Comprehensive Examination

Department of Physics and Astronomy Stony Brook University

August 2018 (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.

Some of the problems may cover multiple pages. 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, if approved by the proctor, a foreign-language dictionary. No other materials may be used.

Classical Mechanics 1

Periodic one-dimensional motion

Part I. Consider one-dimensional motion x(t), as described by the Lagrangian

$$L = \frac{m}{2} \dot{x}^2 - g \left| x \right|.$$

(a) (3 points) First draw a qualitative picture of the motion. Then write down and integrate the equation of motion.

(b) (3 points) Find T(E), the period of the motion at given total nonrelativistic energy E.

(c) (3 points) Find the truncated action per period, $\int_{t_0}^{t_0+T} p \, dx$.

Part II. Same as in Part I, but for the relativistic Lagrangian

$$L = -m\sqrt{1-\dot{x}^2} - g|x|$$
 with $c = 1$.

(a) (5 points) Integrate the equation of motion. Check that the nonrelativistic limit reduces to the solution in I(a).

(b) (2 points) Find T(E), the period of the motion at given total relativistic energy E.

(c) (2 points) Evaluate again the truncated action per period.

(d) (2 points) Compare the relativistic and the nonrelativistic motion of a particle that is momentarily at rest at $x = x_0$.

Solution

Part I:

(a) The equation of motion

$$m\ddot{x} = -g\,\operatorname{sign}(x)$$

describes uniform acceleration -g for positive x, and +g for negative x. The trajectory thus is the juxtaposition of parabolas

$$x(t) - x_0 = -\frac{g}{2m} (t - t_0 + T/4)^2 \quad \text{for} \quad -T/2 \le t - t_0 \le 0,$$

$$x(t) + x_0 = +\frac{g}{2m} (t - t_0 - T/4)^2 \quad \text{for} \quad 0 \le t - t_0 \le T/2,$$

periodically repeated with the period

$$T = 4\sqrt{\frac{2mx_0}{g}}.$$

Here $x_0 \ge 0$ is the amplitude of the oscillations.

(b) The amplitude x_0 relates to the energy E as

$$E = g x_0,$$

hence

$$T(E) = \frac{4\sqrt{2mE}}{g}.$$

(c) Since

$$E = \frac{p^2}{2m} + g\left|x\right|$$

we have

$$p = \pm \sqrt{2m(E - g |x|)}$$

where the sign changes at the turning points $|x| = x_0$. Elementary calculation yields

$$S = \int_{t=t_0}^{t_0+T} p dx = 4 \int_0^{x_0} \sqrt{2mg(x_0-x)} \, dx = \frac{8\sqrt{2m}}{3g} E^{3/2} \tag{P2.1}$$

Part II.

(a) Now the equation of motion is

$$\frac{d}{dt}\left(\frac{m\,\dot{x}}{\sqrt{1-\dot{x}^2}}\right) + g\,\operatorname{sign}(x) = 0\,.$$

As conservative system, it has the first integral

$$E = \frac{m}{\sqrt{1 - \dot{x}^2}} + g\left|x\right|,$$

which allows one to integrate the equation of motion:

$$(X - x)^2 - (t - t_0)^2 = R^2$$
 for $x \ge 0$,
 $(X + x)^2 - (t - t_0)^2 = R^2$ for $x \le 0$.

Here

$$R = \frac{m}{g}, \qquad X = \frac{E}{g},$$

and t_0 is an arbitrary time. For real motion $E \ge m$, hence

 $X \ge R$.

Thus, the trajectory is the periodic (with the period T) extension of the piecewise hyperbolic cycle

$$\begin{aligned} x(t) &= +X - \sqrt{R^2 + (t - t_0 + T/4)^2} & \text{for} & -T/2 \le t - t_0 \le 0, \\ x(t) &= -X + \sqrt{R^2 + (t - t_0 - T/4)^2} & \text{for} & 0 \le t - t_0 \le T/2. \end{aligned}$$

Here

$$T = 4\sqrt{X^2 - R^2}$$

so that $x(t_0) = 0$.

(b) Since X = E/g we have

$$T(E) = \frac{4}{g}\sqrt{E^2 - m^2}.$$

When $E = m + \Delta E$ with $\Delta E \ll m$, this reduces to the result in the Part I, with ΔE replacing E.

(c) In terms of the relativistic momentum

$$p = \frac{m \, \dot{x}}{\sqrt{1 - \dot{x}^2}}$$

we have

$$E = \sqrt{m^2 + p^2} + g |x|.$$

The integral

$$\int_{t=-T/2}^{T/2} p(t) \, dx(t) = 2 \, \int_0^{T/2} \, p(t) \, dx(t)$$

is easy to evaluate with the change of variables

$$t - t_0 - T/4 = R \sinh \tau$$
 for $0 \le t - t_0 \le T/2$,

suggested by the notion of the proper time on the trajectory. Then

$$X - x = R \cosh \tau$$
, $p = -m \sinh \tau$.

When $t - t_0$ changes from 0 to T/2, τ changes from $-\theta$ to θ , where θ is determined from

$$R \sinh \theta = T/4 = \frac{1}{g} \sqrt{E^2 - m^2},$$

or

$$E = m \cosh \theta \,. \tag{P2.2}$$

The integration yields

$$S = \frac{2m^2}{g} \int_{-\theta}^{\theta} d\tau \sinh^2 \tau = \frac{m^2}{g} \left[\sinh 2\theta - 2\theta\right].$$
 (P2.3)

Together with (P1.2) this yields a parametric representation of S(E).

In the non-relativistic limit $\Delta E = E - m \ll m$ we have $\theta \ll 1$, whence

$$\Delta E \approx \frac{m}{2} \theta^2$$
, $S \approx \frac{4m^2}{3g} \theta^3$,

and (P2.2), (P2.3) reduce to (P2.1).

(d) The relativistic orbit encloses the nonrelativistic orbit because for a moving particle a given force accelerates a nonrelativistic particle more than a relativistic particle ("the mass increases with velocity for a relativistic particle").



Classical Mechanics 2

Discretizing canonical transformations

Many physical systems are described by Hamiltonians which give rise to equations of motion that cannot be solved analytically, but must be discretized and solved numerically. Discretizations which preserve the symmetries of the continuum theory are especially effective when numerically integrating the equations of motion for long times. In this problem, we will explore some of the techniques available to describe such systems.

Consider a one-dimensional classical system whose *finite* time evolution is described by a canonical transformation. Specifically, let

$$x \equiv x(t)$$
 , $x' \equiv x(t')$, $p \equiv p(t)$, $p' \equiv p(t')$

and consider a generating function $F_2(x, p')$. Then the evolution from (x, p) to (x', p') is obtained by solving the equations

$$p = \frac{\partial F_2}{\partial x} \quad , \quad x' = \frac{\partial F_2}{\partial p'}$$
 (1)

(a) (5 points)

- (i) Show that this evolution preserves volume in phase space (that is, prove Liouville's theorem for this case).
- (ii) Next show that for

$$F_2 = xp' + \delta t H$$

as $\delta t \equiv t' - t \rightarrow 0$, the evolution equations reduce to Hamilton's equations of motion.

- (b) (5 points) Suppose there is a conserved quantity G(x, p). Noether's theorem states that this means the system has a symmetry.
 - (i) What are the transformations of x, p under this symmetry?
 - (ii) How does the Hamiltonian transform under this symmetry? Explain why this is equivalent to Noether's theorem.
 - (iii) Now compute the transformation of the Lagrangian expressed in the Hamiltonian form:

$$L(x, \dot{x}) = p\dot{x} - H(x, p)$$

Show that L transforms by a total derivative. You should use Hamilton's equations, but do NOT use the Euler-Lagrange equations.

(iv) A simple example of a conserved quantity is the Hamiltonian itself. For this example, what are the transformations of x, p and L? What is the physical interpretation of this symmetry?

(c) (5 points) For a Hamiltonian of the form $\frac{p^2}{2m} + U(x)$, show that the naive discretization of Newton's equations of motion (for δt small but finite)

$$p' = p - \frac{\partial U(x)}{\partial x} \delta t$$
, $x' = x + \frac{p}{m} \delta t$ (2)

does NOT preserve volume in phase space. For a harmonic oscillator, will the volume shrink or grow? What does this say about the long time behavior of this approximation? Estimate the number of iterations before the error is of order one, in terms of the mass m of the particle, the spring constant k, and the finite interval δt .

(d) (5 points) What is the analogous discretization using canonical transformations? Find the right $F_2(x, p')$, and work out the equations corresponding to (2) in part (c). Why is this guaranteed to preserve volume in phase space? What does this say about the long time behavior of this approximation?

Solution

- (a) (5 points)
 - (i) Show that this evolution preserves volume in phase space (that is, prove Liouville's theorem for this case).

Solution: We need to compute the Jacobian determinant of the transformation:

$$\det(\operatorname{Jac}) = \begin{vmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{vmatrix} = \begin{vmatrix} \frac{\partial^2 F_2}{\partial p' \partial x} + \frac{\partial^2 F_2}{\partial p' \partial p'} \frac{\partial p'}{\partial x} & \frac{\partial^2 F_2}{\partial p' \partial p'} \frac{\partial p'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{vmatrix} = \frac{\partial^2 F_2}{\partial p' \partial x} \frac{\partial p'}{\partial p}$$

But differentiating $p = \frac{\partial F_2}{\partial x}$ with respect to p gives

$$1 = \frac{\partial^2 F_2}{\partial p' \partial x} \frac{\partial p'}{\partial p} ,$$

and hence the Jacobian determinant is 1.

Solution: Solution with the volume form:

$$dp \wedge dx = \frac{\partial^2 F_2}{\partial x \partial p'} dp' \wedge dx = dp' \wedge \frac{\partial^2 F_2}{\partial p' \partial x} dx = dp' \wedge dx'$$

is also acceptable.

(ii) Next show that for

$$F_2 = xp' + \delta t H$$

as $\delta t \equiv t' - t \rightarrow 0$, the evolution equations reduce to Hamilton's equations of motion. Solution: Equation (1) becomes:

$$p = p' + \delta t \frac{\partial H}{\partial x}$$
, $x' = x + \delta t \frac{\partial H}{\partial p'}$ \Rightarrow $p' - p = -\delta t \frac{\partial H}{\partial x}$, $x' - x = \delta t \frac{\partial H}{\partial p'}$

which, in the limit $\delta t \to 0, \ p' \to p, \ x' \to x$ reduces to

$$\dot{p} = -\frac{\partial H}{\partial x}$$
, $\dot{x} = \frac{\partial H}{\partial p}$

(b) (5 points) Suppose there is a conserved quantity G(x, p). Noether's theorem states that this means the system has a symmetry.

(i) What are the transformations of x, p under this symmetry? Solution: They given simply by the Poisson brackets with G:

$$\delta p = -\epsilon \frac{\partial G}{\partial x} \quad , \quad \delta x = \epsilon \frac{\partial G}{\partial p}$$

where ϵ is an arbitrary constant small parameter.

(ii) How does the Hamiltonian transform under this symmetry? Explain why this is equivalent to Noether's theorem.

Solution: The statement that this is a symmetry is simply $\delta H = 0$. Then:

$$\delta H \equiv \frac{\partial H}{\partial x} \delta x + \frac{\partial H}{\partial p} \delta p = \epsilon \left(\frac{\partial H}{\partial x} \frac{\partial G}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial G}{\partial x} \right) = \epsilon \left(-\dot{p} \frac{\partial G}{\partial p} - \dot{x} \frac{\partial G}{\partial x} \right) = -\epsilon \dot{G} ,$$

and hence $\delta H = 0 \Leftrightarrow \dot{G} = 0$.

(iii) Now compute the transformation of the Lagrangian in Hamiltonian form:

$$L(x, \dot{x}) = p\dot{x} - H(x, p)$$

Show that L transforms by a total derivative. You should use Hamilton's equations, but do NOT use the Euler-Lagrange equations.

Solution: Because $\delta H = 0$, we have

$$\delta L = \delta p \dot{x} + p \,\delta \dot{x} = \epsilon \left(-\frac{\partial G}{\partial x} \dot{x} + p \frac{d}{dt} \frac{\partial G}{\partial p} \right) = \epsilon \left(-\frac{\partial G}{\partial x} \dot{x} + \frac{d}{dt} \left(p \frac{\partial G}{\partial p} \right) - \dot{p} \frac{\partial G}{\partial p} \right)$$
$$= \epsilon \left(-\dot{G} + \frac{d}{dt} \left(p \frac{\partial G}{\partial p} \right) \right) = \epsilon \frac{d}{dt} \left(p \frac{\partial G}{\partial p} \right) ,$$

where the last step follows from G = 0.

(iv) A simple example of a conserved quantity is the Hamiltonian itself. For this example, what are the transformations of x, p and L? What is the physical interpretation of this symmetry?

Solution: If we take G = H, then from Hamilton's equations we have

$$\delta p = \epsilon \dot{p} \quad , \quad \delta x = \epsilon \dot{x}$$

Plugging into our result, we find

$$\delta L = \epsilon \frac{d}{dt} (p\dot{x})$$

which is correct modulo Hamilton's equations; we are free to subtract a term $0 = \epsilon \dot{H}$, and then we find the more usual result

$$\delta L = \epsilon \dot{L}$$

Physically, this is time translation invariance, and it means that if we find one solution x(t) to the equations of motion, then x(t + a) is also a solution for any constant a.

(c) (5 points) For a Hamiltonian of the form $\frac{p^2}{2m} + U(x)$, show that the naive discretization of Newton's equations of motion (for δt small but finite)

$$p' = p - \frac{\partial U(x)}{\partial x} \delta t \quad , \quad x' = x + \frac{p}{m} \delta t$$
 (2)

does NOT preserve volume in phase space.

Solution: The Jacobian determinant is

$$\det(\operatorname{Jac}) = \begin{vmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{vmatrix} = \begin{vmatrix} 1 & \frac{\delta t}{m} \\ -\delta t \frac{\partial^2 U}{\partial x \partial x} & 1 \end{vmatrix} = 1 + \frac{(\delta t)^2}{m} \frac{\partial^2 U}{\partial x \partial x}$$

For a harmonic oscillator, will the volume shrink or grow?

Solution: For a harmonic oscillator, $U = \frac{1}{2}kx^2$ with k > 0, and hence the Jacobian is $1 + \frac{k}{m}(\delta t)^2 > 1$, which means the volume grows.

What does this say about the long time behavior of this approximation? Estimate the number of iterations before the error is of order one in terms of the mass m of the particle, the spring constant k, and the finite interval δt .

Solution: The approximation is unstable and after approximately

$$N \approx \left(\frac{k}{m} (\delta t)^2\right)^{-1}$$

iterations will deviate from the exact solution by order one.

(d) (5 points) What is the analogous discretization using canonical transformations? Find the right $F_2(x, p')$, and work out the equations corresponding to (2) in part c).

Solution: The right $F_2(x, p')$ follows from part ii) of a):

$$F_2(x, p') = xp' + \delta t \left(\frac{(p')^2}{2m} + U(x) \right)$$

The evolution equations are (1) from above; here they become:

$$p = p' + \delta t \frac{\partial U}{\partial x}$$
, $x' = x + \delta t \frac{p'}{m}$,

which we rewrite as:

$$p' = p - \delta t \frac{\partial U}{\partial x}$$
, $x' = x + \delta t \frac{p'}{m}$

Notice in the second equation, p' appears on the right hand side, rather than p as in (2) of part c).

Why is this *guaranteed* to preserve volume in phase space?

Solution: We proved that *all* canonical transformations preserve volume in phase space.

What does this say about the long time behavior of this approximation?

Solution: We do not expect the errors from the discretization procedure to grow with time (of course, numerical errors can accumulate, though these are typically much smaller than discretization errors).

Classical Mechanics 3

Open system

A particle of mass *m* is attached to an infinite string, with mass μ per unit length, and stretched with tension *T*. The particle is confined to move along the *y* axis normal to the string (see the figure below), in an additional potential U(y), not related to the string, with a minimum at y = 0.



A (5 points). Derive the system of differential equations and boundary conditions describing the dynamics of small deviations of this system from equilibrium.

B (5 points). Assuming that the waves on the string are excited only by the motion of the particle (rather than any external source), reduce this system to an ordinary differential equation for the small displacement of the particle, as a function of time. (Hence consider the case that for x>0 there are only right-moving waves, and for x<0 only left-moving waves.)

C (4 points). Solve this equation for the case U(y) = 0, assuming that the motion was initiated, from equilibrium, by a short external impulse *p* given to the particle. Calculate the final displacement of the particle. Sketch the resulting displacement y(x, t) of some point of the string as a function of time.

D (4 points). For the case of a harmonic oscillator, when $U(y) = m\omega^2 y^2/2$, solve the equation of motion under the same assumptions as in C.

E (2 points). Would you describe this system as a Hamiltonian (energy-conserving) or dissipative?

Solution

A (5 points). For small deviations from equilibrium, with $\partial y/\partial x \rightarrow 0$, the vertical force exerted on the particle by the two parts of the string is

$$F_{y} \approx T\left(\frac{\partial y}{\partial x}\Big|_{x=+0} - \frac{\partial y}{\partial x}\Big|_{x=-0}\right),$$

so that the equation of motion of its vertical coordinate Y(t) is

$$m\ddot{Y} = -\frac{\partial U(Y)}{\partial Y} + T\left(\frac{\partial y}{\partial x}\Big|_{x=+0} - \frac{\partial y}{\partial x}\Big|_{x=-0}\right),\tag{1}$$

where the dot denotes the differentiation over time.

Similarly, the vertical force exerted on to a small fragment, of length dx, of the string by the parts adjacent to it, is

$$dF_{y} \approx T\left(\frac{\partial y}{\partial x}\Big|_{x+dx/2} - \frac{\partial y}{\partial x}\Big|_{x-dx/2}\right) \approx T\left[\frac{\partial^{2} y}{\partial^{2} x}\Big|_{x}\left(+\frac{dx}{2}\right) - \frac{\partial^{2} y}{\partial^{2} x}\Big|_{x}\left(-\frac{dx}{2}\right)\right] = T\frac{\partial^{2} y}{\partial^{2} x}dx$$

Since the mass of this fragment is μdx , this gives us the following equation of the string motion:

$$\mu \frac{\partial^2 y}{\partial t^2} = T \frac{\partial^2 y}{\partial^2 x}.$$
 (2)

Eqs. (1)-(2), together with the boundary condition (evident from the figure above),

$$y(0,t) = Y(t),$$
 (3)

fully describe the system's dynamics, provided that initial conditions are specified.

B (5 points). Eq. (2) is the well-known wave equation, with the general solution

$$y(x,t) = f_{\rightarrow}\left(t - \frac{x}{v}\right) + f_{\leftarrow}\left(t + \frac{x}{v}\right),$$

where $v \equiv (T/\mu)^{1/2} > 0$, is the wave velocity, and $f \rightarrow \text{and } f_{\leftarrow}$ are some functions of a single argument, which are determined by initial and boundary conditions. If the waves on the string are excited only by the motion of the particle (rather than any external sources, in particular any waves arriving from afar), the wave on its right part (x > 0) may travel only to the right, and vice versa:

$$\mathbf{v}(x,t) = \begin{cases} f_{\rightarrow}(t-x/\nu), & \text{at } x \ge 0, \\ f_{\leftarrow}(t+x/\nu), & \text{at } x \le 0, \end{cases}$$

Moreover, according to Eq. (3), at x = 0 these functions have to be equal to each other, and to the particle's coordinate Y(t), so that

$$y(x,t) = \begin{cases} Y(t-x/\nu), & \text{at } x \ge 0, \\ Y(t+x/\nu), & \text{at } x \le 0, \end{cases} \quad \text{and hence} \quad \frac{\partial y}{\partial x} = \begin{cases} (-1/\nu) \dot{Y}(t-x/\nu), & \text{at } x \ge 0, \\ (+1/\nu) \dot{Y}(t+x/\nu), & \text{at } x \le 0. \end{cases}$$
(4)

Plugging the last expressions, for $x = \pm 0$, into Eq. (1), we get the ordinary differential equation

$$m\ddot{Y} = -\frac{\partial U(Y)}{\partial Y} - 2Z\dot{Y}, \quad \text{with } Z \equiv \frac{T}{v} = (\mu T)^{1/2}.$$
 (5)

The constant *Z* is called the *wave impedance* of a string; as Eq. (5) shows, in our case 2*Z* plays the role of the drag coefficient η defined by the relation $F_{\text{drag}} = -\eta u$, where $u \equiv \dot{Y}$ is the particle's velocity.

C (4 points). If U(Y) = 0, Eq. (5) is reduced to a simple linear equation for the velocity of the particle,

$$m\dot{u} + 2Zu = 0,$$

with the solution

$$u(t) = u(0) \exp\left\{-\frac{t}{\tau}\right\}, \quad \text{where } \tau \equiv \frac{m}{2Z}.$$
 (6)

This solution describes the asymptotic approach of the velocity to zero, and of the particle's displacement Y(t) to a constant. For the initial condition specified in the assignment, mu(0) = p, we get

$$Y(t) = \int_{0}^{t} u(t')dt' = \frac{p}{m} \int_{0}^{t} \exp\left\{-\frac{t}{\tau}\right\} dt' = \frac{p\tau}{m} \left(1 - \exp\left\{-\frac{t}{\tau}\right\}\right),$$

so that at $t \to \infty$, $Y \to p \tau/m$. As the first of Eqs. (4) shows, the displacement of each point of any string have the same form, delayed by the wave propagation time $\Delta t = |y|/v$ - see the sketch below.



D (4 points). For the case of a harmonic oscillator, with $U(Y) = m\omega^2 Y^2/2$, Eq. (5) takes the form

$$\ddot{Y} + \frac{1}{\tau}\dot{Y} + \omega^2 Y = 0,$$

where the time constant τ is given by Eq. (6). This is the standard equation of a damped linear oscillator with the *Q*-factor

$$Q = \omega \tau$$
;

in our particular case, $Q = m\omega/2Z$.

E (2 points). This is a good example of an "open" physical system, whose dynamics may be interpreted in two different ways. On one hand, the full energy of the system, with strings extending to infinity,

$$E_{\Sigma} \equiv E + \int_{-\infty}^{+\infty} e dx = \frac{m}{2} \dot{Y}^{2} + U(Y) + \int_{-\infty}^{+\infty} \left[\frac{\mu}{2} \left(\frac{\partial y}{\partial t} \right)^{2} + \frac{T}{2} \left(\frac{\partial y}{\partial x} \right)^{2} \right] dx ,$$

is conserved for any finite *t*. On the other hand, the energy of any sub-system including the particle plus two adjacent segments of the string of any finite length, eventually looses energy, and hence is dissipative. This duality gives a wonderful (and broadly used) opportunity to explore this and similar models to study not only classical, but also quantum dynamical dissipative systems, using reliable theoretical methods developed for Hamiltonian systems.

Comment: One can also derive the equation of motion in (5) from energy conservation. For an arbitrary waveform y(x, t) the kinetic energy of a small fragment dx is

$$\frac{\mu}{2} \left(\frac{\partial y}{\partial t}\right)^2 dx,$$

while its potential energy udx may be calculated as the elementary work, Tdl, necessary for the elongation dl of the fragment - from its equilibrium value dx to the current value

$$\left[1 + \left(\frac{\partial y}{\partial x}\right)^2\right]^{1/2} dx \approx \left[1 + \frac{1}{2}\left(\frac{\partial y}{\partial x}\right)^2\right] dx,$$

where the last form is valid for small elongations, $dl \ll dx$. From here,

$$udx = \frac{T}{2} \left(\frac{\partial y}{\partial x}\right)^2 dx$$

so that the total energy of the fragment is

$$edx = \left[\frac{\mu}{2}\left(\frac{\partial y}{\partial t}\right)^2 + \frac{T}{2}\left(\frac{\partial y}{\partial x}\right)^2\right]dx$$

Traveling with velocities $\pm v$, the waves (4) carry out the power

$$P_{\rightarrow}(x,t) = \pm ve = \pm v \left[\frac{\mu}{2} \left(\frac{\partial Y(t \mp x/v)}{\partial t} \right)^2 + \frac{T}{2} \left(\frac{\partial Y(t \mp x/v)}{\partial x} \right)^2 \right] = \pm v \left[\frac{\mu}{2} + \frac{T}{2} \frac{1}{v^2} \right] \dot{Y}^2 \left(t \mp \frac{x}{v} \right) = \pm Z \dot{Y}^2 \left(t \mp \frac{x}{v} \right)$$

Since both power flows are directed from the particle, its energy balance may be written as

$$\frac{d}{dt}E = -(P_{\rightarrow} - P_{\leftarrow})_{x=0}, \qquad \text{giving } \frac{d}{dt}\left[\frac{m}{2}\dot{Y}^2 + U(Y(t))\right] = -2Z\dot{Y}^2.$$

Carrying out the differentiation in the left-hand side, and cancelling \dot{Y} , we arrive back at Eq. (5).

Electromagnetism 1

Consider two identical rods of length ℓ with charges +q and -q pasted on their ends. The centers of the rods are located on the z-axis which is perpendicular to the length of the rods (see below). The two rods are separated by a distance $d \gg \ell$, with the top and bottom rods located at heights $z = \pm d/2$ respectively. The rods rotate around the z axis with the same frequency ω but are out of phase, and at time t=0 the bottom rod has an azimuthal angle of ϕ_0 while the top rod has $\phi = 0$.



- (a) (8 points) First consider the limit $\omega d/c \ll 1$. Determine the (real) electric and magnetic fields as a function of time at a height z = 3d/2 on the z axis.
- (b) (4 points) Next consider the limit $\omega d/c \gg 1$, but still with $\omega \ell/c \ll 1$. Determine the (real) electric and magnetic fields at a height z = 3d/2 on the z axis.
- (c) (4 points) With the approximations of part (b), determine the phase ϕ_0 when the fields from the two dipoles add destructively. Explain your result physically.
- (d) (4 points) With the approximations of part (b), determine the time averaged electromagnetic power passing through a small area A at a height z = 3d/2 on the z axis, with front face directed towards the origin.

Solution

(a) This is near field regime. In this case we are just supposed to sum the electrostatic fields from the dipoles. The dipoles are

$$\boldsymbol{p}_1 = p_0 e^{-i\omega t} (\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}), \qquad (3)$$

$$\boldsymbol{p}_2 = p_0 e^{-i(\omega t + \phi_0)} (\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}), \qquad (4)$$

where it is understood that we are to take the real part of the expression. Here and below the magnitude of the dipole moment is

$$p_0 = q\ell. (5)$$

The two electrostatic fields are

$$\boldsymbol{E}_{1} = \frac{3\boldsymbol{n}_{1}(\boldsymbol{n}_{1} \cdot \boldsymbol{p}_{1}) - \boldsymbol{p}_{1}}{4\pi r_{1}^{3}}, \qquad (6)$$

$$\boldsymbol{E}_{2} = \frac{3\boldsymbol{n}_{2}(\boldsymbol{n}_{2} \cdot \boldsymbol{p}_{2}) - \boldsymbol{p}_{2}}{4\pi r_{2}^{3}}, \qquad (7)$$

where

$$r_1 = |\boldsymbol{r} - \boldsymbol{r}_1| = d, \qquad (8)$$

$$r_2 = |\mathbf{r} - \mathbf{r}_2| = 2d, \qquad (9)$$

and n_1 (for example) is a unit vector from the center of the dipole to the observation point. Here we note that $n_1 = n_2 = \hat{z}$, and thus n_1 and n_2 are perpendicular to p_1 and p_2 yielding

$$\boldsymbol{E} = \boldsymbol{E}_1 + \boldsymbol{E}_2 \,, \tag{10}$$

$$=\frac{-\boldsymbol{p}_1}{4\pi d^3} + \frac{-\boldsymbol{p}_2}{4\pi (2d)^3}\,,\tag{11}$$

$$= -\frac{p_0}{4\pi d^3} e^{-i\omega t} \left(1 + \frac{e^{-i\phi_0}}{8}\right) \left(\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}\right).$$
(12)

Taking the real part

$$\boldsymbol{E} = -\frac{p_0}{4\pi d^3} \left[\left(\cos(\omega t) + \frac{1}{8}\cos(\omega t + \phi_0) \right) \hat{\boldsymbol{x}} + \left(\sin(\omega t) + \frac{1}{8}\sin(\omega t + \phi_0) \right) \hat{\boldsymbol{y}} \right].$$
(13)

Now we will determine the magnetostatic field. This is given by the Biot-savat law. First we recognize that a time dependent dipole gives a current. Integrating over a small volume including the dipole we find

$$I_1 \Delta \vec{\ell_1} \equiv \boldsymbol{j}_1 \Delta V = \partial_t \boldsymbol{p}_1 = -i\omega p_0 e^{-i\omega t} (\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}), \qquad (14)$$

$$I_2 \Delta \vec{\ell}_2 \equiv \boldsymbol{j}_2 \Delta V = \partial_t \boldsymbol{p}_2 = -i\omega p_0 e^{-i(\omega t + \phi_0)} (\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}).$$
(15)

Then the Biot-savat law gives

$$\boldsymbol{B} = \frac{I_1 \Delta \vec{\ell}_1 / c \times \boldsymbol{n}_1}{4\pi r_1^2} + \frac{I_2 \Delta \vec{\ell}_2 / c \times \boldsymbol{n}_2}{4\pi r_2^2} \,. \tag{16}$$

Thus, since $\boldsymbol{n}_1 = \boldsymbol{n}_2 = \hat{\boldsymbol{z}}$ and

$$(I\Delta \vec{\ell} \times \hat{\boldsymbol{z}}) \propto (\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}) \times \hat{\boldsymbol{z}} = (-\hat{\boldsymbol{y}} + i\hat{\boldsymbol{x}}), \qquad (17)$$

we find:

$$\boldsymbol{B} = \frac{ikp_0e^{-i\omega t}}{4\pi d^2} \left(1 + \frac{e^{-i\phi_0}}{4}\right) \left(\hat{\boldsymbol{y}} - i\hat{\boldsymbol{x}}\right).$$
(18)

Taking the real part we have

$$\boldsymbol{B} = \frac{kp_0}{4\pi d^2} \left[\hat{\boldsymbol{y}} \left(\sin(\omega t) + \frac{1}{4}\sin(\omega t + \phi_0) \right) + \hat{\boldsymbol{x}} \left(\cos(\omega t) + \frac{1}{4}\cos(\omega t + \phi_0) \right) \right]$$
(19)

(b) In this regime the field is radiative. The electric field is just the sum of the radiation fields of two dipoles separated from the observation point by d and 2d respectively. Because of the retardation, the phases of the two dipoles are $e^{-i\omega(t-d/c)}$ and $e^{-i\omega(t-2d/c)+i\phi_0}$ respectively, and thus

$$\boldsymbol{E}_{1} = k^{2} p_{0} \frac{e^{-i\omega(t-d/c)}}{4\pi d} \left(-\boldsymbol{n} \times \boldsymbol{n} \times \left(\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}} \right) \right) , \qquad (20)$$

$$\boldsymbol{E}_{2} = k^{2} p_{0} \frac{e^{-i\omega(t-2d/c)+i\phi_{0}}}{4\pi(2d)} \left(-\boldsymbol{n} \times \boldsymbol{n} \times (\hat{\boldsymbol{x}}+i\hat{\boldsymbol{y}})\right) \,. \tag{21}$$

Then with \boldsymbol{n} in the z direction we have

$$\boldsymbol{E} = \boldsymbol{E}_1 + \boldsymbol{E}_2 \tag{22}$$

$$=k^{2}p_{0}\frac{e^{-i\omega(t-d/c)}}{4\pi d}(\hat{\boldsymbol{x}}+i\hat{\boldsymbol{y}})\left[1+\frac{1}{2}e^{i(\omega d/c-\phi_{0})}\right].$$
(23)

Taking the real part of we determine the radiative electric field

$$\boldsymbol{E} = \frac{k^2 p_0}{4\pi d} \Big[\hat{\boldsymbol{x}} \left(\cos(\omega(t - d/c)) + \frac{1}{2} \cos(\omega(t - 2d/c) + \phi_0) \right) \\ + \hat{\boldsymbol{y}} \left(\sin(\omega(t - d/c)) + \frac{1}{2} \sin(\omega(t - 2d/c) + \phi_0) \right) \Big]. \quad (24)$$

The magnetic field in this region is simply

$$\boldsymbol{B} = -\hat{\boldsymbol{z}} \times \boldsymbol{E} \,. \tag{25}$$

(c) The phase difference between the two oscillators will add destructively when

$$(\omega d/c) - \phi_0 = \pi \tag{26}$$

i.e.

$$\phi_0 = \frac{2\pi d}{\lambda} - \pi \tag{27}$$

Physically we are requiring that the waves from the bottom dipole (which are delayed by a time d/c relative to the top, but ahead by the phase angle ϕ_0) should be 180 degrees out of phase from the waves of the top dipole by the time they reach the observation point.

(d) The time averaged power passing through the detector is

$$P = \langle \boldsymbol{S} \cdot \boldsymbol{n} \, A \rangle = \frac{c}{2} A \, \boldsymbol{E} \cdot \boldsymbol{E}^*$$
(28)

Combining factors we see that

$$\boldsymbol{E} \cdot \boldsymbol{E}^* \propto \left(\hat{\boldsymbol{x}}^2 + \hat{\boldsymbol{y}}^2 \right) \left| 1 + \frac{1}{2} e^{i(\omega d/c) - i\phi_0} \right|^2$$
(29)

$$=2\left(\frac{5}{4} + \cos(\omega d/c - \phi_0)\right) \tag{30}$$

and therefore

$$P = \frac{ck^4 A p_0^2}{16\pi^2 d^2} \left(\frac{5}{4} + \cos(\omega d/c - \phi_0) \right) \,. \tag{31}$$

Electromagnetism 2

A guided wave:

A simple coaxial cable consists of two cylindrical perfect conductors of infinite length as shown below. The inner and outer conducting cylinders have radii a and b respectively. The space between the conductors is filled with a dielectric with electric and magnetic permeablities ϵ and μ respectively. Assume that the currents are on the conducting surfaces and do not penetrate into the interior of the metal. This is an appropriate approximation at high frequency when the skin depth is small compared to the transverse dimensions.



- (a) (2 points) (i) A static potential difference is maintained between the inner and outer conductors. Determine the capacitance per unit length C. (ii) A current runs down the cable on the surface of the inner conductor and returns on the surface of the outer conductor. Determine the inductance per unit length \mathcal{L} . (iii) Determine the product \mathcal{LC} and find a pleasing result.
- (b) (4 points) Now consider an electromagnetic wave propagating down the cable in the z direction. Assume that the electric and magnetic fields are perpendicular to z and take the form

$$\boldsymbol{E}(t,\boldsymbol{x}) = \boldsymbol{E}_{\perp}(\boldsymbol{x}_{\perp}) e^{ikz - i\omega t}, \qquad \boldsymbol{B}(t,\boldsymbol{x}) = \boldsymbol{B}_{\perp}(\boldsymbol{x}_{\perp}) e^{ikz - i\omega t}, \qquad (1)$$

where \boldsymbol{x}_{\perp} denotes the (x, y) coordinates. Show that $\boldsymbol{E}_{\perp}(\boldsymbol{x}_{\perp})$ and $\boldsymbol{B}_{\perp}(\boldsymbol{x}_{\perp})$ satisfy the equations of two-dimensional electro and magneto statics; determine the relation between \boldsymbol{E}_{\perp} and \boldsymbol{B}_{\perp} and the relation between ω and k.

The wave solutions in Eq. (1) are known as transverse electromagnetic (TEM) waves.

- (c) (4 points) Consider the propagating TEM wave of part (c). Show that the current on the conducting surfaces satisfies a one dimensional wave equation.
- (d) (5 points) Determine the power transmitted by the TEM wave. Express your result in terms of the amplitude of current wave, I_0 , and the radii a and b of the cable.
- (e) (5 points) Now assume the walls of the cylinders are not perfect conductors, but have a large but finite conductivity σ . First estimate, and then compute the power lost per length by the TEM wave of part (d). Assume that $kb \ll 1$.

Solution

(a) If the inner conducter has charge per length λ and the outer conductor has charge $-\lambda$, then Gauss law $\int \mathbf{D} \cdot d\mathbf{a} = Q_{\text{enc}}$ gives

$$\epsilon E_{\rho}(2\pi\rho)\ell = \lambda\ell, \qquad E_{\rho} = \frac{\lambda/\epsilon}{2\pi\rho}.$$
 (2)

The potential differnce between the outer and outer conductor is

$$-\Delta V_{ab} = V_b - V_a = -\int_a^b d\rho E_\rho = -\frac{\lambda}{2\pi\epsilon} \log(b/a) \,. \tag{3}$$

Then the capacitance per length is

$$C = \frac{(Q/\ell)}{V_{ab}} = \frac{2\pi\epsilon}{\log(b/a)}.$$
(4)

The inuctance is perhaps most easily found from the energy stored in the region:

$$U_B = \frac{\mu}{2} \int d^3 r \boldsymbol{H}^2 \,, \tag{5}$$

$$= \frac{\mu}{2} \ell(2\pi) \int_{a}^{b} \rho d\rho \frac{I^{2}/c^{2}}{(2\pi)^{2} \rho^{2}}, \qquad (6)$$

$$=\frac{\mu}{2c^2}\ell\frac{I^2}{2\pi}\log(b/a)\,.\tag{7}$$

The energy per length is U_B/ℓ and thus, from the formula $U_B = \frac{1}{2}LI^2$, the inductance per length is

$$\mathcal{L} = \frac{\mu}{2\pi c^2} \log(b/a) \,. \tag{8}$$

Concluding

$$\mathcal{LC} = \frac{\mu\epsilon}{c^2} \,. \tag{9}$$

Although this result result was derived for a cylindrical cable, it actually holds for a coaxial cable of arbitrary transverse cross section. You are invited to prove this statement for yourself.

(b) Now we substitute the provided forms into the Maxwell equations.

We use indices a, b = 1, 2 and ijk = 1, 2, 3. ε^{ijk} is the usual thing, and ε^{ab} is the two dimensional version with $\varepsilon^{12} = +1$. The vectors have only xy components, and thus the divergence and curl take the form:

$$\nabla \cdot \boldsymbol{V} = \partial_a V^a \,, \tag{10a}$$

$$(\nabla \times \boldsymbol{V})^a = \varepsilon^{aij} \partial_i V_j = \varepsilon^{azb} \partial_z V_b \,, \tag{10b}$$

$$= -\varepsilon^{ab}\partial_z V_b, \qquad (10c)$$

$$(\nabla \times \mathbf{V})^z = \varepsilon^{zab} \partial_a V_b \,, \tag{10d}$$

$$=\varepsilon^{ab}\partial_a V_b. \tag{10e}$$

Note

$$\varepsilon_{ab}\varepsilon^{bc} = -\delta_a^c \,. \tag{11}$$

Then breaking up the Maxwell equations with these rules

$$\epsilon \nabla_{\perp} \cdot \boldsymbol{E}_{\perp} = 0 \tag{12a}$$

$$\varepsilon^{ab}\partial_a H_b = 0 \tag{12b}$$

$$-\varepsilon^{ab}\partial_z H_b = -\frac{1}{c}\partial_t(\epsilon E^a) \tag{12c}$$

$$\nabla_{\perp} \cdot (\boldsymbol{B}_{\perp}) = 0 \tag{12d}$$

$$\varepsilon^{ab}\partial_a E_b = 0 \tag{12e}$$

$$\varepsilon^{ab}\partial_z E_b = \frac{1}{c}\partial_t(\mu H^a) \tag{12f}$$

Taking the z derivative of the last equation (and multiplying by ϵ_{ca}) and using it in the time-derivative of the third

$$\left(\frac{\mu\epsilon}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial z^2}\right)\boldsymbol{E}^a(\boldsymbol{x}, z, t) = 0$$
(13)

Similarly, taking the z derivative of the third equation (and multiplying by ϵ_{ca}) and using it in the time-derivative of last gives

$$\left(\frac{\mu\epsilon}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial z^2}\right)\boldsymbol{B}^a(\boldsymbol{x}, z, t) = 0$$
(14)

Thus these equations are solved if

$$\omega^2 = \frac{c^2}{\mu\epsilon}k^2\tag{15}$$

We also can see from the last equation the relation between E and H:

$$\epsilon^{ab}E_b = -ZH^a, \qquad Z \equiv \sqrt{\mu/\epsilon},$$
(16)

i.e.

$$E^x = ZH^y, \qquad E^y = -ZH^x. \tag{17}$$

Finally the perpendicular vector satisfy the equations of 2D electro and magneto statics.

$$\nabla_{\perp} \cdot \boldsymbol{D}_{\perp} = 0, \qquad (18a)$$

$$\epsilon^{ab}\partial_a E_b = 0, \qquad (18b)$$

$$\nabla_{\perp} \cdot \boldsymbol{B}_{\perp} = = 0, \qquad (18c)$$

$$\epsilon^{ab}\partial_a H_b = 0. \tag{18d}$$

(c) Let us examine the boundary conditions. In what follows n is an outward directed normal to the surface (i.e. directed away from the metal.) The charge density is

$$\left. \epsilon \left. \boldsymbol{n} \cdot \left(\boldsymbol{E}_{\text{out}} \right) \right|_{\text{surf}} = \left. \epsilon \left. n_a E^a \right|_{\text{surf}} = \sigma(z, t) \right.$$
 (19)

and the current is in the z direction

$$(\boldsymbol{n} \times \boldsymbol{H}_{\text{out}})^{z}|_{\text{surf}} = \varepsilon^{ab} n_{a} H_{b}|_{\text{surf}} = \frac{K^{z}(z,t)}{c} \,. \tag{20}$$

Then we have the continuity equation:

$$\partial_t \sigma + \partial_z K = 0. \tag{21}$$

Taking the z derivative of this equation

$$\partial_t \partial_z \sigma + \partial_z^2 K = 0, \qquad (22)$$

and using

$$\partial_z \sigma = \epsilon n_a \partial_z E^a = \epsilon n_a \left(-\frac{\mu}{c} \varepsilon^{ab} \partial_t H_b \right) = -\frac{\epsilon \mu}{c^2} \partial_t K \,, \tag{23}$$

we arrive at the wave equation for the surface Current

$$\left(\frac{\mu\epsilon}{c^2}\partial_t^2 - \frac{c^2}{\mu\epsilon}\partial_z^2\right)K = 0.$$
(24)

(d) The electric field is radially outward and equal to

$$E_{\omega}(\boldsymbol{x}) = \frac{\lambda_{\omega}/\epsilon}{2\pi\rho}.$$
(25)

Here and below we use the following notation for the electric field and other physical quantities,

$$E(\boldsymbol{x}, t, z) \equiv E_{\omega}(\boldsymbol{x})e^{-i\omega t + ikz}, \qquad (26)$$

where \boldsymbol{x} denotes the transverse vector $\boldsymbol{x} = (x, y)$. Thus the charge per length is

$$\lambda(t,z) \equiv \lambda_{\omega} e^{-i\omega t + ikz} \,. \tag{27}$$

The magnetic field is azimuthal, and circles around the cylinder

$$H_{\omega} = \frac{I_{\omega}/c}{2\pi\rho} = \frac{I_0/c}{2\pi\rho} \tag{28}$$

where in the last step we used that I_{ω} was called I_0 in the problem statement.

The charge per length λ_{ω} is related to the current through continuity to $I_{|omega|}$

$$\partial_t \sigma + \partial_z K = 0, \tag{29}$$

yielding

$$-i\omega\sigma_{\omega} + ikK_{\omega} = 0.$$
⁽³⁰⁾

Thus the amplitude of the charge wave is

$$\lambda_{\omega} = \frac{\sqrt{\mu\epsilon}}{c} I_0 \,. \tag{31}$$

where $K_{\omega} = I_0/(2\pi a)$ and $K_{\omega} = I_0/(2\pi b)$ on the inner and outer surface respectively.

We then evaluate the (time averaged) Poynting flux

$$\langle \boldsymbol{S} \rangle = c \langle \boldsymbol{E} \times \boldsymbol{H} \rangle = \frac{c}{2} \operatorname{Re}[E_{\omega}^* H_{\omega}] \hat{\boldsymbol{z}}$$
 (32)

$$= \frac{c}{2} \sqrt{\frac{\mu}{\epsilon}} \left(\frac{I_0}{c}\right)^2 \frac{1}{(2\pi\rho)^2} \hat{\boldsymbol{z}}.$$
(33)

Integrating over the transverse area of the cable gives the energy flux carried by the TEM wave

$$\frac{dW}{dt} = \int_{a}^{b} \langle S \rangle 2\pi\rho \,\mathrm{d}\rho \,, \tag{34}$$

$$= \frac{c}{4\pi} \sqrt{\frac{\mu}{\epsilon}} \left(\frac{I_0}{c}\right)^2 \log(b/a) \,. \tag{35}$$

(e) First an estimate. The electric and magnetic fields penetrate a distance of order the skin depth $\delta \sim \sqrt{c/(\omega\sigma)}$ into the metal. Consider a wire with cross sectional area A and length L; the resistance \mathcal{R} per length is

$$\frac{\mathcal{R}}{\ell} = \frac{1}{\sigma A} \,. \tag{36}$$

In this example the effective area is of order $A \sim 2\pi a\delta$, then the energy dissipated per length is of order

$$\frac{dW_{\rm loss}}{dtd\ell} \sim \frac{I^2 \mathcal{R}}{\ell} \sim \frac{I_0^2}{\sigma \delta} \frac{1}{2\pi a} \,. \tag{37}$$

Our computations below will confirm this estimate.

To actually calculate the resistance, we have to evaluate the Poynting flux directed into the ohmic material. Inside the material the magnetic field obeys a diffusion equation

$$\frac{\partial \boldsymbol{H}}{\partial t} = \frac{c^2}{\mu\sigma} \nabla^2 \boldsymbol{H} \,. \tag{38}$$

with diffusion coefficient

$$D = \frac{c^2}{\mu\sigma} \,. \tag{39}$$

Thus, if the system is driven with frequency ω , there is a characteristic length of order

$$\frac{\delta}{\sqrt{2}} \equiv \sqrt{\frac{D}{\omega}} \tag{40}$$

which emerges.

Choosing the normal wall face as the x direction, the parallel direction to the wall face as the y direction, and the longitudinal direction as the z direction. The magnetic field takes the form

$$H_y(t,x) = H_y^o e^{-i\omega t + ikx}, \qquad (41)$$

where

$$k = i^{1/2} \sqrt{\frac{\omega}{D}} = i^{1/2} \frac{\sqrt{2}}{\delta}.$$
 (42)

From the relation

$$\nabla \times H = \frac{\sigma}{c} E \,, \tag{43}$$

we see that the electric field is

$$E_z = \frac{c}{\sigma} \partial_x H_y(t, x) = i \frac{ck}{\sigma} H_y^o e^{-i\omega t + ikx} = i^{3/2} \frac{\sqrt{2}c}{\sigma\delta} H_y^o e^{-i\omega t + ikx}$$
(44)

Next we evaluate the Poynting flux into the wall

$$\langle \boldsymbol{S}_{\text{loss}} \cdot \hat{\boldsymbol{x}} \rangle |_{\text{surf}} = \frac{c}{2} \operatorname{Re}[\boldsymbol{E}_{\omega} \times \boldsymbol{H}_{\omega}^*] \cdot \hat{\boldsymbol{x}} |_{\text{surf}}$$
 (45a)

$$=\frac{c^2|H_y^0|^2}{2\sigma\delta} \tag{45b}$$

$$=\frac{|K_y|^2}{2\sigma\delta} \tag{45c}$$

In the last step we replaced $|H_y^o|$ (the amplitude of the surface field) with the amplitude of the surface current $|K_y|/c$. The surface current is defined as the integral of the volume current

$$\frac{K_z(t)}{c} = \int_0^\infty dx \, \sigma E_z(t, x) = H_y^o e^{-i\omega t} \tag{46}$$

Eq. (45b) and Eq. (45c) are rather general results which can be used in many problems to evaluate losses.

Finally, since the current on the inner and outer surfaces are

$$K_{\rm in} = \frac{I_0}{2\pi a}, \qquad K_{\rm out} = \frac{I_0}{2\pi b},$$
(47)

we may evaluate the energy lost per time per length by integrating Eq. (45c) over the walls of the surface. This yields

$$\frac{dW_{\rm loss}}{dtd\ell} = \frac{I_0^2}{2\sigma\delta} \left(\frac{1}{2\pi a} + \frac{1}{2\pi b}\right) \,,\tag{48}$$

where the first and second terms come from integrating Eq. (45c) over the inner and outer surface respectively

Electromagnetism 3

The Poisson Integral

(a) (5 points) Consider a grounded cylinder of radius a which is infinite in length. A line of charge inside the cylinder has charge per length λ , and is displaced from the center of the cylinder by a distance ρ_0 , with $\rho_0 < a$. Determine the potential $\varphi(\rho, \phi)$ at all points inside the cylinder¹.

Hint: consider an appropriate image line of charge at a distance a/ρ_0^2 from the center, and check that the appropriate boundary conditions are satisfied.

(b) (8 points) Now the line of charge is removed, but the surface cylinder is held at potential

$$V_0(\phi) = \begin{cases} V_0 & 0 < \phi < \pi \\ -V_0 & \pi \le \phi \le 2\pi \end{cases}$$

$$\tag{49}$$

Express the potential inside the cylinder $\varphi(\rho, \phi)$ as a definite integral using the Green function of (a).

(c) (7 points) The potential $\varphi(\rho, \phi)$ of part (b) may also be expressed as a series expansion in the appropriate separated solutions. Determine this expansion and check that the first term in the series agrees with the results of (b) for $\rho \ll a$.

¹Here $\rho = \sqrt{x^2 + y^2}$ and $\phi = \operatorname{atan}(y/x)$, with x, y measured from the center of the cylinder.



Figure 1: Coordinates for determining the potential from a line of charge in a cylinder.

Solution:

(a) The potential is found through inversion. Specifically if the line of charge is at position $\vec{\rho}_1 = (\rho_0, 0)$, then we will take an image line of charge at position $\vec{\rho}_2 = (a^2/\rho_0, 0)$ with charge per length λ' . The full potential is

$$\varphi(\vec{\rho}) = -\frac{\lambda}{4\pi} \log(\vec{\rho} - \vec{\rho}_1)^2 - \frac{\lambda'}{4\pi} \log(\vec{\rho} - \vec{\rho}_2)^2 + \text{const}$$
(50)

Expressing Eq. (50) using the coordinates shown in Fig. 1 we find

$$\log(\vec{\rho} - \vec{\rho}_1)^2 = \log(\rho^2 + \rho_0^2 - 2\rho\rho_0\cos(\phi))$$
(51)

$$\log(\vec{\rho} - \vec{\rho}_2)^2 = \log(\rho^2 + \frac{a^4}{\rho_0^2} - \frac{2a^2\rho}{\rho_0}\cos(\phi))$$
(52)

$$= \log \left((\rho_0 \rho/a)^2 + a^2 - 2\rho \rho_0 \cos(\phi) \right) + \log(a^2/\rho_0^2)$$
(53)

Notice that when $\rho = a$ the two logarithms differ by a constant, $\log a^2/\rho_0^2$. With this result we take $\lambda' = -\lambda$, and set the constant in Eq. (50) to $-\lambda/(4\pi)\log(a^2/\rho_0^2)$, to find the required potential

$$\varphi(\vec{\rho}) = -\frac{\lambda}{4\pi} \log \left(\frac{\rho^2 + \rho_0^2 - 2\rho\rho_0 \cos(\phi))}{(\rho_0 \rho/a)^2 + a^2 - 2\rho\rho_0 \cos(\phi)} \right) \,. \tag{54}$$

This satisfies the Poisson equation $-\nabla^2 \varphi(\vec{\rho}) = \lambda \delta^2(\vec{\rho} - \vec{\rho}_1)$, and the Dirichlet boundary conditions

$$\varphi(\vec{\rho})|_{\rho=a} = 0.$$
(55)

(b) Now we will use Green theorem to determine the potential everywhere in the interior given the Green function and the boundary values of the potential. The Dirichlet Green function is the potential at point $\vec{\rho}$ from a unit charge at point $\vec{\rho}_0 = (\rho_0 \cos(\phi_0), \rho_0 \sin(\phi_0))$. Translating Eq. (50) into this slightly more general geometry, the Dirichlet Green function is

$$G_D(\vec{\rho}, \vec{\rho_0}) = -\frac{1}{4\pi} \log \left(\frac{\rho^2 + \rho_0^2 - 2\rho\rho_0 \cos(\phi - \phi_0))}{(\rho_0 \rho/a)^2 + a^2 - 2\rho\rho_0 \cos(\phi - \phi_0)} \right) \,.$$
(56)

The surface Green function (or boundary to bulk propagator) is the normal derivative of the Dirichlet Green function

$$K(\vec{\rho}, \phi_0) = -\boldsymbol{n} \cdot \frac{\partial G_D(\vec{\rho}, \vec{\rho}_0)}{\partial \vec{\rho}_0} \Big|_{\text{surf}} , \qquad (57)$$

$$= -\frac{\partial G_D}{\partial \rho_0}\Big|_{\rho_0=a} \,. \tag{58}$$

With straightforward algebra we find

$$K(\vec{\rho},\phi_0) = \frac{a}{2\pi} \frac{1 - \rho^2/a^2}{\rho^2 + a^2 - 2\rho a \cos(\phi - \phi_0)}.$$
(59)

The boundary to bulk propagator takes the boundary value of the potential as input and determines the potential in the interior as prescribed by the Green theorem:

$$\varphi(\vec{\rho}) = \int_0^{2\pi} a \, d\phi_0 \, K(\vec{\rho}, \phi_0) V_0(\phi_0) \,. \tag{60}$$

For the problem at hand this integral reads

$$\varphi(\vec{\rho}) = V_0 \int_0^{\pi} a d\phi_0 \left[\frac{a}{2\pi} \frac{1 - \rho^2/a^2}{\rho^2 + a^2 - 2\rho a \cos(\phi - \phi_0)} - \frac{a}{2\pi} \frac{1 - \rho^2/a^2}{\rho^2 + a^2 - 2\rho a \cos(\phi + \phi_0)} \right].$$
(61)

For $\rho \ll a$ we find

$$\varphi(\vec{\rho}) \simeq V_0 \int_0^{\pi} d\phi_0 \frac{1}{2\pi} \frac{2\rho}{a} \left(\cos(\phi - \phi_0) - \cos(\phi + \phi_0) \right) \,, \tag{62}$$

$$=\frac{4V_0}{\pi}\frac{\rho\sin(\phi)}{a}\,.\tag{63}$$

(c) Now we determine the potential using the series expansion of the Laplace equation in cylindrical coordinates

$$\varphi(\vec{\rho}) = A_0 \log \rho + A_1 + \sum_{n=1}^{\infty} \left(C_n \rho^n + \frac{D_n}{\rho^n} \right) \cos(n\phi) + \sum_{n=1}^{\infty} \left(E_n \rho^n + \frac{F_n}{\rho^n} \right) \sin(n\phi) \,. \tag{64}$$

We limit ourselves to sin terms since the potential is odd in this case, and drop the terms which are singular as $\rho \rightarrow 0$, yielding

$$\varphi(\vec{\rho}) = \sum_{n=1}^{\infty} E_n \rho^n \sin(n\phi) \,. \tag{65}$$

Using the orthogonality relation

$$\int_0^{\pi} d\phi \, \sin(n\phi) \sin(m\phi) = \delta_{nm} \frac{\pi}{2} \,, \tag{66}$$

we find the coefficients

$$E_n a^n = \frac{2}{\pi} \int_0^{\pi} d\phi_0 V_0(\phi_0) \,\sin(n\phi_0) \,, \tag{67}$$

$$=\frac{4V_0}{\pi n} \qquad n = 1, 3, 5, \dots,$$
(68)

leading to our final result for the potential

$$\varphi(\rho) = \sum_{n=1,3,5\dots}^{\infty} \frac{4V_0}{\pi n} \left(\frac{\rho}{a}\right)^n \sin(n\phi) \,. \tag{69}$$

The first term in this expansion agrees with Eq. (63) derived in (b).

Quantum Mechanics 1

One dimensional "atoms" and "molecules" in external fields

The purpose of this problem is to study the ionization process of a one-dimensional "atom", and the excitation process of a one-dimensional "molecule" under the action of an external time-dependent interaction.

a. (5 points) Consider a one-dimensional atom composed of a spinless particle of charge e and mass m bound by a delta-function potential $V(x) = -g \,\delta(x)$. Find the normalized energy eigenstates of the bound atom. Find the normalized energy eigenstates of the unbound atom assumed as free particles in a box of size L. Derive their density of states as a function of their energy E_k where k is the wavenumber.

b. (5 points) A time-dependent electric field is applied on the atom,

$$E(t) = E_0 \theta(t) \theta(\tau - t) \tag{1}$$

with $\theta(t)$ a step function. What is the probability $P(E_k)dE_k$ for the charge to be in an unbound state with energy between E_k and $E_k + dE_k$? Discuss the physical nature of this result for small and large k.

c. (5 points) Now, consider a one-dimensional molecule composed of two distinguishable spin- $\frac{1}{2}$ particles with charges $e_{1,2}$ and masses $m_{1,2}$ coupled harmonically:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2} \left(\frac{1}{m_1} + \frac{1}{m_2} \right)^{-1} \omega^2 (x_1 - x_2)^2 + g_S \,\vec{\sigma}_1 \cdot \vec{\sigma}_2 \,. \tag{2}$$

What are the energy levels, wavefunctions and degeneracies of the molecule? Give the explicit form of the normalized wave functions of the two lowest energy levels of the molecule for $g_S/\hbar\omega \ll 1$.

d. (5 points) A time- and spin-dependent interaction is now applied on the molecule

$$V(t) = \left(V_1 + V_2 \frac{(x_1 - x_2)}{L}\right) \sigma_{1x} \theta(t) \sin(\omega t).$$
(3)

Here V_1 and V_2 are constants, x_1 and x_2 are the spatial coordinates of the particles, and σ_{1x} is the spin operator acting on the first particle. The molecule is initially in the ground state when V(t) is applied. What is the transition probability to find the molecule in an excited state if $V_{1,2}$ are small. Comment on any selection rule.

a. If we set $E = -(\hbar k)^2/2m < 0$ and $\alpha = 2mg/\hbar^2$ for the bound state, then the eigenvalue problem is

$$\Psi'' - k^2 \Psi + \alpha \Psi = 0 \tag{4}$$

The normalized bound state solution and energy are

$$E = -\frac{mg^2}{2\hbar^2}$$

$$\Psi(x) = \left(\frac{mg}{\hbar^2}\right)^{\frac{1}{2}} e^{-mg|x|/\hbar^2}$$
(5)

The normalized plane waves in the box of length L with energy $E_k = (\hbar k)^2/2m$ are

$$\Psi_k(x) = \frac{1}{\sqrt{L}} e^{ik_n x} = \frac{1}{\sqrt{L}} e^{i2n\pi x/L} \tag{6}$$

with $n = 0, \pm 1, \pm 2, \dots$ The energy levels are 2-degenerate for $n \neq 0$. The density of free energy levels is

$$n(E_k)dE_k = 2n(k)dk = 2\frac{L\hbar k}{2\pi} = \frac{L}{\pi\hbar} \left(\frac{m}{2E_k}\right)$$
(7)

b. The electric field acts through its dipole form V(t) = -exE(t). The probability to transition from bound to free is

$$P_{k0}(\tau) = \frac{1}{\hbar^2} |\langle k|exE_0|0\rangle|^2 \left| \int_0^\tau dt e^{i\omega_{k0}t} \right|^2 = \frac{1}{\hbar^2} |\langle k|exE_0|0\rangle|^2 \frac{\sin^2(\omega_{k0}\tau/2)}{(\omega_{k0}/2)^2}$$
(8)

with $\omega_{k0} = E_k + mg^2/2\hbar^2$ and

$$\langle k | ex E_0 | 0 \rangle = -\frac{eE_0}{\sqrt{L}} \left(\frac{gm}{\hbar^2}\right) \int_{-\infty}^{+\infty} x e^{-ikx - K|x|} \\ = \left(\frac{gm}{\hbar^2 L^3}\right)^{\frac{3}{2}} \frac{4ieE_0k}{(k^2 + (gm/\hbar^2)^2)^2}$$
(9)

The probability to transit to the interval $[E_k, E_k + dE_k]$ is

$$P(E_k)dE_k = P_{k0}(\tau)n(E_k)dE_k \tag{10}$$

c. The spectrum of the molecule including its translation is

$$E_{P,nS} = \frac{P^2}{2M} + \left(n + \frac{1}{2}\right)\hbar\omega + 2g_S\left(S(S+1) - \frac{3}{2}\right)$$
$$\Psi_{P,nSM_S}(X;x) = \left(\frac{1}{\sqrt{2\pi}}e^{iPX/\hbar}\right)\left(\frac{1}{\pi^{\frac{1}{4}}x_0}H_n(x)e^{-x^2/2x_0^2}\right)\chi_{SM_S}$$
(11)

with $M = m_1 + m_2$ and $\vec{S} = \vec{S}_1 + \vec{S}_2$. Each molecular state is 2S + 1 degenerate. The lowest two states occur for P = 0 and

$$E_{0,00} = \frac{1}{2}\hbar\omega - 3g_S \qquad \Psi_{0,000}(x) \sim e^{-x^2/2x_0^2} \left(\chi_{00} = \frac{1}{\sqrt{2}}(\alpha_1\beta_2 - \alpha_2\beta_1)\right)$$

$$E_{0,01} = \frac{1}{2}\hbar\omega + g_S \qquad \Psi_{0,01M_S}(x) \sim e^{-x^2/2x_0^2} \left(\chi_{1M_S} = (\alpha_1\alpha_2, \frac{1}{\sqrt{2}}(\alpha_1\beta_2 + \alpha_2\beta_1), \beta_1\beta_2)\right)$$
(12)

with $\alpha_{1,2} = \uparrow$ and $\beta_{1,2} = \downarrow$ for each particle.

d. For $V_{1,2}$ small, the transition amplitude follows from the Fermi-Golden rule

$$C_{0\to n}(t=\infty) = \frac{1}{i\hbar} \langle n|V|0\rangle \int_0^\infty dt \sin(\omega t) e^{i\omega_{n0}t}$$
(13)

with $\hbar\omega_{n0} = E_{n,SM_S} - E_{0,00}$. The transition probability is

$$P_{0\to n} = \frac{|\langle n|V|0\rangle|^2}{4\hbar^2} \left(\frac{1}{(\omega+\omega_{n0})^2+\epsilon^2} + \frac{1}{(\omega-\omega_{n0})^2+\epsilon^2}\right) \to \frac{|\langle n|V|0\rangle|^2}{4\hbar^2} \frac{1}{(\omega-\omega_{n0})^2+\epsilon^2} \tag{14}$$

as the second term in the bracket is dominant. Since $\sigma_{1x}\alpha_1 = \beta_1$ and $\sigma_{1x}\beta_1 = \alpha_1$, then

$$\langle n|V|0\rangle \equiv \langle 0, nSM_S|V|0, 000\rangle = \frac{\delta_{S1}}{\sqrt{2}} (\delta_{M_S, +1} - \delta_{M_S, -1}) \left(V_1 \delta_{n0} + V_2 \frac{x_0}{\sqrt{2}L} \delta_{n1} \right)$$
(15)

The transition is to the spin-triplet ground state for the monopole interaction V_1 , i.e $E_{0,00} \rightarrow E_{0,01}$ with $\omega_{10} = 4g_S$, and to the spin-triplet excited state of the harmonic oscilator for the dipole interaction V_2 , i.e. $E_{0,00} \rightarrow E_{1,11}$ with $\omega_{10} = \frac{1}{2}\hbar\omega + 4g_S$.

Quantum Mechanics 2

A complex potential

In this problem we will explore the partial transparency of the nucleus to high energy eutrons, i.e. their partial absorption. For that, a complex potential language will be used. Consider a beam of non-relativistic neutrons of mass m and energy E moving along the z-axis towards a nuclear target. The incoming neutron will be treated as a plane wave with wave number k and the nucleus will be approximated by a constant complex potential $\mathbf{V} = -U - iW$. By analogy with optics, we define n = v/c as the index of refraction, where v and c are the effective velocities of the neutron inside and outside of the nucleus respectively.

a. 4 **points** Derive an expression for n, and express its limit (by Taylor expansion) for high energy neutrons. Derive the intensity of the neutron beam along the z-direction.

b. 4 **points** Derive the equation for the neutron flow of probability and show that it is not conserved. What is the net rate loss of neutrons? Where do the neutrons go?

The nucleus can be thought of as a collection of N (spinless) nucleons, moving in an attractive well potential -U(r) for $r \leq R$, with pair interactions $V(\vec{r_1}, \vec{r_2})$ described by the following Hamiltonian in the second quantized form

$$\mathbf{H} = \sum_{a} e_{a} a_{a}^{\dagger} a_{a} + \frac{1}{2} \sum_{ab,cd} \langle ab | V | cd \rangle \ a_{a}^{\dagger} a_{b}^{\dagger} a_{d} a_{c} , \qquad (16)$$

with $e_a |a\rangle = (\vec{p}^2/2m - U(r)) |a\rangle$. a_a^{\dagger}, a_a are creation and annihilation operators.

c. 6 points Write the commutation relations for a, a^{\dagger} and use them to define the properly symmetrized and normalized ground state $|0_F\rangle$ of the nucleus in zeroth order in V. Use perturbation theory to correct the ground state energy to first order in V.

d. 6 points The neutron in parts **a-b** can be thought to be in an initial state $|\Psi_E\rangle = a_E^{\dagger} |0_F\rangle$ with energy E. Use Fermi Golden rule to express the transition rate between this state and the allowed final states $|\Psi_F\rangle = a_p^{\dagger} a_{p'}^{\dagger} a_h |0_F\rangle$. This rate can be used as a microscopic estimate for W. Explain.

a. The neutron obeys the stationary equation

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + \mathbf{V}\right) \Psi_E(z) = E \Psi_E(z) \tag{17}$$

with a solution $\Psi(z) \approx e^{iKz}$ and $K = \frac{1}{\hbar}\sqrt{2m(E+U+iW)}$. The index of refraction is

$$n = \frac{v}{c} = \frac{K}{k} = \left(\frac{E + U + iW}{E}\right)^{\frac{1}{2}} \approx 1 + \frac{1}{2}\frac{U}{E} + \frac{i}{2}\frac{W}{E}$$
(18)

where the large E limit is the last expression. As in optics K = nk and for large E, the z-attenuation is

$$1 - |\Psi(z)|^2 = 1 - \left|e^{iknz}\right|^2 \approx 1 - e^{-\frac{kW}{E}z}$$
(19)

b. The time evolution of the probability current $(\Psi^{\dagger}\Psi, \Psi^{\dagger}\vec{v}\Psi)$ follows from the time dependent Shrodinger equation

$$i\hbar\Psi(t,\vec{x}) = \left(-\frac{\hbar^2\nabla^2}{2m} + \mathbf{V}\right)\Psi(t,\vec{x})$$
(20)

and its conjugate using the symmetrized velocity $\vec{v} = \hbar \vec{\nabla} / im$. The result is

$$\frac{\partial}{\partial t}|\Psi|^2 = -\vec{\nabla}\cdot\Psi^{\dagger}\vec{v}\Psi - \frac{2W}{\hbar}|\Psi|^2 \tag{21}$$

The rate of neutron loss is

$$\frac{dN}{dt} = -\frac{2}{\hbar} \left\langle \Psi_E | W | \Psi_E \right\rangle = -\frac{2W}{\hbar} N \tag{22}$$

The loss is from the elastic channel to the inelastic channels of the nucleus. In other words, the neutrons get absorbed and excite the nucleus.

c. The a, a^{\dagger} obeys standard anti-commutation rules. For V = 0, the state of N-non-interacting fermions is given by a Slater determinant

$$|0_F\rangle = \prod_{a\in F} a_a^{\dagger} |0\rangle \tag{23}$$

The energy to first order is

$$E_F + E_1 = \sum_{a \in F} e_a + \frac{1}{2} \sum_{ab,cd} \langle ab | V | cd \rangle \ \langle 0_F | a_a^{\dagger} a_b^{\dagger} a_d a_c | 0_F \rangle = \sum_{a \in F} e_a + \frac{1}{2} \sum_{a,b \in F} \langle ab | V | ab \rangle_A$$
(24)

d. The rate of transition from the initial neutron state to the final 2-particles-1-hole state from Fermi Golden rule is (connected part)

$$w_{i \to f} = \frac{2\pi}{\hbar} \sum_{p, p' \notin F; h \in F} \left| \left\langle 0_F \left| a_E \left(\frac{1}{2} \sum_{ab, cd} \left\langle ab | V | cd \right\rangle \, a_a^{\dagger} a_b^{\dagger} a_d a_c \right) a_p^{\dagger} a_{p'}^{\dagger} a_h \right| 0_F \right\rangle \right|^2 \delta(e_p + e_{p'} - e_h - E)$$

$$\tag{25}$$

which is readily reduced by commutation to

$$w_{i \to f} = \frac{2}{\hbar} \left\langle \psi_E | \mathbf{W} | \psi_E \right\rangle \tag{26}$$

with

$$\langle \psi_E | \mathbf{W} | \psi_E \rangle = \sum_{p, p' \notin F; h \in F} \langle Eh | V | pp' \rangle \langle pp' | V | Eh \rangle \times \pi \delta(E + e_h - e_p - e_{p'})$$
(27)

(26) is the rate of transition from the flying neutron with energy E to an excited state of the nucleus with 2 particles labeled by $p, p' \notin F$ and 1 hole labeled by $h \in F$. This rate loss as in (22) with (27) is a microscopic estimate for W which realistically is a non-local potential. Note that energetically $E + e_h = e_p + e_{p'}$ is allowed with $e_{p,p'} > E_F$ and $e_h < E_F$, so the delta-function has a support.

Quantum Mechanics 3

Polarized spin

In this problem, your task is to derive some basic properties of particle's spin, starting exclusively from the commutation relations between the Hermitian Cartesian components \hat{S}_j of its vector operator \hat{S} :

$$\left[\hat{S}_{j},\hat{S}_{k}\right]=i\hbar\hat{S}_{l}\varepsilon_{jkl}$$

(where each of indices *j*, *k*, and *l* may take values from 1 to 3, and ε_{jkl} is the Levi-Civita permutation symbol), plus the fact that the each of these component operators has a set of eigenstates, with eigenvalues separated by multiples of \hbar . Then you would use the derived properties of the operators to analyze properties of a polarized spin.

A (2 points). Calculate the following commutators: $[\hat{S}^2, \hat{S}_j], [\hat{S}_+, \hat{S}_-]$ and $[\hat{S}_3, \hat{S}_{\pm}]$, and prove the operator relation $\hat{S}^2 = \hat{S}_-\hat{S}_+ + \hat{S}_3^2 + \hbar\hat{S}_3$, where $\hat{S}^2 \equiv \hat{S}_1^2 + \hat{S}_2^2 + \hat{S}_2^2$, and $\hat{S}_{\pm} \equiv \hat{S}_1 \pm i\hat{S}_2$.

B (5 points). Prove that for the common eigenstates of the operators \hat{S}^2 and \hat{S}_3 , the eigenvalue of the former operator is $\hbar^2 s(s + 1)$, where *s* is an either integer or half-integer quantum number,¹ which sets the limits for the possible eigenvalues $S_3 = \hbar m$ of the latter operator: $-s \le m \le +s$.

C (3 points). In the basis of the these common eigenstates, calculate all matrix elements of the operators \hat{S}_{\pm} and $\hat{S}_{1,2}$, and then the diagonal matrix elements of operators \hat{S}_1^2 , \hat{S}_2^2 , $\hat{S}_1\hat{S}_2$, and $\hat{S}_2\hat{S}_1$.

D (7 points). A free particle with spin *s* and a gyromagnetic ratio $\gamma \neq 0$ has been placed into an external constant magnetic field, and allowed to relax into its ground state, thus "polarizing" the spin. Use the results of the previous tasks to calculate the expectation value of its spin component along a direction at angle θ with that of the field, and the r.m.s. uncertainty of this value.

E (3 points). Specify your results for $\theta = \pi/2$, and give physical interpretations for their dependence on the spin *s*.

¹ This constant *s* is of course what is called the particle's spin in the narrow sense of the word.

Solutions:

A (2 points). First, let us calculate the commutator of $\hat{S}^2 = \hat{S}_1^2 + \hat{S}_2^2 + \hat{S}_3^2$ with, for example, \hat{S}_1 :

$$\left[\hat{S}^{2},\hat{S}_{1}\right] = \left[\hat{S}_{1}^{2},\hat{S}_{1}\right] + \left[\hat{S}_{2}^{2},\hat{S}_{1}\right] + \left[\hat{S}_{3}^{2},\hat{S}_{1}\right] = 0 + \left(\hat{S}_{2}\hat{S}_{2}\hat{S}_{1} - \hat{S}_{1}\hat{S}_{2}\hat{S}_{2}\right) + \left(\hat{S}_{3}\hat{S}_{3}\hat{S}_{1} - \hat{S}_{1}\hat{S}_{3}\hat{S}_{3}\right),$$

using the commutation rule given in the assignment, which may be spelled out for our cases as:

$$\hat{S}_1\hat{S}_2 = \hat{S}_2\hat{S}_1 + i\hbar\hat{S}_3, \quad \hat{S}_1\hat{S}_3 = \hat{S}_3\hat{S}_1 - i\hbar\hat{S}_2.$$

Applying each of them twice to the corresponding terms, we get

$$\begin{split} \left[\hat{S}^{2},\hat{S}_{1}\right] &= \hat{S}_{2}\hat{S}_{2}\hat{S}_{1} - \left(\hat{S}_{2}\hat{S}_{1} + i\hbar\hat{S}_{3}\right)\hat{S}_{2} + \hat{S}_{3}\hat{S}_{3}\hat{S}_{1} - \left(\hat{S}_{3}\hat{S}_{1} - i\hbar\hat{S}_{2}\right)\hat{S}_{3} \\ &= \hat{S}_{2}\hat{S}_{2}\hat{S}_{1} - \hat{S}_{2}\left(\hat{S}_{2}\hat{S}_{1} + i\hbar\hat{S}_{3}\right) - i\hbar\hat{S}_{3}\hat{S}_{2} + \hat{S}_{3}\hat{S}_{3}\hat{S}_{1} - \hat{S}_{3}\left(\hat{S}_{3}\hat{S}_{1} - i\hbar\hat{S}_{2}\right)\hat{S}_{1}\hat{S}_{3} + i\hbar\hat{S}_{2}\hat{S}_{3} \\ &= -i\hbar\hat{S}_{2}\hat{S}_{3} - i\hbar\hat{S}_{3}\hat{S}_{2} + i\hbar\hat{S}_{3}\hat{S}_{2} + i\hbar\hat{S}_{2}\hat{S}_{3} = 0. \end{split}$$
(1)

Due to the symmetry of \hat{S}^2 , its commutators with \hat{S}_2 and \hat{S}_3 are evidently similar.

Next, using the definition of the operators \hat{S}_+ , we get

$$\left[\hat{S}_{+},\hat{S}_{-}\right] = \left[\left(\hat{S}_{1}+i\hat{S}_{2}\right),\left(\hat{S}_{1}-i\hat{S}_{2}\right)\right] = i\left[\hat{S}_{2},\hat{S}_{1}\right] - i\left[\hat{S}_{1},\hat{S}_{2}\right] = -2i\left[\hat{S}_{1},\hat{S}_{2}\right] = -2i\left(i\hbar\hat{S}_{3}\right) = 2\hbar\hat{S}_{3}$$

The calculation of the last commutator listed in the assignment is also simple:

$$[\hat{S}_{3}, \hat{S}_{\pm}] = [\hat{S}_{3}, (\hat{S}_{1} \pm i\hat{S}_{2})] = [\hat{S}_{3}, \hat{S}_{1}] \pm i[\hat{S}_{3}, \hat{S}_{2}] = i\hbar\hat{S}_{2} \pm i(-i\hbar\hat{S}_{1}) = \pm\hbar(\hat{S}_{1} \pm i\hat{S}_{2}) = \pm\hbar\hat{S}_{\pm}.$$

Finally, spelling out the right-hand side of the relation to be proved, we get

$$\hat{S}_{-}\hat{S}_{+} + \hat{S}_{3}^{2} + \hbar\hat{S}_{3} = (\hat{S}_{1} - i\hat{S}_{2})(\hat{S}_{1} + i\hat{S}_{2}) + \hat{S}_{3}^{2} + \hbar\hat{S}_{3} = \hat{S}_{1}^{2} + \hat{S}_{2}^{2} + i(\hat{S}_{1}\hat{S}_{2} - \hat{S}_{2}\hat{S}_{1}) + \hat{S}_{3}^{2} + \hbar\hat{S}_{3} = \hat{S}_{1}^{2} + \hat{S}_{2}^{2} + i(\hat{h}\hat{S}_{3}) + \hat{S}_{3}^{2} + \hbar\hat{S}_{3} = \hat{S}_{1}^{2} + \hat{S}_{2}^{2} + i(\hat{h}\hat{S}_{3}) + \hat{S}_{3}^{2} + \hbar\hat{S}_{3} = \hat{S}_{1}^{2} + \hat{S}_{2}^{2} + \hat{S}_{3}^{2} + \hat{S}_{3}^{$$

q.e.d.

B (5 points). First of all, since the operators \hat{S}^2 and \hat{S}_3 commute, they may share some eigenstates; let us call their eigenkets $|m\rangle$, where *m* is a certain index ("magnetic quantum number", not necessarily integer) numbering the corresponding eigenvalues sequentially. According to the fact given in the assignment, we may always select the indices *m* so that

$$\hat{S}_{3}|m\rangle = \hbar m |m\rangle, \tag{2}$$

with the adjacent values of *m* different by ± 1 . Let us rewrite the last of the commutation relations derived in part A as

$$\hat{S}_3\hat{S}_{\pm} = \hat{S}_{\pm}\hat{S}_3 \pm \hbar\hat{S}_{\pm},$$

and act by both its parts on any eigenket $|m\rangle$:

$$\hat{S}_{3}\hat{S}_{\pm}|m\rangle = \hat{S}_{\pm}\hat{S}_{3}|m\rangle \pm \hbar\hat{S}_{\pm}|m\rangle.$$

Now applying Eq. (2) to the first term in the right-hand part, we may rewrite the result as

$$\hat{S}_{3}(\hat{S}_{\pm}|m\rangle) = \hbar(m\pm 1)\hat{S}_{\pm}|m\rangle.$$

This equality means that the states $\hat{S}_{\pm}|m\rangle$ are also eigenstates of the operator \hat{S}_3 , corresponding to eigenvalues $m \pm 1$, which are adjacent to the eigenvalue m:

$$\hat{S}_{\pm} | m \rangle = S_{\pm}^{(m)} | m \pm 1 \rangle, \qquad (3)$$

where $S_{\pm}^{(m)}$ are some *c*-numbers (essentially, the only nonvanishing matrix elements of the "ladder operators" \hat{S}_{\pm} in the basis of states *m*), to be calculated later. Thus the operators move the system, respectively, up and down the ladder of the eigenstates *m* – see Fig. on the right.

This state ladder must have ends in both directions, because an infinite increase of |m|, and hence of the modulus

of the expectation value $\hbar m$ of the observable S_3 , would cause the expectation values of the operator

$$\hat{S}_1^2 + S_2^2 = \hat{S}^2 - \hat{S}_3^2$$

which corresponds to a non-negative observable, to become negative. Hence there should be two states on both ends of the ladder, m_{max} and m_{min} , such that

$$\hat{S}_{+} | m_{\max} \rangle = 0, \qquad \hat{S}_{-} | m_{\min} \rangle = 0.$$
⁽⁴⁾

Due to the symmetry of the whole problem with respect to the replacement $m \leftrightarrow -m$, we should have $m_{\min} = -m_{\max}$. The value m_{\max} is exactly what is called the particle's spin *s*, so that the limits of *m* may be represented as

$$-s \le m \le +s$$

Since the difference m_{max} - $m_{\text{min}} = 2s$ should correspond to an integer number of ladder steps, *s* must be either integer of half-integer.

In order to calculate eigenvalues of the operator \hat{S}^2 , we may use the relation proved in part A:

$$\hat{S}^2 = \hat{S}_- \hat{S}_+ + \hat{S}_3^2 + \hbar \hat{S}_3.$$
⁽⁵⁾

Acting by both its sides on the ket-vector $|s\rangle$ of the highest state of the ladder, and then using Eq. (2) and the first of Eqs. (4), we get

$$\hat{S}^{2}|s\rangle = \hat{S}_{-}\hat{S}_{+}|s\rangle + \hat{S}_{3}^{2}|s\rangle + \hbar\hat{S}_{3}|s\rangle = 0 + (\hbar s)^{2}|s\rangle + \hbar(\hbar s)|s\rangle = \hbar^{2}s(s+1)|s\rangle,$$

Next, according to Eq. (1) and its analogs for all other components, the operators \hat{S}^2 and \hat{S}_- commute, so that we may use Eq. (3) twice to write

eigenket eigenvalue of
$$\hat{S}_{3}$$

 $\hat{S}_{+}|m\rangle$ $\xrightarrow{\dots}$ $\hbar(m+1)$
 $|m\rangle$ \hat{S}_{+} \hat{S}_{-} $\hbar m$
 $\hat{S}_{-}|m\rangle$ $\xrightarrow{\dots}$ $\hbar(m-1)$

$$\hat{S}^{2}|s-1\rangle = \hat{S}^{2} \frac{\hat{S}_{-}}{S_{-}^{(s)}}|s\rangle = \frac{\hat{S}_{-}}{S_{-}^{(s)}}\hat{S}^{2}|s\rangle = \frac{\hbar^{2}s(s+1)}{S_{-}^{(s)}}\hat{S}_{-}|s\rangle = \hbar^{2}s(s+1)|s-1\rangle,$$
$$\hat{S}^{2}|s-2\rangle = \hat{S}^{2} \frac{\hat{S}_{-}}{S_{-}^{(s-1)}}|s-1\rangle = \frac{\hat{S}_{-}}{S_{-}^{(s-1)}}\hat{S}^{2}|s-1\rangle = \frac{\hbar^{2}s(s+1)}{S_{-}^{(s-1)}}\hat{S}_{-}|s-1\rangle = \hbar^{2}s(s+1)|s-2\rangle,$$

etc. - until m = -s, where the matrix element *S*₋ turns to zero. This means that the eigenstates of \hat{S}^2 in all available states *m* are indeed the same, equal to $\hbar^2 s(s + 1)$. This fact is very natural, because physically all these states correspond to different spatial orientations of the spin vector **S**, maintaining its effective magnitude.

C (3 points). Let us start from the finding the matrix elements $S_{\pm}^{(m)}$ participating in Eq. (3). First of all, we are speaking essentially about finding just one, rather than two sets of coefficients $S_{\pm}^{(m)}$. Indeed, let us use the general bra-ket conjugation rule to write

$$\langle m | \hat{S}_{+}^{\dagger} | m+1 \rangle = \langle m+1 | \hat{S}_{+} | m \rangle^{*}.$$

Since the spin component operators \hat{S}_{j} are Hermitian, the ladder operators $\hat{S}_{\pm} \equiv \hat{S}_{1} \pm i\hat{S}_{2}$ are Hermitian conjugates of each other, and this equality may be rewritten as

$$\langle m | \hat{S}_{-} | m+1 \rangle = \langle m+1 | \hat{S}_{+} | m \rangle^*.$$

Now applying Eq. (3), and assuming that all eigenstates have the same norm: $\langle m|m\rangle = \langle m+1|m+1\rangle$ (as may always be done by proper normalization), we get

$$S_{-}^{(m+1)} = \left(S_{+}^{(m)}\right)^{*},\tag{6}$$

so that the problem is reduced to finding just one of these coefficient sets, say $S_{+}^{(m)}$.

This may be done, for example, by applying Eq. (5) again, but now to an arbitrary state *m*:

$$\hat{S}^2 |m\rangle = \hat{S}_{-}\hat{S}_{+}|m\rangle + \hat{S}_{3}^2 |m\rangle + \hbar \hat{S}_{3}|m\rangle.$$

Using the eigenvalues calculated above, and Eq. (3), we get

$$\hbar^{2} s(s+1) |m\rangle = \hat{S}_{-} S_{+}^{(m)} |m+1\rangle + (\hbar m)^{2} |m\rangle + \hbar (\hbar m) |m\rangle = \left[\hbar^{2} m(m+1) + S_{-}^{(m+1)} S_{+}^{(m)}\right] |m\rangle.$$

For all existing eigenstates (with $|m| \le s$), this equality may be true only if the *c*-number factors in its first and last forms are equal. Together with Eq. (6), this gives us the final answer:

$$\left|S_{+}^{(m)}\right| = \left|S_{-}^{(m+1)}\right| = \hbar [s(s+1) - m(m+1)]^{1/2}.$$

Other frequently used forms of the same result are

$$\left|S_{\pm}^{(m)}\right| = \hbar \left[s(s+1) - m(m\pm 1)\right]^{1/2} = \hbar \left[\left(s\pm m + 1\right)\left(s\mp m\right)\right]^{1/2}.$$
(7)

As a sanity check, the coefficient $S_{+}^{(m)}$ turns into zero at m = s, while $S_{-}^{(m)}$ does the same at m = -s, thus assuring Eqs. (4). In what follows, we will use Eqs. (7) for $S_{\pm}(m)$, thus dropping possible phase factors $\exp\{\pm i\varphi_m\}$ before these matrix elements, because they are inconsequential for the final results.

Next, from the definition of the ladder operators \hat{S}_+ , we readily get the reciprocal relations

$$\hat{S}_1 = \frac{\hat{S}_+ + \hat{S}_-}{2}, \qquad \hat{S}_2 = \frac{\hat{S}_+ - \hat{S}_-}{2i},$$

so that using Eqs. (7) we may calculate the matrix elements of $\hat{S}_{1,2}$ in two equivalent forms:

$$\langle m | \hat{S}_{1} | m' \rangle = \frac{1}{2} \langle m | \hat{S}_{+} | m' \rangle + \frac{1}{2} \langle m | \hat{S}_{-} | l, m' \rangle$$

$$= \frac{\hbar}{2} \{ [(s+m)(s-m+1)]^{1/2} \delta_{m,m'+1} + [(s-m)(s+m+1)]^{1/2} \delta_{m,m'-1} \}$$

$$= \frac{\hbar}{2} \{ [(s+m'+1)(s-m')]^{1/2} \delta_{m',m-1} + [(s-m'+1)(s+m')]^{1/2} \delta_{m',m+1} \},$$

$$\langle m | \hat{S}_{2} | m' \rangle = \frac{1}{2i} \langle m | \hat{S}_{+} | m' \rangle - \frac{1}{2i} \langle m | \hat{S}_{-} | l, m' \rangle$$

$$= \frac{\hbar}{2i} \{ [(s+m)(s-m+1)]^{1/2} \delta_{m,m'+1} - [(s-m)(s+m+1)]^{1/2} \delta_{m,m'-1} \}$$

$$= \frac{\hbar}{2i} \{ [(s+m'+1)(s-m')]^{1/2} \delta_{m',m-1} - [(s-m'+1)(s+m')]^{1/2} \delta_{m',m+1} \}.$$

$$(8a)$$

$$= \frac{\hbar}{2i} \{ [(s+m'+1)(s-m')]^{1/2} \delta_{m,m'+1} - [(s-m'+1)(s+m')]^{1/2} \delta_{m',m+1} \}.$$

According to these formulas, the diagonal matrix elements of $\hat{S}_{1,2}$ in any of these states are vanishing:

$$\langle m | \hat{S}_{1,2} | m \rangle = 0. \tag{9}$$

For the calculation of the diagonal matrix elements of \hat{S}_1^2 , it is instrumental to represent this operator as the product $\hat{S}_1\hat{S}_1$, and then act by the first of them (a Hermitian operator!) upon the bravector, and with the second one, upon the ket-vector, using Eq. (8a) twice – each time in the most convenient form:

$$\begin{split} \left\langle m \middle| \hat{S}_{1}^{2} \middle| m \right\rangle &= \left\langle m \middle| \hat{S}_{1} \hat{S}_{1} \middle| m \right\rangle \\ &= \frac{\hbar}{2} \left\{ \left\langle m - 1 \left\| [(s+m)(s-m+1)]^{1/2} + \left\langle m + 1 \right| [(s-m)(s+m+1)]^{1/2} \right\} \right. \\ &\times \frac{\hbar}{2} \left\{ \left[(s+m+1)(s-m)]^{1/2} \middle| m + 1 \right\rangle + \left[(s-m+1)(s+m)]^{1/2} \middle| m - 1 \right\rangle \right\} \end{split}$$

Taking into account the orthonormality of the state vectors, this formula yields

$$\left\langle m \left| \hat{S}_{1}^{2} \right| m \right\rangle = \frac{\hbar^{2}}{4} \left[(s+m)(s-m+1) + (s-m)(s+m+1) \right] = \frac{\hbar^{2}}{2} \left[s(s+1) - m^{2} \right].$$
 (10a)

Repeating this calculation for the operator \hat{S}_2 , we get the absolutely similar result (as could be expected from the symmetry of the system with respect to the component swap):

$$\left\langle m \middle| \hat{S}_{2}^{2} \middle| m \right\rangle = \frac{\hbar^{2}}{2} \left[s(s+1) - m^{2} \right].$$
(10b)

Using the same approach to calculate the diagonal matrix elements of the mixed products $\hat{S}_1 \hat{S}_2$ and $\hat{S}_2 \hat{S}_1$, we get

$$\langle m | \hat{S}_1 \hat{S}_2 | m \rangle = \frac{i}{2} \hbar^2 m, \qquad \langle m | \hat{S}_2 \hat{S}_1 | m \rangle = -\frac{i}{2} \hbar^2 m.$$
 (11)

As a sanity check, we may readily calculate the diagonal matrix elements of one of the commutation relations we have started with,

$$\left[\hat{S}_1, \hat{S}_2\right] = i\hbar\hat{S}_3$$

using Eq. (2):

$$\langle m | [\hat{S}_1, \hat{S}_2] | m \rangle = \langle m | i\hbar \hat{S}_3 | m \rangle = i\hbar^2 m$$

- the same result as follows from the subtraction of two Eqs. (11).

D (7 points). Let a classical geometric vector **S** have Cartesian components S_1 , S_2 , S_3 in a certain reference frame { $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ }, i.e.

$$\mathbf{S} = S_1 \mathbf{n}_1 + S_2 \mathbf{n}_2 + S_3 \mathbf{n}_3 \,.$$

Then its projection to the axis **n**', whose direction forms the usual spherical angles θ and φ in this reference frame (see Fig. on the right), so that

$$\mathbf{n}' = \sin\theta\cos\varphi\mathbf{n}_1 + \sin\theta\sin\varphi\mathbf{n}_2 + \cos\theta\mathbf{n}_3,$$

is simply

$$S' \equiv \mathbf{S} \cdot \mathbf{n}' = S_1 \sin \theta \cos \varphi + S_2 \sin \theta \sin \varphi + S_3 \cos \theta \,.$$

According to the correspondence principle, quantum-mechanical vector-operators should follow the same geometric relations as the classical geometric vectors, so that we may write

$$\hat{S}' = \hat{S}_1 \sin \theta \cos \varphi + \hat{S}_2 \sin \theta \sin \varphi + \hat{S}_3 \cos \theta.$$
(12)

Hence the expectation value of this operator in any eigenstate *m* of the operator \hat{S}_3 is:

$$\langle S' \rangle \equiv \langle m | \hat{S} | m \rangle = \langle m | \hat{S}_1 | l, m \rangle \sin \theta \cos \varphi + \langle m | \hat{S}_2 | l, m \rangle \sin \theta \sin \varphi + \langle m | \hat{S}_3 | m \rangle \cos \theta.$$

With Eqs. (2) and (9), this relation yields

$$\langle S' \rangle = \hbar m \cos \theta \,. \tag{13}$$



Next, using Eq. (12) again, we may write:

$$\hat{S}'^{2} \equiv \hat{S}'\hat{S}' = (\hat{S}_{1}\sin\theta\cos\varphi + \hat{S}_{2}\sin\theta\sin\varphi + \hat{S}_{3}\cos\theta)(\hat{S}_{1}\sin\theta\cos\varphi + \hat{S}_{2}\sin\theta\sin\varphi + \hat{S}_{3}\cos\theta)$$
$$= \hat{S}_{1}^{2}\sin^{2}\theta\cos^{2}\varphi + \hat{S}_{2}^{2}\sin^{2}\theta\sin^{2}\varphi + \hat{S}_{3}^{2}\cos^{2}\theta + (\hat{S}_{1}\hat{S}_{2} + \hat{S}_{2}\hat{S}_{1})\sin^{2}\theta\sin\varphi\cos\varphi + (\hat{S}_{1}\hat{S}_{3} + \hat{S}_{3}\hat{S}_{1})\sin\theta\cos\theta\cos\varphi + (\hat{S}_{2}\hat{S}_{3} + \hat{S}_{3}\hat{S}_{2})\sin\theta\cos\theta\sin\varphi.$$

Now using the expectation values calculated in the previous task of the problem, we get

$$\left\langle S'^2 \right\rangle \equiv \left\langle m \left| \hat{S}'^2 \right| m \right\rangle = \frac{\hbar^2}{2} \left[s(s+1) - m^2 \right] \sin^2 \theta \cos^2 \varphi + \frac{\hbar^2}{2} \left[s(s+1) - m^2 \right] \sin^2 \theta \sin^2 \varphi + \hbar^2 m^2 \cos^2 \theta$$
$$= \hbar^2 \left[\frac{s(s+1) - m^2}{2} \sin^2 \theta + m^2 \cos^2 \theta \right].$$

Hence for the variance of this value, i.e. for the square of its uncertainty $\delta S'$, we get

$$\left(\delta S'\right)^2 = \left\langle S'^2 \right\rangle - \left\langle S' \right\rangle^2 = \hbar^2 \frac{s(s+1) - m^2}{2} \sin^2 \theta \,. \tag{14}$$

Let us direct the axis \mathbf{n}_3 along the applied magnetic field. Then the ground state, reached after the system's relaxation, is one of the ultimate steps of the state ladder, i.e. either m = +s or m = -s, depending on the sign of the gyromagnetic ratio γ . For this state, Eqs. (13) and (14) yield

$$\langle S' \rangle = \hbar s \cos \theta, \qquad (\delta S')^2 = \hbar^2 \frac{s(s+1) - s^2}{2} \sin^2 \theta = \frac{\hbar^2}{2} s \sin^2 \theta, \qquad (15)$$

where now θ is the angle between the magnetic field and the spin measurement axis **n**'. As a sanity check, the angle φ shown in Fig. above, i.e. the direction of the axes **n**₁ and **n**₂ of the initial reference frame, do not affect the result.

E (3 points). For the particular case $\theta = \pi/2$, Eqs. (15) are reduced to

$$\langle S' \rangle = 0, \qquad (\delta S')^2 = \frac{\hbar^2}{2} s.$$

The first of these results, valid for any s, is very natural, because we are trying to measure spin in the direction orthogonal to its polarization, and the probabilities to find the spin oriented in either direction along the axis \mathbf{n} ' have to be equal, leading to the cancellation of their contributions to the expectation value.

The second of the results shows that the absolute uncertainty $\delta S'$ of the measured spin grows with spin as $s^{1/2}$, but its fair relative measure,

$$\frac{\delta S'}{\left\langle S^2\right\rangle^{1/2}} = \frac{\hbar (s/2)^{1/2}}{\hbar [s(s+1)]^{1/2}} = \frac{1}{[2(s+1)]^{1/2}},$$

decreases with the growth of *s*, reflecting the effective suppression of the quantum uncertainty in the (essentially, classical) limit $s \rightarrow \infty$.

Statistical Mechanics 1

Dipole interaction

Two similar classical electric dipoles, of a fixed magnitude *d*, are separated by a fixed distance *r*.

A (4 points). Represent the dipole-dipole interaction energy as a function of the angular orientation of each dipole.

B (3 points). Assuming that each dipole may rotate, with negligible mechanical inertia, write a general expression for its statistical sum Z in thermal equilibrium. (The expression may include a specific definite integral.)

C (7 points). Obtain an explicit expression for Z in the high-temperature limit, and use it to calculate the average interaction energy E, heat capacity, and entropy of the system.

D (3 points). Give a brief physical interpretation of the results. In particular, compare the obtained dependence E(r) with the long-range part of the van der Waals interaction¹ between electrically neutral atoms. What are the main handicaps of this simple model for the description of such interaction between real atoms?

E (3 points). Calculate *E* explicitly in the limit $T \rightarrow 0$, and briefly discuss the result.

¹ This part is called the *London dispersion force*.

Solutions:

A (4 points). The electrostatic potential of a dipole **d**, located in the origin, at the point **r** is:²

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{d} \cdot \mathbf{r}}{r^2}.$$

The corresponding electric field is

$$\mathbf{E}(\mathbf{r}) = -\nabla \phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \frac{3\mathbf{r}(\mathbf{r} \cdot \mathbf{d}) - \mathbf{d}r^2}{r^5}$$

On the other hand, the potential energy of the dipole in an external electric field E is

$$U = -\mathbf{d} \cdot \mathbf{E} \ .$$

Combining these formulas, we get the energy of interaction of two independent dipoles:

$$U = -\mathbf{d}_{1} \cdot \mathbf{E}_{2} = -\mathbf{d}_{2} \cdot \mathbf{E}_{1} = \frac{1}{4\pi\varepsilon_{0}} \frac{\mathbf{d}_{1} \cdot \mathbf{d}_{2}r^{2} - 3(\mathbf{r} \cdot \mathbf{d}_{1})(\mathbf{r} \cdot \mathbf{d}_{2})}{r^{5}} = \frac{1}{4\pi\varepsilon_{0}} \frac{d_{1x} \cdot d_{2x} + d_{1y} \cdot d_{2y} - 2d_{1z} \cdot d_{2z}}{r^{3}}$$

where z is the axis directed along vector \mathbf{r} , i.e. along the line connecting the dipoles. Plugging into the last form of this relation the expressions for the Cartesian components of both dipole moments via the polar and azimuthal angles of their orientation,

$$d_{jx} = d\sin\theta_j\cos\varphi_j, \qquad d_{jy} = d\sin\theta_j\sin\varphi_j, \qquad d_{jz} = d\cos\theta_j, \qquad \text{where } j = 1,2,$$

we may rewrite the interaction energy as

$$U = af, \quad \text{with } a \equiv \frac{d^2}{4\pi\varepsilon_0 r^3},$$

$$f = \sin\theta_1 \cos\varphi_1 \sin\theta_2 \cos\varphi_2 + \sin\theta_1 \sin\varphi_1 \sin\theta_2 \sin\varphi_2 - 2\cos\theta_1 \cos\theta_2 \quad (1)$$

$$\equiv \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2) - 2\cos\theta_1 \cos\theta_2.$$

B (4 points). If each dipole is free to rotate, possible states of its orientation are uniformly distributed over the full solid angle $\Omega_j = 4\pi$. In addition, if the kinetic energy of rotation of the physical objects carrying the dipole moments is negligible, as specified in the assignment, the full energy of the system is reduced to the interaction energy Eq. (1) - perhaps plus an inconsequential constant, which may be taken for the energy reference. As a result, the probability density $w \equiv dW/d\Omega_1 d\Omega_2$ to find the system at a certain point $\{\theta_1, \varphi_1; \theta_2, \varphi_2\}$ may be calculated using the Gibbs distribution in the following form:

$$w = \frac{1}{Z} \exp\left\{-\frac{U}{T}\right\} \equiv \frac{1}{Z} e^{-\beta U}$$

where *T* is temperature in energy units, $\beta = 1/T$ is the reciprocal temperature, and *Z* is the statistical sum:

² All formulas in this solution are in the SI units; for the transfer to the Gaussian units it is sufficient to drop the coefficient $1/4\pi\varepsilon_0$.

$$Z = \oint_{4\pi} d\Omega_1 \oint_{4\pi} d\Omega_2 e^{-\beta U} = \int_0^{\pi} \sin \theta_1 d\theta_1 \int_0^{2\pi} d\varphi_1 \int_0^{\pi} \sin \theta_2 d\theta_2 \int_0^{2\pi} d\varphi_2 e^{-\beta U}$$

Due to the 2π -periodicity of the function under the integral with respect to both arguments φ_j , the integral would not change if we replace the integration interval $[0, 2\pi]$ for one of these angles, say φ_1 , to any 2π -long interval, for example $[\varphi_2, \varphi_2 + 2\pi]$. Now in this integral, to be worked out at fixed φ_2 , we may write $d\varphi_1 = d\varphi$, where $\varphi \equiv \varphi_1 - \varphi_2$ is the angle participating in the last form of Eq. (1). Since, according to Eq. (1), the function under the integral depends only on φ but not on φ_2 , we may first take the integral over φ_2 , giving 2π , so that the expression for Z is reduced to

$$Z = 2\pi \int_{0}^{\pi} \sin \theta_1 d\theta_1 \int_{0}^{\pi} \sin \theta_2 d\theta_2 \int_{0}^{2\pi} d\varphi \ e^{-\beta af}, \quad \text{with} \ f = \sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2.$$
(2)

C (7 points). In the high-temperature limit, T >> a, the argument of the exponent in Eq. (2) is small for any dipole orientations, and we may expand it into the Taylor series in this parameter, keeping only three leading terms:

$$e^{-\beta af} \approx 1 - \beta af + \frac{1}{2} (\beta af)^2.$$

The integration (2) of the first term alone yields a β -independent result, $(4\pi)^2$, which gives no contribution to the average interaction energy. The second term is proportional to the function f, which keeps its magnitude but changes sign at any replacement $\theta_j \rightarrow \pi - \theta_j$, i.e. $\theta_j - \pi/2 \rightarrow \pi/2 - \theta_j$. Since the range of integration over each angle θ_j in Eq. (2) is the sum of two equal regions below and above $\pi/2$, the contributions from these regions cancel, and the total integral of this term equals zero. This is exactly why we needed to keep the last, quadratic term in the Taylor expansion: it does give a nonvanishing, β -dependent contribution to Z. Indeed, in this approximation

$$Z - (4\pi)^2 = \pi (\beta a)^2 \int_0^{\pi} \sin \theta_1 d\theta_1 \int_0^{\pi} \sin \theta_2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\varphi (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \cos \varphi - 2\cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \cos \theta_1 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \cos \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \sin \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2 \sin \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2)^2 d\theta (\sin \theta_1 \sin \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2)^2 d\theta (\sin \theta_1 \sin \theta_2)^2 d\theta (\sin \theta_1 \sin \theta_2)^2 d\theta_2 \int_0^{2\pi} d\theta (\sin \theta_1 \sin \theta_2)^2 d\theta (\sin$$

Squaring the parentheses, we see that the mixed term, proportional to $\cos\varphi$, gives a vanishing contribution to the integral over φ , so that we may continue as follows:

$$Z - (4\pi)^2 = \pi (\beta a)^2 \int_0^{\pi} \sin \theta_1 d\theta_1 \int_0^{\pi} \sin \theta_2 d\theta_2 \int_0^{2\pi} d\varphi \left(\sin^2 \theta_1 \sin^2 \theta_2 \cos^2 \varphi + 4\cos^2 \theta_1 \cos^2 \theta_2 \right)$$
$$= (\pi \beta a)^2 \int_0^{\pi} \sin \theta_1 d\theta_1 \int_0^{\pi} \sin \theta_2 d\theta_2 \left(\sin^2 \theta_1 \sin^2 \theta_2 + 8\cos^2 \theta_1 \cos^2 \theta_2 \right)$$
$$= (\pi \beta a)^2 \int_0^{\pi} d(\cos \theta_1) \int_0^{\pi} d(\cos \theta_2) \left[(1 - \cos^2 \theta_1) (1 - \cos^2 \theta_2) + 8\cos^2 \theta_1 \cos^2 \theta_2 \right].$$

Now introducing new variables $\xi_j \equiv \cos \theta_j$, we get

$$\frac{Z - (4\pi)^2}{(\pi\beta a)^2} = \int_{-1}^{+1} d\xi_1 \int_{-1}^{+1} d\xi_2 \left[\left(1 - \xi_1^2\right) \left(1 - \xi_2^2\right) + 8\xi_1^2 \xi_2^2 \right] = \int_{-1}^{+1} d\xi_1 \int_{-1}^{+1} d\xi_2 \left(1 - \xi_1^2 - \xi_2^2 + 9\xi_1^2 \xi_2^2\right) \right] \\ = \left[4 - 4 \int_{-1}^{+1} \xi^2 d\xi + 9 \left(\int_{-1}^{+1} \xi^2 d\xi \right)^2 \right] = \left[4 - 4 \cdot \frac{2}{3} + 9 \cdot \left(\frac{2}{3}\right)^2 \right] = \frac{16}{3},$$

so that, finally,

$$Z = (4\pi)^2 + \frac{16}{3}\pi^2\beta^2 a^2$$

This high-temperature approximation is valid only if the second term on its right-hand side is much smaller than the first one, so that with the accuracy $O(\beta^2)$,

$$\ln Z = \ln \left[\left(4\pi \right)^2 \left(1 + \frac{1}{(4\pi)^2} \frac{16}{3} \pi^2 \beta a^2 \right) \right] \approx \ln(4\pi)^2 + \frac{1}{(4\pi)^2} \frac{16}{3} \pi^2 \beta^2 a^2 \equiv 2\ln(4\pi) + \frac{1}{3} \beta^2 a^2.$$

From here, we may calculate the average interaction energy of the system,

$$E = -\frac{\partial(\ln Z)}{\partial\beta} \approx -\frac{2}{3}a^2\beta \equiv -\frac{2a^2}{3T},$$

its heat capacity

$$C \equiv \frac{\partial E}{\partial T} = \frac{2a^2}{3T^2}$$

and entropy:

$$S = \frac{E}{T} + \ln Z = -\frac{2a^2}{3T^2} + 2\ln(4\pi) + \frac{1}{3}\beta^2 a^2 \equiv \frac{a^2}{3T^2} + \text{const}.$$

(In the last expression, only the first term is due to the dipole-dipole interaction.)

D (3 points). The results show that in the high-temperature limit, all dipole interaction effects are small (proportional to $a^2 \ll T^2$). This is natural, because the probability w is nearly uniformly distributed over all dipole orientations, thus virtually averaging out the interaction energy.

The negative sign of the calculated average interaction energy,

$$E = -\frac{2a^2}{3T} \equiv -\frac{2}{3T} \left(\frac{d^2}{4\pi\varepsilon_0 r^3}\right)^2,$$

and the growth of its magnitude at $r \to 0$ show that the dipoles attract each other. Exactly the same distance dependence of the energy, $E \propto -1/r^6$, is typical for the London dispersion force, which dominates the long-range interaction of electroneutral atoms and molecules.³ This similarity is natural, because the London force is also due to the averaged interaction of electric dipoles.

³ Note that the traditional form, $1/r^{12}$, of the other term in the van der Waals formula, describing molecular/atomic repulsion at small distances, does not have a similarly quantitative physical basis.

However, in contrast to the fixed-magnitude dipole model analyzed in this problem, the London dispersion force between most atoms (having no spontaneous electric dipole moments) is due to weak mutual polarization of their randomly fluctuating dipole moments. The second important feature of this force, not taken into account by this classical model, is that these dipole fluctuations have quantum nature, so that for gas atoms at ambient conditions, the force is virtually temperature-independent.

E (3 points). At $T \ll a$, the system should stay very close to one of its potential energy minima. According to Eq. (1), there are two of them; in both cases the dipole moments **d** are aligned with each other, and the line connecting them:

$$U_{\min} = a f_{\min}, \qquad f_{\min} = -2, \quad \text{at} \quad \theta_1 = \theta_2 = \begin{cases} 0, \\ \pi. \end{cases}$$

(In any of these positions, the angle φ is uncertain.) In this limit,

$$E \approx U_{\min} = a f_{\min} \equiv -2 \frac{1}{4\pi\varepsilon_0} \frac{d^2}{r^3}.$$

This expression shows that in this limit the interaction is also attractive, but temperatureindependent, and much stronger than in the high-temperature limit.

Statistical Mechanics 2

Independent spins in magnetic field

Consider a system of N quantum spins s = 1/2 in magnetic field B. The Hamiltonian of such system is

$$H = -\sum_{i=1}^{N} 2\mu B S_i^z \,. \tag{28}$$

Here μ is the magnetic moment of the particle, S_i^z take values $\pm 1/2$ and we assumed that the magnetic field is in the z-direction.

(a) (2 points) Show that the partition function of such a system at temperature T is given by

$$Z(T, N, B) = [2\cosh(\mu B/T)]^{N}.$$

(b) (3 points) Compute the average value of total magnetization defined as

$$M = \langle \mathcal{\hat{M}} \rangle,$$

as a function of T, N, B. Here the total magnetization operator is given by $\hat{\mathcal{M}} = 2\mu \sum_{i=1}^{N} \hat{S}_{i}^{z}$.

(c) (1 point) Calculate the magnetic susceptibility of the system as a function of T, N, B defined by

$$\chi = \left(\frac{\partial M}{\partial B}\right)_{N,T}$$

(d) (4 points) Find the variance of the magnetization $(\delta M)^2$ as a function of temperature and magnetic field. The variance is defined as

$$(\delta M)^2 = \left\langle \left(\hat{\mathcal{M}} - \langle \hat{\mathcal{M}} \rangle \right)^2 \right\rangle = \left\langle \hat{\mathcal{M}}^2 \right\rangle - \left\langle \hat{\mathcal{M}} \right\rangle^2$$

How is the variance of the magnetization related to the magnetic susceptibility?

- (e) (3 points) Explicitly determine the variance in the limit of high and low temperatures. Interpret these limiting cases physically (i.e. explain why they are almost obvious).
- (f) (8 points) Find the form of the partition function for a system of N classical spins and repeat the calculations of (b), (c), (d), and (e) for *classical* spins. You can take the Hamiltonian of the system to be a classical analogue of (??), i.e.

$$H = -\sum_{i=1}^{N} \boldsymbol{\mu} \cdot \mathbf{B} \,. \tag{29}$$

assuming now that $\boldsymbol{\mu}$ is a classical magnetic moment vector with fixed absolute value $\mu^2 = \boldsymbol{\mu}^2$. Compare the results of part (e) for the classical and spin $\frac{1}{2}$ cases.

Solution:

a) We have

$$Z = \sum_{S_i^z = \pm 1/2} \exp\left\{\frac{1}{T} \sum_{i=1}^N 2\mu B S_i^z\right\} = \prod_{i=1}^N \sum_{S_i^z = \pm 1/2} \exp\left\{\frac{2\mu B}{T} S_i^z\right\} = \prod_{i=1}^N \left(e^{\frac{\mu B}{T}} + e^{-\frac{\mu B}{T}}\right)$$

and

$$Z(T, N, B) = [2\cosh(\mu B/T)]^N$$

b) For magnetization we have

$$M = \left< \hat{\mathcal{M}} \right> = Z^{-1}T \frac{\partial Z}{\partial B} = -\frac{\partial F}{\partial B}$$

with free energy given by

$$F = -T \ln Z = -TN \ln \left(2 \cosh(\mu B/T) \right)$$

Taking derivative with respect to B we obtain

$$M = -\frac{\partial F}{\partial B} = \mu N \tanh \frac{\mu B}{T}.$$

c) The susceptibility is given by

$$\chi = \frac{\partial M}{\partial B} = -\frac{\partial^2 F}{\partial B^2} = \frac{N\mu^2}{T\cosh^2\left(\frac{\mu B}{T}\right)}$$

d) The variance can be calculated as

$$(\delta M)^2 = \left\langle \left\langle \hat{\mathcal{M}}^2 \right\rangle - \left\langle \hat{\mathcal{M}} \right\rangle^2 \right\rangle = \frac{1}{Z} \left(T^2 \frac{\partial^2 Z}{\partial B^2} - \left(T \frac{\partial Z}{\partial B} \right)^2 \right) = T^2 \frac{\partial^2 \ln Z}{\partial B^2} = -T \frac{\partial^2 F}{\partial B^2}$$

We obtained a general relation between fluctuations of magnetization and magnetic susceptibility

$$(\delta M)^2 = \chi T$$
.

We immediately have

$$(\delta M)^2 = \frac{N\mu^2}{\cosh^2\left(\frac{\mu B}{T}\right)}.$$

e) As the temperature gets large $(T \gg \mu B)$ we can use $\cosh(x) \to 1 + x^2/2$ and to the leading order the variance becomes

$$(\delta M)^2 \approx N\mu^2$$

This result is easy to understand. At large temperatures the probability of a spin to be in one of two states is approximately 1/2 and the variance is given by random distribution of particles between two levels (random walk of N steps).

As the temperature gets small $\cosh(x) \rightarrow e^x/2$ and the variance becomes

$$(\delta M)^2 \approx N(2\mu)^2 e^{-2\mu B/T}$$

In this case almost all spins are in the lowest energy state (along the field). Fluctuations are given by probability of exciting spins into the higher state which is $\sim e^{-(2\mu B)/T}$.

f) The partition function can be written as

$$Z = \prod_{i=1}^{N} \int_{0}^{2\pi} d\phi_i \int_{0}^{\pi} \sin\theta_i \, d\theta_i \, \exp\left\{\frac{\mu B}{T}\cos\theta_i\right\} = \prod_{i=1}^{N} 2\pi \frac{T}{2\mu BS} \left(e^{\frac{\mu B}{T}} - e^{-\frac{\mu B}{T}}\right)$$

and

$$Z(T, N, B) = \left[4\pi \frac{T}{\mu B} \sinh(\mu B/T)\right]^{N}.$$

The free energy is given by

$$F = -T \log Z = -TN \log \left[4\pi \frac{T}{\mu B} \sinh(\mu B/T) \right].$$

For magnetization we obtain

$$M = -\frac{\partial F}{\partial B} = \frac{NT}{B} \left[\frac{\mu B}{T} \coth \frac{\mu B}{T} - 1 \right].$$

The magnetic susceptibility is given by

$$\chi = \frac{\partial M}{\partial B} = -\frac{\partial^2 F}{\partial B^2} = \frac{NT}{B^2} \left[1 - \left(\frac{\mu B/T}{\sinh(\mu B/T)}\right)^2 \right]$$

and

$$(\delta M)^2 = \chi T = \frac{NT^2}{B^2} \left[1 - \left(\frac{\mu B/T}{\sinh(\mu B/T)}\right)^2 \right]$$

As the temperature gets large $(T \gg \mu 2\mu BS)$ we have

$$(\delta M)^2 \approx N \frac{\mu^2}{3}$$

corresponding to the Curie's law for susceptibility $\chi = N \frac{\mu^2}{3T}$. For small temperatures sinh is exponentially large and we have approximately

$$(\delta M)^2 \approx \frac{NT^2}{B^2}$$
.

Fluctuations diverge at small B. In fact, the quantization of the magnetic moment (quantum spin) will cut off this divergence when energy level spacing will become of the order of temperature.

Statistical Mechanics 3

Bose-Einstein Condensation:

Consider a non-interacting non-relativistic Bose gas in a macroscopic three-dimensional box of volume V.

- (a) (3 points) Write down the appropriate partition function and derive an equation that gives the occupation number as a function of energy at a given temperature and chemical potential.
- (b) (5 points) Consider a gas composed of a finite number of particles. Make a sketch of the chemical potential as a function of temperature. Does it go to zero? If so, indicate whether this happens at $T \rightarrow 0$ or at some other temperature.

Explicitly determine the chemical potential as a function of temperature in the classical (or high temperature) limit, and also show this approximate result in your sketch.

- (c) (3 points) Compute the critical temperature, T_c , above which practically all the particles are in excited states, but below which a significant number is in the ground state.
- (d) (4 points) Does the pressure at low temperatures $(T < T_c)$ depend on the particle density? If yes, how? If no, explain why. What is limiting behavior of the pressure of the ideal Bose gas as $T \rightarrow 0$?

Consider now what happens for an infinite system $(V \to \infty \text{ with } N/V \text{ fixed})$ in different dimensions, 1d, 2d, and 3d:

(e) (4 points) Can a non-relativistic ideal Bose gas of a given number density of particles undergo Bose condensation in d = 1, 2, 3 dimensions? Explain.

Useful Mathematical Formulas

$$\int_0^\infty x^{n-1} e^{-x} dx = \Gamma(n) \tag{30}$$

$$\Gamma(n+1) = n\Gamma(n); \ \Gamma(1/2) = \sqrt{\pi}$$
(31)

$$\int_0^\infty \frac{x^{s-1}dx}{e^x - 1} = \Gamma(s)\zeta(s) \tag{32}$$

$$\{\zeta(\frac{3}{2}), \zeta(\frac{4}{2}), \zeta(\frac{5}{2}), \zeta(\frac{6}{2}), \zeta(\frac{7}{2}), \zeta(\frac{8}{2}), \ldots\} = \{2.61, 1.64, 1.34, 1.20, 1.13, 1.08, \ldots\}$$
(33)

Solution

(a) Each Fourier mode may be treated separately. The single particle energy of each mode is $\epsilon_p = p^2/2m$. The energy levels are

$$E_n = \left(n + \frac{1}{2}\right)\epsilon_p. \tag{34}$$

Neglecting the zero-point energy, the grand canonical partition function is

$$\mathscr{Q} = \sum_{n} e^{-n\beta(\epsilon_p - \mu)} = \frac{1}{1 - e^{-\beta(\epsilon_p - \mu)}}.$$
(35)

The mean occupation number follows by differentiation:

$$\langle n_p \rangle = \frac{1}{\mathscr{Q}} \sum_n n e^{-n\beta(\epsilon_p - \mu)} = \frac{1}{\beta} \frac{\partial \log \mathscr{Q}}{\partial \mu} = \frac{1}{e^{\beta(\epsilon_p - \mu)} - 1}.$$
 (36)

(b) Ignoring condensation we find

$$N = V \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{e^{\beta(\epsilon_p - \mu)} - 1}$$
(37)

Changing variables to integrate over a dimensionless energy,

$$x \equiv \frac{p^2}{2mT} \tag{38}$$

and defining the thermal wavelength λ , the fugacity z, and the inter-particle spacing ℓ

$$\lambda \equiv \frac{(2\pi\hbar)}{\sqrt{2mT}}, \qquad z \equiv e^{\mu/T}, \qquad \frac{N}{V} \equiv \frac{1}{\ell^3}, \qquad (39)$$

we find

$$\frac{1}{\ell^3} = \frac{\pi^{3/2}}{\lambda^3} g_{3/2}(z) , \qquad (40)$$

where

$$g_{3/2}(z) \equiv \frac{1}{\Gamma(3/2)} \int_0^\infty \frac{y^{1/2} dy}{(1/z)e^y - 1} \,. \tag{41}$$

Eq. (??) implicitly determines μ as a function of T. We will define a temperature T_0 when the thermal wavelength equals the distance between particles

$$T_0 \equiv \frac{1}{2m} \left(\frac{2\pi\hbar}{\ell}\right)^2 \,,\tag{42}$$

and then Eq. (??) can be neatly summarized by the requirement that

$$g_{3/2}(z) = \left(\frac{T_0}{\pi T}\right)^{3/2} \,. \tag{43}$$



Figure 1: The chemical potential (over temperature) versus temperature for a Bose gas at fixed density (solid line). The dashed line gives the approximate result of Eq. (??). T_0 is determined by the density and is given in Eq. (??). The shaded region indicates Bose condensation.

 $g_{3/2}(z)$ is an increasing function of the fugacity z until the point of condensation (see below). For z small, the inversion of Eq. (??) can be done analytically. Specifically for small z (i.e. a classical gas) we have

$$g_{3/2}(z) \simeq \frac{z}{\Gamma(3/2)} \int_0^\infty \sqrt{y} e^{-y} = z ,$$
 (44)

and thus we find

$$\mu = -\frac{3}{2}T\log\left(\frac{\pi T}{T_0}\right). \tag{45}$$

Plotting this last expression gives a qualitative understanding of μ versus T. It is understood that Eq. (??) is only valid for $T \gg T_0$.

At z = 1 (the point of condensation) $g_{3/2}(z)$ reaches its limiting value

$$g_{3/2}(1) = \zeta(\frac{3}{2}) \simeq 2.6$$
. (46)

Thus the left hand size Eq. (??) is an increasing function of z, starting from 0 for z = 0 (a classical gas) and ending at 2.6 for z = 1 (the point of condensation). This information should be enough to qualitatively sketch $z = e^{\mu/T}$ versus T.

Fig. ?? shows the chemical potential versus the temperature. The dashed line shows the approximation given by Eq. (??), while the solid red line is the full (numerical) result found by inverting Eq. (??). The shaded region is below the critical temperature (see below).

(c) When $e^{\mu/T}$ is unity (or $\mu = 0$), this is the point of condensation

$$\zeta(\frac{3}{2}) = \left(\frac{T_0}{\pi T_c}\right)^{3/2} \,. \tag{47}$$

Solving for T_c we find

$$T_c = \frac{1}{\pi(\zeta(\frac{3}{2}))^{2/3}} T_0 = 0.168 T_0.$$
(48)

(d) The condensate and normal parts are in equilibrium. The pressure at $T < T_c$ is simply the contribution of the normal part at zero chemical potential

$$\mathcal{P} = \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{p^i v^i}{3} \frac{1}{e^{p^2/(2mT)} - 1} \,. \tag{49}$$

In writing this expression we have simply used the kinetic theory definition of the stress tensor

$$\mathcal{P} = \frac{1}{3}T_i^i \quad \text{with} \quad T^{ij} = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{p^i v^j}{3} \frac{1}{e^{p^2/(2mT)} - 1} \,. \tag{50}$$

Using the same notation as before

$$\mathcal{P} = \frac{2T}{3} \frac{2\pi\Gamma(5/2)}{\lambda^3} \underbrace{\left[\frac{1}{\Gamma(5/2)} \int_0^\infty \frac{x^{3/2} dx}{e^x - 1}\right]}_{=\zeta(\frac{5}{2})},$$
(51)

yielding

$$\mathcal{P} = \frac{T}{\lambda^3} \pi^{3/2} \zeta(\frac{5}{2}) \,. \tag{52}$$

So we see that the pressure is independent of the density, and goes to zero as $T^{5/2}$. The reason that the pressure is independent of the density is that as we increase the particle number at fixed temperature and volume, the additional particles go to the condensate, and the number of particles in the normal phase (which determines the pressure) remains fixed.

(e) In various dimensions the number of particles per "volume" is

$$\frac{N}{V} = \frac{1}{\lambda^d} \frac{1}{2} \Gamma(d/2) S_{d-1} \frac{1}{\Gamma(d/2)} \int_0^\infty dx \frac{x^{d/2-1}}{(1/z)e^x - 1} \,.$$
(53)

Here S_{d-1} is the surface area of a sphere in d spatial dimensions, *i.e.* $S_{d-1}=2, 2\pi, 4\pi$ for d=1, 2, 3 respectively.

For d=1 and d=2, the dimensionless integral

$$\int_0^\infty dx \frac{x^{d/2-1}}{(1/z)e^x - 1} \,, \tag{54}$$

increases without bound as $z \to 1$ (or $\mu \to 0$). Thus, the density of particles in units of $1/\lambda^d$ can increase without bound before μ/T reaches zero. For this reason, ideal Bose condensation will not occur in one and two dimensions.