Midterm PY 541- Fall 2022

This is a take-home exam for PY541. The exam must be turned in on Blackboard before Wednesday at 11:59pm. Mathematical software such as Mathematica is allowed ONLY for graphing or simple algebraic manipulations. You can consult your book (Sethna) and your notes, and HWs. You also may NOT discuss the exam with each other. This test is meant to be done individually.

You have 3 hours to do test in one setting from the moment you open it up. This time does not include time to scan exam or upload to Blackboard.Please sign the honor pledge on the next page indicating that you have obeyed these rules.

There are 3 problems

I certify that I have read,understand, and followed all rules. In particular, I solemnly pledge that I have tried my best to follow the spirit as well as letter of the rules for this examination.

Signature:

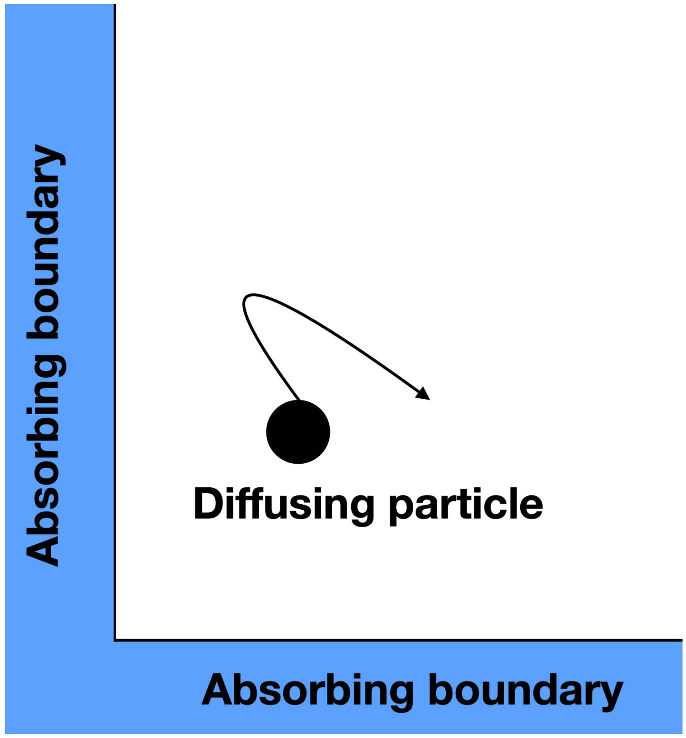

FIG. 1: Particle diffusing in positive quadrant with absorbing boundary conditions.

Problem 1: (20 points)

1. Consider a particle undergoing diffusion in a two dimensional plane with coordinates $\vec{x} = (x, y)$. The particle is confined to the positive quadrant, $x, y \geq 0$, with *absorbing boundary conditions* along the positive x-axis ($y = 0$) and positive y-axis ($x = 0$). If the particle starts at some position $\vec{x}'$, find the resulting probability $p(\vec{x_t}, t|\vec{x}')$ of finding particle at a position $\vec{x_t}$ after a time t? (Hint: think about your electromagnetism class.)

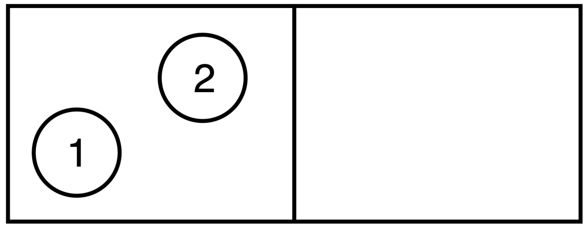

FIG. 2: Two distinguishable particles in a box.

Problem 2 (20 points):

Consider the system illustrated in Figure below (Fig. **??**). The system consists of two distinguishable particles, each of which can be in either of two boxes. The system is in thermal equilibrium with a heat bath at temperature T. Assume that the energy of a particle is zero if it is in the left box and r if it is in the right box. There is also a correlation energy term that increases the energy by Δ if the two particles are in the same box.
(a) Enumerate the $2^2 = 4$ microstates and their corresponding energy.
(b) Calculate the partition function Z for arbitrary values of r and Δ and use your result to find the mean energy.
(c) What is the probability that the system is in a particular microstate?
(d) Suppose that $r = 1$ and $\Delta = 15$. Sketch the qualitative behavior of the heat capacity C as a function of T.

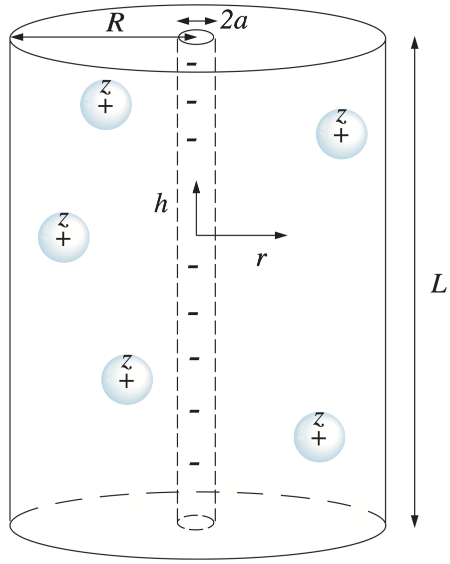

FIG. 3: Geometry of configuration space.

Problem 3 (20 points):

When ionic polymers (polyelectrolytes) such as DNA are immersed in water, the smaller charged counter-ions go into solution, leaving behind an oppositely charged polymer. Because of the electrostatic repulsion of the charges left behind, the polymer is stretched, and shall be modeled as a cylinder of radius a and length L, as depicted in the figure. While thermal fluctuations tend to make the ions wander about in the solvent, electrostatic attractions favor their return and condensation on the polymer.The potential due to a uniform linear charge density is logarithmic, and assuming that the counterions have valence z (chrage ze), their potential energy is given by

$$\mathcal{V} = \frac{2ze^2 n}{\epsilon} \sum_{i=1}^{N} \ln\left(\frac{r_i}{a}\right), \tag{1}$$

where $n = N/V$ is the density of ions and r_i is the radial coordinate of the i-th particle. Note that we have neglected Coulomb repulsion between ions.

(a) For a cylindrical container of radius R, show that at a temperature T, the canonical partition function Z has the form

$$Z = \left(\frac{2\pi L}{a^{-2\xi}}\right)^N \left[\frac{R^{2(1-\xi)} - a^{2(1-\xi)}}{2(1-\xi)}\right]^N, \tag{2}$$

where $\xi = \beta ze^2 n/\epsilon$). (Hint: The volume of thin cylindrical shell dV_r of radius r and length L and thinkness dr is given by $dV_r = 2\pi L r dr$).
(b) Find an expression $p(r)$ for the probability of finding a particle at radius r and use this to calculate $\langle r \rangle$.
(c) Calculate the pressure exerted by counter-ions on the wall of the container. You can assume $R \gg a$. (Hint: Recall that pressure is derivative of free-energy with respect to volume V and that $dV = 2\pi L R dR$).