#### OUTLINE

#### Para- and diamagnetism of metals

- Degenerate Fermi gas (eg: conduction electrons)
- Pauli paramagnetism of a non-interacting FG
- Quantization of a particle motion in the magnetic field
- Landau diamagnetism of a non-interacting FG
- de Haas-Van Alphen effect

#### QUANTUM STATES OF A FREE PARTICLE

Condsider a single particle in a cube  $L \times L \times L$  with periodic boundary conditions (PBC).

$$\widehat{H} = \frac{\widehat{\mathbf{p}}^2}{2m}$$

 $\left[\widehat{H},\widehat{\mathbf{p}}
ight]=0 \;\;\Rightarrow \;\;\;$  momentum  $\mathbf{p}$  is a good quantum number.

$$\mathbf{p} = \hbar \mathbf{k}$$
  $\varepsilon_{\mathbf{k}} = \frac{\hbar^2}{2m} \mathbf{k}^2$   $\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$ 

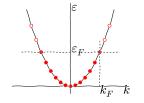
Periodic boundary conditions mean that

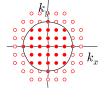
$$k_x, k_y, k_z = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \dots$$

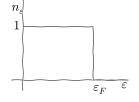
NB: in solids,  $\mathbf{k} \in \mathsf{Brillouin}$  zone

# Non-interacting Fermi gas, T=0

Pauli exclusion principle: one particle per state.  $\Rightarrow$  For N particles, all the states with  $\varepsilon < \varepsilon_F$  are filled, the states with  $\varepsilon > \varepsilon_F$  are empty.







Fermi energy  $\varepsilon_F$ Fermi momentum  $k_F$ Fermi surface (in **k** space)  $\varepsilon(\mathbf{k}) = \varepsilon_F$ 

# Non-interacting Fermi gas, T=0

What is the relation between  $\varepsilon_F$  and N?

In the limit of  $L \to \infty$ 

$$N = (2s+1) \int \frac{\mathrm{d}\mathbf{k}}{(2\pi/L)^d} \Theta(k_F - |\mathbf{k}|) \qquad (d = 3, s = 1/2)$$

$$= 2 \int_0^{k_F} \frac{4\pi k^2 \mathrm{d}k}{8\pi^3/V} = V \frac{k_F^3}{3\pi^2} \qquad \text{(volume } V = L^3\text{)}$$

$$k_F = (3\pi^2 N/V)^{1/3}$$
  $\varepsilon_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m} (3\pi^2 N/V)^{2/3}$ 



# Non-interacting Fermi gas, T = 0, cont'd

What is the energy of a Fermi gas at T=0 and B=0?

$$\frac{E}{N} = \frac{(2s+1)\int_{\text{FS}} \frac{\mathrm{d}\mathbf{k}}{(2\pi/L)^3} \varepsilon_k}{(2s+1)\int_{\text{FS}} \frac{\mathrm{d}\mathbf{k}}{(2\pi/L)^3}} = \frac{(2s+1)\int_{0}^{\kappa_F} \frac{4\pi k^2 \mathrm{d}k}{8\pi^3/V} \frac{\hbar^2 k^2}{2m}}{(2s+1)\int_{0}^{\kappa_F} \frac{4\pi k^2 \mathrm{d}k}{8\pi^3/V}}$$

$$= \frac{\hbar^2}{2m} \int_{\kappa_F}^{0} \frac{k^4 \mathrm{d}k}{k^2 \mathrm{d}k} = \frac{\hbar^2}{2m} \frac{k_F^5/5}{k_F^3/3} = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 = \frac{3}{5} \varepsilon_F$$

4 m b 4 m b 4 m b 4 m b 4 m b 4 m b 4 m b 4 m b 4 m b 4 m b 4 m b 6 m b

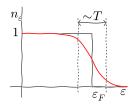
# Non-interacting Fermi gas, finite T

Fermi temperature  $k_B T_F = \varepsilon_F$ 

 $T\gg T_F$  Boltzmann gas (classical)

 $T \sim T_F$  degenerate gas (quantum)

In metals typically  $T_F \sim 1-10\,\mathrm{eV} \sim 10^4\,\mathrm{K}$ 



$$n_{\varepsilon} = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1}$$

Chemical potential  $\mu=\varepsilon_{F}$  at T=0 .  $(\mu/T\to-\infty$  as  $T\to\infty)$ 

Qualitatively: out of N electrons, only  $N(T/T_F)$  are "active",  $\Rightarrow$  paramagnetic susceptibility  $\chi \propto \frac{1}{T} \left( N \frac{T}{T_F} \right)$ 

# Intermezzo: Density of States (DOS)

Density of states (DOS) = # of states per unit energy interval. Depends on (i) the dimension of space,d, and (ii) the dispersion relation,  $\varepsilon_{\mathbf{k}}$ 

$$V \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^d} (\dots) = \int \mathrm{d}\varepsilon \, \mathcal{D}(\varepsilon) (\dots)$$

For example: d = 3,  $\varepsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$ 

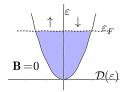
$$d\mathbf{k} = 4\pi k^2 dk$$
,  $k = \left(2m\varepsilon/\hbar^2\right)^{1/2} \Rightarrow$   
$$\mathcal{D}(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}$$

Note that in d = 3

$$\mathcal{D}(\varepsilon_F) = \frac{3}{2} \frac{N}{\varepsilon_F}$$

#### NON-INTERACTING FG: PARAMAGNETISM PAULI

Weak fields, degenerate gas:  $k_BT \ll \mu_BB \ll \varepsilon_F$  .



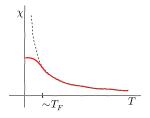
$$\begin{array}{c|c}
\uparrow & \varepsilon \downarrow \\
\hline
\mathbf{B} \neq 0 & \mathcal{D}(\varepsilon)
\end{array}$$

$$\begin{split} N_{\uparrow} &= \frac{1}{2} \int_{-\mu_B B}^{\varepsilon_F} \mathrm{d}\varepsilon \, \mathcal{D}(\varepsilon + \mu_B B) \quad \approx \frac{1}{2} \int_{0}^{\varepsilon_F} \mathrm{d}\varepsilon \, \mathcal{D}(\varepsilon) + \frac{1}{2} \mu_B B \, \mathcal{D}(\varepsilon_F) \\ N_{\downarrow} &= \frac{1}{2} \int_{\mu_B B}^{\varepsilon_F} \mathrm{d}\varepsilon \, \mathcal{D}(\varepsilon - \mu_B B) \quad \approx \frac{1}{2} \int_{0}^{\varepsilon_F} \mathrm{d}\varepsilon \, \mathcal{D}(\varepsilon) - \frac{1}{2} \mu_B B \, \mathcal{D}(\varepsilon_F) \end{split}$$

$$\chi = \frac{M}{B} = \frac{\mu_B (N_{\uparrow} - N_{\downarrow})}{B} = \mu_B^2 \mathcal{D}(\varepsilon_F) = \mu_B^2 \frac{3}{2} \frac{N}{\varepsilon_F} > 0$$



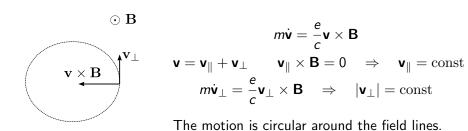
#### NON-INTERACTING FG: PARAMAGNETISM PAULI



$$T\gg T_F$$
  $\chi=rac{N\mu_B^2}{k_BT}$  Curie law  $T< T_F$   $\chi=rac{3}{2}rac{N\mu_B^2}{\epsilon_F}$  Paramagnetism Pauli

But... This is not the end of the story! Diamagnetic contribution is comparable (next step).

# CLASSICAL PARTICLE IN A FIELD: CYCLOTRON ORBITS



eleration 
$$=\omega^2 r$$

$$\left. \begin{array}{c} \operatorname{acceleration} = \omega^2 r \\ \operatorname{velocity} = \omega r \end{array} \right\} \Rightarrow m \omega^2 r = \frac{e}{c} \omega r B$$

cyclotron frequency 
$$\omega_c = \frac{eB}{mc} = 2 \times \text{(Larmor frequency)}$$

cf: Wilson chambers, cosmic rays, Hall effect etc etc



# Intermezzo: Vector potential of a uniform magnetic field

$$\mathbf{B} = \nabla \times \mathbf{A} \qquad \mathbf{B} = B\mathbf{k}$$

Coulomb gauge 
$$\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 0 & 0 & H \\ x & y & z \end{vmatrix} = -\frac{1}{2}\mathbf{i}By + \frac{1}{2}\mathbf{j}Bx$$
Indeed,  $\nabla \times \mathbf{A} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \partial_x & \partial_y & \partial_z \\ -By/2 & Bx/2 & 0 \end{vmatrix} = \mathbf{k}\left(\frac{B}{2} + \frac{B}{2}\right) = \mathbf{k}B$ 

Landau gauge 
$$\mathbf{A} = -\mathbf{i}By$$
  $\nabla \times \mathbf{A} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \partial_x & \partial_y & \partial_z \\ -By & 0 & 0 \end{vmatrix} = \mathbf{k}B$ 

### QUANTUM PARTICLE IN MAGNETIC FIELD

For a particle in a magnetic field, the generalized momentum  $\mathbf{p} = m\mathbf{v} + \frac{e}{c}\mathbf{A}(\mathbf{r})$ .

Kinetic energy 
$$=\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2$$

The Hamiltonian

$$\widehat{H} = \frac{1}{2m} \left( \widehat{\mathbf{p}} - \frac{e}{c} \mathbf{A} \right)^2 + \widehat{\boldsymbol{\mu}} \cdot \mathbf{B}$$

For a spinless particle in a uniform field in z direction, in the Landau gauge

$$\widehat{H} = \frac{1}{2m} \left( \widehat{p}_x + \frac{eB}{c} y \right)^2 + \frac{\widehat{p}_y^2 + \widehat{p}_z^2}{2m}$$

# QUANTUM PARTICLE IN MAGNETIC FIELD II

$$\widehat{H} = \frac{1}{2m} \left( \widehat{p}_x + \frac{eB}{c} y \right)^2 + \frac{\widehat{p}_y^2 + \widehat{p}_z^2}{2m}$$

$$\left[ \widehat{H}, \widehat{p}_x \right] = \left[ \widehat{H}, \widehat{p}_z \right] = 0$$

$$\Rightarrow \psi = e^{i(p_x x + p_z z)/\hbar} \phi(y) \qquad p_x, p_z \in (-\infty, \infty)$$

The Schrödinger equation  $\widehat{H}\psi=E\psi$  is then

$$\phi'' + \frac{2m}{\hbar^2} \left[ \varepsilon - \frac{m}{2} \omega_c^2 (y - y_0)^2 \right] \phi = 0$$

where  $\varepsilon = E - p_z^2/2m$  and  $y_0 = -cp_x/eB$ .

...which is nothing but a harmonic oscillator.



# QUANTUM PARTICLE IN MAGNETIC FIELD III

Landau levels: A quantum counterpart of the cyclotron orbits.

energy spectrum 
$$E=\hbar\omega_c\left(n+rac{1}{2}
ight)+rac{p_z^2}{2m}\;, \qquad n=0,1,\ldots$$
 magnetic length  $a_H=\sqrt{\hbar/m\omega_c}$ 

The motion along the field is not quantized.

Wave functions:

$$\psi_{n,p_z,p_x}(\mathbf{r}) = e^{i(p_x x + p_z z)/\hbar} \times (\text{oscillator w.f.})(y - y_0)$$



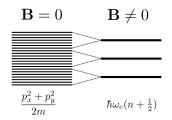
Energy levels do not depend on  $p_x \Rightarrow$  degeneracy.

#### Landau Levels Degeneracy: A closer look

At a given  $p_z$ 

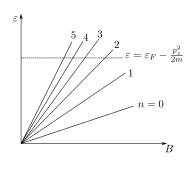
$$\mathcal{N} = \frac{L_x L_y}{2\pi\hbar} \frac{eB}{c} = \frac{L_x L_y}{2\pi\hbar} m\omega_c \qquad \qquad \text{(since } \omega_c = \frac{eB}{mc}\text{)}$$

The level spacing is  $\hbar\omega_c \Rightarrow {\sf DOS} = {\cal N}/\hbar\omega_c = \frac{L_x L_y}{2\pi\hbar^2} m$ , which is exactly the DOS for the 2D motion in the x-y plane!



Energy levels for the transverse motion merge into Landau levels.

#### DE HAAS – VAN ALPHEN EFFECT: THE ORIGIN OF



At a given  $p_z$ , the LL with  $n > n_{\text{max}}$  are empty:

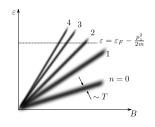
$$\hbar\omega_c \left(n_{\max} + \frac{1}{2}\right) = \varepsilon_F - \frac{p_z^2}{2m}$$
 $\omega_c \propto B \quad \Rightarrow \quad n_{\max} \propto \frac{1}{B}$ 

The degeneracy of LL,

$$\mathcal{N} = \nu B$$
 (where  $\nu = \frac{L_x L_y}{2\pi\hbar} \frac{e}{c}$ )

Upon increasing B, once a LL with  $n=n_{\rm max}$  crosses  $\varepsilon_F-p_z^2/2m$ ,  $n_{\rm max}\longrightarrow n_{\rm max}-1$ .

#### The role of temperature



Recall that  $\varepsilon_F \gg \mu_B B, k_B T$ . Nevertheless,  $\mu_B B \geqslant k_B T$ 

WEAK FIELDS, 
$$\mu_B B \ll k_B T$$
: Landau diamagnetism,  $\chi_{\rm Landau} = -\frac{1}{3} \chi_{\rm Pauli}$ , so that 
$$\chi = \chi_{\rm Landau} + \chi_{\rm Pauli} = \left(1 - \frac{1}{3}\right) \mu_B^2 \frac{3}{2} \frac{N}{\varepsilon_F} = \mu_B^2 \frac{N}{\varepsilon_F}$$

STRONG FIELDS,  $\mu_B B \gg K_B T$ : individual LLs are resolved. de Haas – van Alphen effect: *Magnetisation* oscillates in 1/BShubnikov – de Haas effect: *Resistance* oscillates in 1/B

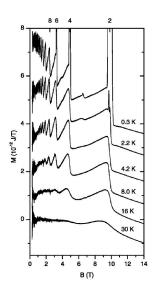
#### A COUPLE OF REMARKS

- We looked at the non-interacting Fermi gas only. In real metals, we need to take into account
  - Diamagnetism of the ionic cores
  - Band effects (Fermi surface is not spherical)
  - Electron-electron interactions

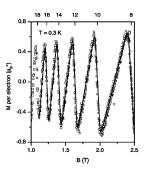
Overall, the combined effect can be comparable to what we've found.

- To observe the de Haas van Alphen effect, one needs
  - Pure samples
  - Magnetic fields of several teslas need very high field stability
  - Temperatures below 20–30 Kelvin
- 2D samples (eg GaAs quantum wells or graphene), in still stronger magnetic field: quantum Hall effect.
   In graphene, observed even at room temperature. Possibly: redefinition of the base SI units.

#### IN REAL LIFE



2D electron gas (AlGaAs/GaAs heterostructure). Exp data from M.P. Schwarz *et al.* Phys. Rev. B **65**, 245315 (2002)



#### FAST-FORWARD TO ROOM TEMPERATURE, WEAK FIELDS

Nothing quantum in this regime (yet)

Edwin Hall, 1879:



Hall resistance:

$$\rho_H = \frac{V_y}{I_x} \propto B$$

typically discussed for semiconductors, not metals.

Typically use *conductivity*,  $\mathbf{j} = \sigma \mathbf{E}$ . With  $\mathbf{B} \neq 0$ ,

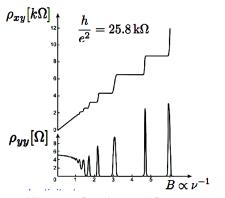
$$j_{\alpha} = \sigma_{\alpha\beta} E_{\beta}$$

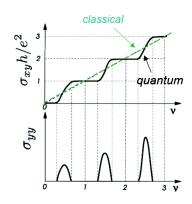
need to distinguish between  $\sigma_{xx}$  and  $\sigma_{xy}$ . (details: e.g., Kittel, Chapter 6, Problem 7)



#### Low temperature, very strong fields

Also confine carriers to two dimensions (jargon: 2DEG)



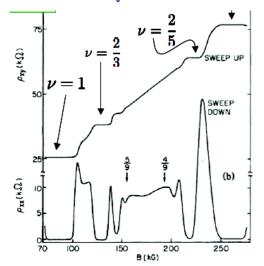


von Klitzing, Dorda, and Pepper, 1980

image from M. Sigrist, ETH Zürich; http://www.itp.phys.ethz.ch/education/fs11/sst/QHE.pdf



#### FRACTIONAL QHE



Störmer, Tsui, and Gossard, 1982

#### **IQHE**

Qualitatively: LL degeneracy  $\propto$  *B*. Carrier density is fixed.

Once a LL is completely full, there's a plateau in  $\rho_{xy}$ .

An alternative picture: each electron has an attached "flux tube".

Electron carry with them integer number of magnetic flux quanta.

#### **FQHE**

Plateaus at a *fractional* occupation of a LL.

Electrons carry a fraction of the flux quantum.