

Random Walkers in an Energy Landscape

We can define some simple repeating energy landscapes where the energy varies from site to site in some way. Examples of such energy landscapes are:

0 0 0 0 0 0 0 0 0 0 0 0 0 0 (Here energy does not change from site to site)

0 1 0 1 0 1 0 1 0 1 0 1 ... (Generate this using $\text{energy}[i]=i\%2$)

0 1 2 0 1 2 0 1 2 0 1 2 ... (Generate using $\text{energy}[i]=i\%3$)

0 1 2 3 0 1 2 3 0 1 2 3 ... (Generate using $\text{energy}[i]=i\%4$)

0 0 1 0 0 1 0 0 1 0 0 1 (Find a way to generate this also)

You can define your own energy landscape

Now, we consider a random walk in the energy landscape as follows:

- Start the walk in the middle. You can choose x to go from 0 to 60 and start the walk at 30.
- At every step there is a probability P that the walker gets an energy kick.
- At every step the walker attempts to move left or right with equal probability.
- If the walker has gotten a kick in that step then the walker has enough energy to go left or right. So, accept the move and update the walker's position.
- If the walker did not get a kick in that step then the walker only moves if there is enough thermal energy. If the attempted move is downhill accept the move and update the position. If the attempted move is up the hill accept the move with probability $\exp(-\Delta E/T)$. Otherwise reject the attempted move. If the move is accepted update the walker's position. If the move is rejected the walker's position stays the same.
- Repeat the move until the walker has reached one of the ends of the walk (in this case 0 or 60).
- Run the simulation many times and find the fraction of times the walker exits left and fraction of times the walker exits right.

We would like a systematic study of the performance of the walker as a function of three things:

- A. The energy landscape
- B. Temperature T
- C. Kicking probability P

1. Repeat the studies for a number of different energy landscapes:
2. Study different Temperatures ($T= 0.1, 1, 10$)
3. Study different kicking Probabilities ($P= 0, 0.2, 0.5, 1.0$)
4. For each case find the fraction of walkers that go left and the fraction that go right and the average number of steps before the walker exits the region. Make a table

Some questions to answer:

1. Examine the different energy landscape by plotting energy[i] vs i for i between 0 to 40. Identify which landscapes have left-right symmetry and which do not.
2. What is the role of temperature T? Does it speed up or slow down the walkers?
3. Examine the role of P and T in breaking the left-right symmetry. Pick a landscape which is not symmetric. Examine
 - (i) Fraction of walkers that go left as a function of P for fixed T=0.1.
 - (ii) Fraction of walkers that go left as a function of T for fixed P=0.2.
4. Can you explain why in some cases walkers preferentially go one way? Why do they go in that particular direction?