

Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

Fall 2023 (in 4 separate parts: CM, EM, QM, SM)

General Instructions:

Three problems are given. If you take this exam as a placement exam, you must work on all three problems. If you take the exam as a qualifying exam, you must work on two problems (if you work on all three problems, only the two problems with the highest scores will be counted).

Each problem counts for 20 points, and the solution should typically take approximately one hour.

Use one exam book for each problem, and label it carefully with the problem topic and number and your ID number.

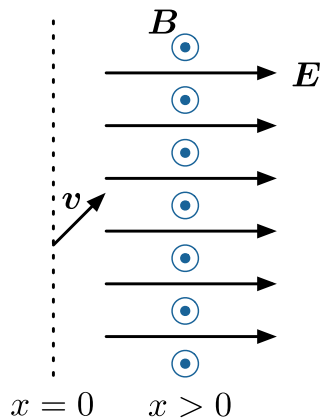
Write your ID number (not your name!) on each exam booklet.

You may use, one sheet (front and back side) of handwritten notes and, with the proctor's approval, a foreign-language dictionary. **No other materials may be used.**

Classical Mechanics 1

Crossed fields

A positively charged particle of charge q and mass m enters a semi-infinite region of crossed homogeneous electric and magnetic fields with \mathbf{E} pointing in the x direction, and \mathbf{B} pointing in the z direction (out of the page as shown below). The particle enters at an angle 45° with velocity $\mathbf{v} = (v_0, v_0)$, so that the initial kinetic energy is mv_0^2 .

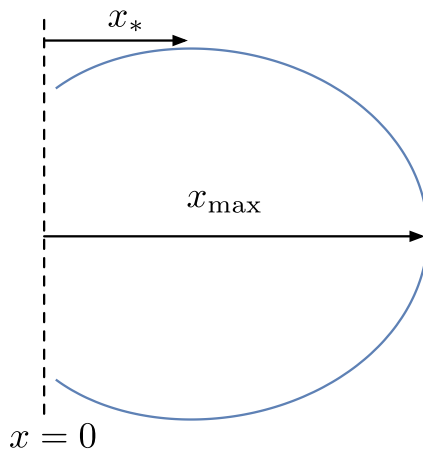


- (a) (3 points) Write down the Lagrangian for the charged particle in the E and B fields, and use it to determine the Hamiltonian of the system.

Hint: The vector potential can be written $\mathbf{A} = B(0, x, 0)$. It is helpful to parametrize B by the cyclotron frequency¹, $\omega_B \equiv qB/m$.

- (b) (5 points) Determine equations of motion in the Hamiltonian formulation and identify all constants of the motion.

A typical trajectory of the particle is shown below.



¹In Gaussian or Heaviside Lorentz units the cyclotron frequency reads $\omega_B \equiv qB/mc$.

- (c) (4 points) Determine the distance of maximum penetration into the fields x_{\max} ?
- (d) (4 points) What is the value of x_* ?
- (e) (4 points) Compute the time it takes to complete an orbit.

Solution

(a) The Lagrangian is

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + q\dot{y}Bx + qEx \quad (1)$$

The term involving B stems from the interaction $\mathbf{v} \cdot \mathbf{A}$.

The Hamiltonian is

$$H = \mathbf{p} \cdot \dot{\mathbf{r}} - L = \frac{(\mathbf{p} - q\mathbf{A})^2}{2m} + q\phi \quad (2)$$

For the problem at hand we have only an A_y component of the vector potential:

$$qA_y = m\omega_B x \quad (3)$$

The Hamiltonian in this case is thus

$$H = \frac{p_x^2}{2m} + \frac{(p_y - m\omega_B x)^2}{2m} + \frac{p_z^2}{2m} - qEx \quad (4)$$

(b) The equations of motion are

$$\frac{dx}{dt} = \frac{p_x}{m}, \quad (5)$$

$$\frac{dp_x}{dt} = qE + (p_y - m\omega_B x)\omega_B, \quad (6)$$

$$\frac{dy}{dt} = \frac{p_y - m\omega_B x}{m}, \quad (7)$$

$$\frac{dp_y}{dt} = 0, \quad (8)$$

$$\frac{dz}{dt} = \frac{p_z}{m}, \quad (9)$$

$$\frac{dp_z}{dt} = 0. \quad (10)$$

We clearly have the cyclic coordinates of y and z leading to

$$p_y = \text{const}, \quad (11)$$

$$p_z = \text{const}. \quad (12)$$

Also the Hamiltonian does not depend on time, and so we have

$$H(\mathbf{r}(t), \mathbf{p}(t)) = \text{const} = \mathcal{H}_0, \quad (13)$$

where $\mathbf{r}(t), \mathbf{p}(t)$ satisfy the equations of motion.

(c) The turning points are at x_{\max} when $\dot{x} = p_x/m = 0$. The initial conditions are such that $\mathcal{H}_0 = mv_0^2$ and $p_y = mv_0$. Using energy conservation we have

$$mv_0^2 = \frac{(mv_0 - m\omega_B x_{\max})^2}{2m} - qEx_{\max} \quad (14)$$

This is a quadratic equation for x_{\max} .

We present the solution by defining $x_E = qE/m\omega_B^2$ and $x_* = v_0/\omega_B$ (see below), yielding:

$$x_{\max} = x_E + x_* + \sqrt{x_*^2 + (x_E + x_*)^2} \quad (15)$$

(d) The point x_* is characterized by $\dot{y} = 0$; \dot{y} is determined by Hamilton's equations:

$$\dot{y} = \frac{\partial H}{\partial p_y} = \frac{p_y - m\omega_B x}{2m} \quad (16)$$

Since $p_y = mv_0$ we find that $\dot{y} = 0$ when

$$x_* = \frac{v_0}{\omega_B} \quad (17)$$

(e) Differentiation gives

$$\frac{d^2 x}{dt^2} = \frac{1}{m} \frac{dp_x}{dt}, \quad (18)$$

$$= \frac{qE + p_y \omega_B}{m} - \omega_B^2 x, \quad (19)$$

$$= \omega_B^2 (x_E + x_* - x). \quad (20)$$

This is a harmonic oscillator with a constant force, with solution

$$\delta x = \mathcal{A} \cos(\omega_B t + \phi), \quad (21)$$

where $\delta x = x - (x_E + x_*)$. Adjusting (\mathcal{A}, ϕ) to reproduce the initial conditions

$$x(0) = 0, \quad \dot{x}(0) = v_0, \quad (22)$$

we require

$$\mathcal{A} \cos(\phi) = -(x_E + x_*), \quad -\mathcal{A} \omega_B \sin(\phi) = v_0. \quad (23)$$

Thus the phase is

$$\tan \phi = \frac{x_*}{x_E + x_*}. \quad (24)$$

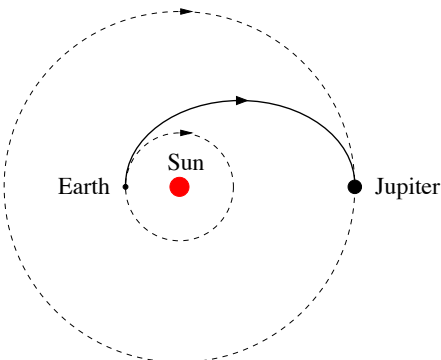
The motion is harmonic with angular frequency ω_B , but we do not make a complete cycle. Using circular motion to represent the harmonic oscillations, the harmonic motion starts at phase angle ϕ (when the particle enters the field at $x = 0$) and stops at phase angle $2\pi - \phi$ (when the particle exits the field at $x = 0$). The duration is thus

$$\tau = \frac{2\pi - 2\phi}{\omega_B}. \quad (25)$$

Classical Mechanics 2

Hohmann Ellipse Transfer Orbit

A spacecraft of mass m is to be sent from the Earth to Jupiter. It is decided to use a Hohmann-ellipse transfer orbit which is tangential to both the orbit of the Earth (assumed circular) at $r = R_1$, and to the orbit (also assumed circular) of Jupiter at $r = R_2$. (There is more than one way of solving this problem. If you decide to use any properties of Kepler orbits, you must derive them to gain full credit.)



- (a) (2 points) Find the orbital velocities v_1 and v_2 of the Earth and Jupiter. Your answer should be expressed in terms of R_1 and R_2 , Newton's constant G and the mass of the sun M .
- (b) (8 points) Find the departure orbital velocity v_D (measured with respect to the Sun and tangential to the Earth's orbit) that must be given to the spacecraft if it is to arrive tangential to Jupiter's orbit, and also the tangential velocity v_A at which it will arrive at this orbit². Again your answer should be expressed in terms of R_1 , R_2 , G and M .
- (c) Find an explicit formula for the time that the journey from the Earth to Jupiter will take:
 - (i) (8 points) Introduce a set of dimensionless variables which describe the trajectory of the spacecraft. Express your result for the time as an overall dimensionful constant times a dimensionless integral, which is explicit enough to be evaluated on a computer given combinations of R_1 , R_2 , G and M .
 - (ii) (2 points) Evaluate the relevant integral.

Note: The following integrals are useful:

$$\int_{\alpha}^{\beta} \frac{dx}{x^2} \frac{1}{\sqrt{(\beta-x)(x-\alpha)}} = \frac{\pi}{2} \frac{\alpha + \beta}{(\alpha\beta)^{3/2}} \quad \int_0^{\pi} \frac{d\theta}{(\alpha + \beta \cos \phi)^2} = \frac{\pi\alpha}{(\alpha^2 - \beta^2)^{3/2}}$$

and recall that the area of an ellipse with semi-major/minor axes a , b is πab .

²You are to neglect the gravitational pull of Earth and Jupiter on the orbit of the satellite

Solution:

(a) The circular orbits have:

$$\frac{mv^2}{R} = \frac{GMm}{R^2}, \quad (1)$$

and so

$$v_{1,2} = \sqrt{\frac{GM}{R_{1,2}}}. \quad (2)$$

(b) The Langrangian for is

$$L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) + \frac{GMm}{r} \quad (3)$$

The integrals of motion are the angular momentum

$$\ell = mr^2\dot{\phi} \quad (4)$$

and the energy

$$E = \frac{1}{2}m\dot{r}^2 + \frac{\ell^2}{2mr^2} - \frac{GMm}{r} \quad (5)$$

The orbital conditions specify the integrals of motion ℓ and E . Since R_1 and R_2 are turning points, $\dot{r} = 0$ here.

$$E = \frac{\ell^2}{2mR_1^2} - \frac{GMm}{R_1} \quad (6)$$

$$E = \frac{\ell^2}{2mR_2^2} - \frac{GMm}{R_2} \quad (7)$$

Subtracting the two equations, and solving for ℓ^2 we find

$$\ell^2 = 2GMm^2 R_1 \left(\frac{1 - R_1/R_2}{1 - R_1^2/R_2^2} \right) = 2GMm^2 \frac{R_1 R_2}{R_1 + R_2} \quad (8)$$

The angular momentum at the turning points inner turning point $\ell = mv_D R_1$ and so

$$v_D = \sqrt{\frac{2GM}{R_1}} \sqrt{\frac{R_1 R_2}{R_1 + R_2}} \quad (9)$$

and so

$$v_D = v_1 \sqrt{\frac{2R_1 R_2}{R_1 + R_2}} \quad (10)$$

Similarly $\ell = mv_A R_2$ and so

$$v_A = v_2 \sqrt{\frac{2R_1 R_2}{R_1 + R_2}} \quad (11)$$

(c) To find the time we need to integrate the equations of motion. We first find the energy in terms of R_1 and R_2 . We multiply by Eq. (6) by R_1^2/R_2^2 and subtract Eq. (7)

$$E = -\frac{GM}{R_1 + R_2} \quad (12)$$

The time is found by integrating the first integral

$$\frac{dr}{dt} = \left(\frac{2}{m} \left(E - \frac{\ell^2}{2mr^2} + \frac{GMm}{r} \right) \right)^{1/2} \quad (13)$$

Introducing some dimensionless variables we set

$$GM = R_1 = m = 1 \quad (14)$$

Then

$$R_2 \Rightarrow \kappa \equiv R_2/R_1 = \text{The outer radius in units of } R_1 \quad (15)$$

$$R_1 \Rightarrow 1 \quad (16)$$

$$E \Rightarrow -\frac{1}{1 + \kappa} \quad (17)$$

$$\ell^2 \Rightarrow \frac{2\kappa}{1 + \kappa} \quad (18)$$

$$r \Rightarrow r \equiv \text{The radius in units of } R_1 \quad (19)$$

$$t \Rightarrow t \equiv \text{The time in units of } R_1/v_1 \quad (20)$$

So

$$\frac{dr}{dt} = \sqrt{2} \left(\frac{-1}{(1 + \kappa)} - \frac{\kappa}{1 + \kappa} \frac{1}{r^2} + \frac{1}{r} \right)^{1/2} \quad (21)$$

We see that when $r = 1$ and when $r = \kappa$ the integrand vanishes. We clean up a little by factoring out a $\kappa/(1 + \kappa)$ so

$$\frac{dr}{dt} = \sqrt{\frac{2\kappa}{1 + \kappa}} \left(\left(\frac{1 + \kappa}{\kappa} \frac{1}{r} - \frac{1}{r^2} - \frac{1}{\kappa} \right) \right)^{1/2} \quad (22)$$

And the time in chosen units is given by

$$t = \int_1^\kappa \frac{dr}{\frac{dr}{dt}} \quad (23)$$

Upon restoring the overall units we have

$$t = \frac{R_1}{v_1} \sqrt{\frac{1 + \kappa}{2\kappa}} \int_1^\kappa \frac{dr}{\left(\frac{(1 + \kappa)}{\kappa} \frac{1}{r} - \frac{1}{r^2} - \frac{1}{\kappa} \right)^{1/2}} \quad (24)$$

(d) The integral is evaluated by changing vars to $u = 1/r$

$$t = \frac{R_1}{v_1} \sqrt{\frac{1+\kappa}{2\kappa}} \int_1^{1/\kappa} \frac{du}{u^2} \frac{1}{\sqrt{(1+\kappa)/\kappa u - u^2 - 1/\kappa}} \quad (25)$$

$$t = \frac{R_1}{v_1} \sqrt{\frac{1+\kappa}{2\kappa}} \int_1^{1/\kappa} \frac{du}{u^2} \frac{1}{\sqrt{(u-1)(1/\kappa - u)}} \quad (26)$$

Using the integral given and minor algebra yields

$$t = \frac{R_1}{v_1} \left(\frac{R_1 + R_2}{2R_1} \right)^{3/2} \pi. \quad (27)$$

When $R_1 = R_2$ this answer is clearly correct.

Classical Mechanics 3

Disk rolling on a string

A solid cylindrical disk of mass M and radius R rolls without slipping along a string of length L fixed at both ends to solid walls separated by a distance W , as shown in Fig. 1. Assume that $R \ll L, W$.

- (a) **[4pts]** Show that the disk is constrained to move along an ellipse.
- (b) **[6pts]** Write the Lagrangian in terms of one generalized coordinate, e.g., the x -coordinate of the disk indicated in Fig. 1.
- (c) **[8pts]** Assuming small oscillations about the equilibrium point, derive the frequency of oscillations.
- (d) **[2pts]** What would change if the disk was replaced by a solid spherical bead threaded along the string? What would be the frequency of oscillations?

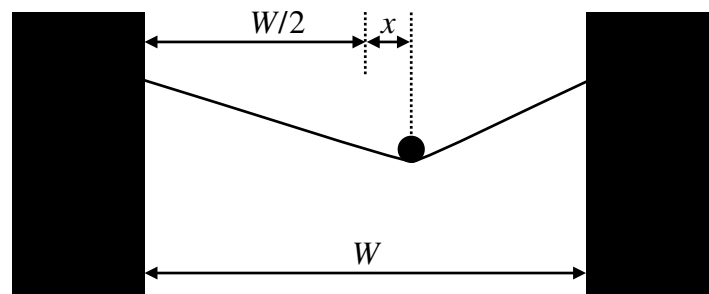


Figure 1: A solid disk rolling along a string.

Solution

(a) **[4pts]** Show that the disk is constrained to move along an ellipse.

Let y be the vertical distance from the ball to the fixed endpoints of the string and x the horizontal distance indicated in Fig. 1. The fixed length of the string imposes the geometric constraint:

$$L = \sqrt{y^2 + \left(\frac{W}{2} + x\right)^2} + \sqrt{y^2 + \left(\frac{W}{2} - x\right)^2} \quad (1)$$

Squaring both sides:

$$L^2 - 2\left(y^2 + \frac{W^2}{4} + x^2\right) = 2\sqrt{\left(y^2 + \left(\frac{W}{2} + x\right)^2\right)\left(y^2 + \left(\frac{W}{2} - x\right)^2\right)} \quad (2)$$

$$= 2\sqrt{\left(y^2 + \frac{W^2}{4} + x^2\right)^2 - W^2x^2} \quad (3)$$

Squaring both sides again and simplifying yields:

$$4L^2y^2 + 4(L^2 - W^2)x^2 = L^4 - L^2W^2, \quad (4)$$

which is an equation for an ellipse.

(b) **[8pts]** Write the Lagrangian in terms of one generalized coordinate, e.g., the x -coordinate of the disk indicated in Fig. 1.

The kinetic energy is a sum of translational and rotational parts:

$$\text{K.E.} = \frac{1}{2}M(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\dot{\phi}^2, \quad (5)$$

where $I = \frac{1}{2}MR^2$ is the moment of inertia. The potential energy comes from gravity:

$$\text{P.E.} = -Mgy \quad (6)$$

To write the Lagrangian in terms of one coordinate requires writing y, ϕ in terms of x . The coordinate y can be written in terms of x using Eq. (4) in part (a),

$$y^2 = \frac{L^2 - W^2}{4} - \left(1 - \frac{W^2}{L^2}\right)x^2 \quad (7)$$

It follows that

$$\dot{y} = \frac{d}{dt}\sqrt{\frac{L^2 - W^2}{4} - \left(1 - \frac{W^2}{L^2}\right)x^2} \quad (8)$$

$$= \frac{-\left(1 - \frac{W^2}{L^2}\right)x\dot{x}}{\sqrt{\frac{L^2 - W^2}{4} - \left(1 - \frac{W^2}{L^2}\right)x^2}} \quad (9)$$

$$= -\frac{2x\dot{x}}{L}\sqrt{\frac{L^2 - W^2}{L^2 - 4x^2}} \quad (10)$$

To write ϕ in terms of x requires the condition that the disk rolls without slipping:

$$R\phi = \sqrt{y^2 + \left(\frac{W}{2} + x\right)^2} \quad (11)$$

Inserting Eq. (7) into Eq. (11) yields:

$$R\phi = \sqrt{\frac{L^2 - W^2}{4} - \left(1 - \frac{W^2}{L^2}\right)x^2 + \left(\frac{W}{2} + x\right)^2} \quad (12)$$

$$= \sqrt{\frac{L^2}{4} + \frac{W^2x^2}{L^2} + xW} = \frac{L}{2} + \frac{xW}{L}, \quad (13)$$

from which it follows:

$$\dot{\phi} = \frac{W}{LR}\dot{x} \quad (14)$$

Inserting Eqs. (7), (10) and (14) into the kinetic and potential energies yields the Lagrangian in terms of only one generalized coordinate, x :

$$\mathcal{L} = \frac{M}{2} \left(1 + \frac{4x^2(L^2 - W^2)}{L^2(L^2 - 4x^2)}\right) \dot{x}^2 + \frac{MW^2}{4L^2} \dot{x}^2 + \frac{Mg}{2L} \sqrt{(L^2 - W^2)(L^2 - 4x^2)} \quad (15)$$

(c) **[8pts]** Assuming small oscillations about the equilibrium point, derive the frequency of oscillations.

The equilibrium point is $x = 0$. Small oscillations implies that x is small, so the Lagrangian can be expanded to quadratic order in x and \dot{x} :

$$\mathcal{L} \approx \left(\frac{M}{2} + \frac{MW^2}{4L^2}\right) \dot{x}^2 + \frac{Mg}{2} \sqrt{L^2 - W^2} \left(1 - \frac{2x^2}{L^2}\right) \quad (16)$$

Applying the Euler-Lagrange equation:

$$-\frac{2Mg}{L^2} \sqrt{L^2 - W^2} x = M \left(1 + \frac{W^2}{2L^2}\right) \ddot{x}, \quad (17)$$

which yields the oscillation frequency Ω given by:

$$\Omega^2 = \frac{2g\sqrt{L^2 - W^2}}{L^2 + \frac{W^2}{2}} \quad (18)$$

(d) **[2pts]** What would change if the disk was replaced by a solid spherical bead threaded along the string? What would be the frequency of oscillations?

If the disk was replaced by a solid bead, there would be no rotational energy, which eliminates the middle term in the Lagrangian in Eq. (15). The final result is that the frequency of oscillations is given by $\Omega = \sqrt{\frac{2g}{L^2} \sqrt{L^2 - W^2}}$.

Electromagnetism 1

(a) (4 points) Preliminaries:

- (i) The electric field \mathbf{E} and the magnetic field \mathbf{B} may be expressed in terms of the vector potential \mathbf{A} and scalar potential ϕ via $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla\phi - \partial\mathbf{A}/\partial t$. Specify the Maxwell equations that are automatically satisfied as a result of these expressions and explain the physical meaning of each equation from its integral form.
- (ii) The potentials \mathbf{A} and ϕ can be constrained to obey a so-called gauge condition. Briefly explain why.
- (iii) Impose on \mathbf{A} and ϕ the *Lorenz gauge condition*, i.e., $\nabla \cdot \mathbf{A} + (c^{-2}\partial\phi/\partial t) = 0$. Show that \mathbf{A} then obeys the driven wave equation, with a driving term proportional to the current density \mathbf{J} .

Now consider a charge distribution consisting of thin line of charge of length $2L$, which at time $t = 0$ is aligned with the x axis and centered at the origin (as shown in the figure below). A charge q is spread uniformly along the line segment $0 < x < L$; a balancing charge $-q$ is spread uniformly along the line segment $-L < x < 0$. The distribution rotates with constant angular velocity Ω around the z axis.

- (b) (2 points) Determine the electric dipole moment $\mathbf{P}(t)$ at times t .
- (c) (2 points) Assume both $L \ll R$ and $L \ll c/\Omega$, where \mathbf{R} is the radius vector from the origin to the location at which the fields are observed, R is its magnitude, and the origin is taken to be close to the region of nonzero current. State briefly the physical meaning of these conditions and the corresponding approximations they permit.
- (d) (8 points) For \mathbf{R} located at a distance Z along the z axis, write down explicit expressions for the Cartesian components of the electric field (E_x, E_y, E_z) in the following two regimes: $L \ll Z \ll c/\Omega$ and $L \ll c/\Omega \ll Z$. Express your answers in terms of Z , t , ϵ_0 , c , q , L , and Ω .
- (e) (4 points) For the second case (i.e., $L \ll c/\Omega \ll X$), explicitly evaluate the instantaneous power absorbed by a small detector of area \mathcal{A} located at a distance X along the x -axis.

NB: This question is expressed in terms of SI units.

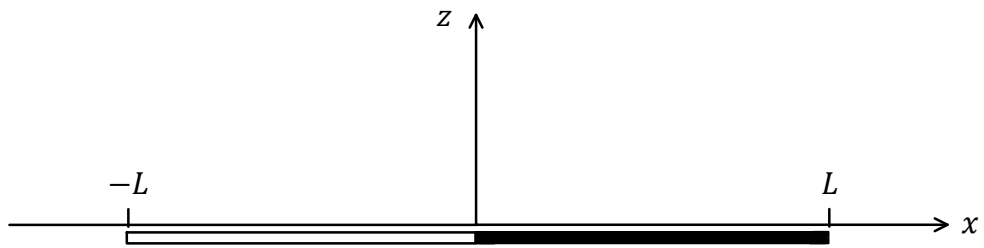


Figure 1: Electromagnetism question

Solution

1. Preliminaries

1(a): $\mathbf{B} = \nabla \times \mathbf{A}$, so (using *div curl* is zero) $\nabla \cdot \mathbf{B} = \nabla \cdot \nabla \times \mathbf{A} = 0$. Thus, we have the Maxwell equation $\nabla \cdot \mathbf{B} = 0$. Obtaining the integral form by integrating over a closed volume V (bounded by the surface S), we have $\int_V dV \nabla \cdot \mathbf{B} = 0$, from which the divergence (or Gauss's) theorem gives $\int_S d\mathbf{S} \cdot \mathbf{B} = 0$. Physical meaning: the net flux of magnetic field through any closed surface is zero which, in particular, implies the absence of magnetic monopoles.

$\mathbf{E} = -(\nabla\phi) - (\partial\mathbf{A}/\partial t)$, so $\nabla \times \mathbf{E} = -(\nabla \times \nabla\phi) - (\nabla \times \partial\mathbf{A}/\partial t)$. Using *curl grad* is zero, re-ordering the space and time derivatives, and applying $\mathbf{B} = \nabla \times \mathbf{A}$, we have the Maxwell equation $\nabla \times \mathbf{E} = -\partial\mathbf{B}/\partial t$. Obtaining the integral form by integrating over a surface S (bounded the closed loop L), we have $\int_S d\mathbf{S} \cdot \nabla \times \mathbf{E} = -\int_S d\mathbf{S} \cdot \partial\mathbf{B}/\partial t$, from which the Stokes theorem gives $\oint_L d\mathbf{r} \cdot \mathbf{E} = -(d/dt) \int_S d\mathbf{S} \cdot \mathbf{B}$. Physical meaning: the electromotive force around the loop equals (minus) the rate of change of the magnetic flux through the loop, i.e. , Faraday's law.

1(b): Under a gauge transformation with $\Lambda(\mathbf{r}, t)$, the potentials transform as: $\phi \rightarrow \tilde{\phi} = \phi - \partial\Lambda/\partial t$ and $\mathbf{A} \rightarrow \tilde{\mathbf{A}} = \mathbf{A} + \nabla\Lambda$. Thus, the electric and magnetic fields transform as $\mathbf{E} \rightarrow \tilde{\mathbf{E}} = -(\nabla\tilde{\phi}) - (\partial\tilde{\mathbf{A}}/\partial t) = -\nabla(\phi - \partial\Lambda/\partial t) - (\partial/\partial t)(\mathbf{A} + \nabla\Lambda) = -(\nabla\phi) - (\partial\mathbf{A}/\partial t) = \mathbf{E}$; and $\mathbf{B} \rightarrow \tilde{\mathbf{B}} = \nabla \times \tilde{\mathbf{A}} = \nabla \times (\mathbf{A} + \nabla\Lambda) = \nabla \times \mathbf{A} = \mathbf{B}$ (using *curl grad* is zero). The electric and magnetic fields are therefore invariant under the gauge transformation, and a gauge condition can be imposed without affecting the electric and magnetic fields.

1(c): Exchange \mathbf{E} and \mathbf{B} for ϕ and \mathbf{A} in the Ampère-Maxwell equation $\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + c^{-2}\partial\mathbf{E}/\partial t$ to obtain: $\nabla \times \nabla \times \mathbf{A} = \mu_0 \mathbf{J} - c^{-2}((\partial/\partial t)\nabla\phi + \partial^2\mathbf{A}/\partial t^2)$. Now use the (Cartesian) identity *curl curl* is *grad div* minus *div grad* , along with the Lorenz gauge condition $\nabla \cdot \mathbf{A} + c^{-2}\partial\phi/\partial t = 0$ to arrive at the wave equation for the vector potential \mathbf{A} , driven by the current \mathbf{J} , namely $c^{-2}\partial^2\mathbf{A}/\partial t^2 - \nabla^2\mathbf{A} = \mu_0 \mathbf{J}$.

2(a): The dipole moment $\mathbf{P}(t)$ at time t is defined via $\mathbf{P}(t) \equiv \int dV \mathbf{r} \rho(\mathbf{r}, t)$, where $\rho(\mathbf{r}, t)$ is the charge density. For the given charge density at time $t = 0$, we have $\mathbf{P}(0) = -\int_{-L}^0 dx x \mathbf{e}_x (q/L) + \int_0^L dx x \mathbf{e}_x (q/L) = qL\mathbf{e}_x$. The rotating distribution produces a similarly rotating dipole moment, so $\mathbf{P}(t) = qL(\mathbf{e}_x \cos \Omega t + \mathbf{e}_y \sin \Omega t)$. Here, $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ are an orthonormal Cartesian basis.

2(b-i): $R \gg L$ is the far-field condition. It validates the omission of terms others than R in the denominator of the expressions for the potentials.

2(b-ii): $(c/\Omega) \gg L$ is the nonrelativistic condition. In one period of rotation of the dipole (i.e., $2\pi/\Omega$), light travels a distance far greater than the size L of the dipole. This allows the neglect of variations of the retarded time as the source-point varies across the dimensions of

the source.

2(c-i): For $L \ll Z \ll (c/\Omega)$ (where $\mathbf{R} = Z\mathbf{e}_z$), the light travel time from source to observation point (i.e., Z/c) is much less than the source variation time (i.e., $2\pi/\Omega$). Thus, the response is essentially instantaneous, so it is as if the electric field is that due to a static electric dipole, but parametrically rotating. Hence,

$$\mathbf{E}(\mathbf{R}, t) \Big|_{\mathbf{R}=Z\mathbf{e}_z} \approx \frac{1}{4\pi\epsilon_0} \frac{1}{|\mathbf{R}|^3} [3\hat{\mathbf{R}} \cdot \mathbf{P}(t) \hat{\mathbf{R}} - \mathbf{P}(t)] \Big|_{\mathbf{R}=Z\mathbf{e}_z}.$$

For the time-dependent dipole moment computed above, this gives

$$\begin{aligned} E_x &= -\frac{1}{4\pi\epsilon_0} \frac{qL}{Z^3} \cos \Omega t; \\ E_y &= -\frac{1}{4\pi\epsilon_0} \frac{qL}{Z^3} \sin \Omega t; \\ E_z &= 0. \end{aligned}$$

2(c-ii): For $L \ll (c/\Omega) \ll Z$ we have

$$\mathbf{E}(\mathbf{R}, t) = \frac{\mu_0}{4\pi} \frac{1}{|\mathbf{R}|} \hat{\mathbf{R}} \times [\hat{\mathbf{R}} \times \ddot{\mathbf{P}}(t - c^{-1}R)] \Big|_{\mathbf{R}=Z\mathbf{e}_z},$$

$$\text{where } \ddot{\mathbf{P}}(t) = -\Omega^2 qL (\mathbf{e}_x \cos \Omega t + \mathbf{e}_y \sin \Omega t).$$

Recalling that $\mu_0\epsilon_0 c^2 = 1$, we have

$$\begin{aligned} E_x &= \frac{1}{4\pi\epsilon_0} qL \frac{\Omega^4}{c^2} \frac{1}{Z} \cos[\Omega(t - c^{-1}Z)]; \\ E_y &= \frac{1}{4\pi\epsilon_0} qL \frac{\Omega^4}{c^2} \frac{1}{Z} \sin[\Omega(t - c^{-1}Z)]; \\ E_z &= 0. \end{aligned}$$

2(d): The energy flux is determined through the Poynting vector \mathbf{S} , defined via $\mathbf{S} \equiv \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}$. In the relevant regime, \mathbf{S} is then given by

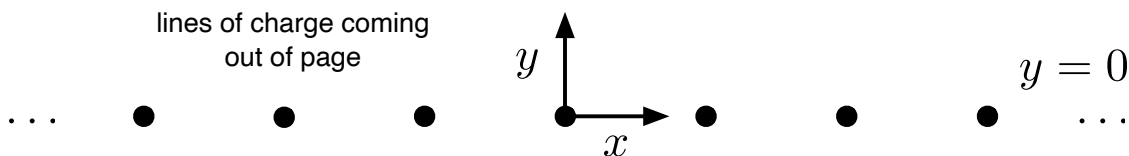
$$\mathbf{S} = \frac{\mu_0}{(4\pi)^2} \frac{1}{c} \frac{1}{|\mathbf{R}|^2} (\hat{\mathbf{R}} \times \ddot{\mathbf{P}}) \times [\hat{\mathbf{R}} \times (\hat{\mathbf{R}} \times \ddot{\mathbf{P}})], \quad (1)$$

where the terms involving the polarization are evaluated at the retarded time [i.e., $t - (R/c)$]. Then, using the form of the polarization computed above, the instantaneous power at a detector of area \mathcal{A} located at $\mathbf{R} = X\mathbf{e}_x$ becomes

$$\frac{1}{(4\pi)^2} \frac{1}{\epsilon_0 c^3} \frac{1}{X^2} \mathcal{A} (qL)^2 \Omega^4 \sin^2[\Omega(t - c^{-1}X)]. \quad (2)$$

Electromagnetism 2

Consider an infinite assembly of long thin wires with linear charge density λ , lying parallel to the z axis and spanning the xz plane (see below). The wire centers are at $y = 0$ and $x = \pm na$ with $n = 0, 1, 2, \dots$



(a) (4 points)

(i) Determine the potential $\varphi(x, y)$ far from the wires, $y \gg a$.

(ii) Determine the potential $\varphi(x, y)$ close to the origin, $x, y \ll a$.

(b) (6 points) Use separation of variables to find a series expansion for the potential $\varphi(x, y)$ in the xy plane. Derive the first correction to part (i) of (a).

(c) (6 points) Sum the series in part (b) to explicitly find the potential, $\varphi(x = 0, y)$, for $x = 0$ and all y . Derive the first correction to part (ii) of (a).

Hint: Recall the series expansion of the natural logarithm.

(d) (4 points) Sum the series of part (b) to explicitly find the potential $\varphi(x, y)$ everywhere in the xy plane. Determine the corresponding electric field.

Hint: Consider a substitution $\cos(\theta) = (e^{i\theta} + e^{-i\theta})/2$ and generalize part (c).

Solution

- (a) (i) For $y \gg a$ the lines of charge act like a surface of charge per area $\sigma = \lambda/a$. The potential from a surface is

$$\varphi(y) = -4\pi\sigma \frac{|y|}{2} = \frac{2\pi\lambda|y|}{a} \quad (1)$$

- (ii) Close to a wire the potential is that of a line of charge

$$\varphi(\rho) = -2\lambda \ln(\rho/a) + \text{const} \quad (2)$$

where $\rho = \sqrt{x^2 + y^2}$.

- (b) The scalar potential solves

$$-\nabla^2 \varphi(x, y) = 4\pi \sigma(x) = 4\pi \sigma(x) = 4\pi\lambda \sum_{n=0}^{\infty} \delta(x \pm na) \quad (3)$$

with the wire charge density $\sigma(x)$. We can seek the solution in separable form, with special attention to the $n = 0$ contribution

$$\varphi(x, y) = a_0|y| + \sum_{n=1}^{\infty} \cos(k_n x) e^{-k_n |y|} \quad (4)$$

with $k_n = \frac{2\pi n}{a}$. The series coefficients are fixed by Gauss law through the wire grid

$$E_y(x, +0) - E_y(x, -0) = 4\pi \sum_{n=0}^{\infty} \delta(x \pm na) \quad (5)$$

which translates to

$$4\pi \lambda \sum_{n=0}^{\infty} \delta(x \pm na) = -2a_0 + \frac{4\pi}{a} \sum_{n=0}^{\infty} na_n \cos\left(\frac{2\pi n x}{a}\right) \quad (6)$$

hence $a_0 = -2\pi\lambda/a$ and $a_n = 2\lambda/n$. The scalar potential in the plane is

$$\varphi(x, y) = -\frac{2\pi\lambda|y|}{a} + 2\lambda \sum_{n=1}^{\infty} \frac{1}{n} \cos(k_n x) e^{-k_n |y|} \quad (7)$$

The first correction comes from the $n = 1$ term

$$\varphi(x, y) \simeq -\frac{2\pi\lambda|y|}{a} + 2\lambda \cos(k_1 x) e^{-k_1 |y|} \quad (8)$$

(c) The series can be resummed using the hint and noting that

$$\begin{aligned}\varphi(x, y) &= -\frac{2\pi\lambda|y|}{a} + 2\lambda \sum_{n=0}^{\infty} \frac{1}{n} e^{-kn|y|} \\ &= -\frac{2\pi\lambda|y|}{a} + 2\lambda \sum_{n=0}^{\infty} \frac{1}{n} z^n = -\frac{2\pi\lambda|y|}{a} - 2\lambda \ln(1 - z)\end{aligned}\quad (9)$$

with $z = e^{-\frac{2\pi}{a}|y|}$. For y small we have

$$\varphi(y) \simeq -2\lambda \ln\left(\frac{2\pi|y|}{a}\right)\quad (10)$$

(d) In general the potential is an analytic function in the lower and upper half planes. Taking the upper half plane for definiteness, to find the sum we just need to replace

$$y \rightarrow -i(x + iy)\quad (11)$$

and take the real part of Eq. (9).

This sophisticated reasoning can be seen concretely using the hint:

$$\begin{aligned}\varphi(x, y) &= -\frac{2\pi\lambda|y|}{a} + 2\lambda \operatorname{Re} \sum_{n=0}^{\infty} \frac{1}{n} e^{kn(ix-|y|)} \\ &= -\frac{2\pi\lambda|y|}{a} + 2\lambda \operatorname{Re} \sum_{n=0}^{\infty} \frac{1}{n} z^n = -\frac{2\pi\lambda|y|}{a} - 2\lambda \operatorname{Re} \ln(1 - z)\end{aligned}\quad (12)$$

with $z = e^{\frac{2\pi}{a}(ix-|y|)}$. The real part is

$$\operatorname{Re} \ln(1 - z) = \ln|1 - z| = \frac{1}{2} \ln\left(1 - 2\cos(2\pi x/a)e^{-2\pi|y|/a} + e^{-4\pi|y|/a}\right)\quad (13)$$

hence the explicit potential

$$\begin{aligned}\varphi(x, y) &= -\lambda \ln e^{2\pi|y|/a} - \ln\left(1 - 2\cos(2\pi x/a)e^{-2\pi|y|/a} + e^{-4\pi|y|/a}\right) \\ &= -\lambda \ln 2 - \lambda \ln(\cosh(2\pi|y|/a) - \cos(2\pi x/a))\end{aligned}\quad (14)$$

The electric field everywhere in the plane is given by

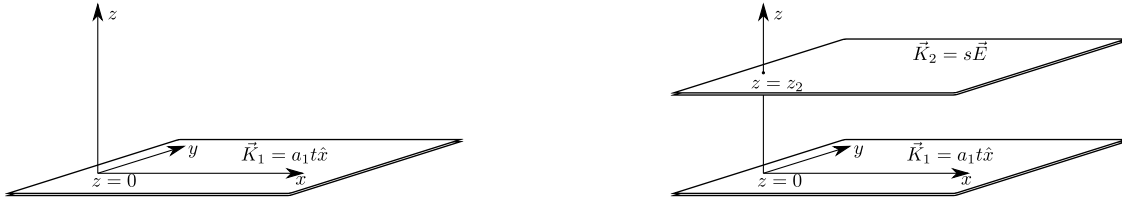
$$\begin{aligned}E_x(x, y) &= -\partial_x \varphi(x, y) = -\frac{2\pi\lambda}{a} \frac{\sin(2\pi x/a)}{(\cosh(2\pi|y|/a) - \cos(2\pi x/a))} \\ E_y(x, y) &= -\partial_y \varphi(x, y) = +\operatorname{sign}(y) \frac{2\pi\lambda}{a} \frac{\sinh(2\pi|y|/a)}{(\cosh(2\pi|y|/a) - \cos(2\pi x/a))}\end{aligned}\quad (15)$$

at large y it asymptotes

$$\begin{aligned}E_x(x, y) &= -\frac{4\pi\lambda}{a} \sin(2\pi x/a) e^{-2\pi|y|/a} \\ E_y(x, y) &= +\operatorname{sign}(y) \frac{4\pi\lambda}{a} \sinh(2\pi|y|/a) e^{-2\pi|y|/a}\end{aligned}\quad (16)$$

Electromagnetism 3

Surface currents



Consider a very large (“infinite”) conductive plate in the $z = 0$ plane that has negligible thickness w . At $t = 0$, an external current source is switched on and the surface density of current on the plate \vec{K} increases linearly with time,

$$\vec{K}_1 = w\vec{J}_1 = (at)\theta(t)\hat{x} = \begin{cases} at\hat{x}, & t > 0 \\ 0, & t \leq 0 \end{cases}$$

First, we will calculate the electromagnetic fields created by the current \vec{K}_1 . Since the fields can depend only on time and z , the wave equation for the (Lorenz gauge) vector potential is

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial z^2} \right) \vec{A}(t, z) = \mu_0 \vec{K}(t) \delta(z)$$

- (a) [3pt] Demonstrate that the following retarded potential is a solution to the wave equation above (t_R is the retarded time):

$$\vec{A}(t, z) = \frac{1}{4} \mu_0 a c t_R^2 \theta(t_R) \hat{x}, \quad t_R = t - |z|/c.$$

- (b) [5pt] Find the electromagnetic fields \vec{E}_1 , \vec{B}_1 , and the Poynting vector \vec{S}_1 at any z and $t \geq |z|/c$.
- (c) [3pt] How much power $P_1(t)$ is required to maintain current $\vec{K}_1(t)$ per unit of the plate area?

Now we will investigate the effect of the second plate at $z = z_2 > 0$, which has surface conductivity s and satisfies the Ohm’s law $\vec{K}_2 = w\vec{J}_2 = s\vec{E}$, where \vec{E} is the total electric field.

- (d) [3pt] Calculate the current $K_2(t)$ for $t \geq |z_2|/c$.

Hint: assume that $\vec{K}_2 = a_2(t - |z_2|/c)\theta(t - |z_2|/c)$ and determine the constant a_2 to satisfy equations in which the total electric field created by both plates is taken into account.

- (e) [3pt] Find the electric and magnetic fields above the second plate at $t > z/c > z_2/c$ and discuss limits $s \rightarrow 0$ and $s \rightarrow \infty$.
- (f) [3pt] Compute the force of the electromagnetic acting on unit area of the second plate.

Surface currents: solution

(a) [3pt]

The second derivative with respect to time of the suggested solution is

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{A}(z, t) = \frac{1}{2c} \mu_0 a \hat{x}, \quad (1)$$

and the second derivative with respect to z for $z \neq 0$ is the same,

$$\left. \frac{\partial^2}{\partial z^2} \vec{A}(z, t) \right|_{z \neq 0} = \frac{1}{2c} \mu_0 a \hat{x}, \quad (2)$$

so for $z \neq 0$ the l.h.s. of wave the equation is zero, and the equation is satisfied. The only interesting part is what happens to A_x at $z = 0$. Its first derivative with respect to z for $z = \pm \varepsilon$ ($\varepsilon \rightarrow 0$) is

$$\left. \frac{\partial}{\partial z} A_x(z, t) \right|_{z=\pm\varepsilon} = \frac{\partial}{\partial z} \left[\frac{1}{4} \mu_0 a c (t \mp z/c)^2 \right]_{z=\pm\varepsilon} = \mp \frac{1}{2} \mu_0 a t, \quad (3)$$

i.e. $\frac{\partial \vec{A}}{\partial z}$ is a step function at $z = 0$. Therefore,

$$\left. \frac{\partial}{\partial z} \left(\frac{\partial A_x}{\partial z} \right) \right|_{z=0} = \delta(z) \left. \frac{\partial A_x}{\partial z} \right|_{z=-\varepsilon}^{z=+\varepsilon} = \delta(z) \cdot \frac{1}{2} \mu_0 a t [(-1) - (+1)] = -\mu_0 a t \delta(z) = -\mu_0 K_x \delta(z) \quad (4)$$

and the equation is also satisfied at $z = 0$.

The step function $\theta(ct - |z|)$ indicates that fields are absent in the region causally disconnected from the event ($t = 0, z = 0$) when/where the current started.

(b) [5pt]

Calculation of the electric and the magnetic fields from the vector potential is straightforward,

$$\vec{E}_1 = -\frac{\partial \vec{A}}{\partial t} = -\frac{1}{2} \mu_0 a c (t - |z|/c) \hat{x}, \quad (5)$$

$$\vec{B}_1 = \vec{\nabla} \times \vec{A}_1 = \frac{\partial A_{1x}}{\partial z} \hat{y} = -\frac{1}{2} \mu_0 a (t - |z|/c) \text{sign}(z) \hat{y} \quad (6)$$

Note that the direction of the magnetic field is different above and below the plate, and that there are no fields prior to $t = |z|$. Also, these fields describe the E&M wave propagating away from the plate in the $\pm \hat{z}$ directions, $\vec{B} = -\frac{1}{c} (\text{sign}(z) \hat{z}) \times \vec{E}$.

The Poynting vector is

$$\vec{S}_1 = \frac{1}{\mu_0} \vec{E}_1 \times \vec{B}_1 = \frac{1}{4} \mu_0 a^2 c (t - |z|/c)^2 \text{sign}(z) \hat{z}, \quad (7)$$

directed away from the plate.

(c) [3pt]

The power that is expended to maintain the current can be computed either from the Poynting vector using the energy conservation,

$$P(t) = S_{1z} \Big|_{z=-\varepsilon}^{z=+\varepsilon} = \frac{1}{4} \mu_0 a^2 c t^2 [(+1) - (-1)] = \frac{1}{2} \mu_0 a^2 c t^2, \quad (8)$$

or noticing that the current is forced against the electric field that it induces,

$$P(t) = -\vec{E}_1(z=0) \cdot \vec{K} = \frac{\mu_0 a c t \hat{x}}{2} \cdot a t \hat{x} = \frac{1}{2} \mu_0 a^2 c t^2 \quad (9)$$

(d) [3pt]

The current in the second plate will be induced by the combination of the electric field $\vec{E}_1(t, z_2)$ but also reduced by the field generated by the plate itself. It is the field $\vec{E}_1(t, z_2) \propto (ct - |z_2|)$ which drives both, so the solution must be proportional to $(ct - |z_2|)$, as suggested in the *Hint*. Let's assume that $\vec{K}_2(t) = a_2(t - |z_2|/c)\hat{x}$; then its own field can be found just as in parts (a,b), with the observation that the linear rise starts at $t = |z_2|/c$:

$$\vec{E}_2(t, z) = -\frac{1}{2}\mu_0 a_2 c \left(t - \frac{1}{c}(|z_2| + |z - z_2|) \right) \theta \left(t - \frac{1}{c}(|z_2| + |z - z_2|) \right), \quad (10)$$

and the fields \vec{E}_2, \vec{B}_2 are zero for $t \leq \frac{1}{c}(|z_2| + |z - z_2|)$. Using the Ohm's law as suggested, and dropping identical factors $(t - |z_2|/c)\hat{x}$ on both sides, one gets

$$\begin{aligned} \vec{K}_2(t) &= s \left(\vec{E}_1(t, z_2) + \vec{E}_2(t, z_2) \right), \\ \text{or } a_2 t &= s \left(-\frac{1}{2}\mu_0 a t - \frac{1}{2}\mu_0 a_2 t \right), \\ \text{therefore } a_2 &= -\frac{\mu_0 s}{2 + \mu_0 s} a \end{aligned}$$

Note that if $s = 0$ (no conductivity in the second plate), there will be no current in the second plate, $\vec{K}_2 = 0$. On the opposite, if $s \rightarrow \infty$ (very good/superconductivity in the second plate) then current \vec{K}_2 will be exactly opposite to \vec{K}_1 for $s \rightarrow \infty$ (very good, or "superconductivity") and reflect the E&M fields from the first plate perfectly.

(e) [3pt]

Computing the fields above the plate is straightforward and similar to part (b); for the special region $ct > z > z_2$, the electric and magnetic fields from both plates add up, so that

$$\begin{aligned} \vec{E}(t > z/c > z_2/c) &= \vec{E}_1 + \vec{E}_2 = -\frac{1}{2}\mu_0(a_1 + a_2)c(t - |z|/c) = -\frac{\mu_0 a c \hat{x}}{2 + \mu_0 s} (t - |z|/c), \\ \vec{B}(t > z/c > z_2/c) &= \frac{1}{c} \hat{z} \times \vec{E} = -\frac{\mu_0 a \hat{y}}{2 + \mu_0 s} (t - |z|/c). \end{aligned}$$

In the second line, the magnetic field was computed assuming that the wave is propagating *away* from the plates, which is the only possibility. However, if one had to compute the fields *between* the plates, this would not work because where there are two waves traveling in the opposite directions ($\pm \hat{z}$). The right answer may be obtained in both cases by simply adding the magnetic fields from both plates with proper signs.

As discussed above, $s = 0$ will result in no current $K_2 = 0$, so the second plate has no effect on the fields. If $s \rightarrow \infty$, then the second plate acts as an ideal reflector and there will be no fields above the second plate ($z > z_2$).

(f) [3pt]

Naturally, the net force of the second plate on itself is zero, so we need to take into account only the fields created by the first plate. The force results from the Ampere's law,

$$\frac{\vec{F}_A}{\text{Area}} = \vec{K}_2 \times \vec{B}_1 = a_2(t - |z_2|/c)\hat{x} \times \left(-\frac{1}{2}\right)\mu_0 a\hat{y}(t - |z_2|/c) = \frac{\mu_0^2 s a^2 \hat{z}}{2(2 + \mu_0 s)} (t - |z_2|/c)^2 \quad (11)$$

The same answer can be obtained by computing the component $T_{zz} = -\sigma_{zz}$ of the stress-energy-momentum tensor of the electromagnetic field, which represents the flux of the mechanical momentum, above and below the second plate:

$$(T_{zz} = -\sigma_{zz})_{z_2 \pm \varepsilon} = \frac{\epsilon_0}{2}(E_{1x} + E_{2x})^2 + \frac{1}{2\mu_0}(B_{1y} \pm B_{2y})^2,$$

where the $E_{1,2}$ ($B_{1,2}$) correspond to the fields *above* the second plate induced by the currents in the first and the second plates, respectively³. T_{zz} represents the density of momentum flowing in the $(+\hat{z})$ direction, so the amount of \hat{z} -momentum absorbed by the second plate per unit area and time is

$$f_z = T_{zz}|_{z_2 - \varepsilon} - T_{zz}|_{z_2 + \varepsilon} = \frac{1}{2\mu_0} \left[(B_{1y} - B_{2y})^2 - (B_{1y} + B_{2y})^2 \right] = -\frac{2}{\mu_0} B_{1y} B_{2y} \quad (12)$$

that leads to the same answer.

³The signs of $E_{1,2x}$ are opposite, as well as the signs of $B_{1,2y}$.

Quantum Mechanics 1

Solvated electrons:

In this problem we will use the variational principle to model solvated electrons. A solvated electron is a separate free electron in a solvent such as ammonia NH_3 , often contributed by alkali metals such as sodium in the solution. (The semi-independent electron can remain in the solution for days.)

In a simple model, the solvent creates a cavity where the free electron lives and is isolated from the rest of the solvent. The cavity potential experienced by the solvated electron is given by:

$$V(r) = \begin{cases} -\frac{\beta e^2}{R} & r < R \\ -\frac{\beta e^2}{r} & r \geq R \end{cases} . \quad (1)$$

Here R is the cavity radius, and β is a constant factor, which depends on the solvent's polarizability.

- (a) (5 points) Consider a variational wave function ϕ for the solvated electron, normalized to unity $\langle \phi | \phi \rangle = 1$. Show $\langle H \rangle_\phi \equiv \langle \phi | H | \phi \rangle$ is greater than or equal to the ground state energy.
- (b) (3 points) Consider a variation of ϕ which maintains the normalization condition and show that $\delta \langle H \rangle_\phi / \delta \phi = 0$ when ϕ satisfies the Schrödinger equation.
- (c) (8 points) Use the variational principle to estimate the ground state energy of a solvated electron.
- (d) (4 points) Take a solvent of ammonia NH_3 with model parameters $\beta = 0.5$ and $R = 3 \text{ \AA}$:
 - (i) Calculate the approximate ground state energy for the solvated electron.
 - (ii) Use your variational ansatz to estimate a typical radius for the solvated electron and compare it to the Bohr radius for the corresponding Coulomb system.

Solution:

- (a) It is possible to decompose the wave-function $|\phi\rangle$ in terms of the eigenstates of the Hamiltonian $|\eta_n\rangle$ as

$$|\phi\rangle = \sum_n c_n |\eta_n\rangle. \quad (2)$$

Then, we find

$$\langle H \rangle_\phi = \sum_n \sum_m c_n c_m^* \langle \eta_m | H | \eta_n \rangle = \sum_n |c_n|^2 \epsilon_n = |c_0|^2 \epsilon_0 + \sum_{n \geq 1} |c_n|^2 \epsilon_n \quad (3)$$

where ϵ_n stands for the n-th eigenvalue of the Hamiltonian. Next, taking into account that the wave function is normalized, i.e., $\sum_n |c_n|^2 = 1$, the previous equation yields

$$\langle H \rangle_\phi = \epsilon_0 + \sum_{n \geq 1} |c_n|^2 (\epsilon_n - \epsilon_0) \geq \epsilon_0. \quad (4)$$

- (b) (3 points) Consider a variation of ϕ , which respects the normalization condition and show that $\delta \langle H \rangle_\phi / \delta \phi = 0$ when ϕ satisfies the Schrödinger equation.

Solution: Assuming that $H|\phi\rangle = E|\phi\rangle$, then $\langle H \rangle_\phi = E \langle \phi | \phi \rangle = E$, then $\delta \langle H \rangle_\phi / \delta \phi = 0$.

- (c) (8 points) Use the variational principle to estimate the ground state energy of a solvated electron.

Solution: The solvated electron is based on a Coulomb-like interaction, so it would be natural to try an ansatz based on the 1s orbitals of the hydrogen atom parametrized with a single free parameter α as

$$\psi(r) = \frac{\alpha^3}{\pi} e^{-\alpha r}. \quad (5)$$

With this trial function, the variational energy is given by

$$\langle H \rangle_\psi = \int_0^\infty -\frac{\hbar^2}{2m_e} \psi(r) \frac{d}{dr} \left(r^2 \frac{d\psi(r)}{dr} \right) 4\pi r dr - \frac{\beta e^2}{R} \int_0^R \psi(r)^2 4\pi r^2 dr - \beta e^2 \int_R^\infty \psi(r)^2 4\pi r dr, \quad (6)$$

which can be further simplified to yield

$$\langle H \rangle_\psi = \frac{\hbar^2 \alpha^2}{2m_e} - \frac{\beta e^2}{R} + \frac{\beta e^2}{R} (1 + \alpha R) e^{-2\alpha R}. \quad (7)$$

Finally, to find the energy, we need to find α^* such that $\frac{d\langle H \rangle_\psi}{d\alpha} \Big|_{\alpha=\alpha^*} = 0$.

(d) (4 points) Take a solvent of ammonia NH_3 with model parameters $\beta = 0.5$ and $R = 3 \text{ \AA}$:

(i) Calculate the approximate ground state energy for the solvated electron.

Solution: From the previous result, it is easy to show that the energy of the solvated electron is -2.160 eV or $3.46 \times 10^{-19} \text{ J}$.

(ii) How does the Bohr radius of the solvated electron compare to the Bohr radius for the corresponding Coulomb system?

Solution: Due to the similitude of the trial wave function with hydrogenic wave functions, it is easy to realize that the typical radius of the solvated electron is $1/\alpha$. Then, in the case at hand, the typical radius for the solvated electron is 4.85 times larger than the Bohr radius.

Quantum Mechanics 2

Dynamics of spin 1/2

A quantum particle with spin 1/2 and magnetic moment is localised in space so that only its spin evolves in time. Magnetic field $\vec{B} = \{B_x, B_y, B_z\}$ is applied to the particle, so that its Hamiltonian is

$$H = -\mu\vec{B} \cdot \vec{\sigma},$$

where μ is the magnitude of the magnetic moment associated with the spin, and $\vec{\sigma}$ is the vector of Pauli matrices, $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$.

(a) (6 pts) Derive the Heisenberg equation of motion for $\vec{\sigma}$. Describe qualitatively (in no more than two sentences) what motion the obtained equation describe in geometric terms.

(b) (6 pts) Write down Hamiltonian H as a matrix in the standard σ_z -representation and find its eigenvalues and the corresponding eigenstates.

Let now the magnetic field be specifically in the x -direction, $\vec{B} = \{B, 0, 0\}$ and use the same σ_z -representation for all results below.

(c) (4 pts) Write down explicitly the ground state of the spin. A strong projective measurement of the σ_z operator is done on the spin at $t = 0$. What is the state $\rho(0)$ of the spin right after the measurement? What is the subsequent time evolution $\rho(t)$ of this state?

(d) (4 pts) One more strong projective measurement of the σ_z operator is done on $\rho(t)$ at time $t = t_0$. What are the possible outcomes of this measurement? If one considers separately the states of the system obtained for different outcomes of the measurement, calculate the time evolution $|\psi(t)\rangle$ of these states?

Solution

(a) In the general form, the Heisenberg equation of motion is

$$\dot{\vec{\sigma}} = \frac{i}{\hbar}[H, \vec{\sigma}] = \frac{-i\mu}{\hbar}[\vec{B} \cdot \vec{\sigma}, \vec{\sigma}].$$

The standard properties of the Pauli matrices mean, e.g., that

$$[\sigma_x, \sigma_x] = 0, \quad [\sigma_y, \sigma_x] = -2i\sigma_z, \quad [\sigma_z, \sigma_x] = 2i\sigma_y,$$

and the x component of the Heisenberg equation of motion takes the following form:

$$\dot{\sigma}_x = \frac{2\mu}{\hbar}(B_z\sigma_y - B_y\sigma_z).$$

Equations for σ_y and σ_z can be obtained either in the same way, or simply by cyclic permutation of indices in the equation for σ_x :

$$\dot{\sigma}_z = \frac{2\mu}{\hbar}(B_y\sigma_x - B_x\sigma_y), \quad \dot{\sigma}_y = \frac{2\mu}{\hbar}(B_x\sigma_z - B_z\sigma_x).$$

One sees immediately that taken together, these equations for components can be combined into the following vector equation:

$$\dot{\vec{\sigma}} = -\frac{2\mu}{\hbar}\vec{B} \times \vec{\sigma}.$$

Geometrically, this equation means that the vector $\vec{\sigma}(t)$ rotates around the vector \vec{B} of magnetic field, i.e. component of $\vec{\sigma}$ along \vec{B} is stationary, while the component orthogonal to \vec{B} rotates clockwise around \vec{B} with frequency

$$\Omega = \frac{2\mu B}{\hbar}, \quad B = (B_x^2 + B_y^2 + B_z^2)^{1/2}.$$

(b) The standard expressions for the Pauli matrices mean that the Hamiltonian has the following matrix form

$$H = -\mu \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix} = -\mu B \begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix},$$

where in the second (optional, but convenient) step we used the standard angles θ and φ of the spherical coordinate system that give the direction of the vector \vec{B} of the magnetic field. From this matrix one gets immediately that its eigenvalues are $\pm\mu B$. The eigenstates follow from the standard eigenstate equations. The ground state with energy $E_- = -\mu B$ is

$$|-\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{pmatrix}.$$

Excited state with energy $E_+ = \mu B$ is

$$|+\rangle = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2)e^{i\varphi} \end{pmatrix}.$$

(c) For \vec{B} in the x -direction (i.e., $\theta = \pi/2$, $\varphi = 0$) expression for the ground state simplifies to

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Since this is the state in the σ_z -representation, and according to the general rules of quantum mechanics, this means that the strong projective measurement of the operator σ_z gives the result $\sigma_z = 1$ with probability $1/2$ and the result $\sigma_z = -1$ also with probability $1/2$. Because of this uncertainty, one needs a density matrix to describe the state of the spin after this measurement. In the same σ_z -representation the density matrix is:

$$\rho(0) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

Since this matrix is proportional to the unit matrix, it commutes with the Hamiltonian, $[H, \rho] = 0$, and does not evolve with time:

$$\rho(t) = \rho(0) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

(d) The outcomes of the subsequent measurement are the same as for the initial measurement. One gets $\sigma_z = 1$ with probability $1/2$ and $\sigma_z = -1$ also with probability $1/2$, regardless of the time t_0 , since $\rho(t)$ is constant. If, however, one considers these two outcomes separately, each state obtained as a result of the measurement does change with time. To see this, we write down the Schrödinger equation σ_z -representation:

$$i\hbar|\dot{\psi}(t)\rangle = H|\psi(t)\rangle, \quad |\psi(t)\rangle = \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix},$$

i.e.,

$$\dot{\alpha} = -i\frac{\Omega}{2}\beta, \quad \dot{\beta} = -i\frac{\Omega}{2}\alpha.$$

If one gets $\sigma_z = 1$ as a result of the measurement at $t = t_0$ the resulting state $|\psi_+(t_0)\rangle$ has $\alpha = 1$, $\beta = 0$. For the measurement outcome $\sigma_z = -1$ the obtained state $|\psi_-(t_0)\rangle$ has $\alpha = 0$, $\beta = 1$. The Schrödinger equation with these initial conditions give directly:

$$|\psi_+(t)\rangle = \begin{pmatrix} \cos \frac{\Omega\tau}{2} \\ -i \sin \frac{\Omega\tau}{2} \end{pmatrix}, \quad |\psi_-(t)\rangle = \begin{pmatrix} \sin \frac{\Omega\tau}{2} \\ i \cos \frac{\Omega\tau}{2} \end{pmatrix}, \quad \tau \equiv t - t_0.$$

We see that the individual states of the spin obtained in the measurement exhibit coherent quantum oscillations between the two σ_z basis states even is the total density matrix $\rho(t)$ remains constant.

Quantum Mechanics 3

Electron in magnetic and electric fields

- (a) (5 points) Consider an electron with charge e and mass m on a two-dimensional plane, in constant uniform magnetic field $\vec{B} = B \hat{z}$ and constant uniform electric field $\vec{E} = E \hat{x}$. Calculate the eigen-energies of the electron. What's the group velocity of the electron in y-direction? (Hint: take a gauge $\vec{A} = B(0, x, 0)$)
- (b) (2 points) Now we confine the electron on a ring with radius R . In absence of magnetic and electric fields ($\vec{B} = 0, \vec{E} = 0$), what is the energy of the electron? Show that the energy is symmetric for clockwise and counterclockwise states.
- (c) (6 points) Still consider the electron on a ring. Now we turn on a magnetic field $\vec{B} = B \hat{z}$ but keep the electric field zero. Calculate the energy of the electron. Show that the clockwise-counterclockwise symmetric is broken by the magnetic field. Quantitatively, how does the magnetic flux affect the energy levels? (Hint: consider symmetric gauge, $\vec{A} = (B/2)(-y, x, 0)$).
- (d) (2 points) If the uniform magnetic field of part(c) is time-dependent, does it induce a transition between different states? Explain. How does your result in (c) compared to the classical physics where a changing magnetic flux will create an electric field which accelerates the electron?
- (e) (5 points) Now with the electron on a ring in constant magnetic field, we turn on an electric field pulse perturbation: $\vec{E} = E_0 \delta(t) \hat{x}$. Calculate the transition probability of the electron between levels M and N .

Solution

(a) The Hamiltonian is:

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m} + Ex \quad (1)$$

For the vector potential, here it is convenient to use the Landau gauge: $\vec{A} = (0, Bx)$. Then

$$\begin{aligned} H &= \frac{p_x^2}{2m} + \frac{(p_y - eBx)^2}{2m} + eEx \\ &= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} - \frac{(eBp_y - eEm)x}{m} + \frac{(eBx)^2}{2m} \\ &= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{(eB)^2}{2m} \left[x - \frac{eBp_y - eEm}{(eB)^2} \right]^2 - \frac{1}{2m} \left(\frac{eBp_y - eEm}{eB} \right)^2 \\ &= \frac{p_x^2}{2m} + \frac{(eB)^2}{2m} \left[x - \frac{eBp_y - eEm}{(eB)^2} \right]^2 + \frac{Ep_y}{B} - \frac{mE^2}{2B^2} \end{aligned} \quad (2)$$

The first two terms correspond to the Hamiltonian of a harmonic oscillation with a offset in the x-axis. The energy is therefore:

$$\epsilon = \hbar\omega_c \left(n + \frac{1}{2} \right) + \frac{Ep_y}{B} - \frac{mE^2}{2B^2} \quad (3)$$

The group velocity in the y-direction is:

$$\frac{\partial \epsilon}{\partial p_y} = \frac{E}{B} \quad (4)$$

(b) The Schrodinger equation for a free electron on a ring is most conveniently expressed in polar coordinate:

$$H\psi = -\frac{\hbar^2}{2mR^2} \frac{\partial^2 \psi}{\partial \phi^2} = \epsilon\psi \quad (5)$$

The wavefunction should satisfy:

$$\psi(\phi) = \psi(\phi + 2\pi) \quad (6)$$

The solution is:

$$\psi = \frac{1}{\sqrt{2\pi}} e^{iN\phi} \quad (7)$$

$$\epsilon = \frac{\hbar^2 N^2}{2mR^2} \quad (8)$$

The momentum has an expectation value of:

$$p = \frac{\hbar N}{R} \quad (9)$$

with its sign (clockwise versus counterclockwise states) determined by the sign of N . Obviously

$$\epsilon(N) = \epsilon(-N) \quad (10)$$

(c) The vector potential in symmetric gauge is: $\vec{A} = \frac{1}{2}(-By, Bx)$, which converts in polar coordinate to: $\vec{A} = \frac{1}{2}(0, BR)$.

The Schrodinger equation is:

$$\hat{H}\psi = \frac{(\vec{p} - e\vec{A})^2}{2m}\psi = \frac{-\hbar^2}{2mR^2} \frac{d^2\psi}{d\phi^2} + \frac{(eBR)^2}{8m} + \frac{i\hbar eB}{2m} \frac{d\psi}{d\phi} \quad (11)$$

We can test see that the same wavefunction as in zero magnetic field is the solution of the above equation:

$$\psi = \frac{1}{\sqrt{2\pi}} e^{iN\phi} \quad (12)$$

$$E = \frac{\hbar^2 N^2}{2mR^2} + \frac{(eBR)^2}{8m} - \frac{\hbar NeB}{2m} = \frac{1}{2m} \left(\frac{N\hbar}{R} - \frac{eBR}{2} \right)^2 \quad (13)$$

Here obviously $\epsilon(N) \neq \epsilon(-N)$ for any non-zero N .

Under $\delta E = 0$

$$\frac{\delta N\hbar}{R} = \frac{eR\delta B}{2} \quad (14)$$

This leads to:

$$\delta N = \frac{e\delta B\pi R^2}{h} = \frac{\delta\Phi}{\Phi_0} \quad (15)$$

(d) To induce a transition between the states, we need a non-zero $\langle M | \hat{H}(t) | N \rangle$ for $M \neq N$. Evidently, this is not the case for an uniform magnetic field where the vector potential (in symmetric gauge) has no angular dependence. So there is no transition under a time-varying magnetic field.

From the energy of the electron: $E = \frac{1}{2m} \left(\frac{N\hbar}{R} - \frac{eBR}{2} \right)^2$, the classical momentum is:

$$p = \frac{N\hbar}{R} - \frac{eBR}{2} \quad (16)$$

It is consistent with the classical case of electron getting accelerated by the electric field generated by a changing magnetic field:

$$\frac{dp}{dt} = \frac{eR}{2} \frac{dB}{dt} = \frac{e}{2\pi R} \frac{d\Phi}{dt} = eE \quad (17)$$

(e) With the electric field pulse as a perturbation, the Halmiltonian is:

$$\hat{H} = \frac{-\hbar^2}{2mR^2} \frac{d^2}{d\phi^2} + \frac{(eBR)^2}{8m} + \frac{i\hbar eB}{2m} \frac{d}{d\phi} + eE(t)R \cos(\phi) = \hat{H} + \hat{H}' \quad (18)$$

Here the perturbation $\hat{H}' = eE(t)R \cos(\phi)$. Then

$$\begin{aligned} \langle M | \hat{H}' | N \rangle &= \frac{1}{2\pi} \int_0^{2\pi} e^{-iM\phi} eE(t)R \cos(\phi) e^{-iN\phi} d\phi \\ &= \frac{1}{2\pi} \int_0^{2\pi} eE(t)R \cos(\phi) [\cos((N-M)\phi) + i \sin((N-M)\phi)] d\phi \\ &= \frac{1}{4\pi} \int_0^{2\pi} eE(t)R [\cos((N-M+1)\phi) + \cos((N-M-1)\phi) \\ &\quad + i \sin((N-M+1)\phi) + i \sin((N-M-1)\phi)] d\phi \\ &= eE(t)R \frac{1}{2} (\delta_{N-M,1} + \delta_{N-M,-1}) \end{aligned} \quad (19)$$

The transition probability is:

$$\begin{aligned} P_{MN}(t) &= \frac{1}{\hbar^2} \left| \int_0^t e^{-i\omega_{MN}t'} \langle M | \hat{H}' | N \rangle dt' \right|^2 \\ &= \frac{1}{4\hbar^2} \left| \int_0^t e^{-i\omega_{MN}t'} eE_0 \delta(t') R (\delta_{N-M,1} + \delta_{N-M,-1}) dt' \right|^2 \\ &= \frac{(eE_0R)^2}{4\hbar^2} (\delta_{N-M,1} + \delta_{N-M,-1}) \end{aligned} \quad (20)$$

Transition happens only between adjacent energy states: $N - M = \pm 1$.

Statistical Mechanics 1

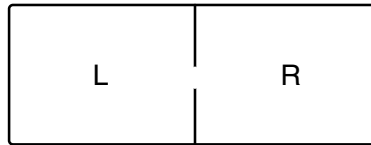
Fluctuations through a small hole

Consider two identical containers labeled as left (L) and right (R), separated by a wall containing a small hole of area A , depicted below. These containers are in equilibrium, exchanging both energy and particles through the hole while being isolated from the external environment. The combined volume of the two vessels is $2V$, and they together contain $2N$ particles of a mono-atomic ideal gas of mass m . The total internal energy of the system is $2E$, meaning each vessel, on average, contains N particles and E units of energy.

However, each container can deviate from this average state and the deviations

$$\delta E \equiv E_R - E_L, \quad \text{and} \quad \delta N \equiv N_R - N_L,$$

can be non-zero, although they are assumed to be small in what follows.



- (a) (6 points) Determine the temperature and chemical potential μ of the system and the variance, $\langle(\delta N)^2\rangle$. Possibly useful integrals are given below.
- (b) (7 points) Possibly useful integrals are given below.
- (i) Determine the particle flux $\Phi_0(T, \mu)$, defined as the number of particles transferred per time to the right container by particles on the left escaping through the hole. *Check that your result is dimensionally correct.*
 - (ii) Show that the energy flux $\Phi_E(T, \mu)$, defined as the energy transferred per time to the right container by particles on the left escaping through the hole, is $\Phi_E(T, \mu) = 2k_B T \Phi_0(T, \mu)$.
- (c) (3 points) The energy and number on the both sides of the container initially deviate from equilibrium by a small amount and $(\delta N, \delta E)$ are non-zero. Show that the relaxation to equilibrium (on average) follows

$$\begin{pmatrix} \frac{d\delta N}{dt} \\ \frac{1}{k_B T} \frac{d\delta E}{dt} \end{pmatrix} = -A\Phi_0 \begin{pmatrix} \lambda_{nn} & \lambda_{ne} \\ \lambda_{en} & \lambda_{ee} \end{pmatrix} \begin{pmatrix} \delta \left(\frac{\mu}{k_B T} \right) \\ \frac{\delta T}{T} \end{pmatrix} \quad (1)$$

where $\delta(\mu/T) \equiv (\mu/T)_R - (\mu/T)_L$ and $\delta T \equiv T_R - T_L$ are the deviations conjugate to δN and δE respectively. Determine the coefficient matrix λ .

- (d) (4 points) The energy and number initially deviate from equilibrium by a small amount as in the previous item. Determine the rate of change in the total entropy, $\dot{S} = \dot{S}_L + \dot{S}_R$. Show that entropy increases regardless of the signs of δN and δE .

We record integrals of the form, $I_n \equiv \int_0^\infty u^n e^{u^2/2} du$:

$$\{I_0, I_1, I_2, I_3, I_4, I_5, I_6\} = \{\sqrt{\pi/2}, 1, \sqrt{\pi/2}, 2, 3\sqrt{\pi/2}, 8, 15\sqrt{\pi/2}\} \quad (2)$$

Solution

Notation: we will denote $\hat{\mu} \equiv \mu/T$ and consider the grand partition function Z_G to be a function of $\hat{\mu}$ and T . We set $k_B = 1$

(a) We will use the grand canonical ensemble, which is natural when both the energy and particle number fluctuate. The grand partition function of an ideal gas is

$$Z_G(T, \hat{\mu}) = \sum_s e^{-\beta E_s + \hat{\mu} N_s} = 1 + e^{\hat{\mu} V} \int \frac{d^3 p}{(2\pi\hbar)^3} e^{-p^2/2mT}, \quad (3)$$

and so

$$\ln Z_G(T, \hat{\mu}) = V e^{\hat{\mu}} \left(\frac{mT}{2\pi\hbar^2} \right)^{3/2}. \quad (4)$$

Differentiation with respect to $\hat{\mu}$ gives

$$\bar{N}(T, \hat{\mu}) = \frac{\partial \ln Z_G}{\partial \hat{\mu}} = V e^{\hat{\mu}} \left(\frac{mT}{2\pi\hbar^2} \right)^{3/2}, \quad (5)$$

and differentiation with respect to $-\beta$ gives

$$\bar{E} = T^2 \frac{\partial \ln Z_G}{\partial T} = \frac{3}{2} \bar{N}(T, \hat{\mu}) T. \quad (6)$$

These two expressions give the temperature and chemical potential in terms of E, N , i.e.

$$T = \frac{2E}{3N}, \quad (7)$$

and

$$\hat{\mu} = \log \left[\frac{N}{V} \left(\frac{2\pi\hbar^2}{mT} \right)^{3/2} \right], \quad (8)$$

where it is understood that the temperature in this last expression is determined by E/N .

The variance

$$\langle (N_R - N)^2 \rangle = \frac{\partial^2 \ln Z_G}{\partial \hat{\mu}^2} = \frac{\partial \bar{N}}{\partial \hat{\mu}} = \bar{N}(T, \hat{\mu}) \quad (9)$$

which reflects the Poissonian character of Maxwell Boltzmann statistics. Note that $\delta N_R = -\delta N_L = \delta N/2$, so

$$\langle (\delta N)^2 \rangle = 4\bar{N} \quad (10)$$

(b) (i) The phase space distribution of a classical ideal gas

$$f(\mathbf{x}, \mathbf{p}) = e^{\hat{\mu}} e^{-p^2/2mT} \quad (11)$$

The flux through the hole is

$$\frac{dN}{dt} = \int_{p_z > 0} \frac{d^3 p}{(2\pi\hbar)^3} f(\mathbf{x}, \mathbf{p}) \mathbf{v} \cdot \hat{\mathbf{z}} A \quad (12)$$

where $A\hat{\mathbf{z}}$ is the area vector of the hole and $\mathbf{v} = \mathbf{p}/m$ is the particle velocity. I find it easiest to switch a dimensionless momentum, $\vec{u} = \mathbf{p}/\sqrt{mT}$:

$$\frac{dN}{dt} = Ae^{\hat{\mu}} \left(\frac{mT}{\hbar^2}\right)^{3/2} \left(\frac{T}{m}\right)^{1/2} \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^1 \frac{d\cos\theta}{2} \cos\theta \int_0^\infty \frac{u^2 du}{2\pi^2} e^{-u^2/2} u. \quad (13)$$

The integration gives

$$\frac{dN}{dt} = Ae^{\hat{\mu}} \left(\frac{mT}{\hbar^2}\right)^{3/2} \left(\frac{T}{m}\right)^{1/2} \frac{1}{4\pi^2} = A\bar{N} \left(\frac{T}{m}\right)^{1/2} \frac{1}{\sqrt{2\pi}}. \quad (14)$$

The flux is $\Phi(T, \hat{\mu}) = (dN/dt)/A$.

(ii) The analysis is identical, but the integral is weighted by the energy of the escaping particles

$$\frac{dE}{dt} = A \int_{p_z > 0} \frac{d^3p}{(2\pi\hbar)^3} f(\mathbf{x}, \mathbf{p}) \mathbf{v} \cdot \hat{\mathbf{z}} \left(\frac{p^2}{2m}\right), \quad (15)$$

In a formula analogous to Eq. (13), the integral over u is we weighted by $Tu^2/2$. We have

$$\frac{T \int_0^\infty u^2 du e^{-u^2/2} u \frac{u^2}{2}}{\int_0^\infty u^2 du e^{-u^2/2} u} = 2T, \quad (16)$$

proving the required result

$$\Phi_E = 2T\Phi_0. \quad (17)$$

(c) We have $\Phi_0 = e^{\hat{\mu}} T^2 C_N$ and $\Phi_E = e^{\hat{\mu}} 2T^3 C_N$. There is an imbalance in the left and right rates of transfer since the chemical potentials and temperatures are unequal on the left and right sides. We define $\delta\hat{\mu}_L \equiv \hat{\mu}_L - \hat{\mu}$ and an analogous shift for the temperature $\delta T_L \equiv T_L - T$. The flux from the left results in a loss of left-sided particles and energy

$$\frac{dN_L}{dt} = -\Phi_0^{(L)}(T + \delta T_L, \hat{\mu} + \delta\hat{\mu}_L) = -\Phi_0 \left[1 + \delta\hat{\mu}_L + 2\frac{\delta T_L}{T}\right], \quad (18)$$

$$\frac{dE_L}{dt} = -\Phi_E^{(L)}(T + \delta T_L, \hat{\mu} + \delta\hat{\mu}_L) = -T\Phi_0 \left[2 + 2\delta\hat{\mu}_L + 6\frac{\delta T_L}{T}\right], \quad (19)$$

with analogous expressions for the right-sided losses. The *difference* in the rates is

$$\begin{pmatrix} \frac{d\delta N}{dt} \\ \frac{1}{T} \frac{d\delta E}{dt} \end{pmatrix} = -A\Phi_0 \begin{pmatrix} 1 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} \delta\hat{\mu} \\ \frac{\delta T}{T} \end{pmatrix} \quad (20)$$

It is not accidental that the matrix is symmetric a positive definite matrix as discussed below.

(d) The rate of entropy production of the left and right sides is respectively

$$\frac{dS_L}{dt} = \frac{1}{T_L} \frac{dE_L}{dt} - \hat{\mu}_L \frac{dN_L}{dt}, \quad (21)$$

$$\frac{dS_R}{dt} = \frac{1}{T_R} \frac{dE_R}{dt} - \hat{\mu}_R \frac{dN_R}{dt}. \quad (22)$$

Then, since $\dot{E}_R = -\dot{E}_L = -\delta E/2$ and $\dot{N}_R = -\dot{N}_L = -\delta N/2$, and noting that

$$\frac{1}{T_R} - \frac{1}{T_L} \simeq -\frac{\delta T}{T^2}, \quad (23)$$

we find

$$\frac{dS}{dt} = -\frac{1}{2}\delta\hat{\mu} \frac{d\delta N}{dt} - \frac{1}{2} \frac{\delta T}{T^2} \frac{d\delta E}{dt} \quad (24)$$

$$= \frac{1}{2} A\Phi_0 \begin{pmatrix} \delta\hat{\mu} & \frac{\delta T}{T} \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} \delta\hat{\mu} \\ \frac{\delta T}{T} \end{pmatrix}. \quad (25)$$

The quadratic form is positive definite since

$$\det \begin{pmatrix} 1 & 2 \\ 2 & 6 \end{pmatrix} = 2, \quad \text{and} \quad \text{tr} \begin{pmatrix} 1 & 2 \\ 2 & 6 \end{pmatrix} = 7, \quad (26)$$

indicate that both eigenvalues are positive. Thus entropy production is positive.

Discussion: The variance is $\langle \delta N^2 \rangle$ in part (a) is part of the covariance matrix which characterizes the fluctuations of the system:

$$\chi \equiv \begin{pmatrix} \langle \delta N \delta N \rangle & \frac{1}{T} \langle \delta N \delta E \rangle \\ \frac{1}{T} \langle \delta E \delta N \rangle & \frac{1}{T^2} \langle \delta E \delta E \rangle \end{pmatrix} = N \begin{pmatrix} 4 & 6 \\ 6 & 15 \end{pmatrix}. \quad (27)$$

The susceptibility matrix χ and the fluctuations can be computed by analyzing the shifts in mean values \bar{N} and \bar{E} with $\hat{\mu}$ and β :

$$\begin{pmatrix} \delta \bar{N} \\ \frac{1}{T} \delta \bar{E} \end{pmatrix} = \begin{pmatrix} \chi_{nn} & \chi_{ee} \\ \chi_{en} & \chi_{ee} \end{pmatrix} \begin{pmatrix} \delta \hat{\mu} \\ \frac{\delta T}{T} \end{pmatrix} \quad (28)$$

We found the first entry χ_{nn} in part (a).

We note entropy takes the form :

$$dS = dS_L + dS_R = -\frac{\delta T}{T^2} d\delta E - \delta\hat{\mu} d\delta N. \quad (29)$$

The purpose of expanding the rate in change $\delta\dot{N}$ and $\delta\dot{E}/T$ in terms of $\delta\hat{\mu}$ and $\delta T/T$ was to simplify the analysis of entropy production. It also simplifies an analysis of the fluctuations as discussed below.

We have discussed only the time evolution of the mean values. The equation of motion Eq. (20) predicts that the deviations δN and δE approach zero. This is true on average, but the variances (such as $\langle \delta N^2 \rangle$) need to approach Eq. (27). For the time evolution to reproduce the variances of the system, the dissipation should be supplemented with stochastic noise

$$\begin{pmatrix} \frac{d\delta N}{dt} \\ \frac{1}{T} \frac{d\delta E}{dt} \end{pmatrix} = -A\Phi_0 \begin{pmatrix} \lambda_{nn} & \lambda_{ne} \\ \lambda_{en} & \lambda_{ee} \end{pmatrix} \begin{pmatrix} \delta \left(\frac{\mu}{T} \right) \\ \frac{\delta T}{T} \end{pmatrix} + \begin{pmatrix} \xi_n \\ \xi_e \end{pmatrix}$$

The variance of the noise is given by the fluctuation dissipation theorem:

$$\begin{pmatrix} \langle \xi_n(t)\xi_n(t') \rangle & \langle \xi_n(t)\xi_e(t') \rangle \\ \langle \xi_e(t)\xi_n(t') \rangle & \langle \xi_e(t)\xi_e(t') \rangle \end{pmatrix} = \delta(t-t')2TA\Phi_0 \begin{pmatrix} \lambda_{nn} & \lambda_{ne} \\ \lambda_{en} & \lambda_{ee} \end{pmatrix}. \quad (30)$$

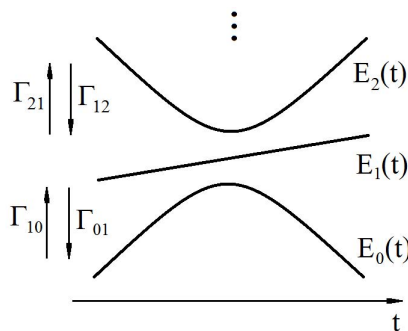
Once the noise is added $(\delta N, \delta E)$ will random walk, and the variances of $(\delta N, \delta E)$ will reproduce the equilibrium covariance matrix. We leave it as a satisfying exercise to show that once the noise is added, the system will evolve in time to reproduce the variances in Eq. (27).

Statistical Mechanics 2

The Landauer principle

This problem discusses Landauer’s erasure principle, a fundamental element of the thermodynamics of computation. A basic model of a classical computing device is a system with an adiabatic (in the sense of quantum mechanics) energy spectrum $E_n(f)$, controlled by a classical external force, $f(t)$. The spectrum can vary in time through the slow time dependence of this force. For example, an individual physical bit is described by a system with two energy levels.

The system interacts weakly with an environment in equilibrium at temperature T , which induces incoherent transitions between the energy states of the system with transition rates Γ_{mn} (see below). As a result, each configuration of the system is characterized by the distribution of occupation probabilities $\{p_n\}$ for the energy eigenstates, $\sum_n p_n = 1$. Note that when the system transitions between its energy levels $n \rightarrow m$, an energy $\Delta E_{mn} = E_m - E_n$ is transferred to the system from the environment. The time evolution of the system is



described then by the usual “rate equation” for the probabilities p_n :

$$\partial p_n / \partial t = \sum_m (\Gamma_{nm} p_m - \Gamma_{mn} p_n). \quad (1)$$

Equilibrium of the environment implies that the rates Γ_{mn} of the transitions from the state n to the state m and those of the reverse transitions from m to n are related by the “detailed balance” condition:

$$\Gamma_{mn} / \Gamma_{nm} = e^{(E_n - E_m) / k_B T}. \quad (2)$$

(a) (3 pts) Show that the system’s equilibrium state is given by the stationary solution of the rate equation.

(b) (4 pts) The internal energy U of the system, and the work dW done on the system by the external force are defined in terms of the energies E_n and probabilities p_n naturally as $U = \sum_n p_n E_n$, and $dW = \sum_n p_n dE_n$. Use the first law of thermodynamics to obtain the expression for the amount of heat dQ transferred from the environment into the system during a small time interval dt .

(c) (6 pts) The total entropy S of the setup we consider consists of the entropy S_{sys} of the system and the entropy S_{env} of the environment, $S = S_{sys} + S_{env}$, where $S_{sys} = -k_B \sum_n p_n \ln p_n$. While S_{env} is not known in absolute terms, the fact that the environment is in equilibrium is sufficient to determine the changes in S_{env} due to processes in the system: $dS_{env} = -dQ/T$, where dQ was found in part (b). Calculate $\partial S/\partial t$ in terms of the probabilities p_n and rates Γ , and show that your result is consistent with the second law of thermodynamics.

Hint: To simplify $\partial S/\partial t$, parametrize the probability $p_n \equiv e^{-\beta E_n} \chi_n$ by χ_n and exploit the detailed balance relation. Symmetrize sums, i.e. $\sum_{m,n} x_{mn} = \sum_{m,n} (x_{mn} + x_{nm})/2$.

(d) (3 pts) If the energy spectrum E_n is changed only very slowly on the time scale set by the transition rates Γ , the probability distribution $\{p_n\}$ determined by the rate equation (1) will maintain equilibrium form at all times throughout the evolution of energies E_n . Use the general result from part (c) to find $\partial S/\partial t$ in this “adiabatic” regime (in the sense of statistical mechanics).

(e) (4 pts) Now consider specifically one physical bit, $n = 0, 1$. The state of the bit with maximal information corresponds to the situation when both states of the bit are equally probable, $p_0 = p_1$, whereas the state with no information is the state with the bit being with certainty in one predetermined state, i.e. $p_0, p_1 = 0, 1$ (it does not matter which is which). Use the results obtained above to find the minimal amount of heat Q that should be released into the environment to transfer the bit from the state with maximal information into the no-information state. This is the Landauer principle, which states, qualitatively, that in a computation process, only erasure of information requires energy dissipation.

Solution

(a) In the stationary state, the probabilities $p_n(t)$ are constant, i.e. $\partial p_n/\partial t = 0$. Equation (1) shows directly that this condition agrees with the equilibrium distribution of the probabilities

$$\partial p_n/\partial t = 0 \Rightarrow \Gamma_{nm}p_m - \Gamma_{mn}p_n = 0 \Rightarrow p_m/p_n = \Gamma_{mn}/\Gamma_{nm} = e^{(E_n - E_m)/k_B T}.$$

From this, after appropriate normalization, one gets the usual equilibrium canonical distribution of probabilities:

$$p_n = \frac{1}{Z} e^{-E_n/k_B T}, \quad Z = \sum_n e^{-E_n/k_B T}.$$

The distribution is canonical, since, by the setup, the system exchanges energy with an external reservoir.

(b) From the first law of thermodynamics, one has:

$$\begin{aligned} \delta Q = dU - \delta W &= \sum_n [d(p_n E_n) - p_n dE_n] = \sum_n dp_n E_n = \sum_{n,m} E_n [\Gamma_{nm}p_m - \Gamma_{mn}p_n] dt = \\ &= \sum_{n,m} (E_m - E_n) \Gamma_{mn} p_n dt. \end{aligned}$$

This expression agrees with the simple understanding that each transition from the state E_n to state E_m transfers the energy $E_m - E_n$ from environment into the system.

(c) Using expression for δQ from part (b) and the rate equation (1) one has

$$\frac{\partial S_{env}}{\partial t} = \frac{1}{T} \sum_{n,m} (E_n - E_m) \Gamma_{mn} p_n = \frac{1}{2T} \sum_{n,m} (E_n - E_m) (\Gamma_{mn} p_n - \Gamma_{nm} p_m),$$

and

$$\frac{1}{k_B} \frac{\partial S_{sys}}{\partial t} = - \sum_n \dot{p}_n (1 + \ln p_n) = \sum_{n,m} (\Gamma_{mn} p_n - \Gamma_{nm} p_m) \ln p_n = \frac{1}{2} \sum_{n,m} (\Gamma_{mn} p_n - \Gamma_{nm} p_m) (\ln p_n - \ln p_m).$$

We took into account that $\sum_n \dot{p}_n = 0$ and also symmetrized these equation by interchanging the summation indices n and m . Taken together, these two equations give:

$$\frac{\partial S}{\partial t} = \frac{1}{2} \sum_{n,m} \left[k_B \ln \frac{p_n}{p_m} + \frac{E_n - E_m}{T} \right] (\Gamma_{mn} p_n - \Gamma_{nm} p_m) = \frac{\partial S}{\partial t} = \frac{k_B}{2} \sum_{n,m} \ln \frac{\Gamma_{mn} p_n}{\Gamma_{nm} p_m} (\Gamma_{mn} p_n - \Gamma_{nm} p_m),$$

where in the last step we used the detailed balance condition (2) for the rates. This equation shows immediately that $\partial S/\partial t \geq 0$, in agreement with the second law of thermodynamics.

(d) If the system evolution is slow, so that the probability distribution maintains equilibrium throughout the evolution, the rate equation gives

$$\Gamma_{mn} p_n = \Gamma_{nm} p_m.$$

From the general expression derived in part (c), one sees then that

$$\frac{\partial S}{\partial t} = 0,$$

in agreement with the basic fact of thermodynamics that adiabatic processes are reversible.

(e) The minimal amount of heat transferred to the environment means that the entropy of the environment is increased as little as possible. Since the maximal information state of a bit has entropy $S_{sys} = k_B \ln 2$, while the no-information state has entropy $S_{sys} = 0$, we see that the minimal heat transfer requires an adiabatic process in which the entropy of the environment is increased by precisely the same amount as the bit entropy is decreased. This means that in this process

$$Q = k_B \ln 2.$$

This is the quantitative form of the Landauer principle: erasure of a bit of information requires, on average, the dissipation of $k_B \ln 2$ of energy.

Statistical Mechanics 3

1D Vibrational Modes

Consider a system of $N \gg 1$ similar particles of mass M , equally spaced on a circle of radius R , and constrained to move only around the circle, as shown in Fig. 1. Nearest neighbor particles are connected by springs with equal spring constants J and corresponding frequency $\Omega_0 \equiv \sqrt{J/M}$

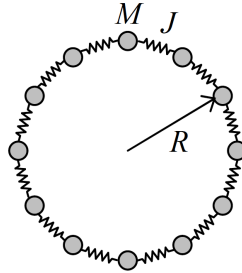


Figure 1: N vibrational modes constrained to a circle.

- (a) **[4pts]** Write down the Lagrangian of the system assuming small oscillations and find an equation of motion for the angular displacement of the n^{th} particle, $\phi_n(t)$. Show that the displacements takes the form

$$\phi_n(t) = \text{Re} \left[\sum_{j=0}^{N-1} c_j(t) e^{2\pi i j n / N} \right], \quad (1)$$

where $c_j(t)$ follows simple harmonic motion with angular frequency:

$$\omega_j^2 = 4\Omega_0^2 \sin^2 \left(\frac{\pi j}{N} \right). \quad (2)$$

What differential equation is obeyed by the $j = 0$ mode and what does it correspond to physically?

- (b) **[4pts]** For a single one-dimensional quantum harmonic oscillator of frequency ω , which is comparable to $k_B T / \hbar$, write down the partition function and calculate its heat capacity $C(T)$ in thermal equilibrium at temperature T . Analyze the low-temperature and high-temperature limits of the function $C(T)$.
- (c) **[4pts]** Returning to the system of N particles on a circle (Fig. 1), calculate its heat capacity in the intermediate temperature range:

$$\frac{\hbar\Omega_0}{N} \ll k_B T \ll \hbar\Omega_0 \quad (3)$$

Why is the contribution from the $j = 0$ mode negligible? Relevant integrals are given below.

- (d) **[4pts]** Now suppose that M is so large that there exists a range of lower temperatures where the oscillator modes contribute negligibly to the heat capacity:

$$\frac{\hbar^2 N}{MR^2} \ll k_B T \ll \frac{\hbar \Omega_0}{N}. \quad (4)$$

In this regime, the $j = 0$ mode dominates. What is the heat capacity of the system in this range?

- (e) **[4pts]** Finally, consider the lowest temperatures, where the $j = 0$ mode not only dominates, but must be quantized. What are the energy levels of the system assuming the particles are distinguishable? Estimate the temperature at which the heat capacity becomes exponentially small in this case. How would your answer change if the particles are indistinguishable bosons?

Hint: you may use the following integrals

$$\int_0^\infty \frac{x dx}{e^x - 1} = \int_0^\infty dx \frac{x^2}{\sinh^2 x} = \frac{\pi^2}{6} \quad (5)$$

Solution

(a) The kinetic energy of the n^{th} particle is:

$$T_n = \frac{1}{2}MR^2\dot{\phi}_n^2, \quad (6)$$

where ϕ_n is the angular displacement of the particle. The potential energy of the spring connecting the n^{th} and $(n+1)^{\text{st}}$ particle due to its small deformation, Δl_n , is

$$U_n = \frac{1}{2}J\Delta l_n^2 = \frac{1}{2}J(R\phi_{n+1} - R\phi_n)^2 \quad (7)$$

It follows that the Lagrangian of the system is given by:

$$L = \sum_{n=1}^N (T_n - U_n) = \frac{R^2}{2} \sum_{n=1}^N \left[M\dot{\phi}_n^2 - J(\phi_{n+1} - \phi_n)^2 \right] \quad (8)$$

(b) From the Lagrangian in Eq. (8), the equation of motion of the n^{th} particle is

$$-J(2\phi_n - \phi_{n-1} - \phi_{n+1}) = M\ddot{\phi}_n \quad (9)$$

Plugging into the ansatz in Eq. (1) yields:

$$\sum_{j=0}^{N-1} \left[M\ddot{c}_j(t) + Jc_j(t) (2 - e^{-2\pi ij/N} - e^{2\pi ij/N}) \right] e^{2\pi ijn/N} = 0, \quad (10)$$

which implies that the functions $c_j(t)$ obey the usual equation for a harmonic oscillator:

$$\ddot{c}_j + \omega_j^2 c_j = 0, \quad (11)$$

with a j -dependent frequency

$$\omega_j = \sqrt{\frac{2J}{M} \left(1 - \cos \frac{2\pi j}{N} \right)} = 2\sqrt{\frac{J}{M}} \left| \sin \frac{\pi j}{N} \right| \equiv 2\omega_0 \left| \sin \frac{\pi j}{N} \right| \quad (12)$$

Notice that $\omega_{j=0} = 0$. Hence, when $j = 0$, Eq. (11) yields $\ddot{c}_0 = 0$, i.e., $c_0(t) = \Omega t + \text{const}$, corresponding to a uniform rotation of the system without any deformation of the springs.

(c) The energy spectrum of a single harmonic oscillator is $E_n = \hbar\omega \left(n + \frac{1}{2} \right)$. Thus its partition function is given by:

$$Z = \sum_{n=0}^{\infty} e^{-E_n/k_B T} = e^{-\hbar\omega/2k_B T} \sum_{n=0}^{\infty} e^{-\hbar\omega n/k_B T} = \frac{e^{-\hbar\omega/2k_B T}}{1 - e^{-\hbar\omega/k_B T}} = \frac{1}{2 \sinh \frac{\hbar\omega}{2k_B T}} = \frac{1}{2 \sinh \frac{\hbar\omega\beta}{2}}, \quad (13)$$

where $\beta \equiv 1/k_B T$. To find the heat capacity, we need the average energy:

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} = \frac{\hbar \omega}{2} \coth \frac{\hbar \omega \beta}{2} \quad (14)$$

From which the heat capacity is given by

$$C(T) = \frac{\partial \langle E \rangle}{\partial T} = k_B \left(\frac{\hbar \omega}{2k_B T \sinh \frac{\hbar \omega}{2k_B T}} \right)^2 \quad (15)$$

At low temperatures,

$$C(k_B T \ll \hbar \omega) \rightarrow k_B \left(\frac{\hbar \omega}{k_B T} \right)^2 e^{-\frac{\hbar \omega}{k_B T}} \quad (16)$$

has an exponential form while at high temperatures $C(k_B T \gg \hbar \omega) \rightarrow k_B$, which follows from the equipartition theorem for the classical harmonic oscillator.

- (d) The heat capacity for N particles is found by summing Eq. (15) over the N frequencies $\omega_j = 2\omega_0 \left| \sin \frac{\pi j}{N} \right|$ found in Eq. (12):

$$C(T) = \sum_{j=1}^N k_B \left(\frac{\hbar \omega_0 \left| \sin \frac{\pi j}{N} \right|}{k_B T \sinh \frac{\hbar \omega_0 \left| \sin \frac{\pi j}{N} \right|}{k_B T}} \right)^2 \quad (17)$$

The constraint $k_B T \ll \hbar \omega_D$ implies that only the linear part of the spectrum will contribute to the energy, i.e., when $\pi j/N \approx 0$ or π . Hence, $\sin \frac{\pi j}{N}$ can be replaced by $\frac{\pi j}{N}$ and the sum can be replaced by twice an integral, where the factor of two comes from accounting for the two linear regimes when $\pi j/N \approx 0$ and $\pi j/N \approx \pi$. Thus,

$$C(T) \approx 2 \int_0^\infty dx k_B \left(\frac{\hbar \omega_0 \frac{\pi x}{N}}{k_B T \sinh \frac{\hbar \omega_0 \frac{\pi x}{N}}{k_B T}} \right)^2 \quad (18)$$

Define $u = \hbar \omega_0 \pi x / N k_B T$, so that $du = \hbar \omega_0 \pi / N k_B T dx$. Then, using the provided dimensionless integral,

$$C(T) \approx \frac{2N k_B^2 T}{\pi \hbar \omega_0} \int_0^\infty du \left(\frac{u}{\sinh u} \right)^2 = \frac{\pi N k_B^2 T}{3 \hbar \omega_0} \quad (19)$$

Notice that the classical $j = 0$ mode contributes $k_B/2$ to the specific heat, which is negligible compared to Eq. (19) in the temperature regime $\hbar \omega_0 / N \ll k_B T$.

- (e) When $k_B T \ll \hbar \omega_0 / N$, the contribution to the heat capacity from the oscillator modes is exponentially small (Eq. (16)). Thus, the specific heat is dominated by the $j = 0$ rotational mode. The constraint $\hbar^2 N / M R^2$ ensures it is in the classical regime. Since the rotational mode does not have any potential energy, it contributes $C(T) = \frac{1}{2} k_B$ by the equipartition theorem.

- (f) The $j = 0$ rotational mode corresponds to $\phi_j = \phi$. Thus, the total energy is given by the kinetic energy

$$T = \sum_{n=1}^N \frac{1}{2} MR^2 \dot{\phi}^2 = \frac{1}{2} NMR^2 \dot{\phi}^2 = \frac{1}{2} \frac{NMR^2 L_z^2}{I^2} = \frac{L_z^2}{2I}, \quad (20)$$

where $L_z = I\dot{\phi}$ is the angular momentum of the system and $I = NMR^2$ its moment of inertia. The quantized angular momentum operator is $\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$. The eigenfunctions of the angular momentum operator are $\psi_m(\phi) = e^{im\phi}$, with eigenvalues $m\hbar$, corresponding to kinetic energy $E_m = \frac{m^2 \hbar^2}{2NMR^2}$. If the particles are distinguishable, then $\psi_m(\phi) = \psi_m(\phi + 2\pi)$ which implies m is an integer. The temperature must be smaller than the gap between the ground state and the first excited state for the heat capacity to be exponentially small

$$k_B T \ll \frac{\hbar^2}{2MNR^2}. \quad (21)$$

On the other hand, if the particles are indistinguishable bosons, then $\psi_m(\phi) = \psi_m(\phi + 2\pi/N)$, which implies m is a multiple of N , $m \equiv \ell N$ with ℓ an integer. Hence the energy levels are $E_\ell = \frac{\hbar^2 \ell^2 N}{2MR^2}$. Thus there is a large gap (proportional to N) between the zero-th and first mode. The specific heat will be exponentially small at a much higher temperature

$$k_B T \ll \frac{\hbar^2 N}{2MR^2}. \quad (22)$$