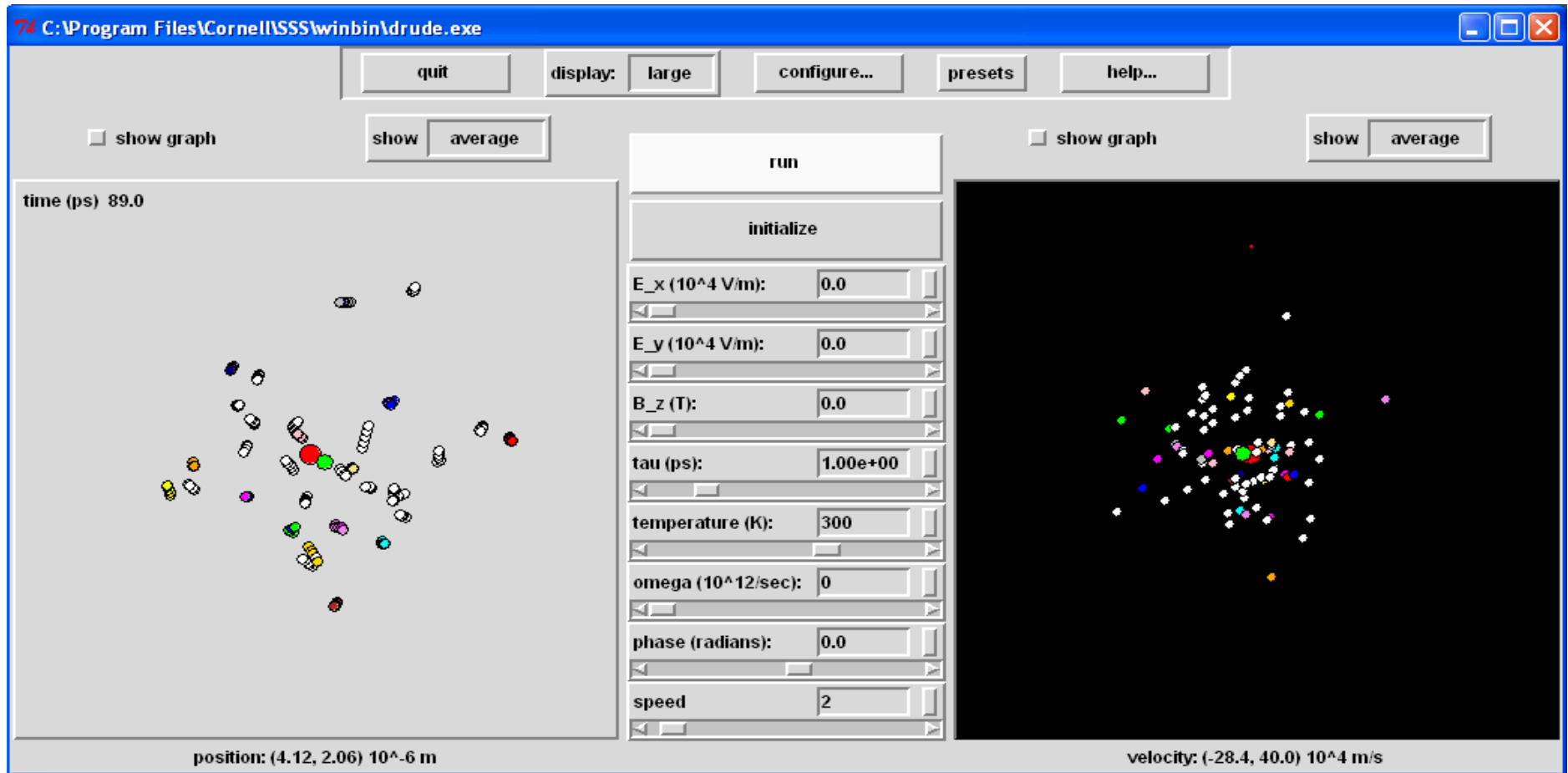


Boltzmann equation

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:

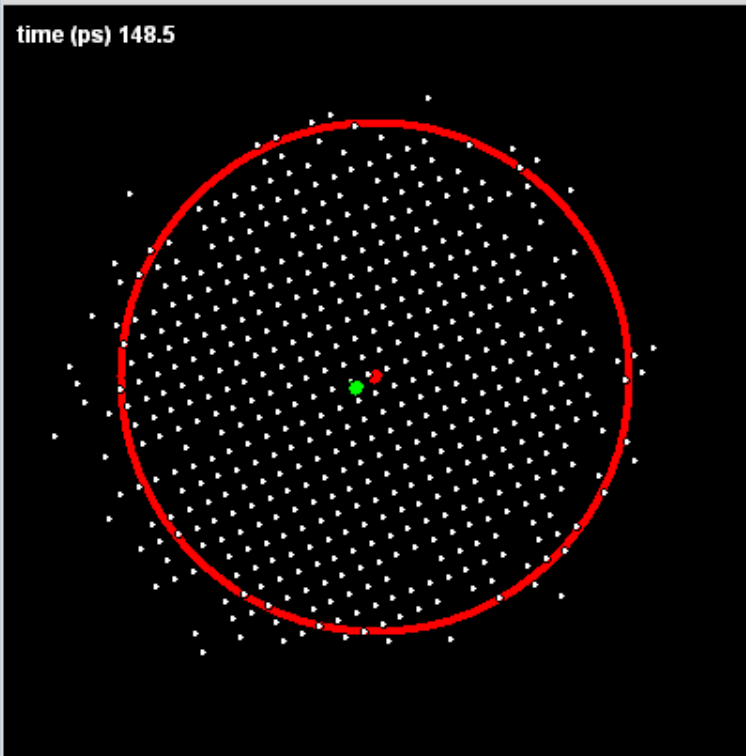
large

configure...

presets

help...

time (ps) 148.5



wave vector (1.88, -1.48) 1/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

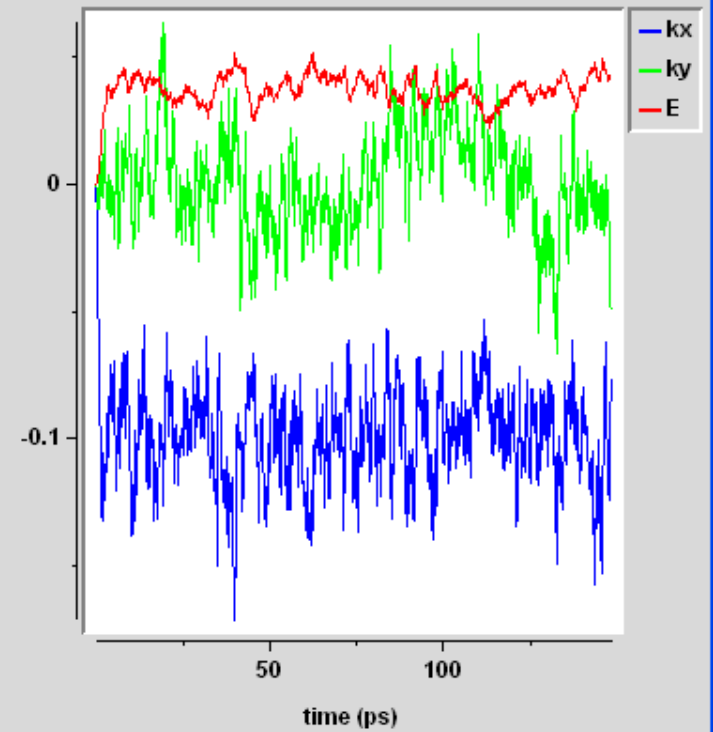
tau_e (ps): 1.00e+04

E_Fermi (eV): 7

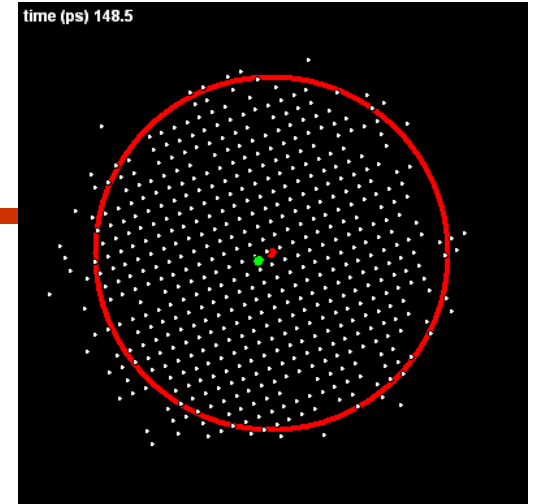
speed: 1

copy graph

<k> (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

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

Current densities

Electrical

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

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

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

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

Liouville's theorem

$f(\vec{r}, \vec{k}, t)$ Probability that state k is occupied at position r and time t .

Number of electrons:
$$N = \int d^3 r \int d^3 k f(\vec{r}, \vec{k}, t).$$

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = 0.$$

If the probability of finding an electron at a particular position with a particular momentum decreases, the probability must increase somewhere else.

Boltzmann Equation

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = 0.$$

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = \frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt} + \frac{\partial f}{\partial k_x} \frac{dk_x}{dt} + \frac{\partial f}{\partial k_y} \frac{dk_y}{dt} + \frac{\partial f}{\partial k_z} \frac{dk_z}{dt} + \frac{\partial f}{\partial t} = 0$$

$$\frac{d}{dt} f(\vec{r}, \vec{k}, t) = \frac{d\vec{r}}{dt} \cdot \nabla_{\vec{r}} f + \frac{d\vec{k}}{dt} \cdot \nabla_{\vec{k}} f + \frac{\partial f}{\partial t} = 0.$$

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

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar} \vec{F}_{\text{ext}} \cdot \nabla_{\vec{k}} f - \vec{v} \cdot \nabla_{\vec{r}} f + \left. \frac{\partial f}{\partial t} \right|_{\text{collisions}}$$

Collision term describes the transitions between k states.

Relaxation time approximation

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \left. \frac{\partial f}{\partial t} \right|_{collisions}$$

In the relaxation time approximation,

$$\left. \frac{\partial f}{\partial t} \right|_{collisions} = \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

If the driving field is turned off, the collision term will drive the system back to equilibrium in time τ .

When $\nabla_k f = \nabla_r f = 0$ and the initial condition is $f = f_1$, the solution to the Boltzmann equation is,

$$f(t) = f_0 + f_1 e^{-t/\tau}$$

Boltzmann equation: relaxation time approx.

The relaxation time approximation:

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext} \cdot \nabla_k f}{\hbar} - \vec{v} \cdot \nabla f + \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

in a stationary state $\frac{\partial f}{\partial t} = 0$

If the system is not far from equilibrium, $f \approx f_0$, and we can substitute f_0 for f on the right

$$f(\vec{k}) = f_0(\vec{k}) - \frac{\tau(\vec{k}) \vec{F}_{ext} \cdot \nabla_k f_0}{\hbar} - \tau(\vec{k}) \vec{v} \cdot \nabla f_0$$

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1}$$

Boltzmann equation: relaxation time approx.

$$f(\vec{k}) \approx f_0(\vec{k}) - \frac{\tau(\vec{k}) \vec{F}_{ext} \cdot \nabla_k f_0}{\hbar} - \tau(\vec{k}) \vec{v} \cdot \nabla f_0$$

$$\nabla f_0 = \frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu$$

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1}$$

Temperature and
chemical potential can
depend on position

$$\vec{F}_{ext} = -e(\vec{E} + \vec{v} \times \vec{B})$$

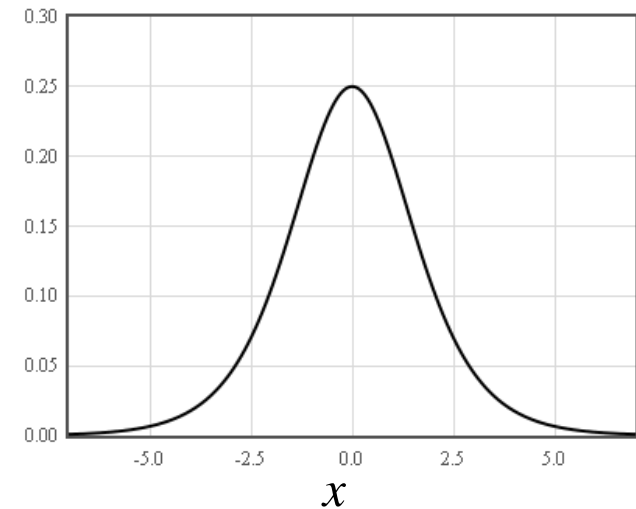
$$f(\vec{k}) \approx f_0(\vec{k}) - \frac{\tau(\vec{k}) (-e) (\vec{v} \times \vec{B} + \vec{E}) \cdot \nabla_k f_0}{\hbar} - \tau(\vec{k}) \vec{v} \cdot \left(\frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu \right)$$

Temperature gradient

Concentration gradient

Boltzmann equation: relaxation time approx.

$$\frac{\partial f_0}{\partial \mu} = \frac{\frac{1}{k_B T} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} = -\frac{\partial f_0}{\partial E} \frac{\exp(x)}{(\exp(x) + 1)^2}$$



$$\begin{aligned} \nabla_k f_0 &= \frac{\frac{-1}{k_B T} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \nabla_k E(\vec{k}) \\ &= \frac{\partial f_0}{\partial E} \nabla_k E(\vec{k}) \end{aligned}$$

$$\begin{aligned} \frac{\partial f_0}{\partial T} &= \frac{\frac{E(\vec{k}) - \mu}{k_B T^2} \exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right)}{\left(\exp\left(\frac{E(\vec{k}) - \mu}{k_B T}\right) + 1\right)^2} \\ &= -\frac{\partial f_0}{\partial E} \frac{E(\vec{k}) - \mu}{T} \end{aligned}$$

Only the states near the Fermi surface contribute.

Boltzmann equation: relaxation time approx.

$$f(\vec{k}, \vec{r}) \approx f_0(\vec{k}, \vec{r}) - \frac{\tau(\vec{k})}{\hbar} \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right)$$

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

density of states $D(\vec{k}) = \frac{2}{(2\pi)^3}$ spin

$$\vec{j}_{elec} = -\frac{e}{4\pi^3 \hbar} \int \nabla_{\vec{k}} E(\vec{k}) \left(f_0(\vec{k}, \vec{r}) - \frac{\tau(\vec{k})}{\hbar} \frac{\partial f_0}{\partial \mu} \nabla_{\vec{k}} E(\vec{k}) \cdot \left(e\vec{E} + \nabla_{\vec{r}} \mu + \frac{E(\vec{k}) - \mu}{T} \nabla_{\vec{r}} T + \frac{e}{\hbar} \nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) \right) d^3k.$$

The contribution of $f_0(k)$ is zero

$$\nabla_{\vec{k}} E(\vec{k}) \cdot \left(\nabla_{\vec{k}} E(\vec{k}) \times \vec{B} \right) = 0$$