Drude simulation report

Name:

The Drude model gives the simplest description of electrical conduction in metals and semiconductors. In this model, electrons are assumed to form a classical gas where there is no interaction between particles but their velocities are randomized by scattering events characterized by a mean time between collisions $\boldsymbol{\tau}$.

In "drude", electrons are moving in two dimensions. An electric field can be applied in the plane of the electron motion and a magnetic field may be applied perpendicular to that plane. Each electron is taken to move independently of all other electrons and its motion is determined by Newton's second law, $\vec{F}(t) = q[\vec{E}(t) + \vec{v}(t) \times \vec{B}(t)]$.
The equations of motion are solved numerically using the Runge-Kutta algorithm.

Thermal equilibrium is maintained through scattering, by assuming that each electron scatters with a probability p= Δt /τ during the interval Δt. In the scattering event, memory of the velocity before the scattering is completely lost, the position of the electron is unchanged and a new velocity is assigned which is consistent with a Maxwellian distribution at temperature T. The Maxwellian probability distribution $P(\vec{v})$ for finding the electron at velocity $\vec{v} = v_x\hat{x} + v_y\hat{y}$ is

$$P(v_x, v_y) = \frac{m}{2\pi k_B T}\exp\left(-m\frac{v_x^2 + v_y^2}{2k_B T}\right)$$

This is a normal (Gaussian) distribution in $v = \sqrt{v_x^2 + v_y^2}$ with mean 0 and variance (mean square deviation) $k_B T / m$.

"drude" uses two complementary displays for characterizing the motion of the electrons: the real-space display shows their position, while the velocity space display shows their velocities, with the large green dot showing the average velocity of all the electrons.

Ex. 1. Run "drude" using PRESET 1. Pick out one electron (by color) and check that the change in direction and speed of its motion in real space correspond correctly to its change in location in velocity space. Why do the electrons move smoothly in real space but remain stationary in velocity space, except for occasional jumps from one point to another?

Ex. 2. Click on SHOW GRAPH over the velocity display. This graph gives the mean square DEVIATION of the electron velocities from their mean (which is zero in this case). RUN briefly at a few TEMPERATURES from 10K to 1000K and determine (and write down) the mean square deviation for each temperature. Is it easy to determine what the average mean square deviation is? How does it depend on the temperature? What else can you observe from the graph?

Ex. 3. Use the SHOW GRAPH over the left hand side display to open a graph which gives the mean square deviations of the electron x- and y-positions from their means. As the system RUNS, the diffusive motion of the electrons gradually increases their dispersion in space. On average the mean square deviation increases linearly with time. COPY GRAPH to save the result, INITIALIZE, and RUN again with a SCATTERING TIME chosen to be larger by a factor of 3. STEAL DATA for comparison. Reduce the TEMPERATURE by a factor of 3, INITIALIZE, and repeat again. What is your conclusion, how does the rate of dispersion change with τ and T?

The spatial distribution of the electrons at time t is approximately

$$\boldsymbol{P(x,y,t) = \frac{1}{2\pi\sigma^2}\exp\left(-\frac{x^2+y^2}{2\sigma^2}\right)}, \text{ with } \boldsymbol{\sigma^2 = \sigma_0^2 + \frac{k_B T\tau}{m}t}$$

This being a normal distribution with variance $\boldsymbol{\sigma^2}$, the expected mean square deviation of the electron x and y positions is $\boldsymbol{\sigma^2}$, which increases linearly in time, with a slope that depends on T and τ the same way.

Ex. 4. PRESET 2 focuses on a single electron with an electric field applied in the positive x –direction and a SCATTERING TIME chosen large enough that no scattering occurs until after the electron has left the real-space screen. How does the position and velocity of the electron change in time?

Shorten the SCATTERING TIME to 3 ps. What happened?

Ex. 5. Use PRESET 3 to find the average behavior of an ensemble of electrons in an electric field. Change the SCATTERING TIME to 1000 ps and see how the average position and velocity vary in response to the field.

Now shorten τ to 3 ps. How does the average position and velocity vary in time now?

The value of the average velocity is called the drift velocity.

Ex. 6. RUN PRESET 4 long enough for the system to reach a steady state, and then STOP. Change E_x to zero and RUN again briefly (without initializing) to allow the average velocity to return to zero. COPY GRAPH, change E_x to a different value, RUN again, then change E_x to zero again, and STEAL DATA. Repeat a couple of times to help distinguish meaningful signal from the noisy fluctuations. Why does the average value not change instantaneously to the appropriate steady state value?

The drift velocity of the Drude electrons follows

$\frac{d\vec{v}}{dt} = -\frac{e\vec{E}}{m} - \frac{\vec{v}}{\tau}$ thus the approach to a steady state is determined by the magnitude of the electric field, while the approach to zero is determined by the scattering.

Ex. 7. Use PRESET 5 to see the electrons' motion in a perpendicular magnetic field. First watch the real-space display. The electrons wander away from the vicinity of the origin and many appear to be lost off screen. Wait a little while and they return to congregate again near the origin. Explain what is going on.

Ex. 8 Look at the graphs for the average position and velocity of the electrons. Check out qualitatively in both spaces how the orbit size and the frequency of circulation of the electrons depend on the magnitude of the MAGNETIC FIELD.

Ex. 9 Explain why all of the orbits in velocity space have a common center, but in real space have different centers.

Since the scattering time is set to very high, the average velocity and position of the electrons satisfy

$\frac{d\vec{v}}{dt} = -\frac{e}{m}\vec{v} \times \vec{B}, \ \frac{d\vec{r}}{dt} = \vec{v}$. The trajectories are referred to as cyclotron orbits

Ex. 10. Reduce the scattering time by several orders of magnitude. What is happening?