Transport phenomena

Crystal momentum

Boltzmann equation

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

Crystal momentum $\hbar\vec{k}$

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

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

$<T>$ 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

$$F_{ext} = -\frac{dU}{dx} \quad \Rightarrow \quad U = -F_{ext}x$$

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

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

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

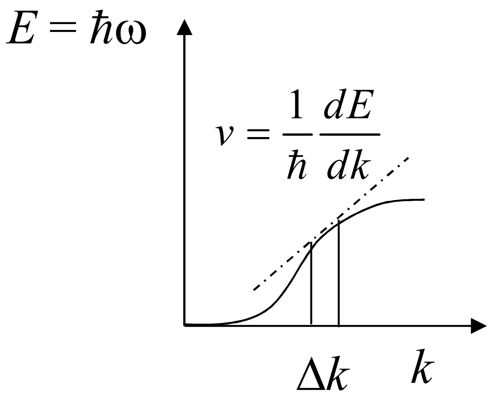
$$\langle T\rangle = \langle e^{-ikx}u_k(x)|T|e^{ikx}u_k(x)\rangle = \langle e^{-ikx}u_k(x)|e^{ik(x+a)}u_k(x+a)\rangle$$

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

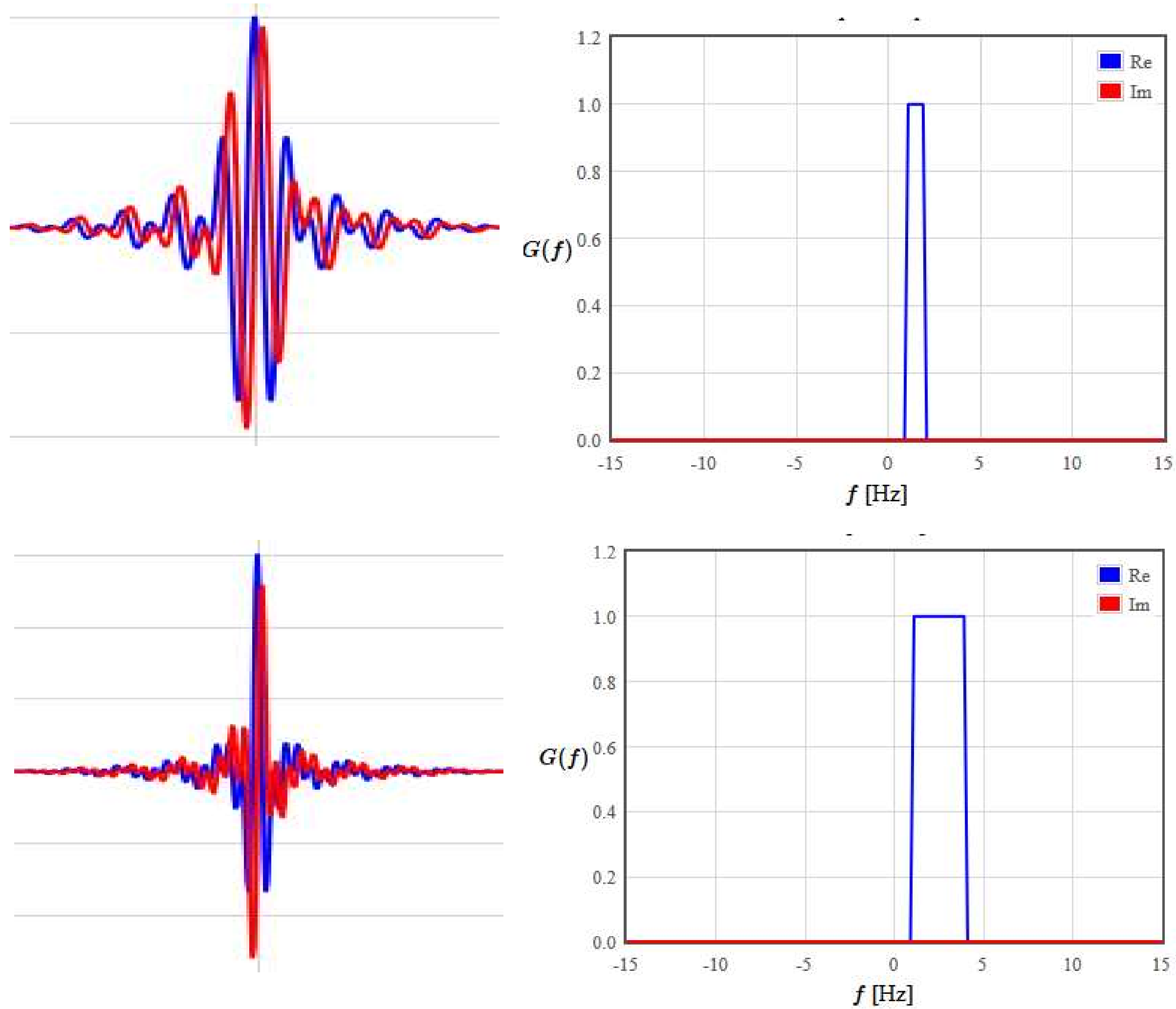
$$i\hbar \frac{d}{dt}e^{ika} = -F_{ext}ae^{ika}$$

$$i\hbar(ia)\frac{dk}{dt}e^{ika} = -F_{ext}ae^{ika} \quad \Longrightarrow \quad \boxed{\hbar\frac{d\vec{k}}{dt} = \vec{F}_{ext}}$$

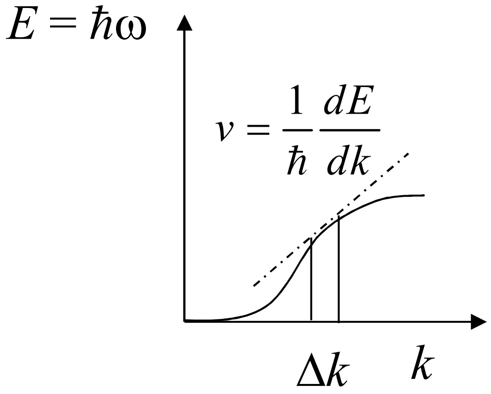
Group velocity



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



Group velocity



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

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

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

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

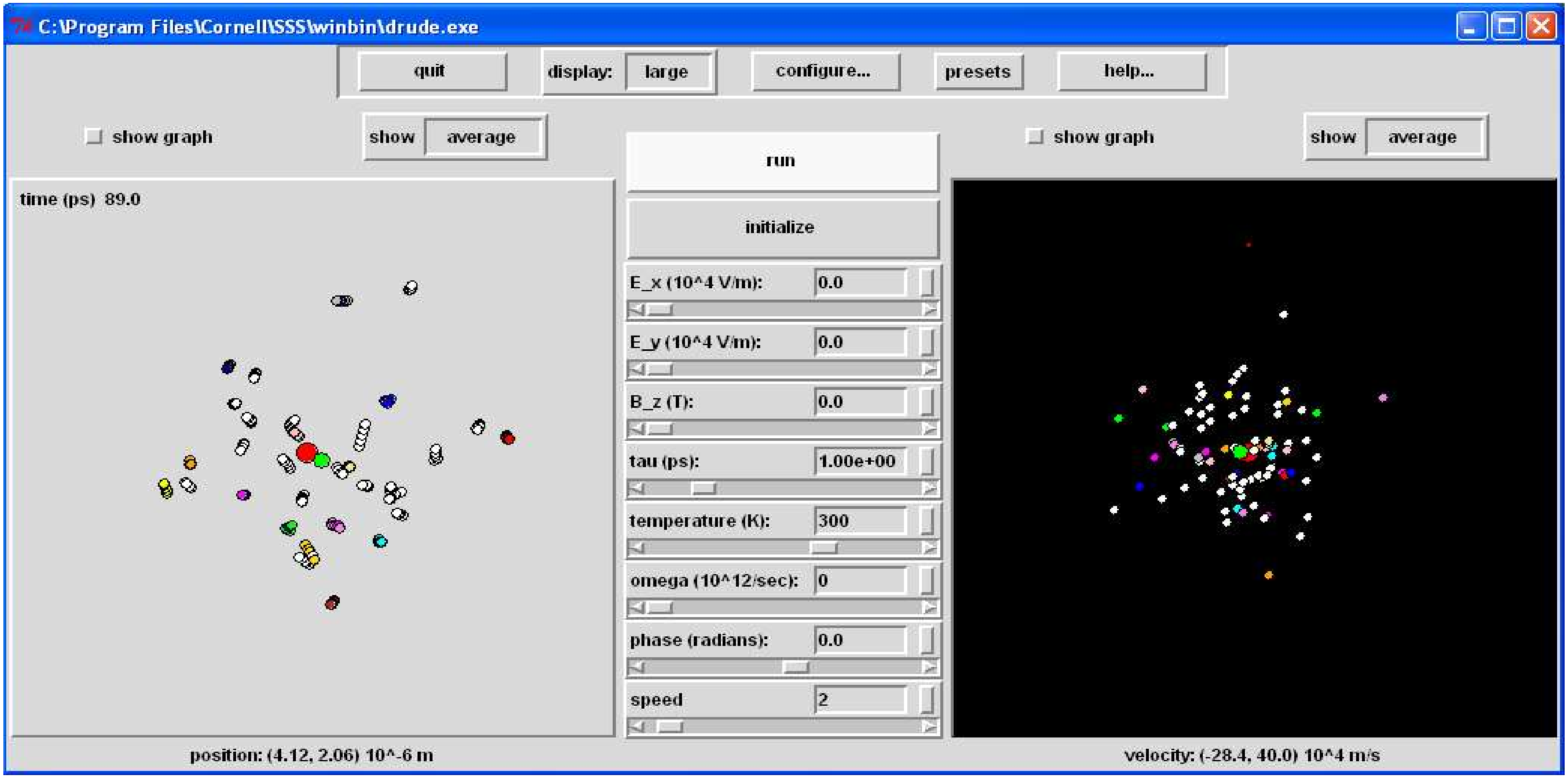
$$\vec{F}_{ext} = \frac{\hbar^2}{\nabla_k^2 E(\vec{k})}\frac{d\vec{v}_g}{dt} = m^*(\vec{k})\vec{a}_g$$

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

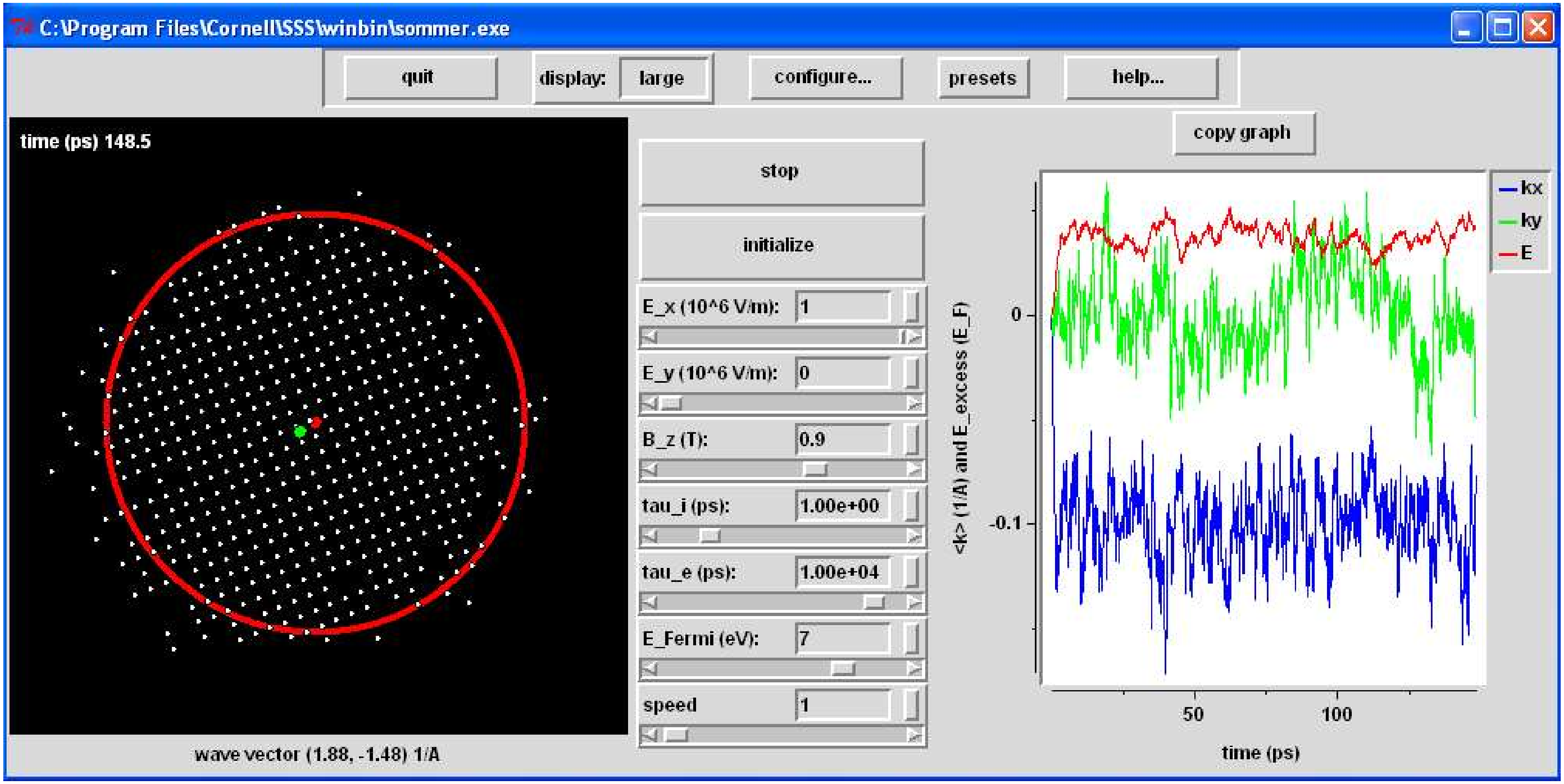
Wave/particle nature of electrons

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.

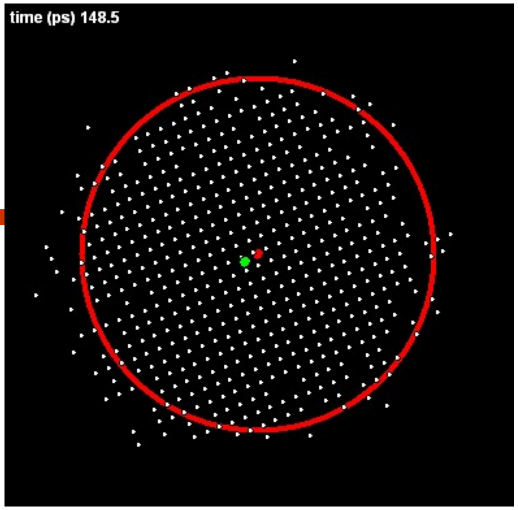


If no forces are applied, the electrons diffuse.
The average velocity moves against an electric field.
In just a magnetic field, the average velocity is zero.
In an electric and magnetic field, the electrons move in a straight line at the Hall angle.



C:\Program Files\Cornell\SSS\winbin\sommer.exe
quit
display:
large
configure...
presets
help...
time (ps) 148.5
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
wave vector (1.88, -1.48) 1/A
copy graph
kx
ky
E
<k> (1/A) and E_excess (E_F)
0
-0.1
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: $\Gamma_{k\to k'} = \frac{2\pi}{\hbar}\left|\langle k' | H | k\rangle\right|^2 \delta\left(E_k - E_{k'}\right)$

Probability current

The probability of finding an electron somewhere is proportional to $\psi^* \psi$

If the probability decreases somewhere it must increase somewhere else.
This can be expressed as a continuity equation,

$$\frac{d(\psi^* \psi)}{dt} = \nabla \cdot \vec{S}$$

probability current

$$\frac{d\psi^*}{dt}\psi + \psi^* \frac{d\psi}{dt} = \nabla \cdot \vec{S}$$

The Schrödinger equation and its complex conjugate

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

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi^* + V(\vec{r})\psi^*$$

Probability current

$$\frac{\partial \psi^* \psi}{\partial t} = i\frac{\hbar}{2m}\nabla^2 \psi^* \psi + i\psi^* \frac{\hbar}{2m}\nabla^2 \psi.$$

The right side can be written as $\nabla \cdot \vec{S}$ if,

$$\vec{S} = -\frac{i\hbar}{2m}(\psi^* \nabla \psi - \psi \nabla \psi^*).$$

Normalized probability current (1-d)

$$S = \frac{-i\hbar}{2m}\frac{\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)}{\int_0^L \psi^* \psi dx}.$$

Probability current in 1-D

The normalize probability current density

$$S = \frac{-i\hbar}{2m} \frac{\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}}{\int_0^L \psi^* \psi \, dx}$$

For Bloch waves, S is constant in space. The larger the crystal, the more spread out the electron and the lower the current density. The velocity is the probability current divided by the average density $1/Na$.

$$v_k = -v_{-k} = \frac{-i\hbar a}{2m} \frac{\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}}{\int_0^a \psi^* \psi \, dx}$$