Problem 1. (40 pts) Two particles are confined to move on frictionless tracks. As depicted in the figure below, m_1 is only allowed to move in the x-direction while m_2 is only allowed to move in the y-direction. These two masses are subjected to gravity $\vec{g} = -g\hat{y}$, and they are connected by a spring of negligible mass, spring constant k and natural length ℓ_0. For simplicity, assume that these two particles have the same mass m. Answer the following questions.

(a) (20 pts) Obtain the equations of motion for the system **with no constraint forces involved**.

(b) (10 pts) In the limit of extremely stiff spring (i.e., fixed spring length, $k \to \infty$), obtain the solution of the system.

(c) (10 pts) Now consider the case where the gravity is negligible (i.e., $g = 0$) but the spring has a finite stiffness, analyze the motion of the system for the non-trivial initial condition that both particles are moving initially.
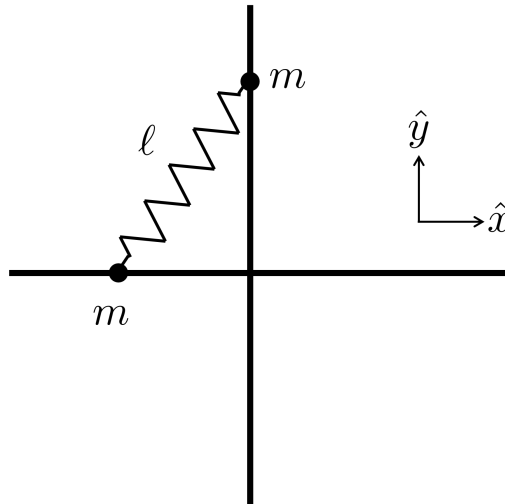
Problem 2. (20 pts) Over-damped dynamics and Brownian motion on the diffusive time scale. Let's consider a particle of mass m moving in one dimension in a viscous solvent. The particle is subject to Brownian forces, $\langle f(t) \rangle = 0$ and $\langle f(t) \cdot f(t') \rangle = 2\gamma k_B T \, \delta(t - t')$, where $\langle \, \rangle$ denotes the ensemble average (i.e., average over many realizations) and γ is the damping coefficient. The equation of motion of the particle is usually written as $\dot{x} = f(t)/\gamma$.

(a) (10 pts) Provide a justification for dropping out the $\ddot{x}$ term in the equation of motion.

(b) (10 pts) Derive the mean squared displacement of the particle.

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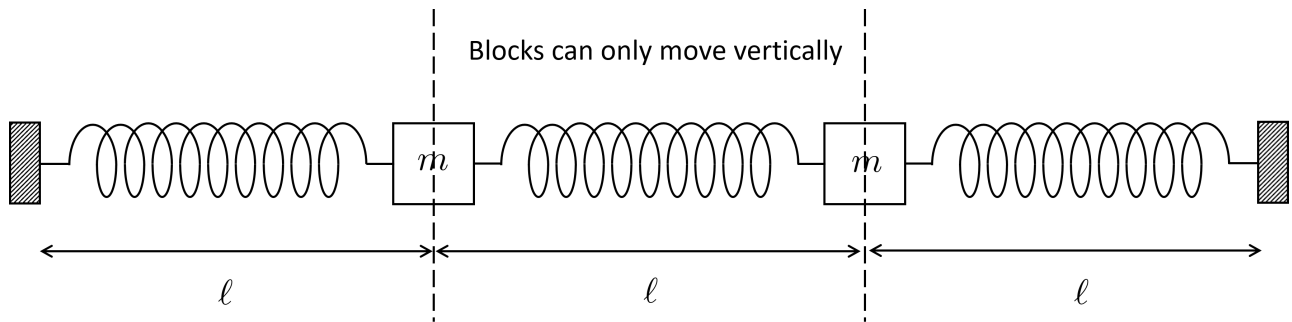
Springs are already stretched to length ℓ when two blocks are at the horizontal ($y_1 = y_2 = 0$).

(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

September 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 and specify your unit system.

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 as volume the whole three-dimensional space. Centered at the origin is a grounded metal sphere with radius R. At $\vec{x} = (0, 0, d)$ we position a point charge with charge q. On the surface of the metal sphere and at $\vec{x} \to \infty$ the electric potential vanishes.

1. (5%) Find the electric potential outside the sphere and check that it fulfills the boundary conditions.

2. (8%) Calculate the surface charge density

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

   with $\hat{n}$ the normal vector on the surface S.

3. (5%) Calculate the total charge

$$Q = \int \sigma \, \mathrm{d}\, S \tag{2}$$

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

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, ϱ.

2. (4%) Calculate the spherical and the Cartesian monopole moment.

3. (5%) Calculate the spherical and the Cartesian dipole moments.

Quantum Mechanics Fall 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 $\dfrac{\hat{\mathbf{p}}^2}{2\mu} + V(\hat{\mathbf{r}})$ and μ is the mass of the particle.

For energy eigenstates, this reduces to the time-independent Schrödinger equation $\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$, where $\psi(\mathbf{r})$ is the energy eigenfunction and E is the energy eigenvalue.

• For a spherically symmetric potential $V(\mathbf{r}) = V(r)$, the energy eigenfunctions can be written as $\psi(\mathbf{r}) = R(r)Y(\theta, \phi)$, and the (radial) time-indepedent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2 u(r)}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2}u(r) + V(r)u(r) = Eu(r),$$

where m is the mass, l is the quantum number for total angular momentum, and $u(r) = rR(r)$. For realistic cases, $u(0) = 0$.

• The general solution for a free particle in 3D is

$$u_l(\rho) = A_l\ \rho j_l(\rho) + B_l\ \rho n_l(\rho),$$

where $\rho = kr$, and the energy of the free particle is $E = \dfrac{\hbar^2 k^2}{2m}$. j_l and n_l are the spherical Bessel and Neumann functions, respectively. In particular,

$$j_0(\rho) = \frac{\sin\rho}{\rho}, \quad n_0(\rho) = -\frac{\cos\rho}{\rho}.$$

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

The raising and lowering operators are

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

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:

$$\sigma_\text{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_\text{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_\text{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- 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

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

where $\left|n^{(0)}\right\rangle$ 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 $\left|n^{(0)}\right\rangle$:

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

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

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

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

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

where the incident wave is in the z-direction. The differential cross section $d\sigma = |f(\theta,\phi)|^2\,d\Omega$. $f(\theta,\phi)$ is called the scattering amplitude, and $d\sigma/d\Omega$ is

often also called the differential cross section.

- The Born series: The solution of $\psi(\mathbf{r})$ scattering off a finite-ranged potential $V(\mathbf{r})$ can be expanded as

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_i \cdot \mathbf{r}} + \int d^3\mathbf{r}' G(\mathbf{r} - \mathbf{r}')U(\mathbf{r}')e^{i\mathbf{k}_i \cdot \mathbf{r}'}$$
$$+ \int d^3\mathbf{r}' G(\mathbf{r} - \mathbf{r}')U(\mathbf{r}') \int d^3\mathbf{r}'' G(\mathbf{r}' - \mathbf{r}'')U(\mathbf{r}'')e^{i\mathbf{k}_i \cdot \mathbf{r}''} + \dots,$$

where $e^{i\mathbf{k}_i \cdot \mathbf{r}}$ is the initial (incident) state, $U(\mathbf{r}) = 2mV(\mathbf{r})/\hbar^2$, and $G(\mathbf{r}-\mathbf{r}') = -\dfrac{1}{4\pi}\dfrac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$ is the Green's function. Under the condition $|\mathbf{r}| \gg |\mathbf{r}'|$, the first order **Born approximation** leads to

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

where m is the mass of the scattering particle, and $\hbar\mathbf{q} = \hbar\mathbf{k}_i - \hbar\mathbf{k}_f$ 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 $V(r)$, the asymptotic form of the wave function $\psi(\mathbf{r})$ can be expanded in spherical waves of different quantum number l

$$\psi(\mathbf{r}) = \frac{\sqrt{4\pi}}{k} \sum_l \sqrt{2l+1}\, i^l\, Y_{l,0}(\theta)\frac{1}{2i}\left[\frac{e^{i(kr-\frac{l\pi}{2})+2i\delta_l}}{r} - \frac{e^{-i(kr-\frac{l\pi}{2})}}{r}\right],$$

where δ_l is the phase shift for the l-th partial wave. The phase shifts are related to the scattering amplitude as

$$f(\theta) = \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1}\, e^{i\delta_l} \sin\delta_l\, Y_{l,0}(\theta),$$

and the total cross section

$$\sigma = \sum_l \sigma_l, \quad \sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l.$$

At $r \gg r_0$ (the effective range of the potential), the form of the wave function for the l-th partial wave is $\psi(r) = [A_l j_l(kr) + B_l n_l(kr)]Y_{l,0}$, and the phase shift can be derived from $\tan\delta_l = -B_l/A_l$.

1. Consider a system made of two spin-1/2 particles: (5 points each)

   (a) 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? Explain your reasoning.

   (b) What is the expectation value of the **total** angular momentum of the system in part (a)?

   (c) Can the system in part (a) be a system of two electrons? Explain your reasoning.

2. The magnetic moment $\boldsymbol{\mu}$ of a charged particle of spin $\mathbf{S}$, mass m, charge q, and g-factor g is $\boldsymbol{\mu} = \dfrac{gq}{2mc}\mathbf{S}$.

   (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

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

   where $\hat{H}$ is the Hamiltonian. (5 points)

   (b) Suppose the particle is a spin-1/2 particle, and it is placed under a magnetic field $\mathbf{B} = B_0\hat{z}$ 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. (10 points)

   [*Hint:* the angular momentum operators satisfy the commutation relation $[\hat{J}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{J}_k$.]

3. 1D Simple Harmonic Oscillator (SHO): Consider a 1D SHO with mass m and frequency ω.

   (a) A coherent state $|\alpha\rangle$ is defined as the eigenstate of the lowering operator $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$. Do α's have to be real? Explain why. (3 points)

   (b) Show that $\Delta x\Delta p_x$ for a coherent state saturates the lowest limit allowed by the Uncertainty Principle. (8 points)

   (c) What is the expectation value of energy for a coherent state $|\alpha\rangle$? (4 points)

   (d) Use the information from part (a) and (b), derive $\Delta x\Delta p_x$ for the ground state of a 1D SHO. (3 points)

(e) The 1D SHO is initially at the ground state. At $t = 0$ a decaying external **force** (*not potential!*) $F_0 e^{-t/\tau}$ is turned on (F_0 and τ are constants). To the lowest order in F_0, what is the probability to find the SHO in an excited state (please specify for any $n \geq 1$) at some later time t_1? (4 points)

(f) Show that your result in part (e) becomes independent of t_1 when the force decays very fast. Is this behavior reasonable? (3 points)

4. A hydrogen atom is placed under a constant external electric field along the z-axis:
$$\mathbf{E} = \mathcal{E}_0 \hat{k},$$
The electron has charge $-e, e > 0$, and $|n, l, m\rangle$ denotes the eigenstates of the hydrogen atom *without* any perturbation. Consider the effects up to the first order in $\mathcal{E}_0$. (5 points each)

(a) Evaluate the commutator $[\hat{L}_z, \hat{z}]$, and use the result to explain the following selection rule: $\langle n', l', m' | \hat{z} | n, l, m \rangle = 0$ if $m \neq m'$.

(b) Make use of the selection rule from part (a), and the fact the parity of the spherical harmonics $Y_{l,m}(\theta, \phi)$ is $(-1)^l$ (you don't need to prove this), write down the perturbing Hamiltonian due to $\mathbf{E}$ as a matrix in the basis of $|n, l, m\rangle$ for $n = 2$. Express the matrix in terms of Δ, which denotes **one of** the non-zero matrix elements (**you don't need to derive it**. Just write down an expression for Δ.)

[*Note:* You only need one symbol Δ. Explain why.]

(c) What is the energy spectrum of the $n = 2$ states of this hydrogen atom, taking into account the first order energy corrections due the external electric field? Again you only need to use Δ to express the answers.

5. 3D Scattering:

(a) Use the **Born approximation**, compute the differential cross section for a 3D potential well
$$V(r) = \begin{cases} -V_0, & r \leq a \\ 0, & \text{elsewhere} \end{cases}$$
where $V_0 > 0$. (5 points)

[*Hint:* $\dfrac{d \sin x}{dx} = \cos x, \dfrac{d \cos x}{dx} = -\sin x$.]

(b) Show that if the incident particles have *low energies*, the differential cross section becomes isotropic. You need to specify what you mean by "low energies". (5 points)

[*Hint:* For small x, $\sin x \approx x - \dfrac{x^3}{3!}$, $\cos x \approx 1 - \dfrac{x^2}{2!}$.]

(c) Compute the total cross section for the potential in part (a) at *low energies* using the Born approximation. What is the condition for your result in to be valid? (5 points)

(d) Show that for the s-wave ($l = 0$), the asymptotic form of the wave function $\psi(\mathbf{r})$ for $r \gg r_0$ (r_0 is the effective range of the potential) is of the form
$$\psi(\mathbf{r}) = \frac{C}{r} \sin\left(kr + \delta_0\right),$$

where C is an overall constant, and δ_0 is the phase shift of the s-wave. (5 points)

(e) Use the result in part (d), evaluate the s-wave scattering cross section of the potential in part (a) using the **partial wave** analysis method . Is your result compatible with your answer in part (c)? (15 points)

[*Hint:* Useful the trigonometric identities for parts (d) and (e):

$$\sin\left(A + B\right) = \sin A \cos B + \cos A \sin B$$
$$\tan\left(A + B\right) = \frac{\tan A + \tan B}{1 - \tan A \tan B}$$

and $\tan x \approx x \approx \sin x$ for small x.]

Qualifying Examination – Statistical Mechanics

Sep 06, 2024

Please explain the logic behind your answers.

Problem 1. *Bosons in Harmonic traps(30 points):* Let us consider a particle in the anisotropic harmonic-oscillator potential $V(\boldsymbol{r}) = \frac{1}{2}\left(K_x x^2 + K_y y^2 + K_z z^2\right)$. Therefore, we can consider the system as three independent harmonic oscillators in three different directions x, y and z. The corresponding energy levels can be parameterized by three non negative integers (n_x, n_y, n_z) as

$$E(n_x, n_y, n_z) = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z. \tag{1}$$

1. Let us consider n_i are continuous variables and neglect the zero-point energies (The $\frac{1}{2}\hbar\omega_i$ in $E(n_x, n_y, n_z)$.), we can simplify the energy as $E \approx \varepsilon_x + \varepsilon_y + \varepsilon_z$ where $\varepsilon_i = n_i\hbar\omega_i$. If we define $G(E)$ as the number of states below energy a specific energy E. Derive the expression of $G(E)$ in terms of $E, \omega_x, \omega_y, \omega_z$ and $\hbar$. (Hint: There are several way to derive this result. One approach is to consider the problem in the (n_x, n_y, n_z) space. What is the geometric meaning of the states below energy E?)

2. Another way to understand density of state is $g(E) = \frac{dG(E)}{dE}$. Use the above expression to get the density of states.

3. We can evaluate the particles in the excited states using

$$N_{ex} = \int_0^\infty dE\, g(E)\frac{1}{e^{E/k_B T} - 1}. \tag{2}$$

Here, we assume N_{ex} reaches its maximum for $\mu = 0$. The definition of the transition temperature, T_c, of Bose-Einstein condensation is when the total number of particles can be just accommodated in excited states. That is,

$$N = N_{ex}(T = T_c, \mu = 0) = \int_0^\infty dE\, g(E)\frac{1}{e^{E/k_B T} - 1}. \tag{3}$$

$\int_0^\infty dx \frac{x^{\alpha-1}}{e^x - 1} = \Gamma(\alpha)\zeta(\alpha)$. Here, $\zeta(\alpha) = \sum_{n=1}^\infty n^{-\alpha}$ is the Riemann zeta function and $\Gamma(\alpha)$ is the gamma function. Derive the transition temperature of this system and express the result using $N, \omega_x, \omega_y, \omega_z$ and the Riemann zeta function.

Problem 2. *Free fermion problem(10 points):* Let the density of states of the electrons in a system be assumed to be a constant D for $\varepsilon > 0$ ($D = 0$ for $\varepsilon < 0$). Here, ε represents the energy. We assume the total number of electrons be equal to N. Here $N = D\int_0^\infty \frac{1}{e^{\beta(\varepsilon-\mu)+1}}d\varepsilon$.

1. Calculate the chemical potential μ at $T = 0K$.

2. When the system is in the regime of quantum degeneracy, estimate or derive the expression of the specific heat and show that it is proportional to T.

Problem 3. *Two-level system(15 points):*   Consider a system of N distinguishable particles, which have two energy levels, $E_0 = -\mu B$ and $E_1 = \mu B$, for each particles. Here μ is the magnetic moment and B is the magnetic field. The particles populate the energy levels according to the classical distribution law.

1. Calculate the average energy of such system at temperature T

2. Calculate the specific heat of the system

3. Calculate the magnetic susceptibility

Problem 4. *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 bounded 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, ϕ, 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.
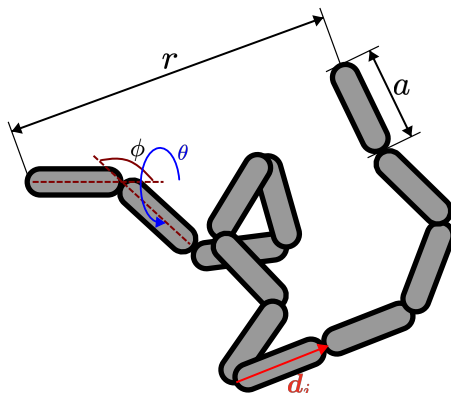

Figure 1: Schematic picture of a single chain polymer molecular formed by the monomers represented by the grey oval.

    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.* $\langle \boldsymbol{d}_i \cdot \boldsymbol{d}_j \rangle_{i \neq j} = 0$. 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 $\langle r^2 \rangle^{\frac{1}{2}}$ 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

$$P_{3D}(r, N) = \frac{\Omega(r, N)}{\int dr \Omega(r, N)} \equiv \frac{\Omega(r, N)}{A_N}. \tag{4}$$

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 (4) 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 anlayze 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?
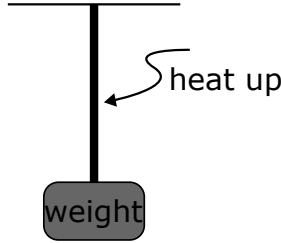
3

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, μ, of the monomers for the polymer as

   $$\mu = \frac{Nv}{r^3}. \tag{5}$$

   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?

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Problem 5. *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., $T_c = 0$.