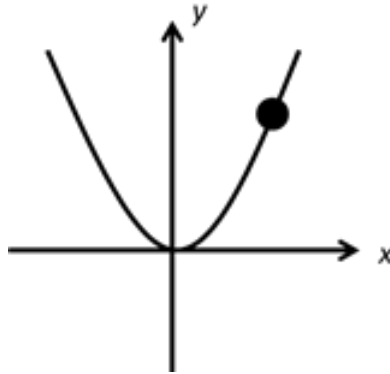


## Qualifying Exam - Classical Mechanics

**Problem 1.** (40 pts) Fundamentals.

(a) (10 pts) Show that one can use the Poisson bracket  $[f, L_z] = 0$  to illustrate  $f$  is an invariant quantity of the system under an infinitesimal rotation around the  $z$  axis.

(b) (10 pts) A particle of mass  $m$  slides under the action of gravity and without friction on a parabolic wire, as shown below. The parabola has the shape  $y = x^2$ . Use the method of Lagrange multipliers to incorporate constraint and to show that the constraint force is perpendicular to the wire.

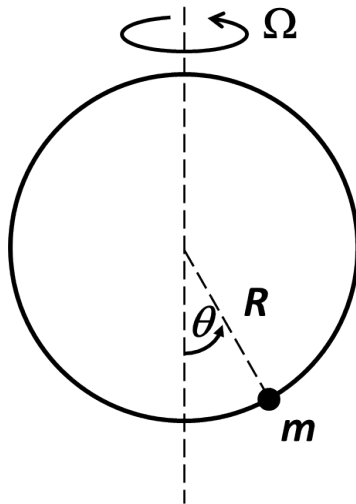


(c) (20 pts) Use the Hamilton-Jacobi equation to solve the trajectory  $\vec{r}(t)$  for a projectile motion of a particle shooting off from the origin at  $t = 0$  with the initial speed  $v_0$  and the launch angle  $\pi/4$  above the horizontal.

**Problem 2.** (20 pts) A bead on a rotating hoop: Consider a bead of mass  $m$  constrained to move on a massless circular hoop of radius  $R$ . The hoop rotates around its central axis (aligned with the  $z$ -axis, the direction of gravity) with a fixed angular velocity  $\Omega$ , as shown in the figure below.

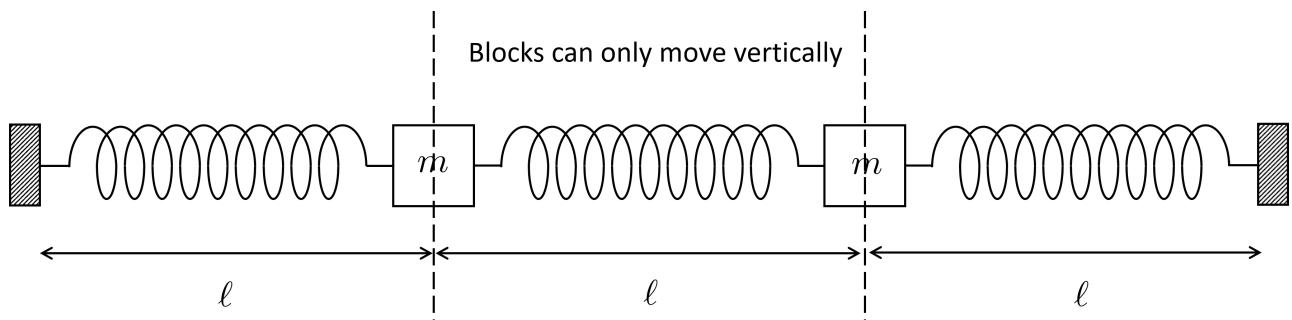
(a) (10 pts) Write the Lagrangian for the system **and** find any constants of the motion.

(b) (10 pts) When the hoop rotates slowly, the system exhibits a stable equilibrium point at  $\theta = 0$ . However, as the angular velocity  $\Omega$  increases beyond a critical value  $\Omega_c$ , this equilibrium point becomes unstable. Determine the critical angular velocity  $\Omega_c$ . In addition, find the new stable equilibrium point for the case where  $\Omega > \Omega_c$ .



**Problem 3.** (40 pts) Coupled oscillation and normal modes.

Two identical blocks of mass  $m$  are connected by three identical massless springs of spring constant  $k$ , as shown in the figure below. **The natural length of springs is  $(\ell/2)$** , therefore, springs are under tension. In addition, the blocks are constrained to move along frictionless vertical tracks. Clearly, the blocks are subject to both gravity and restoring forces of springs. For simplicity, assume that vertical displacements of these two blocks are small.



Springs are already stretched to length  $\ell$  when two blocks are at the horizontal ( $y_1 = y_2 = 0$ ).

(a) (15 pts) Let's define vertical displacements of the blocks away from the horizontal to be  $y_1$  and  $y_2$ . **Write down the Lagrangian of the system.** And use the fact that  $y_1/\ell \ll 1$  and  $y_2/\ell \ll 1$  to obtain **two linear coupled Euler-Lagrange equations** for  $y_1$  and  $y_2$ , respectively.

(b) (15 pts) Find the normal mode frequencies and its corresponding eigenvectors.

(c) (10 pts) If, initially, two blocks are displaced by  $(y_1, y_2) = (-mg/k, -mg/k)$  and released from rest. Obtain the solution for  $y_1(t)$  and  $y_2(t)$ .

# Electrodynamics Qualifying Exams

February 2024

You must provide the details or reasonings to justify your answers.

## Problem 1: Simple Questions (5% each = 35% total)

1. Write down the four Maxwell's equations. Specify all the numerical values of the relevant physical constants and the units you adopt.
2. Why are electromagnetic waves transverse in vacuum?
3. In one particular inertial frame, the electric and magnetic fields are measured as  $\vec{E} = (9, -1, 7)$  and  $c\vec{B} = (5, 0, -2)$  in some units, respectively. For the same field configuration can you measure in a different frame  $\vec{E}' = (2, 0, 4)$  and  $c\vec{B}' = (3, 5, 2)$ ?
4. Explain the terms Lorentz gauge and Coulomb gauge.
5. Explain the term Green's function.
6. Explain the terms Dirichlet and Neumann boundary conditions.
7. How many real degrees of freedom has a quadrupole moment? Explain your answer.

## Problem 2: Simple derivations (10% each = 20% total)

1. Derive the conservation of charge from the Maxwell equations.
2. Derive the wave equation for electromagnetic fields from the Maxwell equations.

## Problem 3: Moving charge (15%)

What are a point charge's electric and magnetic fields at a constant velocity  $\vec{v}$ ?

## Problem 4: Image Charges (18%)

Consider two grounded metal plates at a right angle meeting at the origin. Their position is given by the relation  $y = \pm x$  for all  $z$  and  $x > 0$ . On the surface of the metal plates and at infinity the potential vanishes. In the volume there is a point charge  $q$  at  $\vec{r}_1 = (d, 0, 0)$ .

1. (4%) Find the electric potential  $\phi(\vec{r})$  in the volume  $V$  enclosed by the plates and check that it fulfills the boundary conditions.
2. (6%) Calculate the surface charge density

$$\sigma = -\epsilon_0 \hat{n} \cdot \vec{\nabla} \phi, \quad (1)$$

with  $\hat{n}$  the normal vector on the surface  $S$  pointing out of the volume.

3. (5%) Calculate the total charge

$$Q = \int \sigma \, dS \quad (2)$$

on the plates. You can use Gauss' theorem to calculate  $Q$ .

4. (3%) Calculate the direction of the force on the point charge. Is the point charge pulled towards or away from the origin?

### Problem 5: Multipole Moments (12%)

Consider a homogeneously charged rectangular cuboid with charge  $Q$  and side lengths  $a$ ,  $b$ ,  $b$  with  $a > b$ . Choose the origin of the coordinate system to be in the center of the cuboid and put the axes along the symmetry axes of the object. The length of the cuboid in  $z$ -direction is  $a$ .

1. (3%) Write down an expression for the charge density,  $\rho$ .
2. (4%) Calculate either the spherical or the Cartesian monopole moment.
3. (5%) Calculate either the spherical or the Cartesian dipole moments.

# Quantum Mechanics Spring 2024

## Qualifying Exam

**You must show your work. No credits will be given if you don't show how you get your answers.**

Boldface characters like  $\mathbf{v}$  refer to vectors ( $= \vec{v}$ ).

**You may use the following formula:**

- The Schrödinger equation:

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle$$

where  $\hat{H}$  is the Hamiltonian  $\frac{\hat{\mathbf{p}}^2}{2\mu} + V(\hat{\mathbf{r}})$  and  $\mu$  is the mass of the particle.

For energy eigenstates, this reduces to the time-independent Schrödinger equation (in spherical coordinates)

$$-\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) \psi(\mathbf{r}) + \langle \mathbf{r} | \frac{\hat{\mathbf{L}}^2}{2\mu r^2} | \psi \rangle + V(\mathbf{r}) \psi(\mathbf{r}) = E \psi(\mathbf{r})$$

$\hat{\mathbf{L}}$  is the orbital angular momentum operator,  $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ .

- For a 1-D simple harmonic oscillator (SHO),  $\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2$ :

The raising and lowering operators are

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} - \frac{i}{m\omega} \hat{p}_x \right), \quad \hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left( \hat{x} + \frac{i}{m\omega} \hat{p}_x \right)$$

and  $[\hat{a}, \hat{a}^\dagger] = 1$ . The operators get their names from the facts that

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle, \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle,$$

where  $|n\rangle$ 's are the energy eigenstates of the 1D SHO.

- The Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Time-independent Perturbation: Consider  $\hat{H} = \hat{H}_0 + \hat{H}_1$ , where  $\hat{H}_1$  is a small perturbation. The first order energy correction to the n-th energy eigenvalue of  $\hat{H}_0$  is

$$E_n^{(1)} = \langle n^{(0)} | \hat{H}_1 | n^{(0)} \rangle$$

where  $|n^{(0)}\rangle$  is the n-th eigenstate of  $\hat{H}_0$ .

- Time-dependent Perturbation: Consider  $\hat{H} = \hat{H}_0 + \hat{H}_1(t)$ , where  $\hat{H}_1(t)$  is a small perturbation. The state  $|\psi(t)\rangle$  can be expanded in terms of the unperturbed eigenstates  $|n^{(0)}\rangle$ :

$$|\psi(t)\rangle = \sum_{n=0} d_n(t) e^{-i\frac{E_n^{(0)}t}{\hbar}} |n^{(0)}\rangle.$$

If initially ( $t = 0$ ) the particle is at state  $|i^{(0)}\rangle$ , the transition amplitude for the particle to be in state  $|f^{(0)}\rangle$  at time  $t$  is

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar} \int_0^t dt' \langle f^{(0)} | \hat{H}_1(t') | i^{(0)} \rangle e^{i\frac{(E_f^{(0)} - E_i^{(0)})t'}{\hbar}}.$$

- 3-D Scattering: The wave function  $\psi(\mathbf{r})$  of a particle scattering off a potential  $V(\mathbf{r})$  has the asymptotic behavior

$$\psi(\mathbf{r}) = Ae^{ikz} + Af(\theta, \phi) \frac{e^{ikr}}{r}, \quad r \rightarrow \infty,$$

where the incident wave is in the z-direction.

- Born Approximation: Useful for high-energy scattering.

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int d^3\mathbf{r}' V(\mathbf{r}') e^{-i\mathbf{q}\cdot\mathbf{r}'},$$

where  $m$  is the mass of the scattering particle, and  $\hbar\mathbf{q} = \hbar\mathbf{k}_f - \hbar\mathbf{k}_i$  is the momentum transferred from the initial state  $e^{i\mathbf{k}_i\cdot\mathbf{r}}$  to the final state  $e^{i\mathbf{k}_f\cdot\mathbf{r}}$ .

- Partial wave expansion: Useful for low-energy scattering. For spherically-symmetric  $V(r)$ ,

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) \frac{e^{i\delta_l}}{k} \sin \delta_l P_l(\cos \theta),$$

where  $\delta_l$  is the phase shift of the  $l$ -th partial wave, and  $P_l(\cos \theta)$  is the Legendre polynomial, which relates to the spherical harmonics  $Y_{l,m}(\theta, \phi)$  as

$$Y_{l,0}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta).$$

1. Briefly answer the following questions. **You must explain your reasoning.**:

- (a) Write down the Hermitian conjugate of an operator  $\hat{O}$ , with  $\hat{O}$  being (a)  $3x \frac{d}{dx}$  and (b)  $[\hat{A}, \hat{B}]$ , where  $\hat{A}$  and  $\hat{B}$  are Hermitian operators. (5 points)
- (b) If a system is in an eigenstate of total angular momentum  $\hat{\mathbf{J}}^2$  and angular momentum along the z-axis  $\hat{J}_z$ , what are the expectation values of angular momentum along the x- and the y-axis,  $\langle J_x \rangle$  and  $\langle J_y \rangle$ , and the squares  $\langle J_x^2 \rangle$  and  $\langle J_y^2 \rangle$ , for this system? (5 points)
- (c) Consider a system made of two spin-1/2 particles. The system is in the state

$$|\Phi\rangle = \frac{1}{\sqrt{3}}(|++\rangle + |+-\rangle + |-+\rangle).$$

- (+, - refer to spin along the z-axis). Are the two particles entangled? (3 points)
- (d) What is the expectation value of the *total* angular momentum of the system in part (c)? (3 points)
- (e) Can the system in part (c) be a system of two electrons? (2 points)

2. SHO and perturbation:

- (a) Consider a 1D SHO with mass  $m$  and frequency  $\omega$ . Suppose a perturbation of the form  $H_1 = b\hat{x}^4$  ( $b > 0$ ) is added to the 1D SHO. Find out the first order energy correction to the  $n$ -th energy level of the SHO. What is the condition for this first order result to be a valid energy correction? (5 points)
- (b) From part (a), explain why the first order energy correction must break down when  $n$  is large enough, no matter how small  $b$  is. (2 points)
- (c) If we make the perturbation time-dependent,  $H_1 = b\hat{x}^4 \exp\left(-\frac{t^2}{\tau^2}\right)$  ( $\tau > 0$ ), starting from  $t = -\infty$ . The SHO was originally at the ground state at  $t = -\infty$ . What is the probability for the SHO to transit to an excited state  $|n\rangle$  at  $t = +\infty$ ? (5 points)

3. 3D Scattering: Consider a particle of mass  $m$  and energy  $E$  scattering off a hard sphere in 3D. The potential is thus

$$V(r) = \begin{cases} \infty, & r \leq R \\ 0, & \text{elsewhere} \end{cases}$$

Consider only the s-wave scattering.

- (a) Show that the radial part ( $R(r)$ ) of the wave function for  $r > R$  is of the form

$$U(r) = rR(r) = \sin(kr + \delta_0),$$

where  $k = \frac{\sqrt{2mE}}{\hbar}$  and  $\delta_0$  is the phase shift. (5 points)

- (b) Use the boundary condition at  $r = R$ , prove that  $\sin^2 \delta_0 = \sin^2 kR$ . (5 points)
- (c) Evaluate the total cross section  $\sigma$  of the s-wave scattering, and show that  $\sigma \approx 4\pi R^2$  for low-energy scattering. (10 points)
- [Note: The Legendre polynomial  $P_l(\cos \theta) = 1$  for  $l = 0$ .]

4. The magnetic moment  $\boldsymbol{\mu}$  of a charged particle of spin  $\mathbf{S}$ , mass  $m$ , charge  $q$ , and g-factor  $g$  is  $\boldsymbol{\mu} = \frac{gq}{2mc}\mathbf{S}$ . (5 points each)

- (a) Prove the *Heisenberg equation of motion*: Consider the expectation value of an operator  $\hat{A}$  for a system in a state  $|\psi\rangle$ . Use the Schrödinger equation to prove that

$$\frac{d}{dt}\langle A \rangle = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}] \rangle,$$

where  $\hat{H}$  is the Hamiltonian.

- (b) The particle is placed under a uniform magnetic field  $\mathbf{B}$  with a Hamiltonian  $\hat{H} = -\boldsymbol{\mu} \cdot \mathbf{B}$ . Find the equations of motion of  $\langle S_x \rangle$ ,  $\langle S_y \rangle$ , and  $\langle S_z \rangle$  of the particle.
- (c) Suppose the particle is a spin-1/2 particle, and the magnetic field is  $\mathbf{B} = B_0 \hat{z}$  where  $B_0$  is a constant. At  $t = 0$ , the particle is measured to be spin-up along the  $y$ -axis. Express  $\langle S_x \rangle$  and  $\langle S_z \rangle$  as a function of time  $t$ .

5. Spin-Orbit interactions:

- (a) What is the spin-orbit interaction? Please briefly explain the origin, and show that for each energy level of a hydrogen atom,

$$E_{\text{SO}} \sim \alpha^2 E^{(0)},$$

where  $E_{\text{SO}}$  is the additional energy from the spin-orbit interaction,  $\alpha = \frac{e^2}{\hbar c}$  is the fine structure constant, and  $E^{(0)}$  is the energy eigenvalue from the Coulomb potential. (10 points)

[Hint: The magnetic field produced by a charge  $q$  with velocity  $\mathbf{v}$  is  $\mathbf{B}(\mathbf{r}) = \frac{q}{c} \frac{\mathbf{v} \times \mathbf{r}}{r^3}$ , and  $E^{(0)} \sim \alpha^2(m_e c^2)$  for hydrogen atoms, where  $m_e$  is the mass of the electron.]



- (b) Consider an electron in a hydrogen atom in the state  $Y_1^{+1} |+\rangle$ , express the result of  $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} Y_1^{+1} |+\rangle$  in terms of  $Y_l^m$  and  $(|+\rangle, |-\rangle)$ . (5 points)

6. Probability current:

- (a) Consider a particle of mass  $m$  in 3D, show that integrating its probability current all over the space gives

$$\int d^3\mathbf{r} \mathbf{j}(\mathbf{r}, t) = \frac{\langle \mathbf{p} \rangle}{m},$$

where  $\langle \mathbf{p} \rangle$  is the expectation value of its momentum. (5 points)

- (b) Suppose the particle is moving under an external magnetic field  $\mathbf{B}$  with a vector potential  $\mathbf{A}$ . The Hamiltonian is thus

$$H = \frac{(\mathbf{p}_c - q\mathbf{A}/c)^2}{2m},$$

where  $\mathbf{p}_c$  is the canonical momentum. Prove that the probability current for the particle under the magnetic field is

$$\mathbf{j} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi) - \frac{q}{mc} \mathbf{A} |\psi|^2.$$

[Note:  $\mathbf{p}_c$  and  $\mathbf{A}$  in general do not commute.] (10 points)

- (c) Compare the result in part (a) and part (b), is  $\langle \mathbf{p} \rangle$  in part (a) the same as  $\mathbf{p}_c$  in part (b)? Explain your reasoning. (5 points)

# Qualifying Examination – Statistical Mechanics

Feb 24-25, 2024

*Please explain the logic behind your answers.*

**Problem 1.** *Canonical ensemble at fixed temperature  $T$  (20 points):*

1. Single spin case:

(a) Consider an Ising spin with  $\mu = 1$  with proper unit,  $\sigma_1 = +1$  or  $-1$ , in the external field,  $h$ . The energy of this system is  $H_1 = -h\sigma_1$ . What are the possible energies of this system? What are the microscopic configurations of the Ising spin for the corresponding energies?

(b) Write down the partition function  $Z_1$  of this single spin system.

2. (a) Consider three such Ising spins decoupled from each other. That is, the total energy of the three spin system is  $H = -h(\sigma_1 + \sigma_2 + \sigma_3)$ . What are the possible microscopic configuration of the spins? You can imagine the spins are sitting at real space, so they are distinguishable according to their coordinates. What are the corresponding energies for each configuration?

(b) Write down the partition function  $Z$  of this three-spin system.

3. Show that  $Z = (Z_1)(Z_2)(Z_3) = (Z_1)^3$ . Here  $Z_i$  is the partition function of the  $i$ -th spin.

4. Suppose the Ising spin  $\sigma_1$  does not like to align with spin  $\sigma_2$ , usually it means the system pays more energy to aligning the direction of  $\sigma_1$  and  $\sigma_2$ . We can describe such effect by including a term  $J\sigma_1\sigma_2$  with  $J > 0$ . That is, the total energy is now described by  $H' = -h(\sigma_1 + \sigma_2 + \sigma_3) + J\sigma_1\sigma_2$ . We can construct the corresponding partition function  $Z'$  accordingly. Do you expect to have a factorizable structure as  $Z' = (Z'_1)(Z'_2)(Z'_3)$ ? Why? or Why not? Here  $Z'_i$  is the partition function formed by the degree of freedom  $\sigma_i$ .

**Problem 2.** *Ising model (15 points):* Considering the Ising model  $H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$  where  $\sigma_i = \pm 1$  and  $\langle i,j \rangle$  denotes the nearest-neighbor pairs of sites.

1. For a system of coordinate number  $z$ , use mean-field approximation to find the critical temperature  $T_c$  below which spontaneous magnetization exists.

2. Show that the magnetic susceptibility  $\chi \propto (T - T_c)^{-1}$  at  $T \gg T_c$

3. Use entropy argument to show that in 1D there is no phase transition, i.e.,  $T_c = 0$ .

**Problem 3.** *Free bosons (15 points):* Consider a number conserved Bose gas with energy dispersion  $\varepsilon_p = C|\mathbf{p}|^\alpha$  in  $d$  dimension space:

1. Show that there will be a Bose-Einstein condensation if  $d > \alpha$ .
2. Show that the critical temperature scales with the total number of particles,  $N$ , as  $T_c \propto N^{\alpha/d}$ .  
*Hint: you do not need to do the full calculation and may use dimensional argument for the density of states first.*

**Problem 4.** *Fermions in a two-level system (10 points):* Consider a system of  $N$  independent fermions. Assume that the single-particle Hamiltonian have only two energy levels, with energy 0 and  $\epsilon$ . However, the two levels have degeneracies  $n_0$  and  $n_1$ , which are both integers.

1. For the case of  $n_0 = n_1 = 3$  with  $N = 3$ . Find the chemical potential  $\mu$ , as a function of temperature. What is the Fermi energy  $\epsilon_F = \mu(T = 0)$ ?
2. For the case of arbitrary value of  $n_0$  and  $n_1$ , but with  $N = n_0$ . Find the chemical potential  $\mu$ , as a function of temperature at the low temperature limit. What is the Fermi energy  $\epsilon_F = \mu(T = 0)$ ?

**Problem 5.** *Freely Jointed Chain (Gaussian model) and its mean field picture (40 points)*

Polymers are large (high molar mass) molecules composed of a large number of monomers bonded together to form a chain. In reality, the monomers are bonded covalently. That is, the potential energy between two monomers should be a complex function of the bonding angle between two nearby monomers. Let's make some assumptions to simplify our problem which leads to the freely jointed model. (We might over simplify the problem but let's just try it first to get a feeling about what kind of problem we are facing. Then we can ask how to put back more ingredients to make our analysis more realistic.)

- We assume the joint of the monomers can rotate freely, *i.e.* the potential energy is independent of the bonding angle,  $\phi$ , between two nearby monomers.
- We assume the monomers can overlap with each other in space and have no interaction between each other.

The model with above two assumptions is the freely jointed chain model. It is the idealization of polymers analogous to ideal gas model for gases.

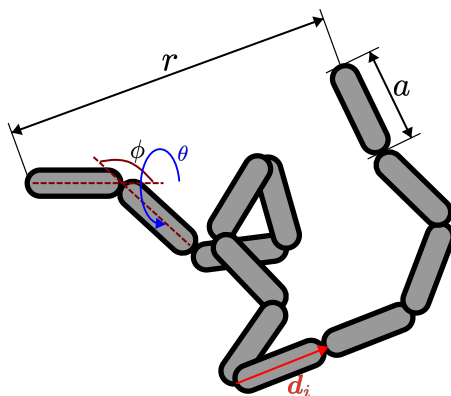


Figure 1: Schematic picture of a single chain polymer molecular formed by the monomers represented by the grey oval.

A key property that we are interested in is the size of the polymer. Usually the polymer coils up. The way they coils up will be a competition between the entropy and the energetics. Therefore,

the size of the polymer is not simply the number of monomers,  $N$ , times the size of the monomer,  $a$ . Instead, we need to use some statistical description to characterize the size of the polymer. Usually, we use the root-mean-square end-to-end distance,  $\langle r^2 \rangle^{1/2}$ , as a measure for the size of the polymer. Here,  $r$  is the distance from one end of the polymer to the other in three-dimensional space. The average is taken over all possible ways the polymer coils. One of the configuration is simple, if all the monomers are aligned in one direction, the end-to-end distance  $r_{straight} = Na$ . However, this is just one of the possible value of  $r$ , once the polymer coils,  $\langle r^2 \rangle^{1/2} < Na$ .

1. It is interesting to observe that the freely jointed model in one-dimension is actually the simple one-dimensional random walk we discussed during the lecture. The step size is just the size of the monomer. The one-dimensional constraint restricts  $\phi = 0/\pi$ . Let's start in this simple limit and use  $x$  to represent the end-to-end distance in one-dimensional case. Derive the probability distribution  $P_{1D}(x, N)$  when the number of monomers  $N$  is large.
2. For the three-dimensional case, we assume the orientation is completely random and the vector from monomer  $i$  and the vector for monomer  $i + 1$  are uncorrelated. *i.e.*  $\langle \mathbf{d}_i \cdot \mathbf{d}_j \rangle_{i \neq j} = 0$ . Therefore, we expect  $N$  to be distributed evenly  $N_x = N_y = N_z = \frac{N}{3}$ . Here,  $N_x$  is a rough definition of the monomer belongs to the monomer in  $x$  direction. We can simply consider the projection of the monomer to the  $x, y, z$  direction. If the projection to  $x$  direction is has the largest size, we said it is a  $x$  monomer that should be counted in  $N_x$ . Derive  $\langle r^2 \rangle^{1/2}$  and express it using  $N$  and  $a$ . This is a simple estimation for the size of the polymer. (Sometimes you will see people use the radius of gyration  $r_g^2$  to estimate the size of the polymer.  $r_g$  is the average distance between monomers and the center of mass. It turns out the length scale,  $\langle r_g^2 \rangle$ , will be proportional with  $\langle r^2 \rangle$ . We will not discuss the calculation here, but just mention the fact that using the root mean square of the end-to-end distance capture the essential information for the size of the polymer.)
3. Now we have a rough idea about the freely jointed model. Let's assume we are in three-dimensional world. In the last problem, we should be able to have the probability distribution function  $P_{3D}(r, N)$ . Using the microcanonical ensemble, we should expect the probability distribution to related to the phase space volume as

$$P_{3D}(r, N) = \frac{\Omega(r, N)}{\int dr \Omega(r, N)} \equiv \frac{\Omega(r, N)}{A_N}. \quad (1)$$

Here,  $\Omega(r, N)$  is the phase space volume for the size  $N$  polymer with the end-to-end distance  $r$ .  $A_N$  is the integral of  $\Omega(r, N)$  over  $r$ . Use (1) to find the expression of the entropy,  $S(r, N)$ , for the size  $N$  polymer with the end-to-end distance  $r$  using  $N, a, r, k_B$  and  $A_N$ .

4. With the expression of entropy, we can derive the Helmholtz free energy of the system using  $F(r, N) = U(r, N) - TS(r, N)$ . Here, we are considering the freely jointed model, so there is no internal energy. The Helmholtz free energy is just  $F(r, N) = -TS(r, N)$ . Here is the interesting part, the free energy depends on  $r$  just like the spring with elastic energy ( $E \propto k(\delta x)^2$ ). We can have the elasticity constant of the polymer. Find the expression of the elasticity constant  $k$  for the polymer described by the freely jointed model.
5. A rubber is an composite object with entangled polymers. They are difficult to analyze during the qualify exam. However, from the simple calculation we achieved here we can explain some interesting physics. Consider a piece of rubber hanging a massive object below it. Suppose the rubber is strong enough such that the massive object just hang in the air. Next, if we

heat up the rubber (hopefully we did not melt it.), what would you expect? Will the massive object be lifted higher? Or the other way around?

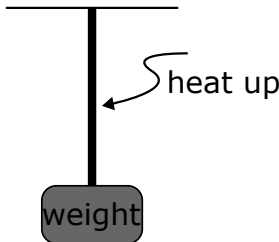


Figure 2: Schematic plot for the massive object hanging in the air.

6. Till now, we assume the non-interacting limit. So the free energy only consider the entropic effect. Now, we would like to extend the understanding to the case that the monomers can actually interact with each other. In order to proceed, we make the following assumptions:

- In Fig. 1, we can clearly see the monomer is a rod like object which does not have rotational symmetry (it is not a sphere). However, **let's put that aside and assume the monomers are spherically symmetric objects with volume  $v$  that forbidden the overlap of two monomers.**
- We can define the packing ratio,  $\mu$ , of the monomers for the polymer as

$$\mu = \frac{Nv}{r^3}. \quad (2)$$

We drop the irrelevant coefficients just to get an estimation about the physics. It is the ratio of the total volume of the monomers and the volume given by the "size" of the polymer.

Since the interaction avoids two monomers to overlap in space. We can assume that the interaction between the monomers are pair-wise interaction. (They are just one monomer interacts with another one to satisfy the no-overlapping condition.) Estimate the interaction energy,  $U_{int}(r, N, T)$ , at temperature  $T$  for a polymer with length  $N$  at large  $N$ . (Hint: Think about the meaning of the packing ratio. How to estimate the pair-wise interactions using the packing ratio?)

7. Before we do any calculation, let's think about the effect of each term. The entropic contribution favors the value of small  $r$  to minimize the improved free energy. On the other hand, since the monomers repel each other due to the interaction energy, the  $U_{int}(r, N, T)$  term prefers the value of large  $r$  in order to minimize the  $F_{improved}(r, N, T)$ . Therefore, the two effects competes with each other and fix the characteristic size of the polymer with length scale  $r^*$ . Use the above result to improve the free energy estimation by including the interaction between the monomers. We should have  $F_{improved}(r, N, T) = U_{int}(r, N, T) + F_{entropic}(r, N, T)$ . Find  $r^*$  as a function of  $v, a, N$ .

8.  $r_{ideal} \sim N^{\frac{1}{2}}$ ,  $r^* \sim N^\alpha$ . Compare  $r_{ideal}$  and  $r^*$  at large  $N$  limit. Is  $\alpha > \frac{1}{2}$ ,  $\alpha < \frac{1}{2}$  or  $\alpha = \frac{1}{2}$ ?  
Why is it a reasonable result?