Assignment 2 — Computer Simulation I: Computational Methods (Mitchison)

November 14, 2023

Instructions:

- Write Python code to complete the exercises below.
- Write a brief report (max. 4 pages) describing your results. The report should include all figures that you are asked to make, with informative captions.
- Submit your report (as a PDF file) electronically via Blackboard. Also submit your code as a single file (either a .py or .ipynb is fine). When executed, your code should generate output to solve each of the exercises below. Both file names (report and Python code) should include your full name. **It is crucial that you include an executable Python file in your submission, e.g. do not just submit a PDF copy of a Jupyter notebook.**

Exercise 1

Consider a large system of electrons, in contact with an external reservoir at temperature T and chemical potential μ. The average electron density ρ and the average energy density ε are given by the integrals

$$\rho = \int_0^\infty \mathrm{d}w\, d(w) f(w), \qquad \varepsilon = \int_0^\infty \mathrm{d}w\, w d(w) f(w),$$

where $f(w) = (\mathrm{e}^{(w-\mu)/k_B T} + 1)^{-1}$ is the Fermi-Dirac distribution and $d(w)$ is the density of states per unit energy per unit volume. The 3D electron gas is described by the density of states

$$d(w) = \frac{m_e^{3/2}\sqrt{w}}{\sqrt{2}\pi^2\hbar^3},$$

where m_e is the electron mass.

(a) Plot the energy density of the 3D electron gas as a function of temperature at fixed chemical potential of $\mu = 1$ eV. Consider temperatures in the range $T \in [0\ \mathrm{K}, 10^4\ \mathrm{K}]$.
Hint: choose an appropriate unit system to avoid absurdly small or large values. It is sensible to measure lengths in nanometres, masses in units of the electron mass, and energies in electronvolts. In this unit system, $k_B \approx 8.62 \times 10^{-5}\ \mathrm{eV/K}$ **and** $\hbar \approx 0.276\ \mathrm{nm}\sqrt{\mathrm{eV}\, m_e}$**.**

(b) On the same axes, plot the energy density of the 3D electron gas as a function of temperature at fixed electron density $\rho = 2.27\ \mathrm{nm}^{-3}$. Consider the same temperature range as part (a).

Exercise 2

The Aubry-Andre-Harper (AAH) model is a 1D tight-binding model defined by the Hamiltonian

$$\hat{H} = \begin{pmatrix} \epsilon_0 & -\hbar\lambda & 0 & 0 & \cdots \\ -\hbar\lambda & \epsilon_1 & -\hbar\lambda & 0 & \cdots \\ 0 & -\hbar\lambda & \epsilon_2 & -\hbar\lambda & \cdots \\ 0 & 0 & -\hbar\lambda & \epsilon_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

with a tunnelling rate λ between nearest-neighbour lattice sites, and an on-site energy $\epsilon_l = u\cos(2\pi\alpha l)$.

(a) First we will consider the case where α is a *rational* number. Specifically, we will consider three cases: $\alpha = 1$, $\alpha = 1/2$ and $\alpha = 1/3$. For each value of α, find the eigenvalues and plot them in increasing order. In addition, find and plot the (unnormalised) density of states (DOS) $\nu(w)$, which is defined as the number of eigenstates within an energy interval $w \in [w - \delta w/2, w + \delta w/2]$. Choose parameters $L = 500$, $u = 2\hbar\lambda$, and $\delta w = \hbar\lambda/10$.

(b) Now we will consider the AAH model for an irrational value of α: specifically, the golden ratio

$$\alpha = \frac{1+\sqrt{5}}{2}.$$

Depending on the value of u, the eigenstates of this model are *extended* over the entire lattice or *localised* near a particular lattice site. The degree of localisation is quantified more precisely by the inverse participation ratio (IPR). The IPR of an energy eigenstate $|\psi\rangle = \sum_{l=0}^{L-1} \psi_l |l\rangle$ is defined by

$$I = \sum_{l=0}^{L-1} |\psi_l|^4.$$

For localised states we expect $I \sim 1$, while for extended states we expect $I \sim L^{-1} \ll 1$.

Compute the mean IPR, i.e. find the IPR I_k for each eigenstate $|\phi_k\rangle$ and then take the average $\bar{I} = \frac{1}{L}\sum_k I_k$. Repeat this analysis for different values of u and plot your result for $\bar{I}$ as a function of u in the range $u/\hbar\lambda = [0.0, 5.0]$, with $L = 500$. Identify the critical disorder strength u_c where the system transitions from extended to localised. Plot an example of the spatial probability distribution for an eigenstate in the extended phase, and compare it with the probability distribution for an eigenstate in the localised phase.

Exercise 3

Now consider a tight-binding model where the on-site energy is the same everywhere except for on one particular site of the lattice, $l = l_0$. This represents a localised impurity that affects the energy of nearby electrons. Mathematically, we represent this as a position-dependent on-site energy

$$\epsilon_l = \langle l|\hat{H}|l\rangle = \begin{cases} u & (l \neq l_0) \\ v & (l = l_0). \end{cases}$$

Construct the Hamiltonian matrix for such a tight-binding model with $L = 500$ sites, tunneling rate λ, and with $u = 2\hbar\lambda$ and $v = 5\hbar\lambda$. Put the impurity in the centre of the system, $l_0 = 249$. Simulate the time evolution of the quantum state $|\psi(t)\rangle$ under the Schrödinger equation, starting from the initial condition

$$|\psi(0)\rangle = \frac{|99\rangle + \mathrm{i}|100\rangle}{\sqrt{2}},$$

where the states $|99\rangle$ and $|100\rangle$ denote the states $|l\rangle$ localised on sites $l = 99$ and $l = 100$ of the lattice, respectively. Discuss what happens before, during, and after the electron's interaction with the impurity at $l = l_0$. Back up your discussion with appropriate plots, e.g. of the spatial probability distribution $|\langle l|\psi(t)\rangle|^2$ at different points in time.