Handout 2

Sommerfeld Model for Metals – Free Fermion Gas

In this lecture you will learn:

- Sommerfeld theory of metals

Arnold Sommerfeld (1868-1951)

Problems with the Drude Theory

$$\frac{d\vec{p}(t)}{dt} = m\frac{d\vec{v}(t)}{dt} = \vec{F} - \frac{m\vec{v}(t)}{\tau}$$

$$= -e\left[\vec{E} + \vec{v}(t)x\vec{B}\right] - \frac{m\vec{v}(t)}{\tau}$$

- Does not say anything about the electron energy distribution in metals
  - Are all electrons moving around with about the same energy?
- Does not take into account Pauli's exclusion principle

To account for these shortcomings Sommerfeld in 1927 developed a model for electrons in metals that took into consideration the Fermi-Dirac statistics of electrons

Note added:

Six of Sommerfeld's students - Werner Heisenberg, Wolfgang Pauli, Peter Debye, Hans Bethe, Linus Pauling, and Isidor I. Rabi - went on to win Nobel prize in Physics.

Sommerfeld himself was nominated 81 times (more than any other person) but was never awarded the Nobel prize.

Quantum Mechanics and the Schrodinger Equation

The quantum state of an electron is described by the Schrodinger equation:

$$\hat{H}\,\psi(\vec{r},t) = i\hbar\,\frac{\partial\,\psi(\vec{r},t)}{\partial t}$$

Where the Hamiltonian operator is: $\hat{H} = \frac{\hat{P}^2}{2m} + V\left(\hat{\vec{r}}\right) = \frac{\hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2}{2m} + V\left(\hat{\vec{r}}\right)$

Suppose: $\psi(\vec{r},t) = \psi(\vec{r})\,e^{-i\frac{E}{\hbar}t}$ then we get: $\hat{H}\,\psi(\vec{r}) = E\,\psi(\vec{r})$

(Time independent form)

The momentum operator is: $\hat{\vec{P}} = \frac{\hbar}{i}\nabla$

Therefore: $\frac{\hat{P}^2}{2m} = \frac{\hat{\vec{P}}\,.\,\hat{\vec{P}}}{2m} = \frac{1}{2m}\frac{\hbar}{i}\nabla\,.\,\frac{\hbar}{i}\nabla = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]$

The time independent form of the Schrodinger equation is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r})$$

Schrodinger Equation for a Free Electron

The time independent form of the Schrodinger equation is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r})$$

For a free-electron: $V(\vec{r}) = 0$

We have:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) = E\,\psi(\vec{r})$$

Solution is a plane wave (i.e. plane wave is an energy eigenstate):

$$\psi_{\vec{k}}(\vec{r}) = \sqrt{\frac{1}{V}}\;e^{i\,\vec{k}\,.\,\vec{r}} = \sqrt{\frac{1}{V}}\;e^{i\left(k_x x + k_y y + k_z z\right)} \longrightarrow \left[\int d^3\vec{r}\;\left|\psi_{\vec{k}}(\vec{r})\right|^2 = 1\right]$$

Energy:

The energy of the free-electron state is: $E = \frac{\hbar^2\left(k_x^2 + k_y^2 + k_z^2\right)}{2\,m} = \frac{\hbar^2 k^2}{2\,m}$

Note: The energy is entirely kinetic (due to motion)

Momentum:

The energy eigenstates are also momentum eigenstates:

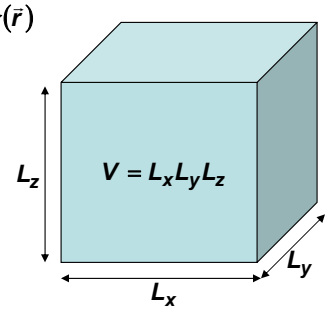
$$\hat{\vec{p}} = \frac{\hbar}{i}\nabla \quad \Rightarrow \quad \hat{\vec{p}}\,\psi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i}\nabla\psi_{\vec{k}}(\vec{r}) = \hbar\vec{k}\,\psi_{\vec{k}}(\vec{r})$$

Electrons in Metals: The Free Electron Model

The quantum state of an electron is described by the time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})+V(\vec{r})\psi(\vec{r})=E\,\psi(\vec{r})$$

Consider a large metal box of volume $V = L_x L_y L_z$:



In the Sommerfeld model:

- The electrons inside the box are confined in a three-dimensional infinite potential well with zero potential inside the box and infinite potential outside the box

$$V(\vec{r})=0 \quad \text{for } |\vec{r}| \text{ inside the box}$$
$$V(\vec{r})=\infty \quad \text{for } |\vec{r}| \text{ outside the box}$$

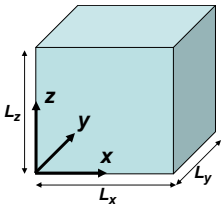
free electrons (experience no potential when inside the box)

- The electron states inside the box are given by the Schrodinger equation

Electrons in Metals: The Free Electron Model

Need to solve: $-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})=E\,\psi(\vec{r})$

With the boundary condition that the wavefunction $\psi(\vec{r})$ is zero at the boundary of the box



$V = L_xL_yL_z$

Solution is: $\psi_{\vec{k}}(\vec{r})=\sqrt{\frac{8}{V}}\sin(k_x x)\sin(k_y y)\sin(k_z z)$

Where: $k_x = n\frac{\pi}{L_x} \qquad k_y = m\frac{\pi}{L_y} \qquad k_z = p\frac{\pi}{L_z}$

And *n*, *m*, and *p* are non-zero positive integers taking values 1, 2, 3, 4, …….

Normalization:

The wavefunction is properly normalized: $\int d^3\vec{r}\;\left|\psi_{\vec{k}}(\vec{r})\right|^2 = 1$

Energy:

The energy of the electron states is: $E=\frac{\hbar^2\left(k_x^2+k_y^2+k_z^2\right)}{2m}=\frac{\hbar^2k^2}{2m}$

Note: The energy is entirely kinetic (due to motion)

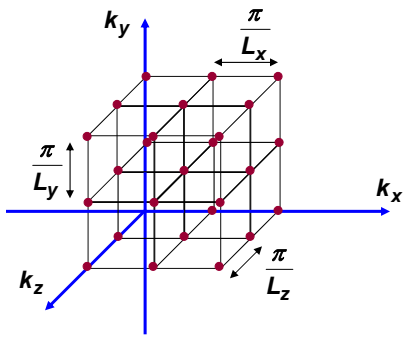
Electrons in Metals: The Free Electron Model

Labeling Scheme:

All electron states and energies can be labeled by the corresponding k-vector

$$\psi_{\vec{k}}(\vec{r}) = \sqrt{\frac{8}{V}}\sin(k_x x)\sin(k_y y)\sin(k_z z)$$

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m}$$



k-space Visualization:

The allowed quantum states can be visualized as a 3D grid of points in the first quadrant of the "k-space"

$$k_x = n\frac{\pi}{L_x} \qquad k_y = m\frac{\pi}{L_y} \qquad k_z = p\frac{\pi}{L_z}$$

$n, m, p = 1, 2, 3, 4, \ldots\ldots$

Problems:

- **The "sine" solutions are difficult to work with – need to choose better solutions**
- **The "sine" solutions come from the boundary conditions – and most of the electrons inside the metal hardly ever see the boundary**

Born Von Karman Periodic Boundary Conditions

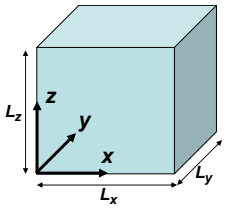
Solve: $-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) = E\,\psi(\vec{r})$

Instead of using the boundary condition: $\psi(\vec{r})\,|_{\text{boundary}} = 0$

Use periodic boundary conditions:

$$\psi(x+L_x, y, z) = \psi(x, y, z)$$
$$\psi(x, y+L_y, z) = \psi(x, y, z)$$
$$\psi(x, y, z+L_z) = \psi(x, y, z)$$

These imply that each facet of the box is folded and joined to the opposite facet



Solution is: $\psi_{\vec{k}}(\vec{r}) = \sqrt{\frac{1}{V}}\,e^{i\vec{k}\cdot\vec{r}} = \sqrt{\frac{1}{V}}\,e^{i(k_x x + k_y y + k_z z)}$

The boundary conditions dictate that the allowed values of k_x, k_y, and k_z, are such that:

$$e^{ik_x(x+L_x)} = e^{ik_x x} \Rightarrow e^{ik_x L_x} = 1 \Rightarrow k_x = n\frac{2\pi}{L_x} \qquad n = 0, \pm1, \pm2, \ldots.$$

$$e^{ik_y(y+L_y)} = e^{ik_y y} \Rightarrow e^{ik_y L_y} = 1 \Rightarrow k_y = m\frac{2\pi}{L_y} \qquad m = 0, \pm1, \pm2, \ldots.$$

$$e^{ik_z(z+L_z)} = e^{ik_z z} \Rightarrow e^{ik_z L_z} = 1 \Rightarrow k_z = p\frac{2\pi}{L_z} \qquad p = 0, \pm1, \pm2, \ldots.$$

Born Von Karman Periodic Boundary Conditions

Labeling Scheme:

All electron states and energies can be labeled by the corresponding k-vector

$$\psi_{\vec{k}}(\vec{r}) = \sqrt{\frac{1}{V}}\; e^{i\,\vec{k}\,.\,\vec{r}} \qquad E(\vec{k}) = \frac{\hbar^2 k^2}{2m}$$

Normalization: The wavefunction is properly normalized: $\int d^3\vec{r}\;\left|\psi_{\vec{k}}(\vec{r})\right|^2 = 1$

Orthogonality: Wavefunctions of two different states are orthogonal:

$$\int d^3\vec{r}\;\psi^*_{\vec{k}'}(\vec{r})\,\psi_{\vec{k}}(\vec{r}) = \int d^3\vec{r}\;\frac{e^{i\,(\vec{k}-\vec{k}')\,.\,\vec{r}}}{V} = \delta_{\vec{k}',\,\vec{k}}$$

Momentum Eigenstates:

Another advantage of using the plane-wave energy eigenstates (as opposed to the "sine" energy eigenstates) is that the plane-wave states are also momentum eigenstates

Momentum operator: $\hat{\vec{p}} = \frac{\hbar}{i}\nabla \quad \Rightarrow \quad \hat{\vec{p}}\,\psi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i}\nabla\psi_{\vec{k}}(\vec{r}) = \hbar\vec{k}\,\psi_{\vec{k}}(\vec{r})$

Velocity:

Velocity of eigenstates is: $\vec{v}(\vec{k}) = \frac{\hbar\vec{k}}{m} = \frac{1}{\hbar}\nabla_{\vec{k}}\,E(\vec{k})$

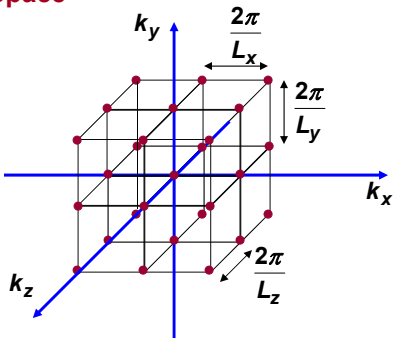
States in k-Space

k-space Visualization:

The allowed quantum states states can be visualized as a 3D grid of points in the entire "k-space"

$$k_x = n\frac{2\pi}{L_x} \qquad k_y = m\frac{2\pi}{L_y} \qquad k_z = p\frac{2\pi}{L_z}$$

$n, m, p = 0, \pm1, \pm2, \pm3, \ldots\ldots$



Density of Grid Points in k-space:

Looking at the figure, in k-space there is only one grid point in every small volume of size:

$$\left(\frac{2\pi}{L_x}\right)\left(\frac{2\pi}{L_y}\right)\left(\frac{2\pi}{L_z}\right) = \frac{(2\pi)^3}{V}$$

$\Rightarrow$ There are $\frac{V}{(2\pi)^3}$ grid points per unit volume of k-space } Very important result

Electron Spin

Electron Spin:

Electrons also have spin degrees of freedom. An electron can have spin up or down.

So we can write the full quantum state of the electron as follows:

$$\psi_{\vec{k}\uparrow}(\vec{r}) = \sqrt{\frac{1}{V}}\; e^{i\,\vec{k}\,.\,\vec{r}}\,|\uparrow\rangle \qquad \text{or} \qquad \psi_{\vec{k}\downarrow}(\vec{r}) = \sqrt{\frac{1}{V}}\; e^{i\,\vec{k}\,.\,\vec{r}}\,|\downarrow\rangle$$

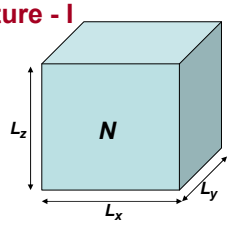
The energy does not depend on the spin (at least for the case at hand) and therefore

$$E(\vec{k}\uparrow) = E(\vec{k}\downarrow) = \frac{\hbar^2 k^2}{2m}$$

For the most part in this course, spin will be something extra that tags along and one can normally forget about it provided it is taken into account when counting all the available states

The Electron Gas at Zero Temperature - I

- Suppose we have *N* electrons in the box.



- Then how do we start filling the allowed quantum states?

- Suppose *T*~0K and we are interested in a filling scheme that gives the lowest total energy.

The energy of a quantum state is:

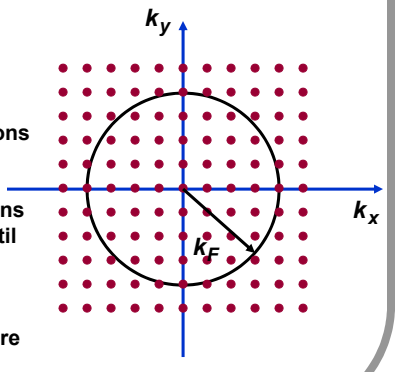
$$E(\vec{k}) = \frac{\hbar^2\left(k_x^2 + k_y^2 + k_z^2\right)}{2m} = \frac{\hbar^2 k^2}{2m}$$

Strategy:

- Each grid-point can be occupied by two electrons (spin up and spin down)

- Start filling up the grid-points (with two electrons each) in spherical regions of increasing radii until you have a total of *N* electrons

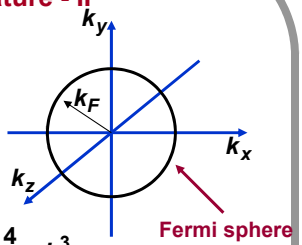
- When we are done, all filled (i.e. occupied) quantum states correspond to grid-points that are inside a spherical region of radius k_F



The Electron Gas at Zero Temperature - II

• Each grid-point can be occupied by two electrons (spin up and spin down)

• All filled quantum states correspond to grid-points that are inside a spherical region of radius k_F



Volume of the spherical region = $\frac{4}{3}\pi k_F^3$

Number of grid-points in the spherical region = $\frac{V}{(2\pi)^3} \times \frac{4}{3}\pi k_F^3$

Number of quantum states (including spin) inside the spherical shell = $2 \times \frac{V}{(2\pi)^3} \times \frac{4}{3}\pi k_F^3 = \frac{V}{3\pi^2} k_F^3$

But the above must equal the total number N of electrons inside the box:

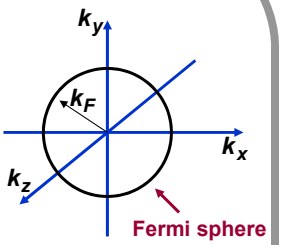
$$N = \frac{V}{3\pi^2} k_F^3$$

$$\Rightarrow \quad n = \text{electron density} = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

$$\Rightarrow \quad k_F = \left(3\pi^2 n\right)^{\frac{1}{3}}$$

The Electron Gas at Zero Temperature - III

• All quantum states inside the Fermi sphere are filled (i.e. occupied by electrons)
• All quantum states outside the Fermi sphere are empty



Fermi Momentum:
The largest momentum of the electrons is: $\hbar k_F$
This is called the Fermi momentum
Fermi momentum can be found if one knows the electron density:

$$k_F = \left(3\pi^2 n\right)^{\frac{1}{3}}$$

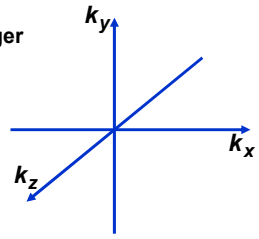
Fermi Energy:
The largest energy of the electrons is: $\frac{\hbar^2 k_F^2}{2m}$

This is called the Fermi energy E_F : $E_F = \frac{\hbar^2 k_F^2}{2m}$

Also: $E_F = \frac{\hbar^2 \left(3\pi^2 n\right)^{\frac{2}{3}}}{2m}$ or $n = \frac{1}{3\pi^2}\left(\frac{2m\,E_F}{\hbar^2}\right)^{\frac{3}{2}}$

Fermi Velocity:
The largest velocity of the electrons is called the Fermi velocity v_F : $v_F = \frac{\hbar k_F}{m}$

The Electron Gas at Non-Zero Temperature - I



- Since T≠0K, the filling scheme used for T=0K will no longer work

- For T≠0K one can only speak of the "probability" that a particular quantum state is occupied

Suppose the probability that the quantum state of wavevector $\vec{k}$ is occupied by an electron is $f(\vec{k})$

Then the total number N of electrons must equal the following sum over all grid-points in k-space:

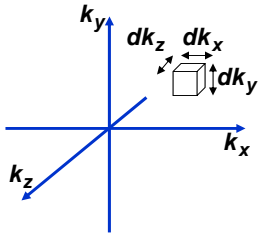
$$N = 2 \times \sum_{\text{all } \vec{k}} f(\vec{k})$$

spin

- By assumption $f(\vec{k})$ does not depend on the spin. That is why spin is taken into account by just adding the factor of 2 outside the sum

- $f(\vec{k})$ can have any value between 0 and 1

The Electron Gas at Non-Zero Temperature - II



Recall that there are $\frac{V}{(2\pi)^3}$ grid points per unit volume of k-space

$\Rightarrow$ So in volume $dk_x\, dk_y\, dk_z$ of k-space the number of grid points is:

$$\frac{V}{(2\pi)^3} dk_x\, dk_y\, dk_z = \frac{V}{(2\pi)^3} d^3\vec{k}$$

$\Rightarrow$ The summation over all grid points in k-space can be replaced by a volume integral

$$\sum_{\text{all } \vec{k}} \rightarrow V \int \frac{d^3\vec{k}}{(2\pi)^3}$$

Therefore:

$$N = 2 \times \sum_{\text{all } \vec{k}} f(\vec{k}) = 2 \times V \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k})$$

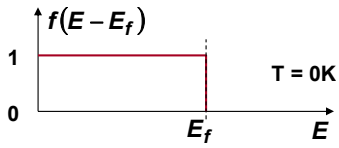
Question: What is $f(\vec{k})$?

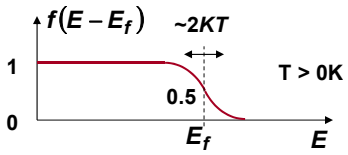
The Fermi-Dirac Distribution - I

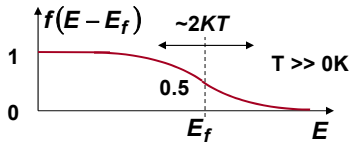
A fermion (such as an electron) at temperature T occupies a quantum state with energy E with a probability $f(E-E_f)$ given by the Fermi-Dirac distribution function:

$$f(E-E_f)=\frac{1}{1+e^{(E-E_f)/KT}}$$

E_f = chemical potential or the Fermi level (do not confuse Fermi energy with Fermi level)
K = Boltzmann constant = 1.38 X 10^{-23} Joules/Kelvin







The Fermi level E_f is determined by invoking some physical argument …(as we shall see)

Distribution Functions: Notation

The following notation will be used in this course:

• The notation $f(\vec{k})$ will be used to indicate a general k-space distribution function (not necessarily an equilibrium Fermi-Dirac distribution function)

• The notation $f(E-E_f)$ will be used to indicate an equilibrium Fermi-Dirac distribution function with Fermi-level E_f. Note that the Fermi-level is explicitly indicated. Note also that the Fermi-Dirac distribution depends only on the energy and not on the exact point in k-space

• Sometimes the notations $f_o(E-E_f)$ or $f_o(E)$ or $f_o(\vec{k})$ are also used to indicate equilibrium Fermi-Dirac distribution functions

The Electron Gas at Non-Zero Temperature - III

The probability $f(\vec{k})$ that the quantum state of wavevector $\vec{k}$ is occupied by an electron is given by the Fermi-Dirac distribution function:

$$f(\vec{k}) = \frac{1}{1+e^{(E(\vec{k})-E_f)/KT}} = f(E(\vec{k})-E_f) \qquad \text{Where: } E(\vec{k}) = \frac{\hbar^2(k_x^2+k_y^2+k_z^2)}{2m} = \frac{\hbar^2 k^2}{2m}$$

Therefore:

$$N = 2\times V\int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k}) = 2\times V\int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{1+e^{(E(\vec{k})-E_f)/KT}}$$

Density of States:

The k-space volume integral is cumbersome. We need to convert into a simpler form – an energy space integral – using the following steps:

$$d^3\vec{k} = 4\pi k^2\, dk \qquad \text{and} \qquad E = \frac{\hbar^2 k^2}{2m} \Rightarrow dE = \frac{\hbar^2 k}{m} dk$$

Therefore:

$$d^3\vec{k} = 4\pi k^2\, dk = 4\pi \frac{m\,k}{\hbar^2} dE \qquad \text{But: } k = \sqrt{\frac{2mE}{\hbar^2}}$$

It follows that:

$$d^3\vec{k} = 4\pi \frac{m\,k}{\hbar^2} dE = \frac{4\pi}{\hbar^3}\sqrt{2m^3E}\, dE$$

The Electron Gas at Non-Zero Temperature - IV

$$N = 2\times V\int \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{1+e^{(E(\vec{k})-E_f)/KT}} = V\int_0^\infty dE\; g(E) \frac{1}{1+e^{(E-E_f)/KT}}$$

Where: $g(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}$ ← Density of states function

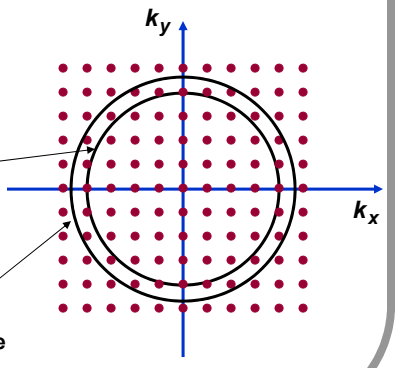
$g(E)$ has units: # / Joule-cm^3

The product $g(E)\,dE$ represents the number of quantum states available in the energy interval between E and $(E+dE)$ per cm^3 of the metal

Suppose E corresponds to the inner spherical shell from the relation:

$$E = \frac{\hbar^2 k^2}{2m}$$

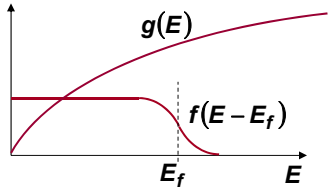
And suppose $(E+dE)$ corresponds to the outer spherical shell, then $g(E)\,dE$ corresponds to twice the number of the grid points between the two spherical shells



The Electron Gas at Non-Zero Temperature - V

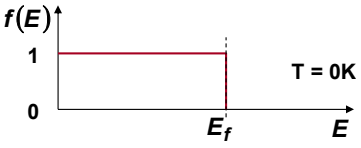
$$N = V\int_0^\infty dE\ \ g(E)\ \frac{1}{1+e^{(E-E_f)/KT}} = V\int_0^\infty dE\ \ g(E)\ f(E-E_f)$$

Where: $g(E) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}$



The expression for N can be visualized as the integration over the product of the two functions:

Check: Suppose T=0K:



$$N = V\int_0^\infty dE\ \ g(E)\ f(E-E_f) = V\int_0^{E_f} dE\ \ g(E)$$

$$= V\frac{1}{3\pi^2}\left(\frac{2m\,E_f}{\hbar^2}\right)^{\frac{3}{2}}$$

$$\Rightarrow\quad n = \frac{1}{3\pi^2}\left(\frac{2m\,E_f}{\hbar^2}\right)^{\frac{3}{2}}$$

Compare with the previous result at T=0K:

$$n = \frac{1}{3\pi^2}\left(\frac{2m\,E_F}{\hbar^2}\right)^{\frac{3}{2}} \quad\Rightarrow$$

At T=0K (and only at T=0K) the Fermi level E_f is the same as the Fermi energy E_F

The Electron Gas at Non-Zero Temperature - VI

For $T \neq 0$K:

Since the carrier density is known, and does not change with temperature, the Fermi level at temperature T is found from the expression

$$n = \int_0^\infty dE\ \ g(E)\ \frac{1}{1+e^{(E-E_f)/KT}}$$

In general, the Fermi level E_f is a function of temperature and decreases from E_F as the temperature increases

$$E_f(T=0) = E_F$$
$$\&\quad E_f(T>0) < E_F$$

For small temperatures ($KT << E_F$), a useful approximation is:

$$E_f(T) \approx E_F\left[1 - \frac{1}{3}\left(\frac{\pi\,K\,T}{2\,E_F}\right)^2\right]$$

Total Energy of the Fermion Gas

The total energy U of the electron gas can be written as:

$$U = 2 \times \sum_{\text{all } \vec{k}} f(\vec{k}) E(\vec{k}) = 2 \times V \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k}) E(\vec{k})$$

Convert the k-space integral to energy integral: $U = V \int_0^\infty dE \;\; g(E) \;\; f(E - E_f) \, E$

The energy density u is: $u = \frac{U}{V} = \int_0^\infty dE \;\; g(E) \;\; f(E - E_f) \, E$

Suppose T=0K:

$$u = \int_0^{E_F} dE \;\; g(E) \;\; E = \frac{1}{5\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E_F)^{\frac{5}{2}}$$

Since: $n = \frac{1}{3\pi^2} \left(\frac{2m \, E_F}{\hbar^2} \right)^{\frac{3}{2}}$

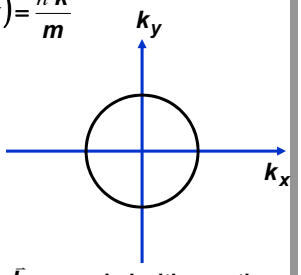
We have: $u = \frac{3}{5} n \, E_F$

Equilibrium Current Density of the Electron Gas

In the Drude model we had:

$$\vec{J} = n(-e)\vec{v}$$

- But now we have a Fermi gas in which electrons move with different velocities
- The velocity of the electron with wavevector $\vec{k}$ is: $\vec{v}(\vec{k}) = \frac{\hbar \vec{k}}{m}$



So the current density expression can be written as:

$$\vec{J} = (-e)\frac{2}{V} \times \sum_{\text{all } \vec{k}} f(\vec{k}) \vec{v}(\vec{k}) = -2\,e \times \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k}) \vec{v}(\vec{k})$$

$$\vec{J} = -2\,e \times \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k}) \, \frac{\hbar \vec{k}}{m}$$

In the sum, for every occupied state $\vec{k}$ there is a state $-\vec{k}$ occupied with exactly the same probability. Therefore:

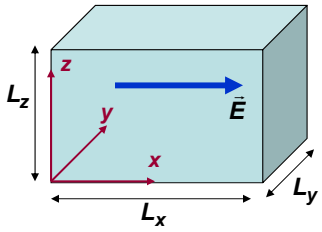
$$\vec{J} = -2\,e \times \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k}) \, \frac{\hbar \vec{k}}{m} = 0$$

Makes sense - metals do not have net current densities flowing in equilibrium

Electron Gas in an Applied Electric Field - I

- Now suppose there is an electric field inside the metal
- Also assume, as in the Drude model, that the scattering time of the electrons is τ and the scattering rate is $1/\tau$
- The time-independent Schrodinger equation is a good point to start:

$$\hat{H}\,\psi(\vec{r},t) = i\hbar\,\frac{\partial\,\psi(\vec{r},t)}{\partial t}$$



Where: $\hat{H} = \frac{\hat{P}^2}{2m} + V\left(\hat{\vec{r}}\right) = \frac{\hat{P}^2}{2m} + e\,\vec{E}\,.\,\vec{r} = -\frac{\hbar^2}{2m}\nabla^2 + e\,\vec{E}\,.\,\vec{r}$

Assume a solution: $\psi(\vec{r},t) = \sqrt{\frac{1}{V}}\;e^{\,i\left(\vec{k}\,-\,\frac{e\,\vec{E}}{\hbar}\,t\right).\,\vec{r}}\;e^{\,-i\,\frac{\int_{-\infty}^{t} E(t')\,dt'}{\hbar}}$ and plug it in to get:

$$E(t) = \frac{\hbar^2\left|\vec{k} - \frac{e\,\vec{E}}{\hbar}\,t\right|^2}{2m}$$

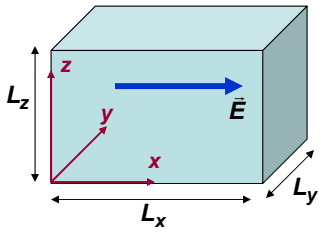
The energy of the electron shows that its wavevector (and momentum) is increasing with time

The wavevector is now time dependent!

Electron Gas in an Applied Electric Field - II

- An equation for the time-dependent electron wavevector can be written as:

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



Now we need to add the effect of electron scattering. As in the Drude model, assume that scattering adds damping:

$$\frac{d\;\hbar\vec{k}(t)}{dt} = -e\,\vec{E} - \frac{\hbar\left[\vec{k}(t) - \vec{k}\right]}{\tau}$$

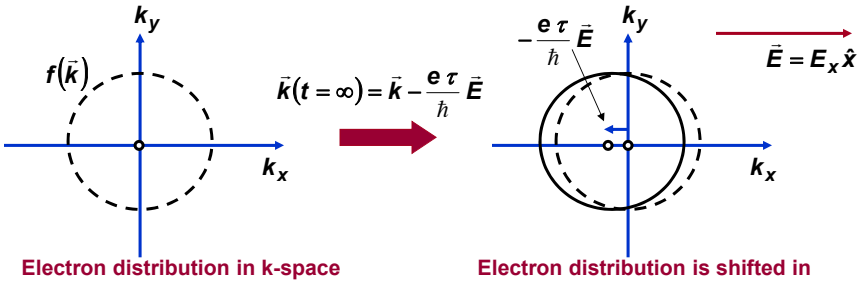
The boundary condition is that: $\vec{k}(t=0) = \vec{k}$

Note: the damping term ensures that when the field is turned off, the wavevector of the electron goes back to its original value

Steady State Solution: $\vec{k}(t=\infty) = \vec{k} - \frac{e\,\tau}{\hbar}\,\vec{E}$

In the presence of an electric field, the wavevector of every electron is shifted by an equal amount that is determined by the scattering time and the field strength

Electron Gas in an Applied Electric Field - III



Electron distribution in k-space when E-field is zero

Distribution function: $f(\vec{k})$

Electron distribution is shifted in k-space when E-field is not zero

Distribution function: $f\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right)$

Since the wavevector of each electron is shifted by the same amount in the presence of the E-field, the net effect in k-space is that the entire electron distribution is shifted as shown

Electron Gas in an Applied Electric Field - IV

Current Density:

$$\vec{J} = -2\,e \times \int \frac{d^3\vec{k}}{(2\pi)^3} f\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right)\vec{v}(\vec{k})$$

Do a shift in the integration variable:

$$\vec{J} = -2\,e \times \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k})\vec{v}\left(\vec{k} - \frac{e\tau}{\hbar}\vec{E}\right)$$

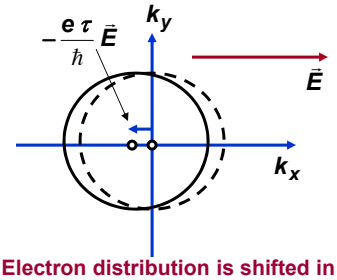
$$\vec{J} = -2\,e \times \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k})\frac{\hbar\left(\vec{k} - \frac{e\tau}{\hbar}\vec{E}\right)}{m}$$

$$\vec{J} = \frac{e^2\tau}{m}\left[2 \times \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k})\right]\vec{E}$$

electron density = n

$$\vec{J} = \frac{n\,e^2\tau}{m}\vec{E} = \sigma\,\vec{E}$$

Where: $\sigma = \frac{n\,e^2\tau}{m}$ → Same as the Drude result!



Electron distribution is shifted in k-space when E-field is not zero

Distribution function: $f\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right)$