Physics III – Workshop – Introduction to Statistical Physics
Simulating a spin system

1 Activity introduction

We have N spins in an external magnetic field H. The energy of a particular microstate $\{s_i\}$ of this system is given by

$$E(\{s_i\}) = -\mu H \sum_{i=1}^{N} s_i, \tag{1}$$

where μ is the magnetic dipole moment of the spin.
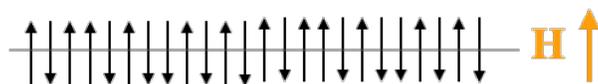
Figure 1: Particular microstate of the system we're simulating.

In this activity, we will simulate this system for $N = 10$ spin by applying the previously derived transition probability result

$$\frac{\pi_{j \to k}}{\pi_{k \to j}} = e^{-(E_k - E_j)/k_B T} \tag{2}$$

to a computational algorithm. Your group will use some basic random number generators provided online and each person will act as a particular part of a larger program in order to simulate this system.

2 Setup and Description of Algorithm

(a) Each group is given a deck of 10 numbered cards each of which is black (representing a +1 spin) on one side and white (representing a -1 spin) on the other. Arrange the cards in numerical order, with the **black side facing up** for all cards. This will be the initial spin configuration of our system.

(b) For this activity, your group will need to select **four people** to perform different roles:

- **Spin-selector:** This person uses an integer-based random number generator to randomly select a number between 1 and 10 inclusive. The selected number determines the spin to be flipped. Go to https://www.random.org/ for your random number generator.

- **Random number-generator:** This person uses a real-number based random number generator to select a number between 0 and 1. The selected number is denoted u in what follows. Go to https://www.random.org/decimal-fractions/

- **Flip Acceptor/Denier:** This person uses Eq.(1) to calculate $\exp(-\Delta E/k_B T)$ and compares the result with the random number u to determine whether the spin flip is accepted or rejected.

- **Recorder:** After each cycle of the algorithm, this person records the total spin $\sum_{i=1}^{N} s_i$ of the system. Go to Google Sheets and open a new document. Title the document with the last names of the group and the year (e.g. "Nyovanie_Workie_Gilbert_Lee_Lopez_2018". In the left most, column record the total spin of the system for each cycle of the algorithm.

(For groups with five people, the extra person should serve as a second recorder to check the data set.)

(c) Beginning from your initial spin configuration, the algorithm you will implement is as follows:

Simulating a lattice of spins at a temperature T and energy $E(\{s_j\})$

 (a) Start in an initial spin microstate given $s_1, s_2, \ldots, s_N$ represented by 10 cards. This microstate is denoted $\{s_j\}_0$. The colors denote $+1$ or -1 states as follows:

$$+1 \text{ spins are black cards}$$
$$-1 \text{ spins are white cards.}$$

 (b) The **Spin-selector** uses the random integer generator to randomly select a spin j (between 1 and 10), and prepares to flip the spin to black, if spin is white, or to white, if spin is black; The potential microstate is denoted $\{s_j\}_{\text{new}}$.

 (c) The **Random number-generator** and the **Flip Acceptor/Denier** determine whether to accept or reject the potential transition in 2. according to the following:

   i. The **Flip Acceptor/Denier** uses Eq.(1) to calculated the energy difference

$$\Delta E = E(\{s_j\}_{\text{new}}) - E(\{s_j\}_0) \tag{3}$$

   between the initial and final microstate. *Hint: You should only have two terms in this difference.*

   ii. **Random number-generator** draws a random real number u between $[0, 1]$.

   iii. If $u < e^{-\Delta E/k_B T}$, then **Flip Acceptor/Denier** <u>accepts</u> the potential microstate;
   If $u \geq e^{-\Delta E/k_B T}$, then **Flip Acceptor/Denier** <u>rejects</u> the potential microstate.

 (d) If the transition is accepted, then $\{s_j\}_{\text{new}}$ becomes the new $\{s_j\}_0$. If the transition is rejected, then $\{s_j\}_0$ remains as $\{s_j\}_0$ for the next iteration.

 (e) The **Recorder** computes

$$S_{\text{tot}} = \sum_{i=1}^{N} s_i, \tag{4}$$

 for this cycle and records the result in the Google Doc.

 (f) Return to step 1; cycle through procedure until you have proceeded through the desired number of iterations.

A graphical summary of this algorithm is given on the last page.

3   Submission: Rounds of Simulation

We will implement at least a single round (i.e., a single simulation) of this algorithm, and will implement a second round if there is time.

 1. **First Round – High Temperature Simulation:**

   (a) Let $\mu = 1.0$ and $H = 1.0$ for simplicity. We choose $k_B T$ to have the high temperature given by

$$k_B T_{\text{high}} = \frac{2}{\ln \dfrac{4}{3}}. \tag{5}$$

   Suggestion: It will help you later if you use Eq.(5) to compute $e^{-2\mu H/k_B T}$ now.

(b) Implement the simulation algorithm outlined in (c) of the previous section, for **30 cycles**. **Recorder** should make sure to record the total spin after each cycle.

(c) After all 30 cycles, click "Insert Chart" on Google Sheets toolbar to create a line plot of S_{tot}.

 – Title the chart, the horizontal axes, and the vertical axes.
 – Indicate whether this is a low or high temperature simulation.
 – Save the document and share it with williams.mobolaji@gmail.com.

2. **Second Round – Low Temperature Simulation**

(a) Let $\mu = 1.0$ and $H = 1.0$ for simplicity. We choose $k_B T$ to have the high temperature given by

$$k_B T_{\text{low}} = \frac{2}{\ln 4}. \tag{6}$$

It will help you later if you use Eq.(6) to compute $e^{-2\mu H/k_B T}$ now.

(b) Implement the simulation algorithm outlined in (c) of the previous section, for **30 cycles**. **Recorder** should make sure to record the total spin after each cycle.

(c) After all 30 cycles, click "Insert Chart" on Google Sheets toolbar to create a line plot of S_{tot}.

 – Title the chart, the horizontal axes, and the vertical axes.
 – Indicate whether this is a low or high temperature simulation.
 – Save the document and share it with williams.mobolaji@gmail.com.

Summary of Algorithm
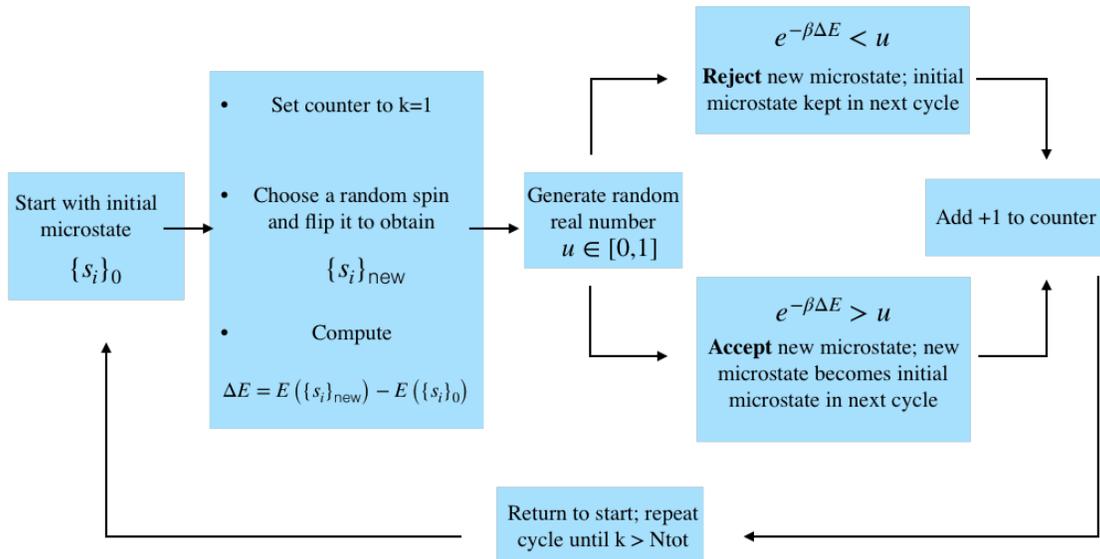
Figure 2: Algorithm for simulating lattice of spins in statistical physics. This simulation assumes a chosen temperature T (related to β through $\beta = 1/k_B T$) and a given energy of a microstate $E(\{s_i\})$. Simulation iterates for N_{tot} time steps.

Resource: Introduction to Statistical Physics
Mobolaji Williams