10^{12-13}\),
  wave length \(\lambda \sim 0.01\) mm - 0.1mm
(Waschke et al, PRL, 1993)
Quantization of Bloch oscillation:

Wannier-stark ladders \( n\hbar \omega \)

Mendez and Bastard, Phys Today 1993
Bloch electron in an uniform magnetic field

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

\[ \rightarrow \dot{\vec{k}} \cdot \vec{B} = 0, \quad \dot{\vec{k}} \cdot \vec{v}_k = \frac{1}{\hbar} \frac{d \varepsilon(\vec{k})}{dt} = 0 \]

Therefore, 1. Change of \( k \) is perpendicular to \( B \), \( k_\parallel \) does not change
and 2. \( \varepsilon(k) \) is a constant of motion

This determines uniquely an orbit on the FS (given I.C.):

- For a spherical FS, it just gives the cyclotron orbit.
- For a connected FS, there might be open orbit.
Cyclotron orbit in real space

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

\[
\dot{\hbar}k = -\frac{e}{c} \dot{r} \times \vec{B} \rightarrow \dot{r} = -\frac{\hbar c}{eB^2} \vec{B} \times \dot{k} + \dot{r}_\parallel
\]

\[
\rightarrow \vec{r}_\perp(t) - \vec{r}_\perp(0) = -\frac{\hbar c}{eB} \vec{B} \times [\vec{k}(t) - \vec{k}(0)]
\]

- \( r \)-orbit rotates by 90 degrees w.r.t the \( k \)-orbit and scaled by \( \hbar c/eB \equiv \lambda_B^2 \)
- \( \lambda_B = 256 \) A at \( B = 1 \) T. magnetic length.
• Higher BZ, Fermi surface
• Semiclassical electron dynamics
• de Haas-van Alphen effect
De Haas-van Alphen effect (1930)

In a strong 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

These are all due to the quantization of electron energy levels in a magnetic field (Landau levels, 1930)
• 1927 Pauli, paramagnetism (electron gas)
• 1928 Heisenberg, ferromagnetism (exchange interaction)
• 1930 Landau, diamagnetism (electron gas)

Along the way, he (Landau) noted that the diamagnetic moment should have a strong periodicity in the field.

... Landau himself despaired of observing this effect, suggesting in his paper that inhomogeneities would wash it out.  

\[ \hbar \omega \approx 1.16 \cdot 10^{-4} \left[ \frac{B}{T} \right] \text{ eV} \]
Quantization of cyclotron orbits

In the discussion earlier, the radius of a cyclotron orbit can be varied continuously, but the orbit should be quantized due to quantum effect.

- **Bohr-Sommerfeld quantization rule** (Onsager, 1952)
  for a *closed* cyclotron orbit,

\[
\oint d\vec{r} \cdot \vec{p} = \left( n + \frac{1}{2} \right) \hbar
\]

where \( \vec{p} = \vec{p}_{\text{kin}} + \vec{p}_{\text{field}} = \vec{\hbar}k + \frac{q}{c} \vec{A} \), \( q = -e \)

\[
\oint d\vec{r} \cdot \vec{\hbar}k = -\frac{e}{c} \oint d\vec{r} \cdot \vec{r} \times \vec{B} = 2\frac{e}{c} \Phi
\]

also

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

\[
\Rightarrow \Phi_n = \left( n + \frac{1}{2} \right) \frac{hc}{e}, \quad A_n = \frac{\Phi_n}{B} = \left( n + \frac{1}{2} \right) 2\pi\lambda_B^2
\]

- The flux through an \( r \)-orbit is quantized in units of
  flux quantum: \( \hbar c/e \equiv \Phi_0 = 4.14 \cdot 10^{-7} \) gauss \( \cdot \) 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 (Onsager, 1952)

\[
S_n = \frac{A_n}{\lambda_B^4} = \left( n + \frac{1}{2} \right) \frac{2\pi e}{\hbar c} B = \left( n + \frac{1}{2} \right) \frac{2\pi}{\lambda_B^2}
\]

• Energy of the orbit (for a spherical FS)

\[
\mathcal{E}_n = \frac{(\hbar k_n)^2}{2m} = \left( n + \frac{1}{2} \right) \hbar \omega_c
\]

Landau levels
Degeneracy of Landau level

\[ D = 2 \frac{2\pi eB / \hbar c}{(2\pi / L)^2} \]

\[
\text{spin} = 2 \frac{BL^2}{hc / e} = 2 \frac{\Phi_{\text{sample}}}{\Phi_0}
\]

Highly degenerate

In the presence of \( B \), the Fermi sphere becomes a stack of cylinders.

In 3D, the \( k_z \) direction is not quantized

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

- Fermi energy \( \sim 1 \text{ eV} \), cyclotron energy \( \sim 0.1 \text{ meV} \) (for \( B = 1 \text{ T} \))
- the number of cylinders \( \sim 10000 \)
- need low \( T \) and high \( B \) to observe the quantization.
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:

$$S_n = \frac{(n+1/2) 2\pi e}{\hbar c} B$$

$$S_{n-1}' = \frac{(n-1/2) 2\pi e}{\hbar c} B' \quad (B' > B)$$
Quantitative details (2D)

$\frac{D}{\partial B} = - \frac{\partial}{\partial B}$

$N=50$

$D \propto B$

Fermi surface

Semiclassical dynamics

de Haas-van Alphen effect
Oscillation of DOS at Fermi energy (3D)

On top of the variation in 2D, there is also the $k_z$ variation.

- Number of states in $d\varepsilon$ are proportional to area of cylinder in an energy shell.

- Number of states at $E_F$ is highly enhanced when there is extremal orbit on FS.
- There are extremal orbits (and enhanced DOS) at regular interval of $1/B$.
- This oscillation of DOS (in $1/B$) can be detected in any physical quantity that depends on DOS.
Extremal orbits for a cylindrical Fermi surface. The quantum oscillations can be approximated as a sum of oscillations from short cylindrical sections. At the “extremal orbits” (the gray ellipses) the oscillations from adjacent cylinders are nearly in phase (upper zoomed section, with the Landau levels shown as dashed gray lines), so there is a large contribution. At a non-extremal region (lower zoomed region) the oscillations from nearby cylindrical sections have different phase, so there is no net contribution. For a warped cylinder there are two extremal orbits, so the resulting oscillations have two contributions that beat against each other, as in a and b. At certain ‘magic angles’, as in c, the maximum and minimum orbits are identical in area, and the oscillations interfere constructively over the whole surface, giving rise to a large amplitude signal with no beats.
In the dHvA experiment of silver, the two different periods of oscillation are due to 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 "neck" and "belly".

\[ \frac{A_{111}(\text{belly})}{A_{111}(\text{neck})} = 27 \]

\[ \frac{A_{111}(\text{belly})}{A_{111}(\text{neck})} = 51 \]

\[ \frac{A_{111}(\text{belly})}{A_{111}(\text{neck})} = 29 \]
Determination of FS

- **dHvA**
- **ARPES** *(Angle-resolved photoemission spectroscopy)*
- **ACAR** *(Angular Correlation of Electron-Positron Annihilation Radiation)*
- ...

Fermi surface and electron momentum density of Copper (wiki)

F.Baumberger's webpage