

Transport

Transport phenomena

Crystal momentum

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

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

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

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

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

Bloch waves are eigenfunctions of the Hamiltonian

Crystal momentum $\hbar\vec{k}$

Ehrenfest theorem:
$$i\hbar \frac{d}{dt} \langle A \rangle = \langle AH - HA \rangle$$

translation operator
$$T\psi(x) = \psi(x+a)T$$

$\langle T \rangle$ is a constant of motion
for a perfect crystal
$$i\hbar \frac{d}{dt} \langle T \rangle = \langle TH_0 - H_0T \rangle = 0$$

Consider an external
force in the x -direction
$$F_{ext} = -\frac{dU}{dx} \Rightarrow U = -F_{ext}x$$

$$i\hbar \frac{d}{dt} \langle T \rangle = \langle T (H_0 - F_{ext}x) - (H_0 - F_{ext}x)T \rangle$$

$$i\hbar \frac{d}{dt} \langle T \rangle = \langle -TF_{ext}x + F_{ext}xT \rangle$$

Crystal momentum

$$i\hbar \frac{d}{dt} \langle T \rangle = \langle -F_{ext} (x+a)T + F_{ext} xT \rangle$$

$$i\hbar \frac{d}{dt} \langle T \rangle = \langle -F_{ext} aT \rangle = -F_{ext} a \langle T \rangle$$

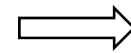
The expectation value of T for a Bloch state is

$$\langle T \rangle = \langle e^{-ikx} u_k(x) | T | e^{ikx} u_k(x) \rangle = \langle e^{-ikx} u_k(x) | e^{ik(x+a)} u_k(x+a) \rangle$$

$$\langle T \rangle = e^{ika} \langle e^{-ikx} u_k(x) | e^{ikx} u_k(x) \rangle = e^{ika}$$

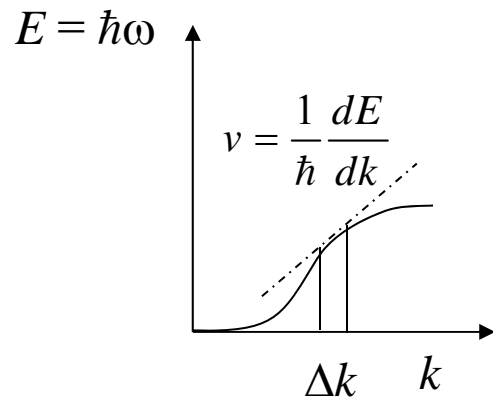
$$i\hbar \frac{d}{dt} e^{ika} = -F_{ext} a e^{ika}$$

$$i\hbar (ia) \frac{dk}{dt} e^{ika} = -F_{ext} a e^{ika}$$

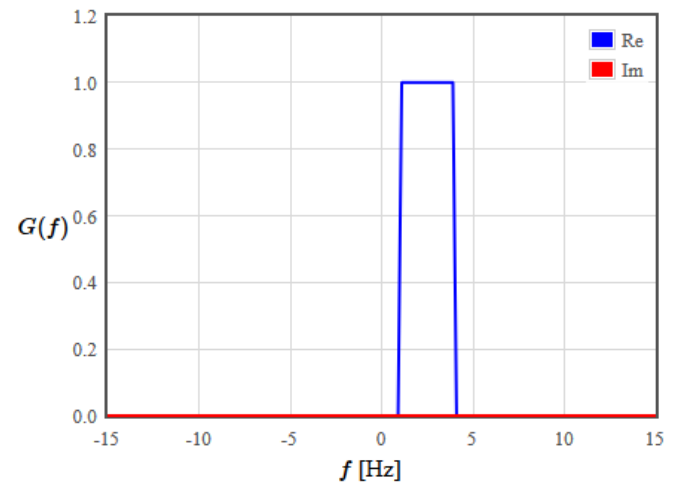
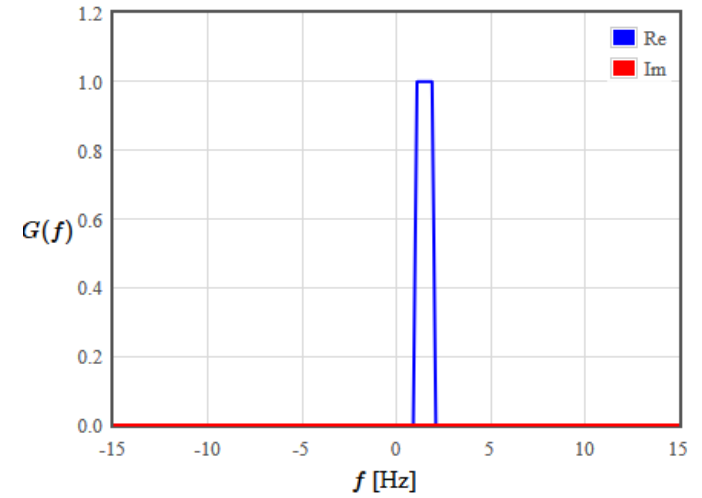
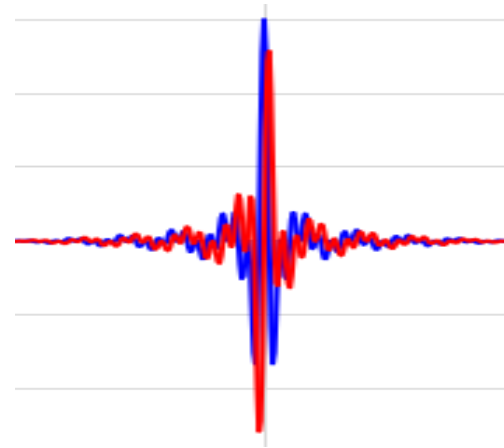
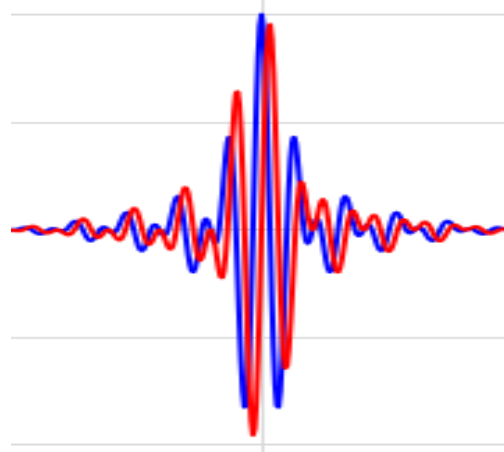


$$\hbar \frac{d\vec{k}}{dt} = \vec{F}_{ext}$$

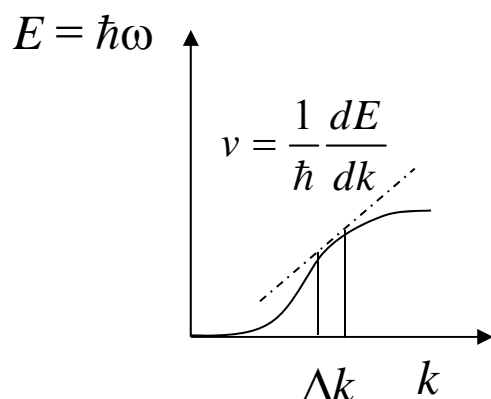
Group velocity



v_g is the velocity
of a wave packet
 $\Delta x \Delta k \sim 1$



Group velocity



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

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

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

v_g is the velocity of a wave packet

$$\Delta x \Delta k \sim 1$$

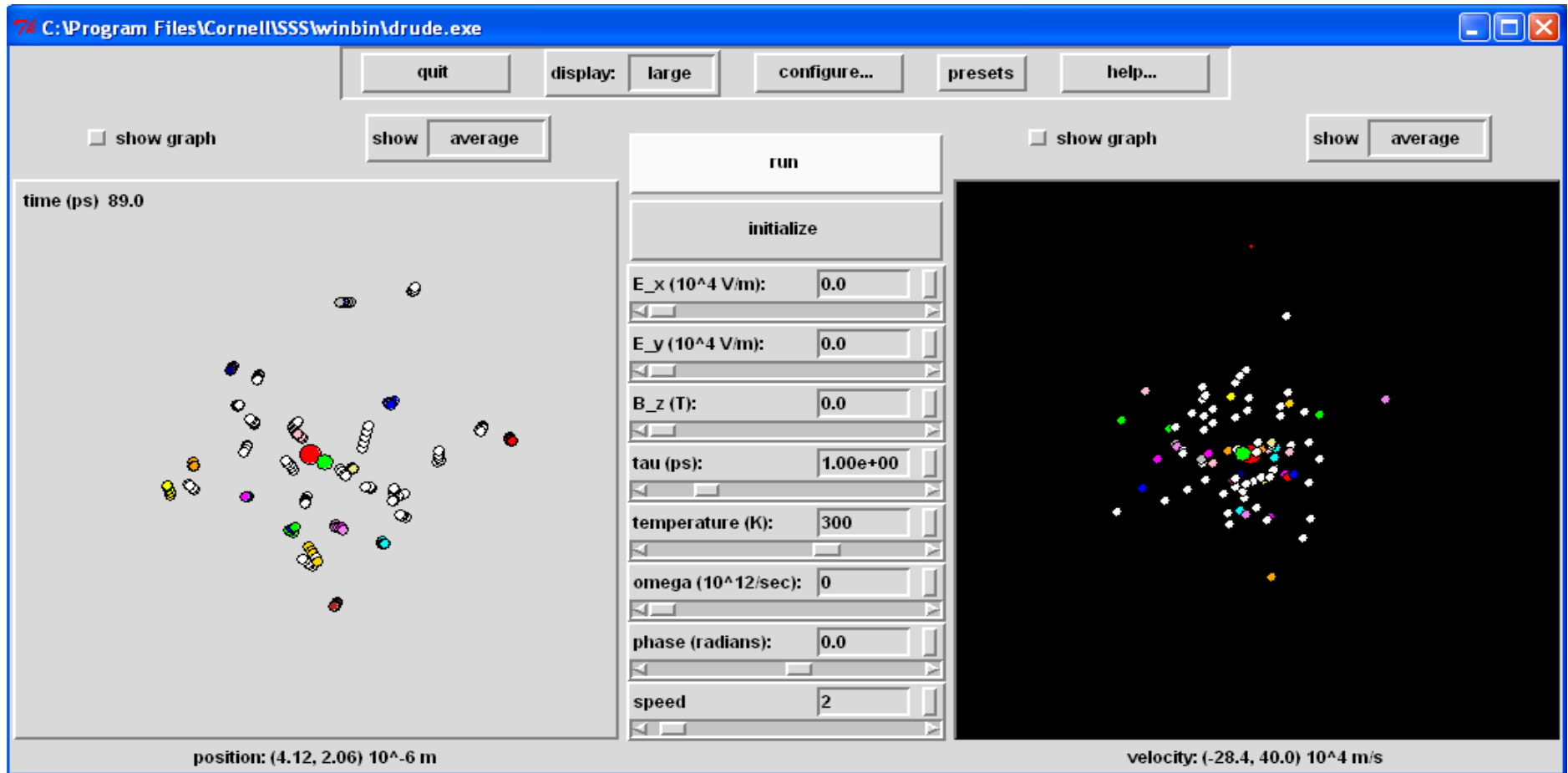
$$\vec{F}_{ext} = \frac{\hbar^2}{\nabla_{\vec{k}}^2 E(\vec{k})} \frac{d\vec{v}_g}{dt} = m^*(\vec{k}) \vec{a}_g$$

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

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:

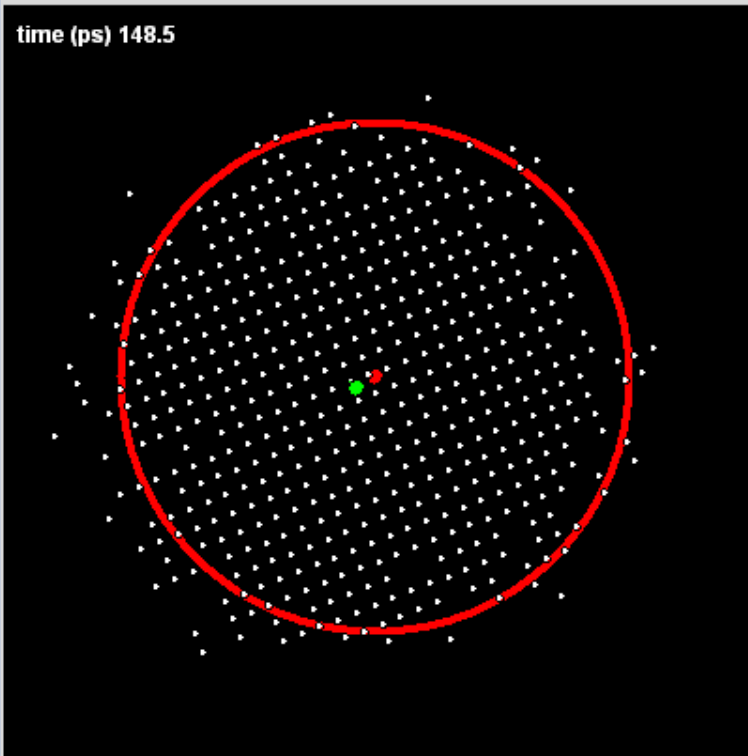
large

configure...

presets

help...

time (ps) 148.5



wave vector (1.88, -1.48) 1/Å

stop

initialize

E_x (10⁶ V/m): 1

E_y (10⁶ V/m): 0

B_z (T): 0.9

tau_i (ps): 1.00e+00

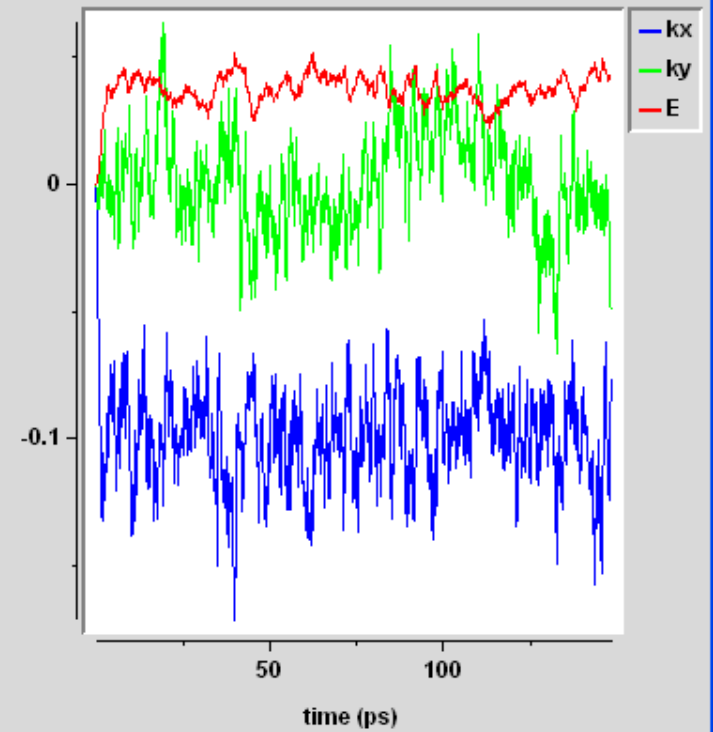
tau_e (ps): 1.00e+04

E_Fermi (eV): 7

speed: 1

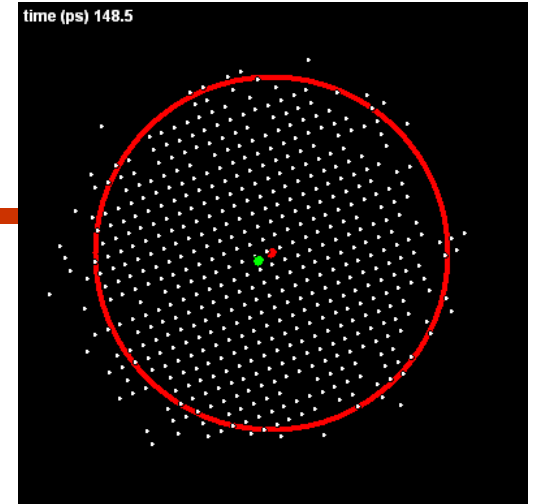
copy graph

$\langle k \rangle$ (1/Å) and E_excess (E_F)



Master equation

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



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

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

Current densities

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

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

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

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

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