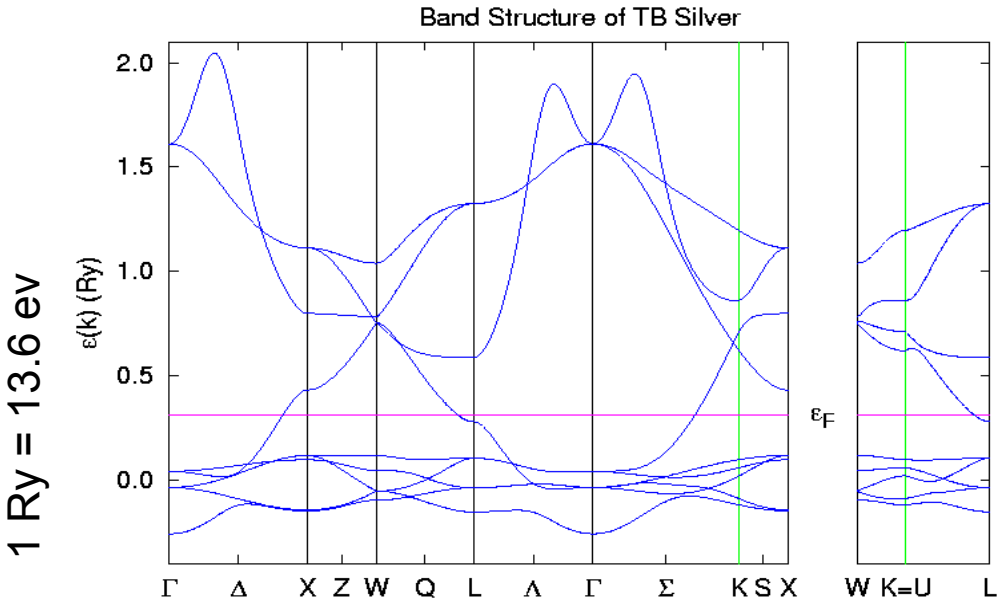
Microwave Engineering

Intraband transitions

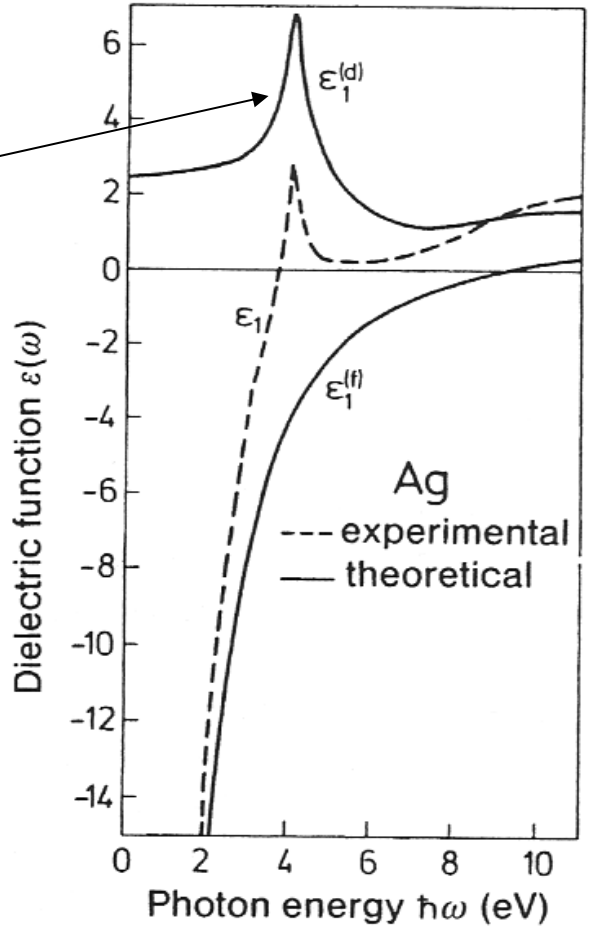
When the bands are parallel, there is a peak in the absorption (ε")

$$\hbar\omega = E_c(\vec{k}) - E_v(\vec{k})$$

Intraband (d-band) absorption

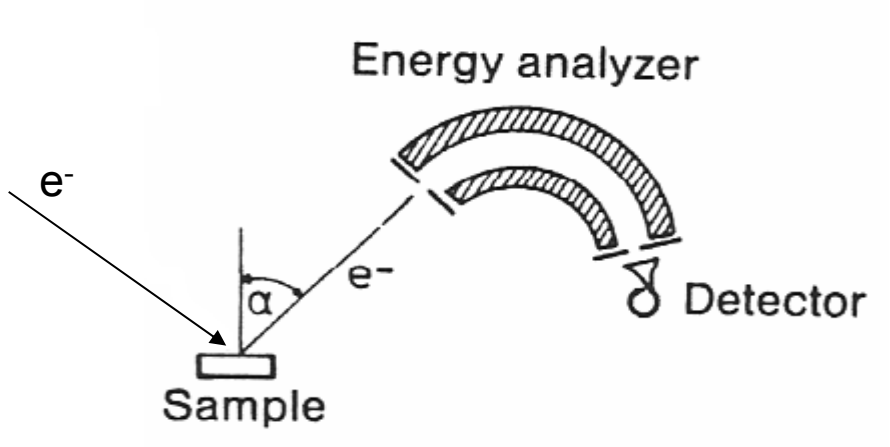


1 Ry = 13.6 ev



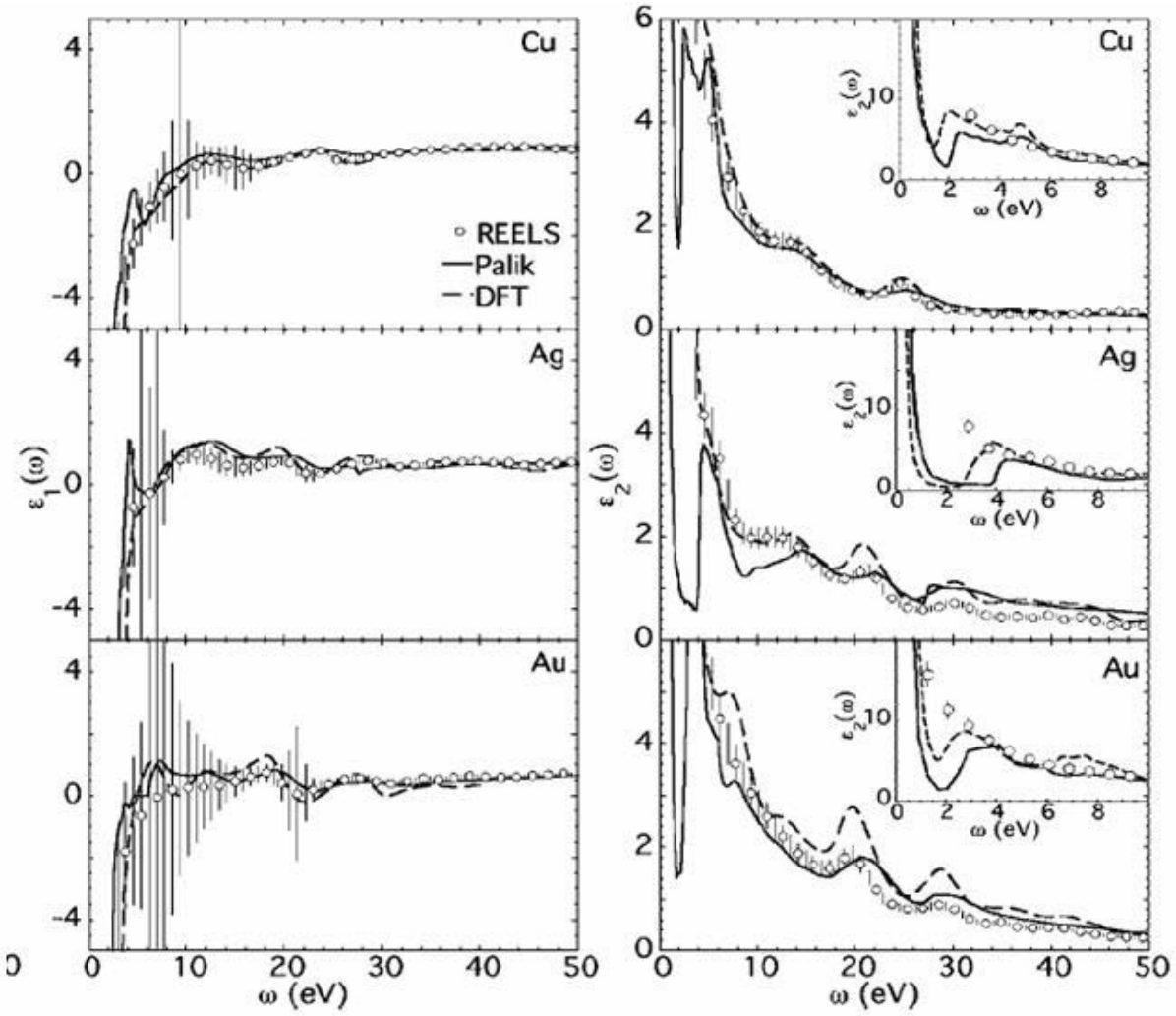
Ibach &Lueth

Reflection Electron Energy Loss Spectroscopy



Fast electrons moving through the solid generate and a time dependent electric field. If the polarization moves out of phase with this field, energy will be lost. This is detected in the reflected electrons.

Dielectric function of Cu, Ag, and Au obtained from reflection electron energy loss spectra, optical measurements, and density functional theory



Werner (TU Vienna) APL 89 213106 (2006)

Microwave engineering

Microwave frequencies are a few GHz

The wavelength is smaller than the circuit

Losses in metals increase with increasing frequency

Losses in dielectrics increase with increasing frequency

There is a characteristic length scale called the skin depth which tells us how far into a metal fields penetrate before they are reflected out.

Skin depth $\omega\tau << 1$

$$\sigma(\omega) = ne\mu\left(\frac{1 - i\omega\tau}{1 + \omega^2\tau^2}\right) \approx ne\mu = \sigma_0 \qquad \omega\tau << 1$$

Ohm's law $$\vec{J} = \sigma_0 \vec{E}$$

Take the curl $$\frac{1}{\sigma_0}\nabla \times \vec{J} = \nabla \times \vec{E} = -\frac{d\vec{B}}{dt}$$ Faraday's law

$$\nabla \times \vec{B} = \mu_0 \vec{J}$$ Ampere's law

$$\frac{1}{\sigma_0\mu_0}\nabla \times \nabla \times \vec{B} = -\frac{d\vec{B}}{dt}$$

Vector identity $$\nabla \times \nabla \times \vec{B} = \nabla\left(\cancelto{0}{\nabla \cdot \vec{B}}\right) - \nabla^2 \vec{B}$$

$$\frac{1}{\sigma_0\mu_0}\nabla^2 \vec{B} = \frac{d\vec{B}}{dt}$$

Skin depth

$$\frac{1}{\sigma_0 \mu_0} \nabla^2 \vec{B} = \frac{d\vec{B}}{dt}$$

Assume harmonic dependence $B_0 e^{i(kx-\omega t)}$

$$\frac{k^2}{\sigma_0 \mu_0} = i\omega$$

$$k = \sqrt{i\omega\sigma_0\mu_0} = \sqrt{\frac{\omega\sigma_0\mu_0}{2}} + i\sqrt{\frac{\omega\sigma_0\mu_0}{2}}$$

Exponential decay

Skin depth $\delta = \sqrt{\frac{2}{\mu_0\sigma_0\omega}}$

Light $\omega < \omega_p$ is reflected out of a metal. The waves penetrate a length δ.

Skin depth

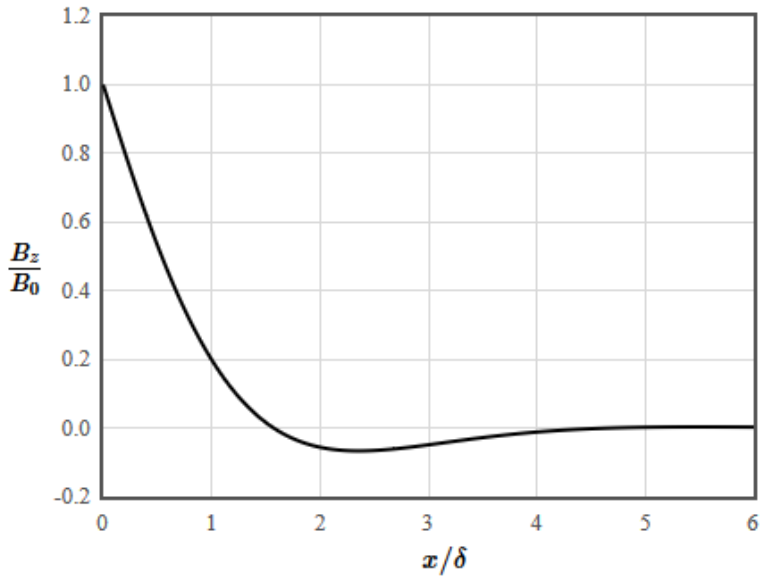
$$\vec{B} = B_0 e^{-x/\delta} e^{i(x/\delta - \omega t)} \hat{z}$$

$$\vec{J} = \frac{1}{\mu_0} \nabla \times \vec{B} = \frac{B_0 (1-i)}{\mu_0 \delta} e^{-x/\delta} e^{i(x/\delta - \omega t)} \hat{y}$$

$$1 - i = \sqrt{2} e^{-i\pi/4}$$

$$\vec{J} = \frac{\sqrt{2} B_0}{\mu_0 \delta} e^{-x/\delta} e^{i(x/\delta - \omega t - \pi/4)} \hat{y}$$

$$\vec{E} = \frac{\vec{J}}{\sigma_0} = \frac{\sqrt{2} B_0}{\mu_0 \delta \sigma_0} e^{-x/\delta} e^{i(x/\delta - \omega t - \pi/4)} \hat{y}$$



The electric field lags behind the magnetic field by 45 degrees.

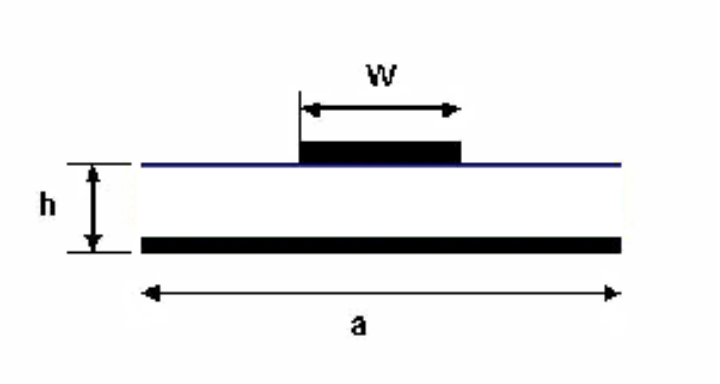
Surface resistance

At low frequencies: $$R = \frac{\rho \ell}{wt} = \frac{\ell}{\sigma_0 wt}$$

When $\delta < t$: $$R = \frac{\ell}{\sigma_0 w \delta}$$

for $$\ell = w$$

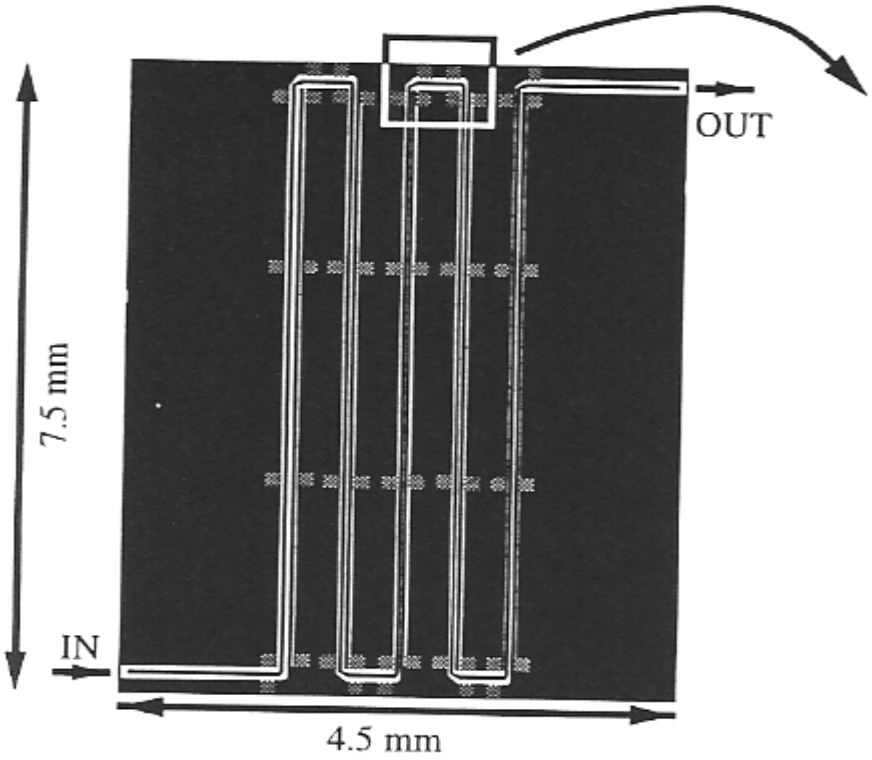
$$R_s = \frac{1}{\sigma_0 \delta} \propto \sqrt{\omega}$$

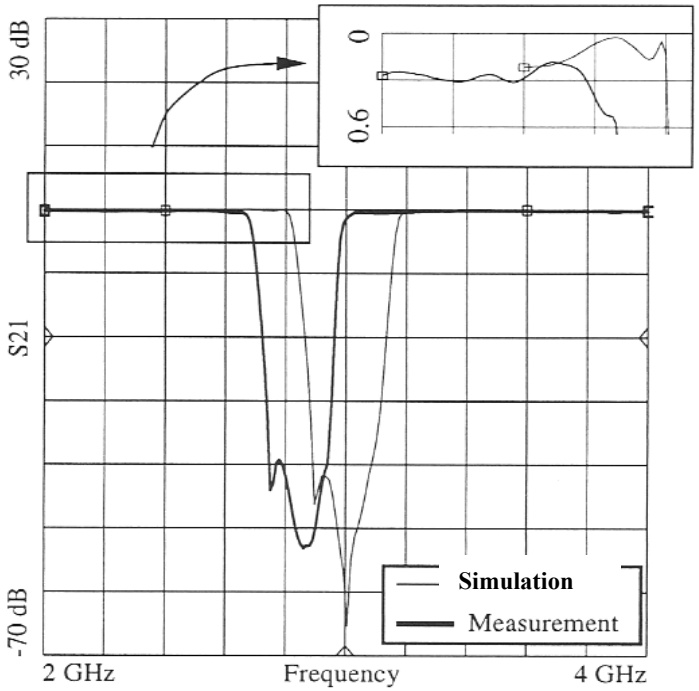


Complex signal processing at high frequencies > 1 GHz is difficult because the losses increase with frequency.

Usually you mix down to a lower frequency as soon as possible.

Superconducting filter





Complex signal processing at high frequencies > 1 GHz is difficult because the losses increase with frequency.

Transport

Transport phenomena

Bloch waves
Crystal momentum
Group velocity

Boltzmann equation
Electrical conductivity
Thermal conductivity
Hall effect
Peltier effect
Seebeck effect
Ettingshausen effect
Nerst effect

- **Transport**
  - Thermoelectric effects
  - Crystal momentum
  - Boltzmann equation
  - Relaxation time approximation
  - Current densities
  - Electrochemical potential
  - Electrical conductivity
  - Thermoelectric currents
  - Seebeck effect
  - Hall effect
  - Nernst effect
  - Free-electron model
    - Electrical conductivity
    - Electrical contribution to the thermal conductivity
    - Wiedemann–Franz law
  - Transport in 1-D crystals
    - Current of Bloch waves in 1-D

Bloch waves

Any wave function: $\psi(\vec{r}) = \sum_{\vec{k}} c_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$

$$\psi(\vec{r}) = \sum_{\vec{k}\in 1\mathrm{BZ}} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i(\vec{k}+\vec{G})\cdot\vec{r}}$$

Bloch wave: $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} c_{\vec{k}+\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$

$$\psi(\vec{r}) = \sum_{\vec{k}\in 1\mathrm{BZ}} \psi_{\vec{k}}(\vec{r})$$

$$\mathbf{T}\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot(\vec{r}+\vec{a})} u_{\vec{k}}(\vec{r}+\vec{a}) = e^{i\vec{k}\cdot\vec{a}} e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{a}} \psi_{\vec{k}}(\vec{r})$$

Bloch waves are eigenfunctions of the Hamiltonian

http://lampx.tugraz.at/~hadley/ss2/transport/crystalmomentum.php

Bloch waves in 1-D

It is instructive to consider a one-dimensional crystal at this point since the dispersion relation $E(\vec{k})$ can be readily calculated numerically in one-dimension. Consider an electron moving in a periodic potential $V(x)$. The period of the potential is a, $V(x+a) = V(x)$. The Schrödinger equation for this case is,

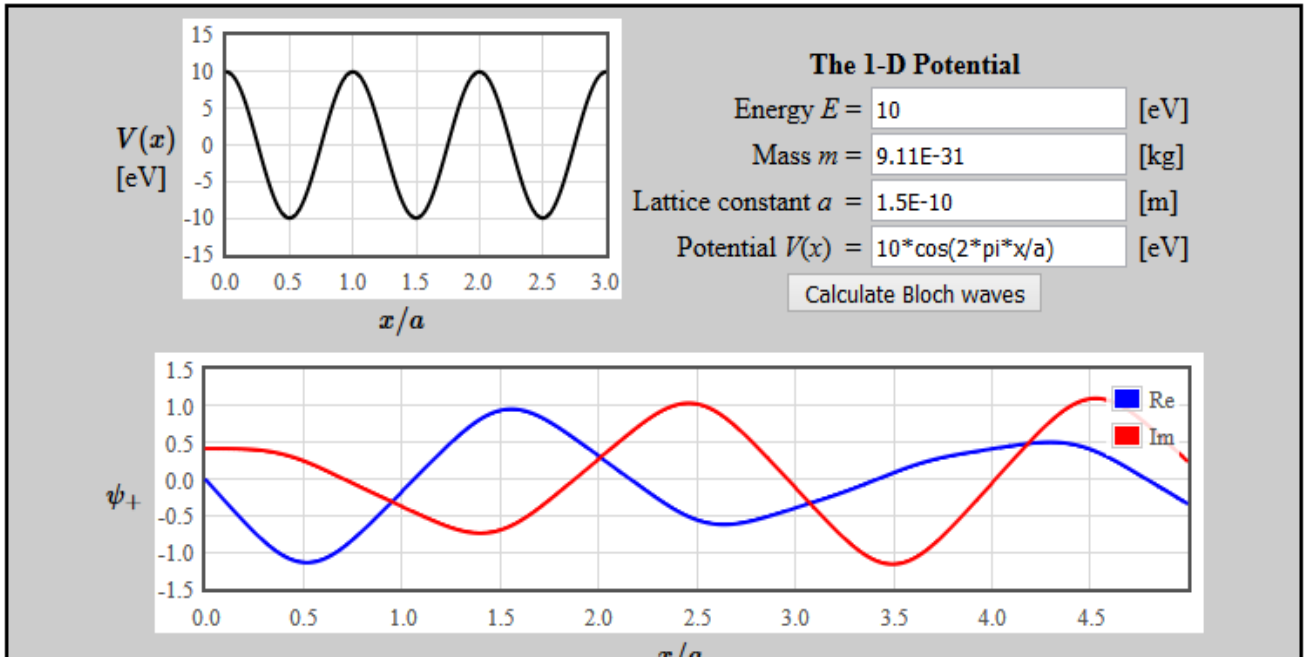
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

Quantum mechanically, the electron moves as a wave through the potential. Due to the diffraction of these waves, there are bands of energies where the electron is allowed to propagate through the potential and bands of energies where no propagating solutions are possible. The Bloch theorem states that the propagating states have the form,

$$\psi = e^{ikx}u_k(x).$$

where k is the wavenumber and $u_k(x)$ is a periodic function with periodicity a.

There is a left moving Bloch wave $\psi_- = e^{-ikx}u_{k-}$ and a right moving Bloch wave $\psi_+ = e^{ikx}u_{k+}$ for every energy. The following form calculates the Bloch waves for a potential $V(x)$ that is specified in the interval between 0 and a. A discussion of the calculation can be found below the form.



Crystal momentum $\hbar\vec{k}$

Ehrenfest theorem: $$i\hbar\frac{d}{dt}\langle \mathbf{A}\rangle = \langle[\mathbf{A},\mathbf{H}]\rangle$$

translation operator $T\psi(\vec{r}) = \psi(\vec{r}+\vec{a})T$

<*T*> is a constant of motion for a perfect crystal $$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle[\mathbf{T},\mathbf{H}_0]\rangle = 0$$

Consider an external force $\vec{F} = -\nabla U \quad U = -F_x x - F_y y - F_z z$

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle[\mathbf{T},\mathbf{H}_0 - F_x x - F_y y - F_z z]\rangle$$

Since $[\mathbf{T},\mathbf{H}_0] = [\mathbf{H}_0,\mathbf{T}] = 0$, this is,

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle -\mathbf{T}(F_x x + F_y y + F_z z) + (F_x x + F_y y + F_z z)\mathbf{T}\rangle$$

http://lampx.tugraz.at/~hadley/ss2/transport/crystalmomentum.php

Crystal momentum

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle -\mathbf{T}(F_x x + F_y y + F_z z) + (F_x x + F_y y + F_z z)\mathbf{T}\rangle.$$

Allow $\mathbf{T}$ to act on $(F_x x + F_y y + F_z z)$,

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle -(F_x(x + a_x) + F_y(y + a_y) + F_z(z + a_z))\mathbf{T} + (F_x x + F_y y + F_z z)\mathbf{T}\rangle$$

$$= \langle -(F_x a_x + F_y a_y + F_z a_z)\mathbf{T}\rangle$$

Here a_x, a_y, a_z are integer steps in the periodic lattice. As $(F_x a_x + F_y a_y + F_z a_z)$ is a constant,

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = -(F_x a_x + F_y a_y + F_z a_z)\langle \mathbf{T}\rangle.$$

Crystal momentum

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = -(F_x a_x + F_y a_y + F_z a_z)\langle \mathbf{T}\rangle.$$

For a Bloch wave $\langle \mathbf{T}\rangle = \langle e^{-i\vec{k}\cdot\vec{r}}u^*_{\vec{k}}|\mathbf{T}|e^{i\vec{k}\cdot\vec{r}}u_{\vec{k}}\rangle = e^{i\vec{k}\cdot\vec{a}}\langle e^{-i\vec{k}\cdot\vec{r}}u^*_{\vec{k}}|e^{i\vec{k}\cdot\vec{r}}u_{\vec{k}}\rangle = e^{i\vec{k}\cdot\vec{a}}$,

$$i\hbar\frac{d}{dt}e^{i\vec{k}\cdot\vec{a}} = -(F_x a_x + F_y a_y + F_z a_z)e^{i\vec{k}\cdot\vec{a}}.$$

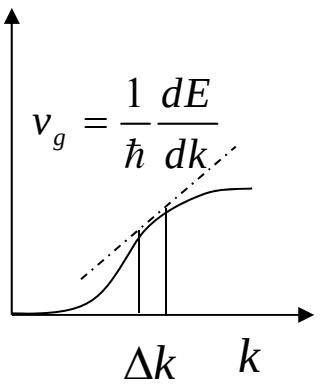
The external force will cause the momentum of the electron to change so $\vec{k}$ will be time dependent. Performing the differentiation with respect to time,

$$-\hbar\left(\frac{dk_x}{dt}a_x + \frac{dk_y}{dt}a_y + \frac{dk_z}{dt}a_z\right)e^{i\vec{k}\cdot\vec{a}} = -(F_x a_x + F_y a_y + F_z a_z)e^{i\vec{k}\cdot\vec{a}}.$$

$$\boxed{\hbar\frac{d\vec{k}}{dt} = \vec{F}_{\text{ext}}.}$$

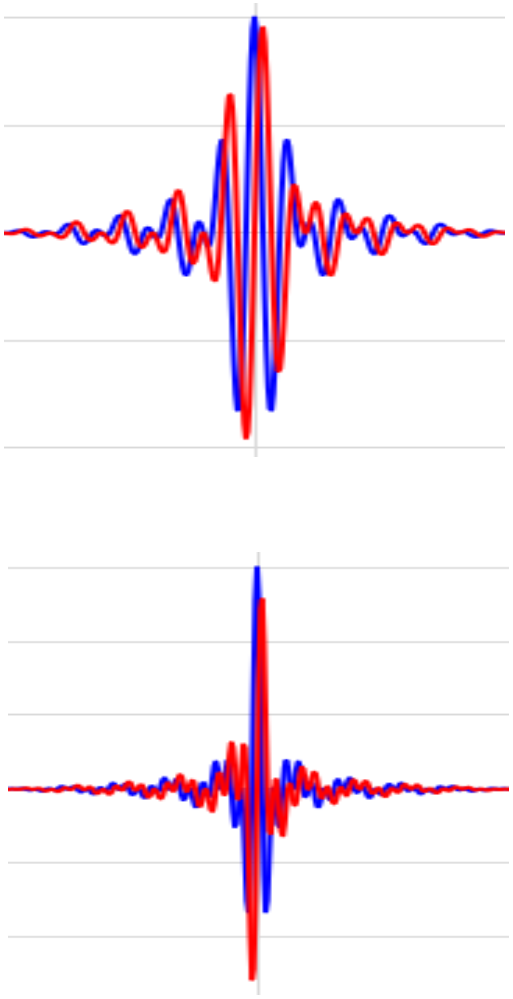
Group velocity

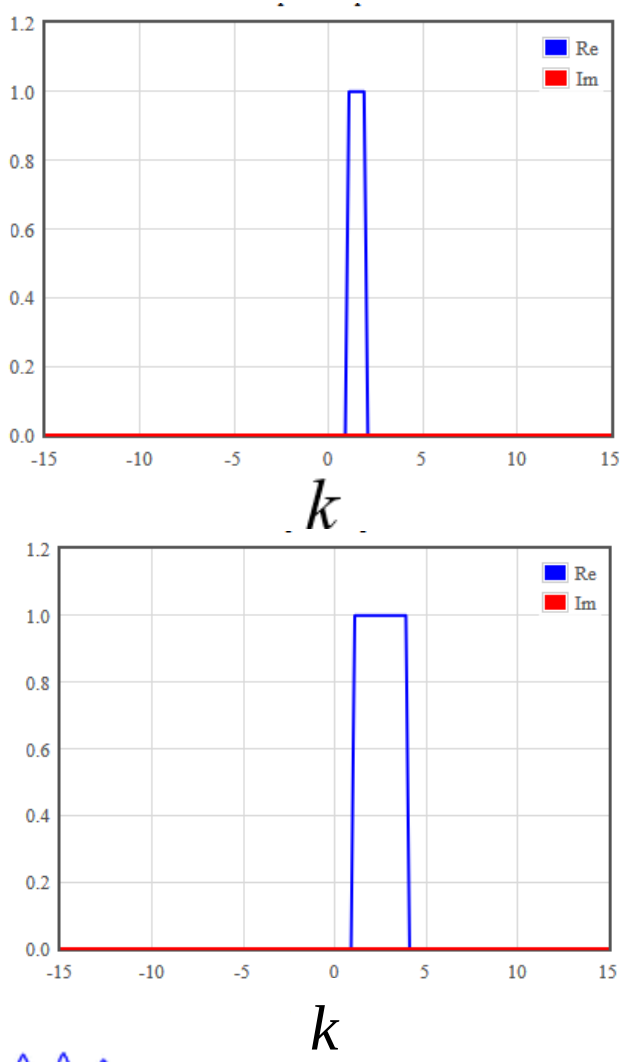
$E = \hbar\omega$

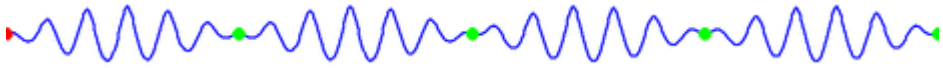


v_g is the velocity of a wave packet

$\Delta x \Delta k \sim 1$



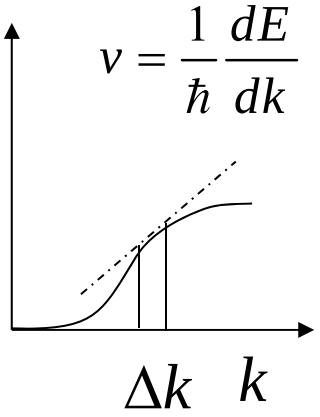




https://en.wikipedia.org/wiki/Phase_velocity

Group velocity

$$E = \hbar\omega$$



$$\vec{v}_g = \frac{1}{\hbar}\nabla_{\vec{k}} E$$

$$\frac{d\vec{v}_g}{dt} = \frac{1}{\hbar}\left(\frac{d^2E}{dk_x dt}\hat{k}_x + \frac{d^2E}{dk_y dt}\hat{k}_y + \frac{d^2E}{dk_z dt}\hat{k}_z\right) = \frac{1}{\hbar}\nabla_k^2 E\,\frac{d\vec{k}}{dt}$$

$$\frac{d\vec{v}_g}{dt} = \frac{1}{\hbar^2}\nabla_k^2 E\vec{F}_{ext}$$

v_g is the velocity of a wave packet

$\Delta x \Delta k \sim 1$

$$\vec{F}_{ext} = \frac{\hbar^2}{\nabla_k^2 E(\vec{k})}\frac{d\vec{v}_g}{dt} = m^*(\vec{k})\vec{a}_g$$

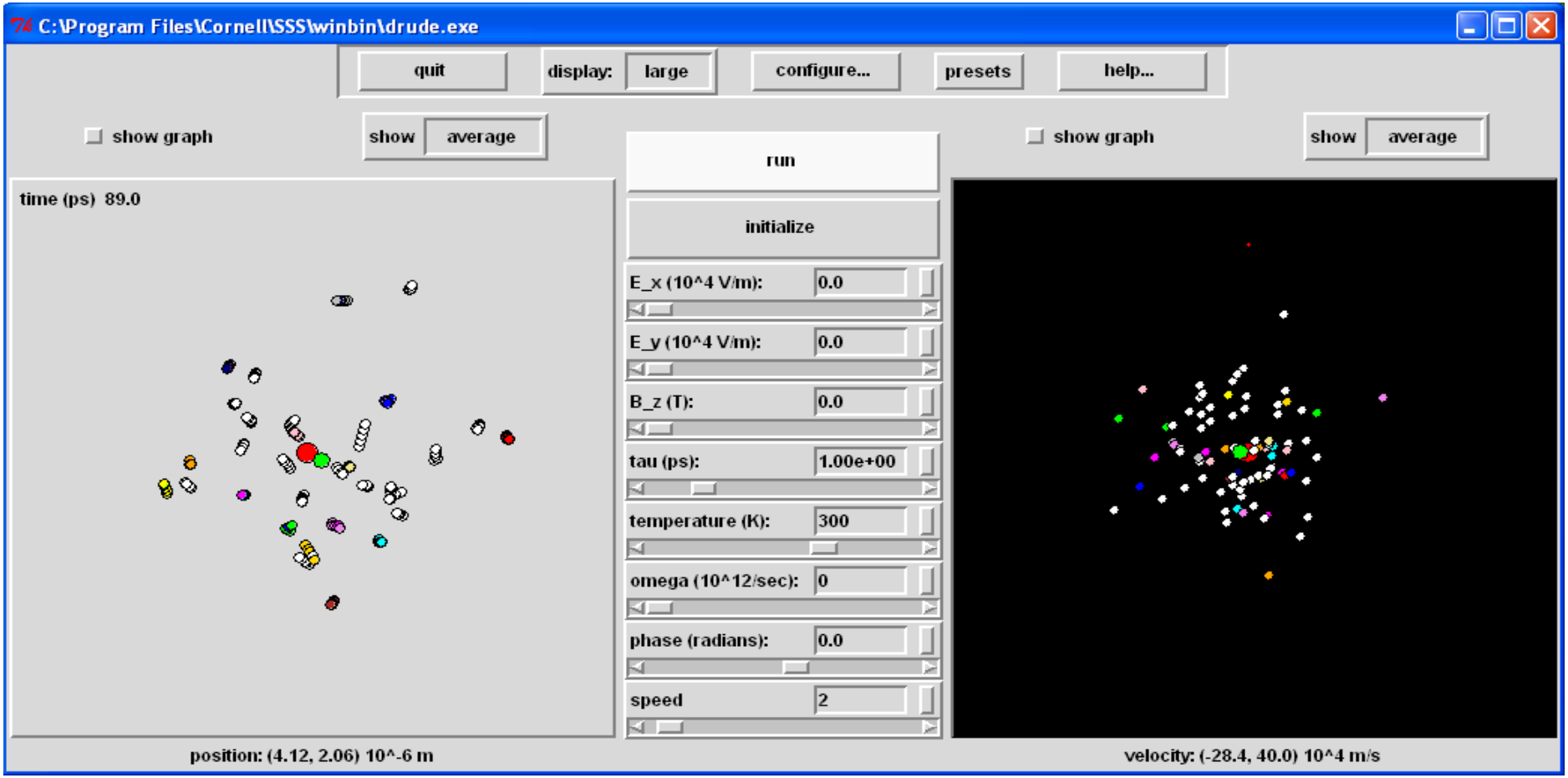
Particles in a semiconductor can be thought of as free particles with an effective mass.

Boltzmann equation

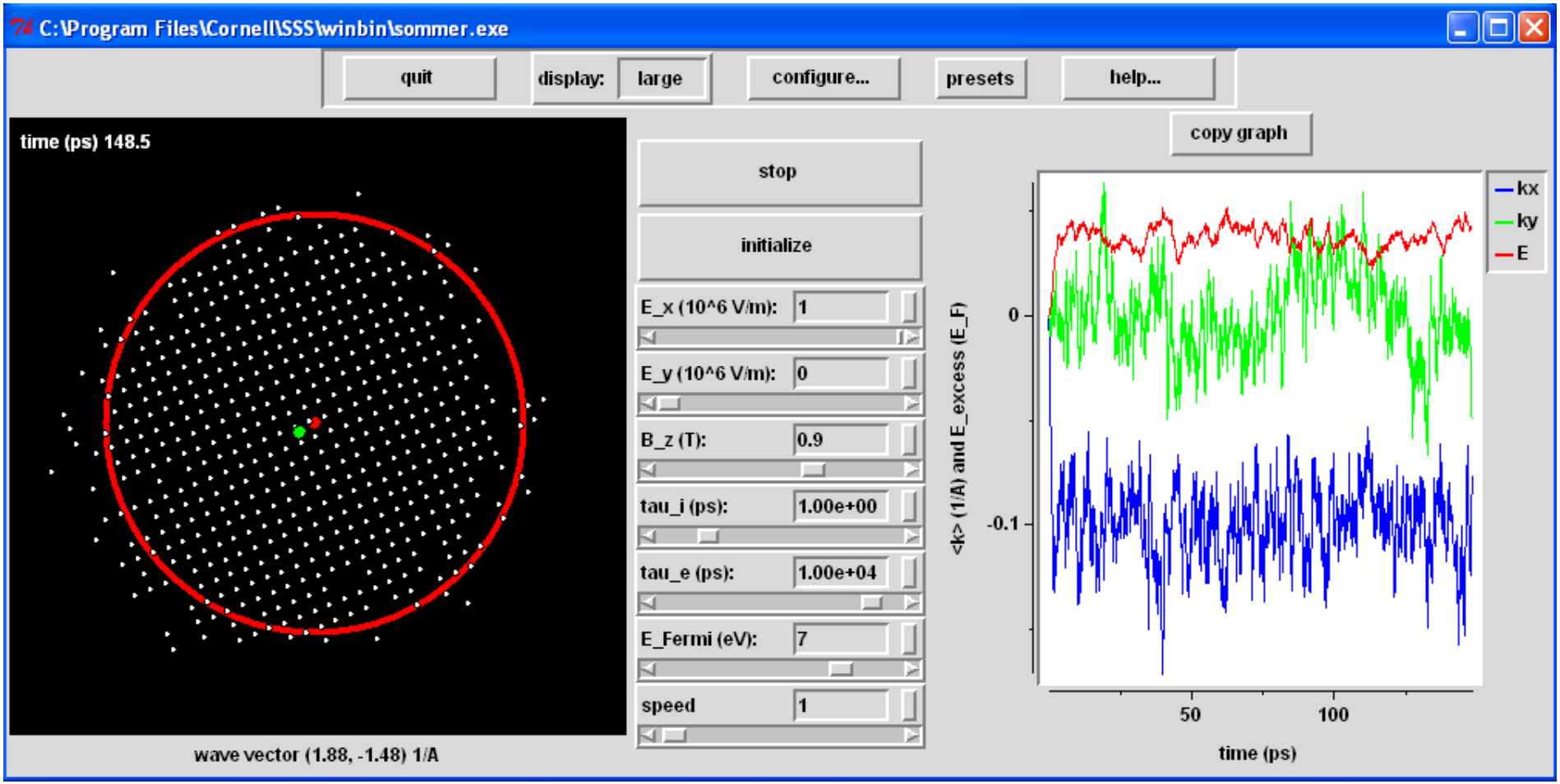
Wave/particle nature of electrons

Usually when we think about a current flowing, we imagine the electrons as particles moving along. Really we should be thinking about how the occupation of the wave like eigenstates are changing.

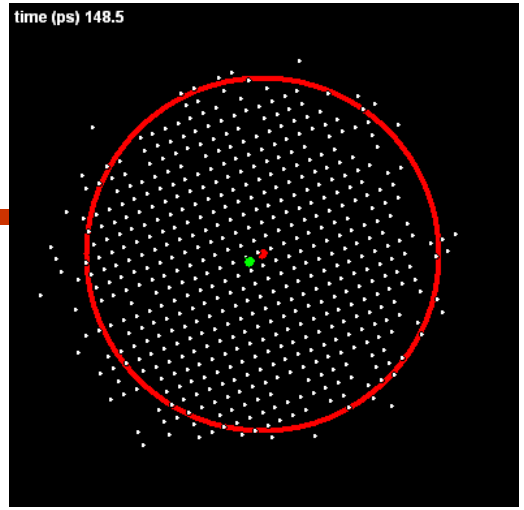
When wave packets are built from the eigenstates, they move like particles with an effective mass.



If no forces are applied, the electrons diffuse.
The average velocity moves against an electric field.
In just a magnetic field, the average velocity is zero.
In an electric and magnetic field, the electrons move in a straight line at the Hall angle.


C:\Program Files\Cornell\SSS\winbin\sommer.exe
quit
display:
large
configure...
presets
help...
time (ps) 148.5
wave vector (1.88, -1.48) 1/A
stop
initialize
E_x (10^6 V/m):
1
E_y (10^6 V/m):
0
B_z (T):
0.9
tau_i (ps):
1.00e+00
tau_e (ps):
1.00e+04
E_Fermi (eV):
7
speed
1
copy graph
kx
ky
E
0
-0.1
<k> (1/A) and E_excess (E_F)
50
100
time (ps)

Master equation



$$\vec{j}_{elec} = -e\int \vec{v}(\vec{k})D(\vec{k})\,f(\vec{k})\,d\vec{k}$$

$$\frac{d}{dt}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} = \begin{bmatrix} -\sum_{j\neq 1}\Gamma_{1\to j} & \Gamma_{2\to 1} & \Gamma_{3\to 1} & \Gamma_{4\to 1} \\ \Gamma_{1\to 2} & -\sum_{j\neq 2}\Gamma_{2\to j} & \Gamma_{3\to 2} & \Gamma_{4\to 2} \\ \Gamma_{1\to 3} & \Gamma_{2\to 3} & -\sum_{j\neq 3}\Gamma_{3\to j} & \Gamma_{4\to 3} \\ \Gamma_{1\to 4} & \Gamma_{2\to 4} & \Gamma_{3\to 4} & -\sum_{j\neq 4}\Gamma_{4\to j} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

Fermi's golden rule: $$\Gamma_{k\to k'} = \frac{2\pi}{\hbar}\left|\langle k'|H|k\rangle\right|^2 \delta\left(E_k - E_{k'}\right)$$

Current densities

Electrical $\vec{j}_{\text{elec}} = -e \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3k$

Particle $\vec{j}_n = \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3k$

Energy $\vec{j}_U = \int \vec{v}_{\vec{k}} E(\vec{k}) D(\vec{k}) f(\vec{k}) d^3k.$

1st law: $dU = dQ - dW + \mu dN.$

Heat $\vec{j}_Q = \int \vec{v}_{\vec{k}} \left(E(\vec{k}) - \mu \right) D(\vec{k}) f(\vec{k}) d^3k.$

http://lampx.tugraz.at/~hadley/ss2/transport/intro.php

Current densities

Electrical

$$\vec{j}_{\text{elec}} = -e \int \vec{v}_{\vec{k}} D(\vec{k}) f(\vec{k}) d^3k$$

$$D(\vec{k}) = \frac{2}{(2\pi)^3} \longleftarrow \text{spin}$$

$$\vec{v}_{\vec{k}} = \frac{\nabla_{\vec{k}} E(\vec{k})}{\hbar}$$

$f(\vec{k})$ Probability that state *k* is occupied.

http://lampx.tugraz.at/~hadley/ss2/transport/intro.php