Transport

Transport phenomena

Crystal momentum

Boltzmann equation

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

- **Transport**
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  - Crystal momentum
  - Boltzmann equation
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  - Electrochemical potential
  - Electrical conductivity
  - Thermoelectric currents
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    - 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,

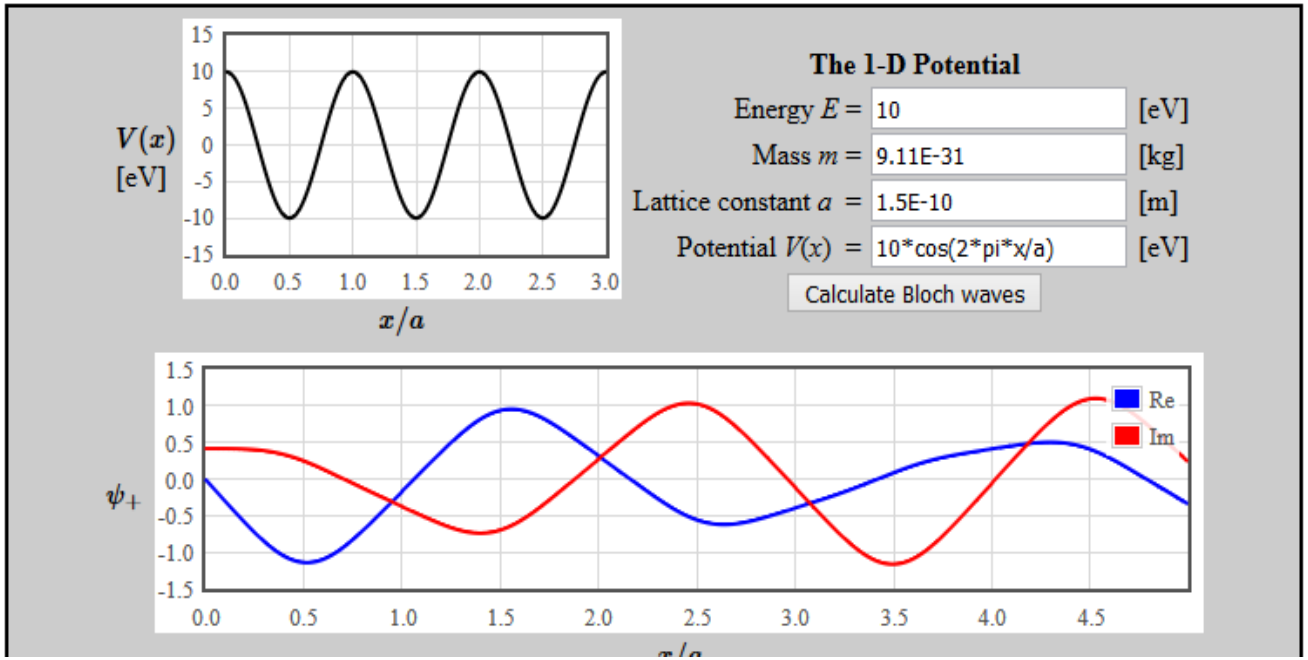
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi.$$

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 $\vec{F} = -\nabla U$ $U = -\vec{F}_{\text{ext}}\cdot\vec{r}$

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle [\mathbf{T},\mathbf{H}_0 - \vec{F}_{\text{ext}}\cdot\vec{r}]\rangle$$

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

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle -\mathbf{T}\vec{F}_{\text{ext}}\cdot\vec{r} + \vec{F}_{\text{ext}}\cdot\vec{r}\mathbf{T}\rangle$$

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

Crystal momentum

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle -\mathbf{T}\vec{F}_{\text{ext}}\cdot\vec{r} + \vec{F}_{\text{ext}}\cdot\vec{r}\mathbf{T}\rangle.$$

Allow $\mathbf{T}$ to act on the $\vec{F}_{\text{ext}}\cdot\vec{r}$ term,

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = \langle -\vec{F}_{\text{ext}}\cdot(\vec{r}+\vec{a})\mathbf{T} + \vec{F}_{\text{ext}}\cdot\vec{r}\mathbf{T}\rangle = \langle -\vec{F}_{\text{ext}}\cdot\vec{a}\mathbf{T}\rangle.$$

$\vec{F}_{\text{ext}}\cdot\vec{a}$ is a constant,

$$i\hbar\frac{d}{dt}\langle \mathbf{T}\rangle = -\vec{F}_{\text{ext}}\cdot\vec{a}\langle \mathbf{T}\rangle.$$

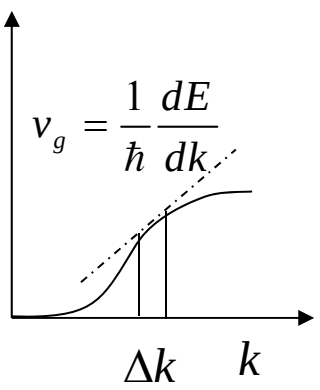
For a Bloch wave $\langle \mathbf{T}\rangle = e^{i\vec{k}\cdot\vec{a}}$,

$$i\hbar\frac{d}{dt}e^{i\vec{k}\cdot\vec{a}} = -\vec{F}_{\text{ext}}\cdot\vec{a}e^{i\vec{k}\cdot\vec{a}}.$$

$$-\hbar\frac{d\vec{k}}{dt}\cdot\vec{a}e^{i\vec{k}\cdot\vec{a}} = -\vec{F}_{\text{ext}}\cdot\vec{a}e^{i\vec{k}\cdot\vec{a}} \quad \Longrightarrow \quad \boxed{\hbar\frac{d\vec{k}}{dt} = \vec{F}_{ext}}$$

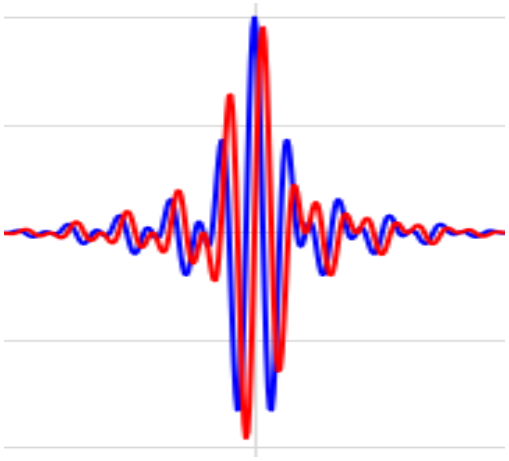
Group velocity

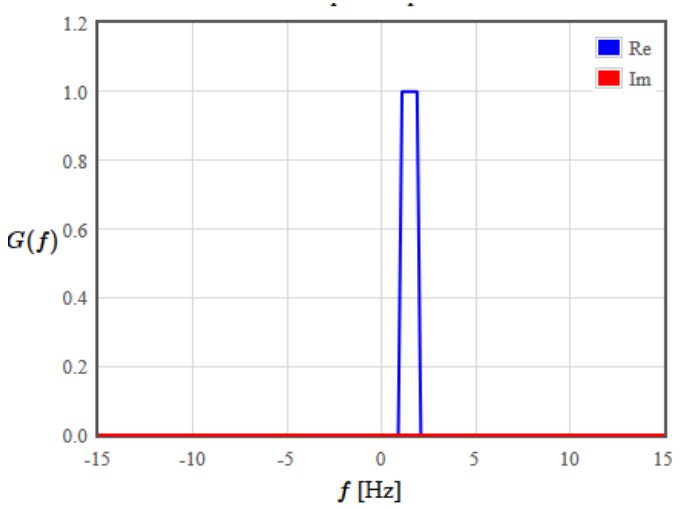
$E = \hbar\omega$

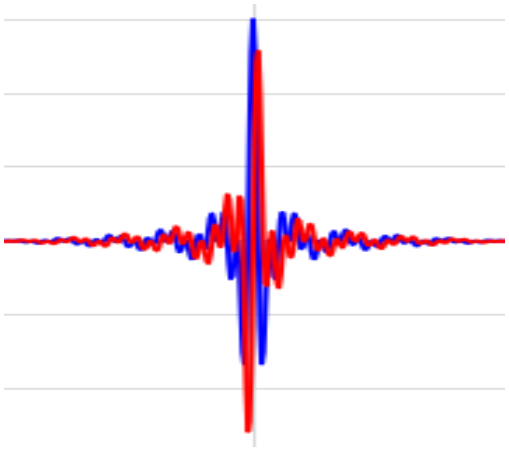


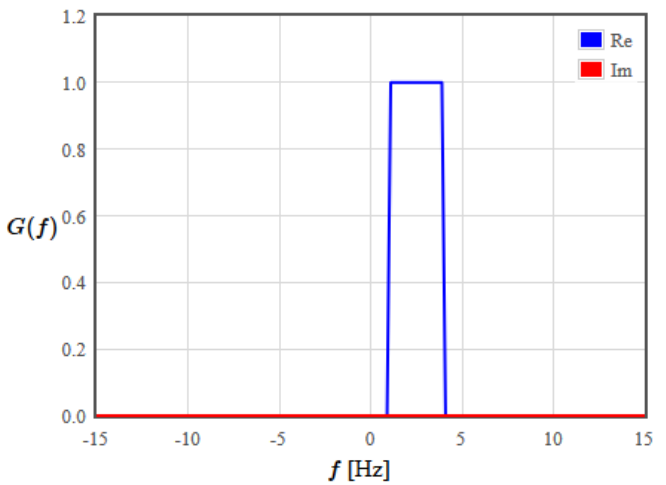
v_g is the velocity of a wave packet

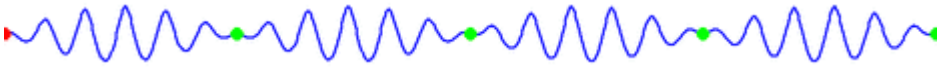
$\Delta x \Delta k \sim 1$





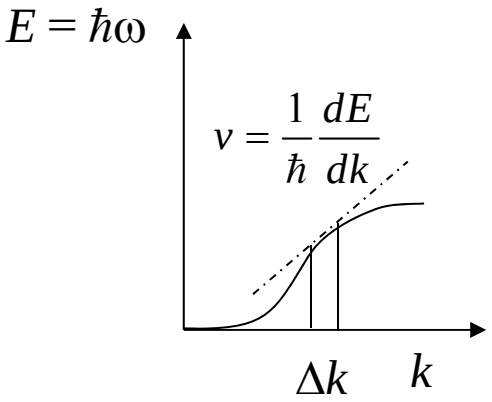






https://en.wikipedia.org/wiki/Phase_velocity

Group velocity



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

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

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

v_g is the velocity of a wave packet

$\Delta x \Delta k \sim 1$

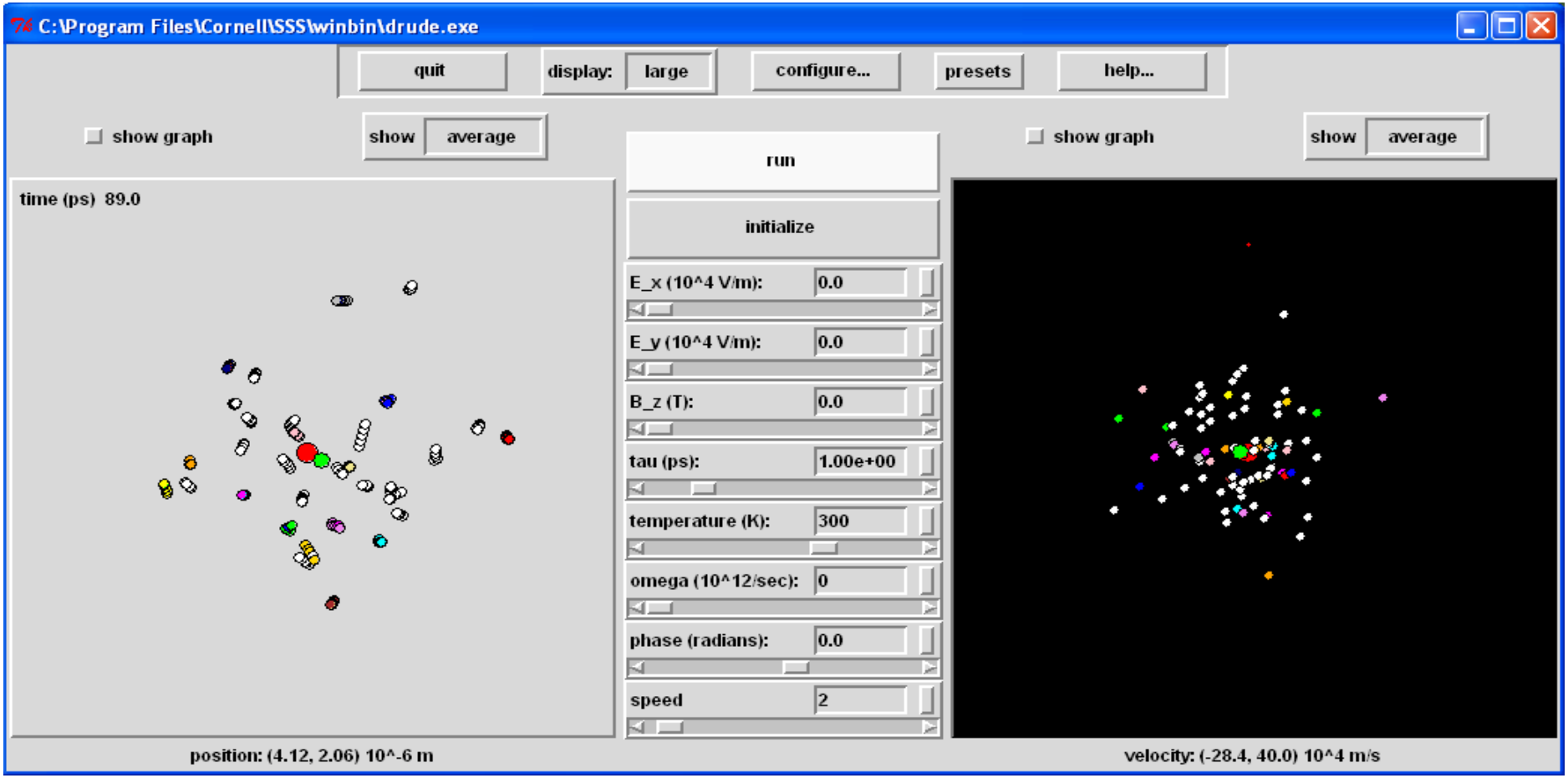
$$\vec{F}_{ext} = \frac{\hbar^2}{\nabla_k^2 E(\vec{k})}\frac{d\vec{v}_g}{dt} = m^*(\vec{k})\vec{a}_g$$

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

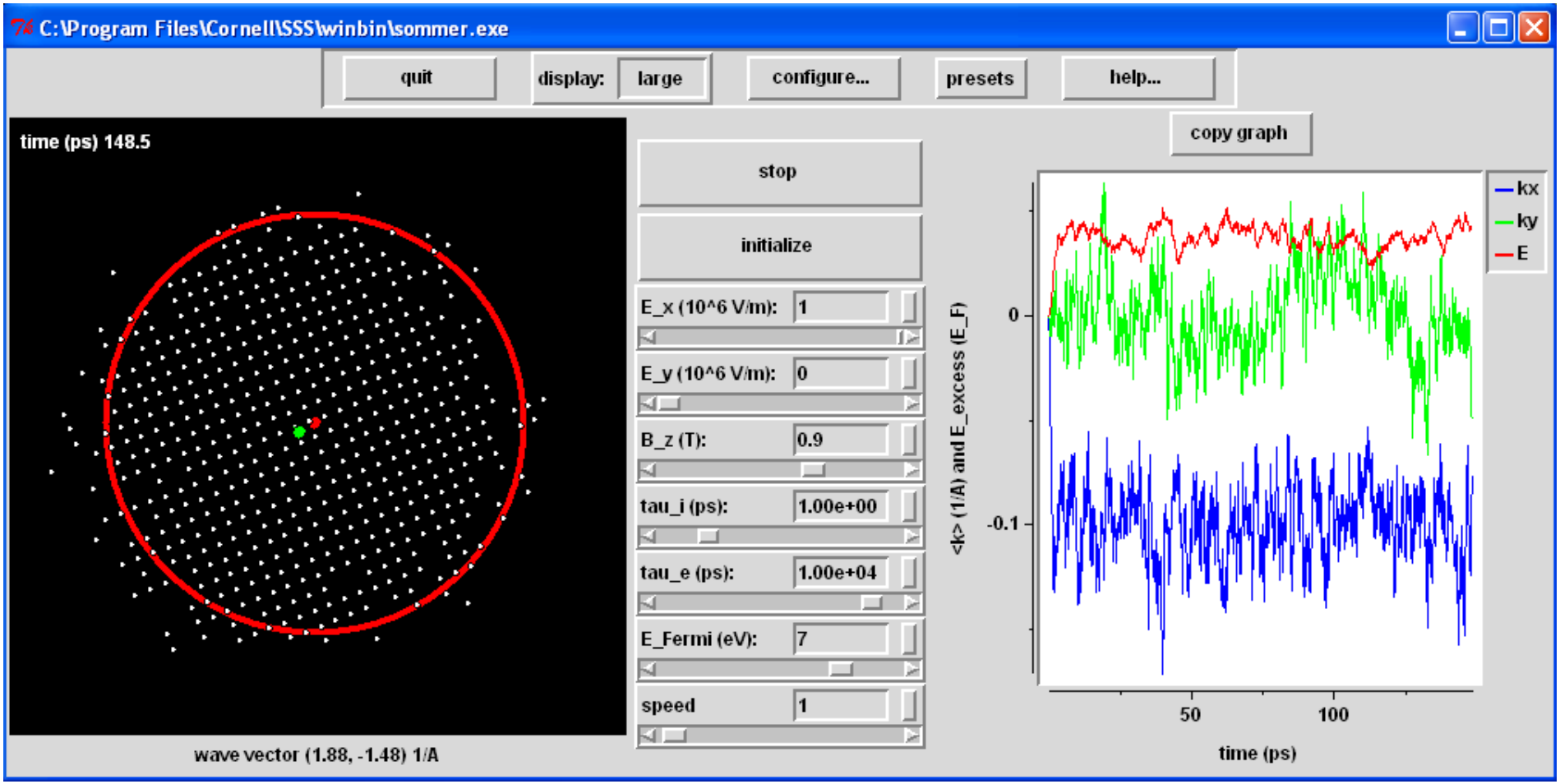
Wave/particle nature of electrons

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.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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)