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

October 18, 2022

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 $\epsilon_l = u\cos(2\pi\alpha l)$. In this exercise 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 $\delta w = \hbar\lambda/10$.

Exercise 3

The generalised Aubry-Andre-Harper (GAAH) model is a tight-binding model with nearest-neighbour tunnelling rate λ and on-site energy

$$\epsilon_l = \frac{u\cos(2\pi\alpha l)}{1 + \beta\cos(2\pi\alpha l)}.$$

(a) Find the inverse participation ratio (IPR) for each eigenstate of the GAAH model, with $\alpha = \frac{1}{2}\left(1 + \sqrt{5}\right)$, $\beta = 0.6$, $u = 2\hbar\lambda$, and $L = 500$. Recall that the IPR of a normalised eigenstate $|\psi\rangle = \sum_l c_l|l\rangle$ is defined as

$$I = \sum_l |c_l|^4.$$

Plot the IPR versus the corresponding energy eigenvalue.

(b) Choose an example of an eigenstate with low and high IPR and plot the corresponding spatial probability distribution $|c_l|^2$ for each state. Discuss the differences between the two distributions.