Random Walk Simulation: Exploring Clustering and Ordering in a 1D System

Objective

To study the dynamics of a 1D system of red and blue particles performing random walks, exploring how clustering and ordering emerge based on interaction energies and temperature.

System Description

- **Lattice:** A 1D lattice with $N = 50$ sites arranged in a line with periodic boundary conditions.
- **Particles:** Two types of particles, red and blue, are distributed on the lattice:
  - Initially, the lattice contains an equal number of red and blue particles ($N_{\text{red}} = N_{\text{blue}} = 25$).
  - Each site is occupied by exactly one particle.
- **Interaction Energies:**

$$J_{\text{red-red}} = -1.0\,\text{eV}, \quad \text{(favorable interaction between red particles)}$$
$$J_{\text{blue-blue}} = -1.0\,\text{eV}, \quad \text{(favorable interaction between blue particles)}$$
$$J_{\text{red-blue}} = \begin{cases} +0.5\,\text{eV} & \text{(unfavorable interaction for clustering)} \\ -1.5\,\text{eV} & \text{(favorable interaction for ordering)} \end{cases}$$

- **Temperature:** Perform simulations at two temperatures:

- $T_1 = 100\,\mathrm{K}$: Promotes clustering or ordering.
- $T_2 = 1000\,\mathrm{K}$: Promotes mixing.

Random Walk Dynamics

1. Each particle performs a random walk on the lattice by swapping places with a randomly chosen neighbor.

2. The **total energy** E of the system is given by:

$$E = \sum_{i=1}^{N} \sum_{j \in \text{neighbors}(i)} J_{ij} \delta(c_i, c_j),$$

   where c_i and c_j are the types of particles at sites i and j, and $\delta(c_i, c_j)$ is 1 if $c_i = c_j$, otherwise 0.

3. During a random walk step:

   - Select a random particle and a neighboring site.
   - Calculate the change in energy ΔE if the particle swaps with its neighbor.
   - Accept the swap using the **Metropolis criterion**:

$$P = \begin{cases} 1 & \text{if } \Delta E \leq 0, \\ \exp\left(-\frac{\Delta E}{k_B T}\right) & \text{if } \Delta E > 0. \end{cases}$$

4. Repeat this process for 10^5 steps.

Tasks

1. **Simulation:**

   - Write a Python program to simulate the random walk dynamics of red and blue particles on the lattice.
   - Perform the simulation for $T_1 = 100\,\mathrm{K}$ and $T_2 = 1000\,\mathrm{K}$.

2. **Visualization:**

- Plot the final configuration of the lattice. Use red dots for red particles and blue dots for blue particles.
- Plot the **pair correlation function** $g(r)$:

$$g(r) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \delta(|r_i - r_j| - r),$$

  normalized by the total number of sites.

3. **Order Parameter:** Calculate the **order parameter** for the alternating red-blue pattern:

$$\eta = \frac{1}{N} \sum_{i=1}^{N} (-1)^i \cdot c_i,$$

   where $c_i = +1$ for red particles and $c_i = -1$ for blue particles.

Experimentation

- **Clustering:** Set $J_{\text{red-blue}} = +0.5\,\text{eV}$ and observe clustering at T_1.
- **Ordering:** Set $J_{\text{red-blue}} = -1.5\,\text{eV}$ and observe alternating patterns at T_1.
- **Temperature Effects:** Compare results at T_1 and T_2.
- **Critical Interaction Energy:** Experiment with varying $J_{\text{red-blue}}$ to identify the transition from clustering to ordering.

Expected Results

1. For $J_{\text{red-blue}} > 0$: Clustering of red and blue particles into separate regions at low temperature.
2. For $J_{\text{red-blue}} < 0$: Alternating red-blue pattern with a high order parameter at low temperature.
3. At high temperature: Random distribution of red and blue particles due to thermal agitation.

Deliverables

1. Final lattice configuration plots for all cases.
2. Pair correlation function, $g(r)$, for each configuration.
3. Order parameter, η, for $J_{\text{red-blue}} < 0$.