1. Consider a 1D or 2D array of a total of $N$ spins subject to an external magnetic field and a nearest-neighbor exchange interaction, with a Hamiltonian given by:

$$
\mathcal{H} = M \sum_i \sigma_i + J \sum_{\langle ij \rangle} \sigma_i \sigma_j,
$$

where the angular brackets denote a sum over the nearest neighbors in the chosen dimensionality. The Hamiltonian can then be applied to the eigenproblem $\mathcal{H}\Psi = E\Psi$, where $E$ is the energy eigenvalue.

1a. For the 1D case: if $N = 32$, $M = 0$ and $J = -1$, what are the lowest and highest energy and associated eigenvectors? What if $M = 1$ and $J = 1$? Which case(s) would correspond to the behavior of a ferromagnet (e.g., iron), and why?

1b. Now consider the behavior of the related 2D system with $N = 64$, $M = 0.01$ and $J = -1$ at a finite temperature. We will implement this using the Metropolis algorithm, in which any initial spin configuration $\{\sigma_i\}$ is modified by the following steps, repeated 1000 times:

1. Randomly choose a single spin $\sigma_i$.
2. Calculate the energy change $\Delta E$ associated with flipping its sign.
3. If $\Delta E \leq 0$, accept the flip; otherwise, accept with probability $e^{-\Delta E/kT}$.
4. Calculate the new average magnetization $\langle \mu \rangle = \frac{1}{N} \sum_i \sigma_i$.

Plot $\langle \mu \rangle$ versus trial number when $kT = 0.5$, $kT = 2.269$, and $kT = 3$. What is different in these various cases, and why?
2. Recall the Kronig-Penney model: it describes electrons traveling in a 1D periodic potential, consisting of barriers of width $a/2$ and potential height $U$, with wells of width $a/2$ and 0 potential. Assume that the electron energy $E < U$. In this case, it can be shown that the periodic portion of the wavefunction

$$\psi_1(x) = (A e^{i\alpha x} + B e^{-i\alpha x}) e^{-ikx}$$

in the wells, while

$$\psi_2(x) = (C e^{i\beta x} + D e^{-i\beta x}) e^{-ikx}$$

inside barriers. Here, $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$, and $\beta = \sqrt{\frac{2m(U-E)}{\hbar^2}}$. Note that this system is subject to Bloch’s theorem.

Figure 2: Kronig-Penney model describing 1D periodic potential for electrons.

2a. Write down four equations for the coefficients ($A, B, C, D$) using the continuity of $\Psi$ and its derivatives at $x = 0$ and $x = a/2$. Formulate this as a matrix problem that could be written as:

$$Q \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (1)$$

2b. Now set the determinant of $Q = 0$, and assume that $U = 10$, $a = 1$, $m = 1$, and $\hbar = 1$. Now solve for the possible real values of the energy $E$ when $k = 0$ and $k = \pi/a$. What is the bandgap for this system, defined as the smallest difference between $E$ values associated with a given value of $k$?