Ising simulation report

Name:

“sommerfeld” – Dynamics of quantum free electrons

“sommerfeld” simulates the response of a two-dimensional quantum free-electron gas to applied DC electric and magnetic fields. As in “drude”, electrons do not interact, but their velocities are randomized by scattering events characterized by a mean time between collisions $\boldsymbol{\tau}$. In contrast to “drude”, the electrons are quantum particles and obey the Pauli Exclusion Principle. This does not change the electrical conductivity dramatically. However, it gives a qualitatively new point of view that is important when considering the implications of band structure: rather than working with average properties of the electrons, we focus on the behavior of the electrons of highest energy, the ones with energies near the Fermi energy. Electrons of lower energies, because of the exclusion principle, effectively play no role.

It is straightforward to find the quantum-mechanical one-electron energy states for an electron confined to a volume V. The ground state of the many-electron system is defined by assigning the electrons one by one to these energy states in order of increasing energy.

Ex.1. Consider a square of edge length L. Verify that plane wave solutions $\psi(\boldsymbol{k}) = exp(i\boldsymbol{k}\cdot\boldsymbol{r})/L$ to the Schrodinger equation will satisfy the PBC if $\boldsymbol{k}$ is chosen to be $\boldsymbol{k} = \frac{2\pi n_1}{L}\hat{\boldsymbol{x}} + \frac{2\pi n_2}{L}\hat{\boldsymbol{y}}$, with the n_i integers.

“sommerfeld” defines a two-dimensional grid of points in reciprocal space by the above relation and specifies the initial state of the system in terms of which of these allowed $\boldsymbol{k}$ states are occupied. The occupied states are the white dots in the “sommerfeld” display. “sommerfeld” pretends the electrons have no spin and limits the occupation of each $\boldsymbol{k}$ state to one electron.

PRESET 1 shows the occupied states for a few electrons in a small box.

Ex. 2. Deduce the dimensions of the 2D box to which these electrons are confined. Hint: measure the spacing of the grid of allowed $\boldsymbol{k}$ values. Is the box rectangular or square

shaped? Change the box size in the CONFIGURE dialog box. How does the spacing change?

The maximum energy of the filled states is called the Fermi energy; the surface separating the filled states from the empty states is the Fermi surface.

Ex. 3. Because of the simplicity of the dispersion relation, $E(\boldsymbol{k}) = \hbar^2 |\boldsymbol{k}|^2 / 2m$, the Fermi surface in 2D is a circle. Express the Fermi wave vector as a function of the electron density $n=N/L^2$, knowing that the Fermi circle must contain N/2 $\boldsymbol{k}$- states.

Ex. 4. Run PRESET 1 to see the occupied states change due to thermal motion (scattering) at nonzero temperatures. Do all states have the same chance to become empty? Does the exclusion principle inhibit scattering?

Ex. 5. Select PRESET 2 and run to see the effect of an electric field in the x direction for the case of a long relaxation time $\boldsymbol{\tau}$. What happens to the Fermi circle? Does the exclusion principle restrict the ability of an electric field to accelerate the electrons?

Reduce τ_i to 1 ps and run again. What happens to the Fermi circle now?

Read pages 144 – 145, “Displaced Fermi sea” to understanding why the current is being carried by a tiny minority of the total number of electrons.

“ising” – Ising model and ferromagnetism

Let us imagine a collection of atoms, each having a permanent magnetic moment, with no interaction between the moments. The system is characterized by its magnetization, or its magnetic moment per unit volume. The response of the system to an external magnetic field can be quantified by a dimensionless quantity called magnetic susceptibility, defined as the ratio of the magnetization and the intensity of the magnetic field. According to the Curie law, the magnetic susceptibility is inversely proportional to the temperature for a non-interacting system. At room temperature, achievable magnetic fields produce only a weak alignment of the spins. However, if there are interactions between the spins which favor their parallel alignment, then at high temperatures the susceptibility of the system is enhanced. Even more interestingly, the interactions lead to a spontaneous alignment of the spins at low temperatures, a phenomenon called ferromagnetism.

“ising” is a simulation of one of the classic models for ferromagnetic systems, the two-dimensional Ising model. The Ising model is a system of N atoms distributed on a square lattice, with spin variables which can take on only the values +1 and -1, corresponding to “up” and “down” orientations. The spins are assumed to interact with their nearest neighbors with an exchange energy $-J$ if the neighbor is parallel, and $+J$ if the neighbor is anti-parallel. Each spin also interacts with the applied magnetic field. The energy of the full system is $\boldsymbol{E = -\frac{1}{2}\sum_{ij} J_{ij} S_i S_j - \sum_i S_i H,}$ where $J_{ij}=J$ if i and j are neighbors and zero otherwise.

“ising” selects a spin at random and determines an effective field at the selected spin, equal to the sum of the applied field and an exchange field from the neighbors. If both the external field and chosen spin point upwards, $\boldsymbol{H^{eff} = (n_+ - n_-)J + H}$, where n_+ and n_- are the numbers of up and down-oriented neighbors. “ising” makes the spin point up with the probability

$$\boldsymbol{p(S_i = 1) = \frac{\exp(H_i^{eff}/T)}{\exp(-H_i^{eff}/T) + \exp(H_i^{eff}/T)}},$$

and point down with the probability $\mathbf{1 - p(S_i = 1)}$, regardless of its previous orientation. These formulas do not contain the Boltzman constant because both the *T* and *H* are measured in units of *J*.

This process is repeated for a number of sweeps, during which each spin is selected in once, on average. This algorithm is an example of a **Monte Carlo simulation.**

Ex. 1. Open PRESET 1 to see the array of spins on the left, with red and white indicating the up and down orientations of the spins. Click RUN and drag the EXTERNAL FIELD slider slowly to both positive and negative values. What color of spin in the display corresponds to alignment parallel to a positive magnetic field?

Ex. 2. Leave the EXTERNAL FIELD at 1 J and RUN, varying the TEMPERATURE in the range T>3 J. STOP to see on the right a graphical history of the magnetization during your variation of the temperature. Why does the magnetization increase as the temperature is lowered?

T>3 J means that the thermal energy (k_BT) is three times larger than the interaction energy. The magnetization and magnetic susceptibility are normalized by their saturation values, obtained when all the spins are aligned in parallel.

Ex. 3 Use PRESET 2 and take a data series recording T, H and <M>, starting at T=20 J and H= 4 J. Work down in T until you feel the data no longer makes sense. Choose H values large enough that the magnetization is easily measurable, but small enough that M<0.25, to avoid nonlinearities. You will need to decrease H as you reduce T in order to continue to satisfy these conditions. Note that you can have H values between 0 and 1 if you write them in instead of using the slider. It is useful to take smaller spacings in T as T is lowered. Also, repeat measurements to see how well successive runs agree. The readouts of <M> are average values over the time interval displayed in the graph. Be sure to RESET the graph before each change in temperature!

Divide <M> by H to find the magnetic susceptibility. If the spins were independent,

$\chi = 1/T$, or the inverse susceptibility, χ^{-1}, is proportional with T. Plot the inverse susceptibility you obtained (e.g. use Excel). Is the x-intercept equal to zero? If not, what value do you obtain?

The Curie-Weiss law gives $\chi = 1/(T - \theta)$, and the Curie temperature, θ , is predicted by the mean-field theory of ferromagnetism to be $\theta = 4J$. Does your result agree with that?

Ex. 4. Use PRESET 3, where the temperature is below the Curie temperature and the external field is zero. When you RUN, the spins quickly condense into a state with most of the spins in the same direction. Increase both the NUMBER OF SWEEPS and the SPEED by a factor of 10. While running, click on INIT whenever the system decided on a preferred orientation. Is the result always the same when repeating the experiment? Why?

Ex. 5. In PRESET 4 the Ising system is initialized in a random T=inf array in zero field, but then runs at T= 1J. With each RUN, only a single sweep is performed. Already after the first RUN you see that the spins have preferentially aligned in the direction of the majority of their neighbors. Click RUN a number of times to see a coarsening of the parallel-spin clusters. The larger clusters grow at the expense of the smaller ones. Increase the NUMBER OF SWEEPS as time increases. Watch the clusters. Does “ising” use open or periodic boundary conditions?

Ex. 6. CONFIGURE the array of spins to 20x20. Watch the coarsening process again. Focus your attention on a small cluster of oriented spins on a background of spins in the other orientation. Can you argue why the small cluster is more likely to shrink than to grow?

Ex. 9 Now let's see if an external magnetic field can flip a system that is oriented in the other direction. In PRESET 5 the low external field of H=0.1 J is unlikely to flip spins surrounded by parallel neighbors. RUN and watch how thermal fluctuations collaborate with the magnetic field to form nuclei of field-oriented spins. How large a nucleus can ultimately flip the whole array? Try to vary the temperature and magnetic field slightly and record the time needed for flipping the system. What do you find?