SCIENCE II
CLASS ASSIGNMENTS

1. Random Walk

① TWO DRUNKS START OUT TOGETHER AT THE ORIGIN, EACH HAVING EQUAL PROBABILITY OF MAKING A STEP TO THE LEFT OR RIGHT ALONG THE X-AXIS. FIND THE PROBABILITY THAT THEY MEET AGAIN AFTER N STEPS. IT IS TO BE UNTERSTOOD THAT THE MEN MAKE THEIR STEPS SIMULTANEOUSLY.

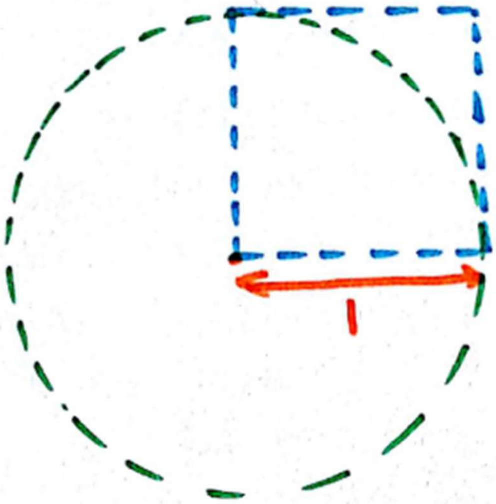
RELATED QUESTIONS :-

⇒ WHAT IS THE PROBABILITY FOR A DRUNK TO BE AT THE ORIGIN AFTER TAKING N STEPS?

⇒ MEAN DISPLACEMENT OF THE DRUNK ?

⇒ MEAN SQUARE DISPLACEMENT OF THE DRUNK ?

2. Estimating Pi using Monte Carlo



YOU HAVE BEEN GIVEN N POINT PEBBLES.
HOW DO YOU DETERMINE THE VALUE OF
π USING THESE INPUTS?
WRITE A CODE TO DETERMINE THE
VALUE OF π.

Note: Although you have submitted these assignments already, include them in this submission.

3. Phase space trajectory of a 1D harmonic oscillator

CONSIDER ONE. DIMENSIONAL OSCILLATOR

$$H(x, P) = \frac{1}{2} k x^2 + \frac{P^2}{2m}$$

SOLVE THE HAMILTON'S EQUATION AND SHOW THE PHASE SPACE TRAJECTORY.

- Calculate $\frac{dp}{dt}$ and $\frac{dx}{dt}$ from the Hamiltonian (hint: use Hamilton's equations)
- Get the time evolution P and X using these equations and plot the phase space (p vs x). Do this for different initial values of H (defined by constants **m** and **k**)
- Plot the mean square displacement vs time, where mean square displacement at time t is given by:

$$\mathrm{MSD}(t) = \langle \mathbf{r}^2(t) \rangle = \left\langle \, |\mathbf{r_i}(t) - \mathbf{r_i}(0)|^2 \right\rangle$$

Since we are dealing with just one particle in this case, MSD is just square displacement, you don't need to calculate any average.

4. Numerical Solution of 1D Diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial x^2}$$

$\Delta t \rightarrow$ TIME STEP

$\Delta x \rightarrow$ STEP LENGTH

$$-L \le x \le L \quad ; \quad 0 \le t \le T$$

INITIAL CONDITION: $P(x,0) = 1$ for $x = 0$
$= 0$ otherwise

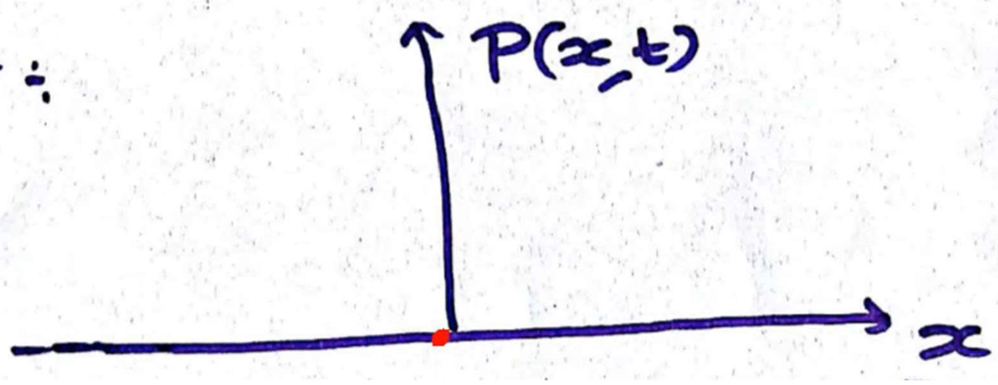
BOUNDARY CONDITIONS: $P(-L,t) = 0 \quad ; t > 0$
$P(L,t) = 0 \quad ; t > 0$

FORWARD EULER SCHEME:

$$t = n\Delta t, \quad n = 0, 1, 2, \ldots N_t$$

$$P(i, n+1) = P(i,n) + \frac{D\Delta t}{(\Delta x)^2}\left[P(i+1, n) - 2P(i,n) + P(i-1, n)\right]$$

PLOT:



- Repeat this for 2D diffusion equation:

$$\frac{\partial P(x,y,t)}{\partial t} = D_x \frac{\partial^2 P(x,y,t)}{\partial x^2} + D_y \frac{\partial^2 P(x,y,t)}{\partial y^2}$$

  Plot different 2D density plots for different number of timesteps (n = 10, 100, 1000, 10000) for three different cases (take suitable values):

    i. $D_x = D_y$
    ii. $D_x > D_y$
    iii. $D_x < D_y$

5. Calculating Potential energy of a system of water molecules

Provided with the PSF and PDB files for a system of water molecules, calculate the total potential energy of the system. This total potential energy is the sum of pairwise potentials. The potential for a pair of molecules **a** and **b** is given by:

$$E_{ab} = \sum_{i}^{\text{on } a} \sum_{j}^{\text{on } b} \frac{k_C q_i q_j}{r_{ij}^2} + \frac{A}{r_{\text{OO}}^{12}} - \frac{B}{r_{\text{OO}}^{6}},$$

$$k_c = \ 332.1 \text{ Å} \cdot kcal/(mol \cdot e^2)$$

$$A = 582.0 * 10^3 kcal\text{Å}^{12}/mol$$

$$B = 595.0\ kcal\text{Å}^6/mol$$

You need to use periodic boundary conditions (hard code the length as Lx=23.623; Ly=22.406; Lz=27.1759) and the minimum image convention as explained in the lecture.

6. Integration using Monte Carlo

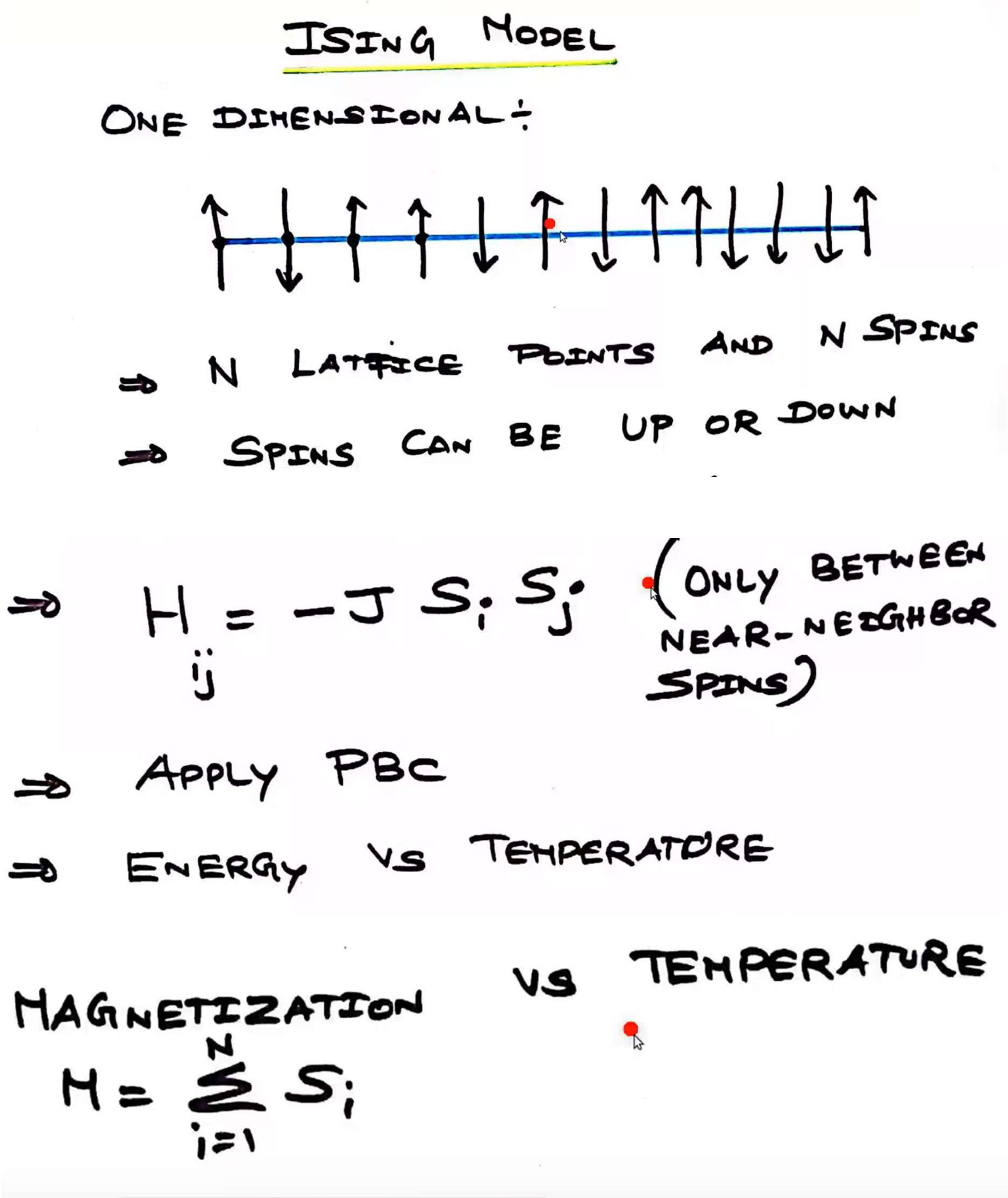
Calculate following integrals using the Monte Carlo method:

- $I = \int_0^1 3x^2 \; dx$
- $I = \int_0^1 \int_0^1 x^2 y \; dxdy$

For each integral

- Plot I vs Number of pointes (N)
- Fix N=20; 100 trials; Plot I vs trials; calculate std deviation.
- Fix N=1000; 100 trials; Plot I vs trials; calculate std. deviation.
- Plot standard deviation (Of I vs trials) vs N for a fixed number of trials; Check if STD is proportional to sqrt(N) [Hint: increase number of trials if the plot deviates from sqrt(N)]

7. Ising Model (1D spin system)



Use the Monte Carlo method explained in class to simulate an N particle Ising model at a given temperature. Plot:

- Energy vs Temperature
- Magnetization vs Temperature

8. Predator – Prey Model

$$\frac{dN_1(t)}{dt} = r N_1(t)\left[1 - \frac{N_1(t)}{K}\right] - \alpha N_1 N_2$$

$$\frac{dN_2(t)}{dt} = -c\, N_2(t) + \beta N_1 N_2$$

CONSTANTS

$\alpha, \beta \Rightarrow$ POSITIVE CONSTANT

$\alpha \Rightarrow$ RATE AT WHICH THE PREDATOR CAPTURES ITS PREY

$\beta \Rightarrow$ GROWTH RATE OF THE PREDATOR

$c \Rightarrow$ DECAY RATE OF THE PREDATOR (IF $N_1 = 0$)

Solve the set differential equations for different starting values and parameters.

Plot N1 and N2 against time.

Report any observations regarding the nature of trajectory.

PROJECT - PART A

① INITIAL CONFIGURATION :

$$N = 108$$

$$L_x = L_y = L_z = 18.0\ \text{Å}$$

$$\epsilon = 0.238\ \text{KCAL/MOL}$$

$$\sigma = 3.4\ \text{Å}$$

GENERATE A RANDOM INITIAL CONFIGURATION

$$(r_{ij} \geq 3.4\ \text{Å})$$

② $$U_{LJ}(r_{ij}) = 4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

$\Downarrow$

INTERACTION ENERGY PER PAIR

③ MINIMIZE THE TOTAL POTENTIAL ENERGY OF THE SYSTEM $\quad -\nabla U\Big|_{min} = 0$

(USE PERIODIC BOUNDARY CONDITIONS)

④ CALCULATE THE HESSIAN MATRIX AND GET THE EIGEN VALUES AND EIGEN VECTORS.

⑤ GET THE HISTOGRAM OF VIBRATIONAL FREQUENCIES