

Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

Fall 2025 (in 4 separate parts: CM, EM, QM, SM)

General Instructions:

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

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

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

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

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

CLASSICAL MECHANICS 1

A boy on a swing

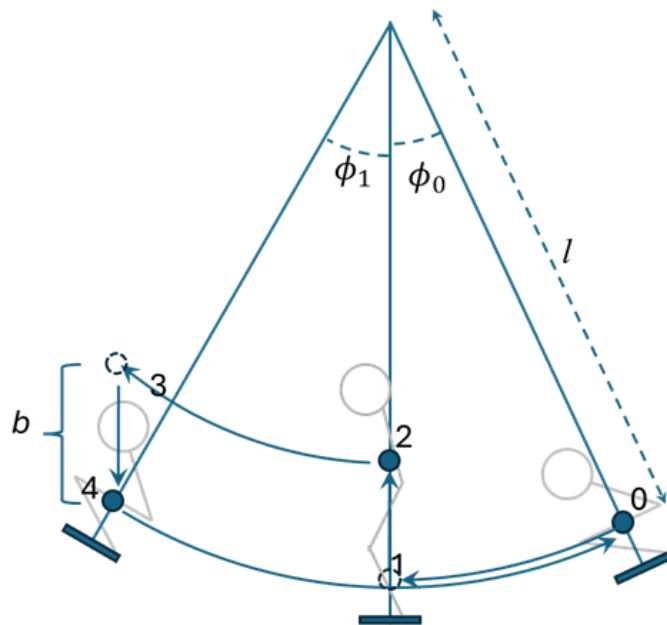
A boy of mass m stands on a swing and moves his body as shown in the figure. Every time he is at the lowest point while swinging *left*, he quickly raises his center of mass by a small distance b . Once he reaches the highest point on the left, he quickly lowers his center of mass back and then keeps his position while swinging to the highest point on the right. In each extremal position, the distance between the center of mass and the pivot point of the swing is l . Assume that $b \ll l$, the swing angles ϕ are small, and that the swing period is much longer than the time it takes him to change his body position.

(a)[6pt] Given an initial angle of ϕ_0 , calculate the extremal angle ϕ_1 after half a period from point 0 to 4. Ignore any friction for now.

(b)[6pt] Prove that over many swing cycles the energy of the swing grows exponentially according to $dE/dt = \gamma E$ and determine the constant γ .

(c)[8pt] Now consider a more realistic situation in which there is tiny amount of air friction proportional to the velocity of the child at his center of mass, $f = \alpha v$. Assume weak damping, find the value of α so that the swing returns to the same angle of ϕ_0 after each swing cycle.

Hint: the swing angle of a weakly-damped pendulum follows: $\phi(t) = A \cos(\omega t) e^{-\beta t}$, with $\beta \ll \omega$. You can solve for ω and β .



Solution

(a) Consider half a period of swinging motion between points 0-1-2-3-4. From 0-1, energy is conserved: $E_0 = E_1$.

$$mgl(1 - \cos(\phi_0)) = mv_1^2/2 \quad (1)$$

where ϕ_0 is the initial angle. From 1-2, angular momentum is conserved:

$$mlv_1 = m(l - b)v_2 \quad (2)$$

$$v_2 = \frac{v_1 l}{(l - b)} \quad (3)$$

From 2-3, again energy is conserved:

$$mv_2^2/2 = mg(l - b)(1 - \cos(\phi_1)) \quad (4)$$

With these we can obtain the relation between the angles:

$$mgl(1 - \cos(\phi_0)) \left(\frac{l}{l - b} \right)^2 = mg(l - b)(1 - \cos(\phi_1)) \quad (5)$$

$$1 - \cos(\phi_1) = (1 - \cos(\phi_0)) \left(\frac{l}{l - b} \right)^3 \quad (6)$$

The work done from 0 to 3 is the change of the potential energy at the extremals:

$$\Delta P_{13} = mg[l - (l - b) \cos(\phi_1)] - mgl[1 - \cos(\phi_0)] = mgl[1 - \cos(\phi_0)] \left[\left(\frac{l}{l - b} \right)^2 - 1 \right] + mgb \quad (7)$$

The ΔE can also be directly calculated from the work done between points 1 and 2. As the child raises the center of mass to a radius of r , from conservation of angular momentum the velocity is:

$$v(r) = v_1 l / r \quad (8)$$

The force to raise the center of mass does a work which is

$$W = \int_{l-b}^l \left[\frac{mv^2(r)}{r} + mg \right] dr = \frac{1}{2} mv_1^2 \left[\left(\frac{l}{l-b} \right)^2 - 1 \right] + mgb = mgl[1 - \cos(\phi_0)] \left[\left(\frac{l}{l-b} \right)^2 - 1 \right] + mgb \quad (9)$$

We see that $W = \Delta P_{13}$.

From 3 to 4, the center of gravity is lowered by b . Finally, return to 0 from 4 to complete one period, the total energy change is:

$$\Delta E = mgl[1 - \cos(\phi_0)][(\frac{l}{l-b})^2 - 1] = E_0[(\frac{l}{l-b})^2 - 1] \quad (10)$$

(b) Considering the swing has an approximately constant period of $T = 2\pi\sqrt{l/g}$, we can estimate that the energy of the system follows:

$$dE/dt \approx \Delta E/T = \frac{E}{2\pi}\sqrt{\frac{g}{l}}[(\frac{l}{l-b})^2 - 1] \quad (11)$$

Therefore the energy increases exponentially with:

$$\alpha = \frac{1}{2\pi}\sqrt{\frac{g}{l}}[(\frac{l}{l-b})^2 - 1] \quad (12)$$

(c) In the presence of friction the equation of motion for a swing with length r is (under small swing angle):

$$mg\phi + \alpha r \frac{d\phi}{dt} + mr \frac{d^2\phi}{dt^2} = 0 \quad (13)$$

With $\phi = \phi_0 \cos(\omega t)e^{-\beta t}$, we have:

$$mg\phi_0 \cos(\omega t)e^{-\beta t} - \alpha r \phi_0 [\omega \sin(\omega t) + \beta \cos(\omega t)]e^{-\beta t} + mr \phi_0 e^{-\beta t} [-\omega^2 \cos(\omega t) + 2\omega\beta \sin(\omega t) + \beta^2 \cos(\omega t)] = 0 \quad (14)$$

Hence:

$$mg - \alpha r \beta - mr\omega^2 + mr\beta^2 = 0 \quad (15)$$

$$-\alpha r \omega + 2mr\omega\beta = 0 \quad (16)$$

From these equation we obtain:

$$\beta = \frac{\alpha}{2m} \quad (17)$$

$$\omega = \sqrt{\frac{g}{r} - \frac{\alpha^2}{4m^2}} \quad (18)$$

Applying the above to the problem here, the swing reaches vertical position 1 when $t = t_1 = \frac{\pi}{2\omega}$ with $\omega = \sqrt{\frac{g}{l} - \frac{\alpha^2}{4m^2}}$. There the velocity of the center of mass is

$$v_1 = l \frac{d\phi}{dt} = -l\phi_0\omega e^{-\frac{\beta\pi}{2\omega}} \quad (19)$$

from 1 to 2, the angular velocity becomes:

$$\frac{d\phi}{dt} = \frac{v_2}{l-b} = \frac{v_1 l}{(l-b)^2} = -\phi_0\omega \frac{l^2}{(l-b)^2} e^{-\frac{\beta\pi}{2\omega}} \quad (20)$$

Generally the angular velocity of a non-driven swing is:

$$\frac{d\phi}{dt} = -\phi_0[\omega \sin(\omega t) + \beta \cos(\omega t)]e^{-\beta t} \quad (21)$$

Matching the angular momentum with that of the continued motion $\phi' \propto \phi'_0 (-\sin \omega'(t - t_1)) e^{-\beta(t-t_1)}$ for $t > t_1$

$$\frac{d\phi'}{dt} = -\phi'_0\omega' = -\phi_0\omega \frac{l^2}{(l-b)^2} e^{-\frac{\beta\pi}{2\omega}} \quad (22)$$

where $\omega' = \sqrt{\frac{g}{l-b} - \frac{\alpha^2}{4m^2}}$, and

$$\phi'_0 = \phi_0 \frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} e^{-\frac{\beta\pi}{2\omega}} \quad (23)$$

Hence from 2 to 3, the motion of the swing follows:

$$\phi' = \phi_0 \frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} (-\sin \omega'(t - t_1)) e^{-\frac{\beta\pi}{2\omega} - \beta(t-t_1)} \quad (24)$$

The extremal swing angle ϕ'_3 is reached when $\frac{d\phi'}{dt} = 0$ which, with $\beta \ll \omega$, happens at when $t = t_3 = t_1 + \frac{\pi}{2\omega'}$:

$$\phi'_3 = -\phi_0 \frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} e^{-\frac{\beta\pi}{2\omega} - \frac{\beta\pi}{2\omega'}} \quad (25)$$

From 3 to 4, the swing remains stationary. From 4 back to 0, the swing motion follows:

$$\phi = \phi'_3 \cos \omega(t - t_3) e^{-\beta(t-t_3)} \quad (26)$$

and reaches back to the original ϕ_0 at $t = t_4 = t_3 + \frac{\pi}{\omega}$:

$$\phi_0 \frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} e^{-\frac{\beta\pi}{2\omega} - \frac{\beta\pi}{2\omega'} - \frac{\beta\pi}{\omega}} = \phi_0 \quad (27)$$

Hence we get the equation for α :

$$\frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} e^{-\beta(\frac{3\pi}{2\omega} + \frac{\pi}{2\omega'})} = 1 \quad (28)$$

$$\ln \left[\frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} \right] = \frac{1}{2} \beta \pi \left(\frac{3}{\omega} + \frac{1}{\omega'} \right) = \frac{\alpha \pi}{4m} \left(\frac{3}{\omega} + \frac{1}{\omega'} \right) \quad (29)$$

and

$$\alpha = \frac{4m\omega\omega'}{\pi(3\omega' + \omega)} \ln \left[\frac{\omega}{\omega'} \frac{l^2}{(l-b)^2} \right] \quad (30)$$

The answer can be expanded in the small difference $(\omega'/\omega - 1)$ and b/l :

$$\alpha \approx \frac{m\omega}{\pi} \ln \left[\left(1 - \frac{gb}{2\omega^2 l^2} \right) \left(1 + 2\frac{b}{l} \right) \right] \approx \frac{m\omega}{\pi} \left[-\frac{gb}{2\omega^2 l^2} + 2\frac{b}{l} \right] \approx \frac{m\omega}{\pi} \frac{3b}{2l} \quad (31)$$

where the higher-order in the difference between ω and ω' has been neglected. In the right-most approximation, the difference between ω^2 and g/l has also been neglected.

CLASSICAL MECHANICS 2

Orbiting stars

In this problem, we model a binary star system as two point-like bodies of mass M_1 and M_2 separated by distance d orbiting around each other in circular orbits.

(a)[6pt] Write an expression for total angular momentum in terms of the parameters given and any fundamental constants.

(b)[2pt] Explain why angular momentum is conserved (without using an equation).

In a simple model of mass transfer, the masses change adiabatically in time so that $dM_1/dt = -dM_2/dt = \alpha$, where $\alpha > 0$ is constant. Suppose that after some time T (before the second star is completely consumed), the mass transfer ends and the orbit remains circular.

(c)[6pt] What is the distance between the bodies at times $t \geq T$?

(d)[6pt] What is the change in energy after the mass transfer?

Solution

(a) The angular momentum of the system can be shown to be

$$L = \mu d^2 \omega, \quad (1)$$

where $\mu = (M_1 M_2)/(M_1 + M_2)$ is the reduced mass and ω is the angular frequency of the orbit.

The angular frequency can be determined from the force law. Specifically,

$$\ddot{\mathbf{r}} = \ddot{\mathbf{r}}_2 - \ddot{\mathbf{r}}_1 \quad (2)$$

$$= \frac{1}{M_2} \mathbf{F}_2 - \frac{1}{M_1} \mathbf{F}_1 \quad (3)$$

$$= - \left(\frac{1}{M_2} + \frac{1}{M_1} \right) \left(\frac{GM_1 M_2}{r^2} \right) \frac{\mathbf{r}}{r} \quad (4)$$

$$= - \frac{(M_1 + M_2)G}{r^3} \mathbf{r} \quad (5)$$

where $\mathbf{r}_{1,2}$ denote the position vectors of the bodies, \mathbf{r} their relative position, and $\mathbf{F}_{2(1)}$ the force on mass 2(1) from mass 1(2). G denotes the gravitational constant. Since for circular motion, $\ddot{\mathbf{r}} = -\omega^2 \mathbf{r}$, it follows that:

$$\omega = \sqrt{\frac{(M_1 + M_2)G}{r^3}} \quad (6)$$

Hence

$$\boxed{L = \mu \sqrt{(M_1 + M_2)Gd}, \quad \mu = \frac{M_1 M_2}{M_1 + M_2}} \quad (7)$$

(b) Angular momentum is conserved because there is no net torque on the system (all the forces are internal to the system and central).

(c)

Using the fact that the angular momentum is conserved and the total mass $M_1 + M_2$ remains constant, it is evident that the product $\mu_f \sqrt{d_f} = \mu_i \sqrt{d}$ remains constant, which implies

$$d_f = \left(\frac{\mu_i}{\mu_f} \right)^2 d = \left(\frac{M_1 M_2}{M_{1f} M_{2f}} \right)^2 d, \quad (8)$$

where i, f indicate initial ($t = 0$) and final ($t = T$) values. Thus

$$\boxed{d_f = \left[\frac{M_1 M_2}{(M_1 + \alpha T)(M_2 - \alpha T)} \right]^2 d} \quad (9)$$

(d)

For a circular orbit:

$$E = \frac{L^2}{2\mu r^2} - \frac{GM_1(t)M_2(t)}{r} \quad (10)$$

Using the value of angular momentum in Eq. (7),

$$E = \frac{\mu(M_1(t) + M_2(t))G}{2r} - \frac{GM_1(t)M_2(t)}{r} = -\frac{GM_1(t)M_2(t)}{2r} \quad (11)$$

Hence,

$$E_f - E_i = -\frac{G}{2} \left(\frac{M_1(t)M_2(t)}{d_f} - \frac{M_1M_2}{d} \right) = \frac{GM_1M_2}{2d} \left(1 - \frac{M_{1f}M_{2f}}{M_1M_2} \frac{d}{d_f} \right) \quad (12)$$

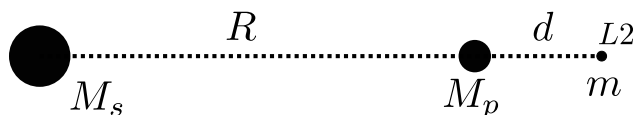
Using d_f from Eq. (9),

$$E_f - E_i = \frac{GM_1M_2}{2d} \left(1 - \left[\frac{M_{1f}M_{2f}}{M_1M_2} \right]^3 \right) = \boxed{\frac{GM_1M_2}{2d} \left(1 - \left[\frac{(M_1 + \alpha T)(M_2 - \alpha T)}{M_1M_2} \right]^3 \right)} \quad (13)$$

If the smaller star is consumed by the larger one, $M_1 > M_2$, it would appear that the total (kinetic + potential) energy is increased. However, this does not take into account the energy of gravitational attraction within the stars themselves, $U_{self} \propto (-GM^2/R)$, where their radii $R_{1,2} < d$.

CLASSICAL MECHANICS 3

Lagrange points – a restricted three body problem



Consider a solar system with one planet of mass M_p and a star of mass M_s separated by distance R . They move in the circular orbit around the center of mass in the (\hat{x}, \hat{y}) plane. A small third body, a satellite, which also moves *only in the (\hat{x}, \hat{y}) plane*, has negligible mass and does not impact the equation of motion of the star and the planet.

(a)[3pt] Find the orbital period of the planet and star motion neglecting the effects of the satellite.

Now consider the reference frame co-rotating with the star and the planet such that they stay on the \hat{x}' axis and their center of mass is at $(x', y') = (0, 0)$.

(b)[4pt] Write the Lagrangian for the motion of the satellite in the co-rotating reference frame using the new coordinates (x', y') . Find the canonical momentum, the Hamiltonian, and write the equations of motion in terms of (x', y') , (\dot{x}', \dot{y}') , and derivatives of the effective potential $U'(x', y')$.

The Lagrange point L2 is one of the equilibrium points in line with the star and the planet with $y' = 0$ (see the figure).

(c)[6pt] Using the effective potential, write the condition for the Lagrange point L2. Assuming that the planet is much lighter than the star, show that the distance from the planet to L2 is

$$d \approx R \left(\frac{\alpha}{3} \right)^{1/3} \ll R,$$

where $\alpha = M_p / (M_s + M_p) \ll 1$.

(d)[7pt] Would the satellite be dynamically stable at L2? If yes, prove it. If not, estimate how fast the satellite would fall out of L2 in the case of Earth/Sun system neglecting all other bodies in the Solar system.

Hint: Expand the effective potential $U'(x', y')$ to the lowest relevant order and analyze the equations derived in part (b). Here and above, you may find useful the following Taylor series

$$(1 + \varepsilon)^{-2} = 1 - 2\varepsilon + O(\varepsilon^2), \quad (1 + \varepsilon)^{-1/2} = 1 - \frac{1}{2}\varepsilon + \frac{3}{8}\varepsilon^2 + O(\varepsilon^3).$$

Solution

(a) The bound two-body system would rotate around the common center of mass on the line between them at distances αR and $(1 - \alpha)R$ from the star and the planet. The period of the circular motion is most easily found using the reduced mass of the system $\mu = (M_s^{-1} + M_p^{-1})^{-1}$,

$$\mu\omega^2 R = \frac{GM_s M_p}{R^2} \implies \omega = \sqrt{\frac{GM}{R^3}}.$$

where $M = M_s + M_p$ and the period $T = 2\pi/\omega$.

(b) The Lagrangian for the satellite is most easily written in the inertial (non-rotating) reference frame first,

$$\mathcal{L}(\vec{r}, \vec{v}) = T(\vec{v}) - U(\vec{r}) = \frac{1}{2}m\vec{v}^2 + \frac{GM_s m}{|\vec{r} - \vec{r}_s(t)|} + \frac{GM_p m}{|\vec{r} - \vec{r}_p(t)|}$$

where $\vec{r}_s(t)$ and $\vec{r}_p(t)$ are time-dependent positions of the star and the planet. Only the kinetic term is affected when changing to the co-rotating RF, and it will yield the Coriolis and the centrifugal forces below. Using the angular velocity vector $\vec{\omega} = \omega \hat{z} \perp (\hat{x}, \hat{y})$ to specify the rotation, the inertial-frame velocity can be expressed as $\vec{v} = \vec{v}' + \omega \times \vec{r}'$ and the Lagrangian

$$\mathcal{L} = \frac{1}{2}m(\vec{v}')^2 + m\vec{v}' \cdot (\vec{\omega} \times \vec{r}') - U'(\vec{r}')$$

where the new effective potential is

$$U'(\vec{r}') = -\frac{1}{2}m\omega^2(\vec{r}')^2 - \frac{GM_s m}{|\vec{r}' - \vec{r}'_s|} + \frac{GM_p m}{|\vec{r}' - \vec{r}'_p|}$$

and where $\vec{r}'_s = (-\alpha R, 0)$ $\vec{r}'_p = ((1 - \alpha)R, 0)$ are now constant positions of the star and the planet. The satellite's canonical momentum is

$$\vec{p}' = \frac{\partial \mathcal{L}}{\partial \vec{v}'} = m\vec{v}' + m\vec{\omega} \times \vec{r}'$$

and the Hamiltonian

$$\mathcal{H} = \vec{p}' \cdot \vec{v}' - \mathcal{L} = \frac{1}{2}m\vec{v}'^2 + U'(\vec{r}') = \frac{1}{2m}(\vec{p}' - m\vec{\omega} \times \vec{r}')^2 + U'(\vec{r}')$$

The equations of motion can be derived from either the Lagrangian for $\dot{\vec{v}}' = (\ddot{x}', \ddot{y}')$,

$$\begin{aligned} \frac{d}{dt}(m\vec{v}' + m\vec{\omega} \times \vec{r}') &= \frac{\partial \mathcal{L}}{\partial \vec{r}'} = m\vec{v}' \times \vec{\omega} - \frac{\partial U'}{\partial \vec{r}'}, \\ m\dot{\vec{v}}' &= 2m\vec{v}' \times \vec{\omega} - \frac{\partial U'}{\partial \vec{r}'} \end{aligned}$$

or from the Hamiltonian for $\dot{\vec{p}}'$.

(c) For the satellite to remain static at any point in the co-rotating RF, its velocity must be $\vec{v}' = 0 = \text{const}$ and its effective potential satisfy $\frac{\partial U'}{\partial \vec{r}'} = 0$. For L2, the y' -dependence is trivial because of symmetry, and the x' dependence requires

$$\begin{aligned} 0 &= \frac{\partial}{\partial x'} \left[-\frac{1}{2}\omega^2 x'^2 - \frac{GM_s}{x' + \alpha R} - \frac{GM_p}{x' - (1 - \alpha R)} \right] \\ &= \frac{\partial}{\partial d} \left[-\frac{1}{2}\omega^2 ((1 - \alpha)R + d)^2 - \frac{GM_s}{R + d} - \frac{GM_p}{d} \right], \\ &= -\omega^2 ((1 - \alpha)R + d) + \frac{GM_s}{(R + d)^2} + \frac{GM_p}{d^2} \end{aligned}$$

where $x' > (1 - \alpha)R$ and $d > 0$. In the case of $\alpha \ll 1$ and $d \ll R$, expanding the r.h.s. in $\delta = d/R$ and using $\omega^2 R = GM/R^2$ we get

$$0 \approx \omega^2 R \left[-(1 - \alpha) - \delta + (1 - \alpha)(1 - 2\delta) + \frac{\alpha}{\delta^2} \right] \implies \delta^3 \approx \frac{\alpha}{3 - 2\alpha} \approx \alpha/3$$

or $d = R\delta = R(\alpha/3)^{1/3}$.

(d) This part is a little bit tedious. One can proceed by either calculating the second derivatives of U' with respect to (x', y') around the L2 point $([1 - \alpha + \delta]R, 0)$ or, more thoughtfully, find the second-order terms in the series

$$\begin{aligned} U'(x', y')/m &= U([1 - \alpha + \delta]R + a, b)/m \\ &= -\frac{1}{2}\omega^2 [((1 - \alpha)R + d + a)^2 + b^2] - \frac{GM(1 - \alpha)}{\sqrt{(R + d + a)^2 + b^2}} - \frac{GM\alpha}{\sqrt{(d + a)^2 + b^2}} \end{aligned}$$

because it is already known that all the first-order terms cancel. Using the provided (or hopefully remembered) Taylor series for $(1 + \varepsilon)^{-1/2}$ and some algebra yields

$$U'/m \approx (U'/m)_{L2} + \omega^2 \left(-\frac{9}{2}a^2 + \frac{3}{2}b^2 \right)$$

so it is obvious that the effective potential as a saddle point at L2 and it is a point of unstable equilibrium.

One can roughly estimate the lifetime at L2 using the negative eigenvalue of the potential Hessian in the direction \hat{x}' , $\tau \propto 1/\omega_x = 1/(3\omega)$ i.e. 1/3 of a year. A more careful approach should take into account the Coriolis force $\propto \vec{v}' \times \vec{\omega}$, which results in the following equations of motion

$$\begin{cases} \ddot{a} = 9\omega^2 a + 2\omega \dot{b} \\ \ddot{b} = -3\omega^2 b - 2\omega \dot{a} \end{cases} .$$

Looking for solution in the form $(a_{0\lambda}, b_{0\lambda})e^{\lambda t}$ results in the eigenvalue equation

$$\det \begin{pmatrix} \lambda^2 - 9\omega^2 & -2\lambda\omega \\ 2\lambda\omega & \lambda^2 + 3\omega^2 \end{pmatrix} = 0 \iff \lambda^4 - 2\omega^2\lambda^2 - 27\omega^4 = 0$$

and two eigenvalues $\lambda^2 = \omega^2(1 \pm 2\sqrt{7})$. The largest real eigenvalue $\lambda = \omega\sqrt{(1 + 2\sqrt{7})} \approx 2.5\omega$ yields slightly longer L2 lifetime of about $\approx (2.5)^{-1} = 0.4$ year.

ELECTROMAGNETISM 1

Mutual inductance

Consider a static situation in which electromagnetic fields and their sources (charges and currents) do not vary in time.

(a)[3pt] By using Maxwell's equations and expressing the magnetic induction as $\mathbf{B} = \nabla \times \mathbf{A}$, show that the Cartesian components of the vector potential \mathbf{A} obey Poisson's equation, $-\nabla^2 \mathbf{A} = \mu_0 \mathbf{J}$, where \mathbf{J} is the current density and $\nabla \cdot \mathbf{A} = 0$ (i.e., the Coulomb gauge is adopted).

(b)[3pt] Explain why the vector potential due to the current density is given by

$$\mathbf{A}(\mathbf{r}) = C_1 \int d^3 r' \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},$$

and determine the necessary constant C_1 .

(c)[4pt] When the current density is held steady by some external source, the equilibrium can be studied using the magnetostatic energy \mathcal{E} ,

$$\mathcal{E}[\mathbf{J}] = \int d^3 r \left[\frac{1}{2\mu_0} |\nabla \times \mathbf{A}|^2 - \mathbf{J} \cdot \mathbf{A} \right],$$

where the first term on the right hand side is the energy of the magnetic field and the second term accounts for the work done maintaining the currents. Show that (upon neglecting the surface terms) \mathcal{E} can be expressed as

$$\mathcal{E}[\mathbf{J}] = -C_2 \int d^3 r \mathbf{J} \cdot \mathbf{A},$$

and determine the necessary constant C_2 .

(d)[6pt] It is now specified that the current density arises from a collection of N nonintersecting closed-loop filaments, and that filament n carries current I_n along spatial path $\mathbf{R}_n(s)$, where s is a parameter along the filament. Show that the *interaction energy* among the current loops \mathcal{E}_{int} is given by

$$\mathcal{E}_{\text{int}}[\{I_n\}] = -\frac{1}{2} \sum_{\substack{n=1 \\ n \neq m}}^N \sum_{m=1}^N L_{n,m} I_n I_m,$$

where the coefficients of induction $L_{n,m}$ are given by

$$L_{n,m} = C_3 \int ds \int dt \frac{\dot{\mathbf{R}}_n(s) \cdot \dot{\mathbf{R}}_m(t)}{|\mathbf{R}_n(s) - \mathbf{R}_m(t)|},$$

in which the overdots represent derivatives with respect to the parameter and the integrals are taken around the loops. Obtain the necessary constant C_3 . [Note: A *filament* is defined

to be a single, threadlike object.]

(e)[6pt] A pair of wires lie parallel to one another, separated by a distance Σ . They carry currents I_1 and I_2 , flowing in the same direction. Show that the interaction energy of the two-wire system is given by $\mathcal{E}_{\text{int}} = -C_4 I_1 I_2 \Lambda \ln(2\Lambda/\Sigma e)$, provided the length of the system, Λ , is much greater than Σ , and determine the necessary constant C_4 .

You may use the following result without deriving it:

$$\int_{-W/2}^{W/2} du \int_{-W/2}^{W/2} dv \frac{1}{\sqrt{1+(u-v)^2}} \approx 2W \ln(2W/e), \quad \text{for } W \gg 1.$$

(f)[6pt] With reference to the magnetic field and your answer to part (e), explain whether or not like currents attract.

Solution

(a) Maxwell's equations (in SI units) read

$$\begin{aligned}\nabla \cdot \mathbf{E} &= \frac{\rho}{\epsilon_0} & \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{B} &= \mu_0 \mathbf{J} + \frac{1}{c^2} \partial_t \mathbf{E} & \nabla \times \mathbf{E} &= -\partial_t \mathbf{B}\end{aligned}$$

For static situations, $\partial_t \rightarrow 0$, so that

$$\begin{aligned}\nabla \cdot \mathbf{E} &= \frac{\rho}{\epsilon_0} & \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{B} &= \mu_0 \mathbf{J} & \nabla \times \mathbf{E} &= \mathbf{0}\end{aligned}$$

As $\nabla \cdot \mathbf{B} = 0$, we can introduce the vector potential \mathbf{A} such that $\mathbf{B} = \nabla \times \mathbf{A}$. Then the Ampère-Maxwell law $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$ becomes $\nabla \times \nabla \times \mathbf{A} = \mu_0 \mathbf{J}$. Now, for Cartesian components of \mathbf{F} we have the identity $\nabla \times \nabla \times \mathbf{F} = \nabla(\nabla \cdot \mathbf{F}) - \nabla^2 \mathbf{F}$, so the Cartesian components of \mathbf{A} obey $\nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} = \mu_0 \mathbf{J}$. Then, in Coulomb gauge (*i.e.*, $\nabla \cdot \mathbf{A} = 0$), the Ampère-Maxwell equation for the Cartesian components of \mathbf{A} becomes

$$-\nabla^2 \mathbf{A} = \mu_0 \mathbf{J}.$$

Thus, each component of \mathbf{A} obeys Poisson's equation, sourced by the corresponding Cartesian components of \mathbf{J} .

(b) The solution for \mathbf{A} is therefore given by the analog of Coulomb's law for point charges, together with superposition, and thus reads

$$\mathbf{A}(\mathbf{r}) = C_1 \int d^3 r' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \mathbf{J}(\mathbf{r}'), \quad C_1 = \frac{\mu_0}{4\pi}.$$

(c) The \mathcal{E} energy is given by

$$\mathcal{E} = - \int d^3 r \left\{ \mathbf{J} \cdot \mathbf{A} - \frac{1}{2\mu_0} |\nabla \times \mathbf{A}|^2 \right\}.$$

To arrive at the specified form, we replace one factor of $\nabla \times \mathbf{A}$ by \mathbf{B} to obtain

$$\mathcal{E} = - \int d^3 r \left\{ \mathbf{J} \cdot \mathbf{A} - \frac{1}{2\mu_0} \mathbf{B} \cdot (\nabla \times \mathbf{A}) \right\}.$$

We then integrate by parts and drop the surface term to arrive at

$$\mathcal{E} = - \int d^3 r \left\{ \mathbf{J} \cdot \mathbf{A} - \frac{1}{2\mu_0} (\nabla \times \mathbf{B}) \cdot \mathbf{A} \right\}.$$

Finally, we use the Ampère-Maxwell law, $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$, to eliminate $\nabla \times \mathbf{B}$ in favor of \mathbf{J} , thus arriving at

$$\mathcal{E} = -C_2 \int d^3r \mathbf{J} \cdot \mathbf{A}, \quad C_2 = \frac{1}{2}.$$

(d) In the equation for \mathcal{E} in terms of \mathbf{J} and \mathbf{A} , we use the specified filamentary current distributions to make the following replacements:

$$\begin{aligned} \mathbf{J}(\mathbf{r}) &\rightarrow \sum_{n=1}^N I_n \int ds \dot{\mathbf{R}}_n(s) \delta(\mathbf{r} - \mathbf{R}_n(s)), \\ \mathbf{A}(\mathbf{r}) &= \frac{\mu_0}{4\pi} \int d^3r' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \mathbf{J}(\mathbf{r}') \rightarrow \frac{\mu_0}{4\pi} \sum_{m=1}^N I_m \int dt \frac{\dot{\mathbf{R}}_m(t)}{|\mathbf{r} - \mathbf{R}_m(t)|}. \end{aligned}$$

Then, omitting the self-interaction (i.e., $n = m$) terms, and using the delta function to perform the volume integration, we arrive at interaction contribution to the energy \mathcal{E}_{int} , expressed in terms of the coefficients of induction $L_{n,m}$, i.e.:

$$\begin{aligned} \mathcal{E}_{\text{int}} &= \frac{1}{2} \sum_{\substack{n=1 \\ n \neq m}}^N \sum_{m=1}^N L_{n,m} I_n I_m, \\ L_{n,m} &= C_3 \int ds \int dt \frac{\dot{\mathbf{R}}_n(s) \cdot \dot{\mathbf{R}}_m(t)}{|\mathbf{R}_n(s) - \mathbf{R}_m(t)|}, \quad C_3 = \frac{\mu_0}{4\pi}. \end{aligned}$$

(e) Let the wires run along the z axis and be displaced from one another along the x axis. Then we may choose to write $\mathbf{R}_1(s) = \mathbf{e}_z s$ and $\mathbf{R}_2(t) = \mathbf{e}_z t + \mathbf{e}_x \Sigma$, where $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ are the Cartesian basis unit vectors. For the coefficients of induction, we need the ingredients $\dot{\mathbf{R}}_1(s) \cdot \dot{\mathbf{R}}_2(t) = 1$ and $|\mathbf{R}_1(s) - \mathbf{R}_2(t)|^2 = \Sigma^2 + (s - t)^2$. The integrals over the filaments then give

$$L_{n,m} = \frac{\mu_0}{4\pi} \int_{-\Lambda/2}^{\Lambda/2} ds \int_{-\Lambda/2}^{\Lambda/2} dt \frac{1}{\sqrt{\Sigma^2 + (s - t)^2}}.$$

Rescaling the integration variables from s and t to $u \equiv s/\Sigma$ and $v \equiv t/\Sigma$ gives the equivalent formula:

$$L_{n,m} = \frac{\mu_0}{4\pi} \Sigma \int_{-\Lambda/2\Sigma}^{\Lambda/2\Sigma} du \int_{-\Lambda/2\Sigma}^{\Lambda/2\Sigma} dv \frac{1}{\sqrt{1 + (u - v)^2}},$$

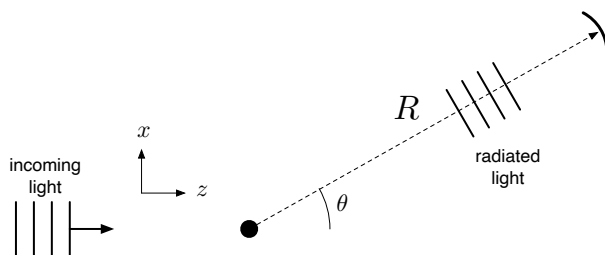
to which we may apply the approximate result provided in the problem statement, thus obtaining:

$$\mathcal{E}_{\text{int}} \approx C_4 I_1 I_2 \Lambda \ln \left(\frac{2\Lambda}{e\Sigma} \right), \quad C_4 = \frac{\mu_0}{2\pi}.$$

(f) For *like* currents, I_1 and I_2 have the *same* sign as one another. The energy therefore *decreases* with decreasing separation Σ , indicating that the currents *attract* one another. In terms of field energy, this is because in the region between the wires the Ampère magnetic fields due to the like currents tend to *cancel* (rather than reinforce) one another, leading to a more pronounced lowering of the field energy for closer wires.

ELECTROMAGNETISM 2

Scattering from a Dielectric Sphere



Consider a monochromatic beam of light propagating in the z -direction. The light is linearly polarized along the x -axis, with polarization vector $\epsilon_0 = \hat{x}$. The wave number is $k = \omega/c$, and the electric field has amplitude E_0 . This light is incident on a small dielectric sphere of radius a and dielectric constant ϵ . Assume $ka \ll 1$.

You may assume without proof that a dielectric sphere placed in an approximately uniform electric field \mathbf{E} develops an induced dipole moment given by:

$$\mathbf{p} = 4\pi a^3 \left(\frac{\epsilon_r - 1}{\epsilon_r + 2} \right) \mathbf{E},$$

where $\epsilon_r = \epsilon/\epsilon_0$ is the relative permittivity.

(a)[3pt] Determine the *incident* photon flux, i.e., the average number of photons per unit area per second arriving at the sphere.

(b)[5pt] Determine the total radiated power P by the dielectric sphere.

(c)[3pt] Determine the scattering cross-section $\sigma = P/I$, defined as the ratio of the radiated power P to the incident intensity I (power per unit area). Alternatively, it is the ratio of the number of photons scattered per second to the incident photon flux. Is σ large or small compared to the geometric cross section of the sphere? Explain the answer.

(d)[4pt] Consider a small photon counter with collecting area A positioned at distance R from the dielectric sphere at an angle θ in the xz -plane (see the figure). The detector is located very far from the sphere and lies outside the direct path of the incoming light.

Determine the average number of photons detected per second.

(e)[5pt] Now consider two identical small spheres placed along the z -axis, separated by a distance $b \gg a$, where a is the radius of each sphere. The separation b is comparable to the wavelength of the incident light, $kb \sim 1$.

Determine how the second sphere modifies the count rate found in part (c). Assume that the radiated field from one sphere does not affect the dipole moment of the other.

Hint: The dipole moments of the two spheres are not in phase. Begin by determining the dipole moments of both spheres.

Solution

Preliminaries:

The solution will use Heaviside-Lorentz units. With this system of units (which is common in nuclear and particle physics), a plane wave of light has $E = B$ and the Poynting vector is $\boldsymbol{\xi} = c\mathbf{E} \times \mathbf{B}$. The squared field E^2 and B^2 have units of energy per volume.

The fields have a harmonic time dependence and we will use a complex notation, e.g. for a signal $V(t)$, we have

$$V(t) = V_\omega e^{-i\omega t} = |V_\omega| e^{-i\omega t + \varphi}. \quad (1)$$

It is understood that the physical signal is the real part of this expression:

$$V_{\text{phys}}(t) = \text{Re}V(t) = \frac{1}{2} (V(t) + V^*(t)) = |V_\omega| \cos(\omega t - \varphi). \quad (2)$$

The time average of two harmonic fields is

$$\langle V_{\text{phys}}(t)W_{\text{phys}}(t) \rangle \equiv \frac{1}{4} (V(t)W^*(t) + V^*(t)W(t)) = \frac{1}{4} [V_\omega W_\omega^* + V_\omega^* W_\omega] = \frac{1}{2} \text{Re} [V(t)W^*(t)] \quad (3)$$

So, in what follows you will see expressions such as:

$$\langle \mathbf{S}_{\text{phys}} \rangle \equiv \frac{1}{2} \text{Re} [c\mathbf{E} \times \mathbf{B}^*] \quad \text{and} \quad \langle \mathbf{p}_{\text{phys}}^2 \rangle = \frac{1}{2} |\mathbf{p}|^2 \quad (4)$$

(a) The incoming fields are

$$\mathbf{E} = E_0 e^{-i\omega t + ikx} \hat{\mathbf{x}}, \quad (5)$$

$$\mathbf{B} = E_0 e^{-i\omega t + ikx} \hat{\mathbf{y}}, \quad (6)$$

and thus $\mathbf{E}_\omega = E_0 e^{ikx} \hat{\mathbf{x}}$ etc. The time averaged Poynting vector records the time-averaged energy per area per time and reads

$$\langle \hat{\mathbf{z}} \cdot \mathbf{S}_{\text{phys}} \rangle = \frac{c}{2} \text{Re} [\mathbf{E}(t) \times \mathbf{B}^*(t)] = \frac{c}{2} E_0^2. \quad (7)$$

Dividing by the energy $\hbar\omega$ of each photon, we get the number of photons per area per time

$$\Phi = \frac{\langle \hat{\mathbf{z}} \cdot \mathbf{S}_{\text{phys}} \rangle}{\hbar\omega} = \frac{c}{2\hbar\omega} E_0^2. \quad (8)$$

(b) The (complex) dipole moment as a function of time is

$$\mathbf{p}(t) = 4\pi a^3 \left(\frac{\epsilon_r - 1}{\epsilon_r + 1} \right) E_0 e^{-i\omega t} \hat{\mathbf{x}} \equiv p_0 e^{-i\omega t} \hat{\mathbf{x}}. \quad (9)$$

where we defined the real number

$$p_0 \equiv 4\pi a^3 \left(\frac{\epsilon_r - 1}{\epsilon_r + 1} \right) E_0. \quad (10)$$

The time average power passing through a sphere of (large) radius r at time t is

$$P(t, r) = \left(\frac{1}{6\pi c^3} \right) \frac{1}{2} |\ddot{\mathbf{p}}(t_r)|^2. \quad (11)$$

Here the dipole moment is evaluated at *the retarded time*

$$t_r = t - \frac{r}{c}, \quad (12)$$

which is the time when the light was emitted in order to arrive at the sphere of radius r at time t . However, this distinction is just an irrelevant phase in this case

$$\ddot{\mathbf{p}}(t_r) = -\omega^2 p_0 e^{-i\omega(t-r/c)} \hat{\mathbf{x}}, \quad \text{and} \quad |\ddot{\mathbf{p}}(t_r)|^2 = \omega^4 p_0^4, \quad (13)$$

but will be significant in part (d). Thus

$$P = \frac{4\pi a^6}{3 c^3} E_0^2 \left(\frac{\epsilon_r - 1}{\epsilon_r + 1} \right)^2 \omega^4. \quad (14)$$

(c) Dividing by the incoming intensity we find

$$\sigma = \frac{P}{c|E_0^2|/2} = \frac{8\pi a^6 \omega^4}{3 c^4} \left(\frac{\epsilon_r - 1}{\epsilon_r + 1} \right)^2. \quad (15)$$

We see that the cross section is of order

$$\sigma \sim (\pi a^2)(ka)^4, \quad (16)$$

where $k = \omega/c$. In the dipole approximation the wavelength is large compared to a and thus $ka \ll 1$. We see that the dipole cross section is much smaller than the geometric cross section. Physically this is because the long wavelength barely resolves the small sphere.

(d) The electric field in the radiation zone is at the observation time t and position $\mathbf{r} = r\hat{\mathbf{n}}$ is

$$\mathbf{E}_{\text{rad}}(t, r, \mathbf{n}) = \frac{1}{4\pi r c^2} (-\ddot{\mathbf{p}}_T(t_r)). \quad (17)$$

Here $\hat{\mathbf{n}}$ is the unit vector pointing from the origin to the observation point, $\mathbf{r} = r\hat{\mathbf{n}}$ (see figure). The transverse dipole moment is

$$\mathbf{p}_T = \mathbf{p} - (\mathbf{p} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}, \quad (18)$$

which is the vector component of \mathbf{p} , which is transverse to $\hat{\mathbf{n}}$ (see figure). From the figure

$$\mathbf{p}_T(t) = p_0 e^{-i\omega t} \cos(\theta) \hat{\mathbf{e}}_1 \quad (19)$$

Here \mathbf{e}_1 is the unit vector parallel to \mathbf{p}_T , which is shown in the figure.

The dipole is evaluated at the retarded time t_r , which is the observation time minus the time it takes travel from the dipole to the observation point

$$t_r = t - \frac{|\mathbf{r} - \mathbf{r}_0|}{c} \simeq t - \frac{r}{c} + \frac{\hat{\mathbf{n}} \cdot \mathbf{r}_0}{c} \quad (20)$$

Here \mathbf{r}_0 is the position of the dipole. For the case of one dipole we have $\mathbf{r}_0 = 0$. Thus

$$\ddot{\mathbf{p}}_T(t_r) = -\omega^2 p_0 e^{-i\omega(t-r/c)} \cos(\theta) \hat{\mathbf{e}}_1 \quad |\ddot{\mathbf{p}}_T|^2 = \omega^4 p_0^2 \cos^2(\theta) \quad (21)$$

The time averaged Poynting vector along the "line of sight" $\hat{\mathbf{n}}$ is

$$\langle \hat{\mathbf{n}} \cdot \hat{\mathbf{S}}_{\text{phys}} \rangle = \frac{c}{2} |\mathbf{E}_{\text{rad}}|^2 = \frac{1}{32\pi^2 R^2 c^3} p_0^2 \omega^4 \cos^2 \theta. \quad (22)$$

Multiplying by the collecting area and dividing by the energy of each photon $\hbar\omega$, we find the count rate

$$\Gamma = \frac{\langle \hat{\mathbf{n}} \cdot \hat{\mathbf{S}}_{\text{phys}} \rangle A}{\hbar\omega} \propto \omega^3 \frac{A}{R^2} \frac{p_0^2}{c^3} \cos^2 \theta. \quad (23)$$

From a physical perspective, it is clear that the count rate should vanish at $\theta = \pi/2$. In this case the oscillating currents $\mathbf{J} \sim \partial_t \mathbf{p}$ are parallel to the direction of the outgoing radiation, i.e. for $\theta = \pi/2$ in the oscillating current is in the $\hat{\mathbf{x}}$ direction (imagine Fig 1 for $\theta = \pi/2$). However, the outgoing radiated electric field must be transverse to the direction of propagation. There is no components of the oscillating currents which are transverse to \mathbf{n} , which can drive the transverse electromagnetic wave. Thus the resulting radiation is zero.

(e) The two dipoles A and B each contribute to the radiation field

$$\mathbf{E}_{\text{rad}}(t, r, \mathbf{n}) = \frac{-1}{4\pi r c^2} [(\ddot{\mathbf{p}}_T^A(t_r^A) + (\ddot{\mathbf{p}}_T^B(t_r^B))] . \quad (24)$$

The first dipole is driven by the field at $x = 0$

$$\mathbf{p}^A(t) = p_0 e^{-i\omega t + ikx} \Big|_{x=0} \hat{\mathbf{x}} = p_0 e^{-i\omega t} \hat{\mathbf{x}}. \quad (25)$$

The second dipole is driven by the field at $x = b$ and is out of phase due to the displacement:

$$\mathbf{p}^B(t) = p_0 e^{-i\omega t + ikx} \Big|_{x=b} \hat{\mathbf{x}} = p_0 e^{ikb} e^{-i\omega t} \hat{\mathbf{x}}. \quad (26)$$

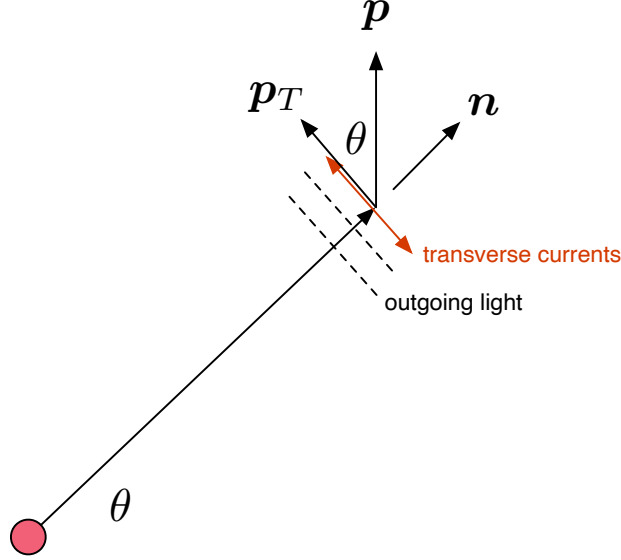


FIG. 1. Geometry of the radiation.

In addition, the retarded times are different as the propagation times between the two dipoles and the observation point are different. The retarded time of dipole A is $t_r^A = t - r/c$, but the retarded time of dipole B is

$$t_r^B = t - \frac{r}{c} + \frac{\hat{\mathbf{n}} \cdot \mathbf{r}_0}{c} = t - \frac{r}{c} + \frac{b}{c} \cos \theta. \quad (27)$$

The difference in propagation times has a clear geometric significance

$$t_r^B - t_r^A = (b/c) \cos \theta, \quad (28)$$

which is studied in Fig. 2.

Putting together the ingredients, we have as before

$$\mathbf{p}^A(t_r^A) = p_0 e^{-i\omega(t-r/c)} \hat{\mathbf{x}}, \quad (29)$$

while for B

$$\mathbf{p}^B(t_r^B) = p_0 e^{ikb} e^{-i\omega(t-r/c+b/c \cos \theta)} \hat{\mathbf{x}}, \quad (30)$$

$$= e^{ikb(1-\cos \theta)} [p_0 e^{-i\omega(t-r/c)} \hat{\mathbf{x}}]. \quad (31)$$

Thus

$$[\mathbf{p}^A(t_r^A) + \mathbf{p}^B(t_r^B)] = \mathbf{p}^A(t_r^A) (1 + e^{ikb(1-\cos \theta)}), \quad (32)$$

The count rate is modified by the interference

$$\Gamma_{(d)} = \Gamma_{(c)} |1 + e^{ikb(1-\cos \theta)}|^2 = \Gamma_{(c)} [2 + 2 \cos(kb(1 - \cos \theta))]. \quad (33)$$

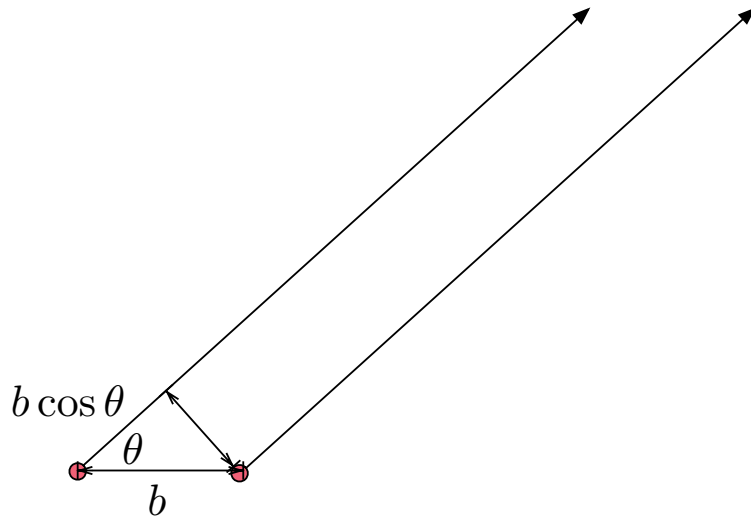


FIG. 2. The distance that the light from dipole A (the left circle) needs to travel to the observation point is longer by $b \cos \theta$ than for dipole B (the right circle). Thus, the retarded time (sometimes called the emission time) of dipole B is later by $(b \cos \theta)/c$ so that the two signals arrive at the observation point at the same time.

ELECTROMAGNETISM 3

Reflection from plasma

In this problem, we will consider electromagnetic waves propagating in and reflected from the boundary of a region filled with plasma. Consider non-relativistic ionized gas consisting of light particles having mass m and charge q with number density n as well as heavy particles (atoms) with the same density but carrying charge $(-q)$, so that the whole gas is electrically-neutral. The motion of the atoms can be neglected.

(a)[4pt] Describe the motion of the light charges in presence of electric field $\vec{E}(r, t) = \vec{E}_0 e^{-i\omega t}$. Calculate the polarization density of the plasma $\vec{P} = qn\vec{r}$ where \vec{r} is the displacement of the light charges from the equilibrium in the absence of electric field.

(b)[4pt] Calculate the phase velocity $v_{ph}(\omega)$ of an electromagnetic wave with frequency ω propagating through the plasma. Express your answer using the plasma frequency $\omega_p = \sqrt{nq^2/m\epsilon_0}$. *Hint: one way to do it is to use the previous section result to evaluate the (relative) frequency-dependent dielectric permittivity $\epsilon(\omega) = 1 + \chi_r(\omega)$ of the plasma, where $\chi(\omega)$ is the (relative) electric susceptibility, $\vec{P} = \chi(\omega)\epsilon_0\vec{E}$.*

(c)[2pt] Calculate the group velocity $v_g(\omega)$; at which frequencies electromagnetic waves can freely propagate through plasma? What happens at the other frequencies?

Now consider a plane wave $\vec{E}(z, t) = E_0 \hat{x} e^{ikz - i\omega t}$ traveling in vacuum ($z < 0$) and incident on the boundary of plasma ($z > 0$) at $z = 0$.

(d)[5pt] For the frequencies at which *the wave can propagate through the plasma*, find the electric and magnetic fields in the reflected and transmitted waves. Compute the reflection coefficient $R = \frac{\text{Energy incident}}{\text{Energy reflected}}$ and sketch it as a function of ω .

(e)[5pt] For the frequencies at which *the wave cannot propagate through the plasma*, calculate the phase shift δ of the reflected wave, $E_r = |E_{0r}| e^{-ikz - i\omega t + i\delta}$, and sketch it as a function of ω .

Solution

(a) In the presence of oscillating electric field, the light charges will also oscillate with the same frequency. Writing the dynamic equation for a single charge's displacement $\vec{r} = \vec{r}_0 e^{-i\omega t}$

$$m\ddot{\vec{r}} = q\vec{E} \implies \vec{r}_{(0)} = -\frac{q}{m\omega^2}\vec{E}_{(0)},$$

(the relation holds both for the amplitudes and the time-dependent complex values) hence the polarisation density $\vec{P} = nq\vec{r} = P_0 e^{-i\omega t}$ is

$$\vec{P}_{(0)} = nq\vec{r}_{(0)} = -\frac{1}{\omega^2} \frac{nq^2}{m} \vec{E}_{(0)} = -\frac{\omega_p^2}{\omega^2} \varepsilon_0 \vec{E}_{(0)}$$

(b) The electric displacement vector $\vec{D} = \varepsilon_0 \vec{E} + \vec{P}$ yields the dielectric permittivity

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$

and in absence of magnetic effects the phase velocity is reduced by $n(\omega) = \sqrt{\varepsilon(\omega)}$,

$$v_{ph}(\omega) = \frac{\omega}{k(\omega)} = \frac{c}{\sqrt{1 - \omega_p^2/\omega^2}}$$

The wave can propagate only if $\omega > \omega_p$. If $\omega < \omega_p$, the wave can exist only as a special kind of standing wave with amplitude exponentially decreasing away from the plasma boundary.

(c) The group velocity $v_g(\omega) = d\omega/dk$ is calculated using $k(\omega) = \omega/v_{ph}(\omega) = (\omega/c)\sqrt{1 - \omega_p^2/\omega^2}$:

$$v_g(\omega) = \left(\frac{dk}{d\omega}\right)^{-1} = c\sqrt{1 - \omega_p^2/\omega^2}.$$

For $\omega > \omega_p$ the group velocity $v_g < c$ as expected but for $\omega < \omega_p$ the velocity is imaginary and the wave cannot propagate.

(d) Using the relation between the electric and magnetic fields $\vec{k} \times \vec{E} = \omega \vec{B}$ in any plane wave $\{\vec{E}, \vec{B}\} \propto e^{i\vec{k}\cdot\vec{r} - i\omega t}$, the field amplitudes in the incident, reflected, and transmitted waves

$$\begin{aligned} \vec{E}_i &= E_{0i} \hat{x} e^{ikz - i\omega t} & \vec{B}_i &= \frac{k}{\omega} E_{0i} \hat{y} e^{-ikz - i\omega t} \\ \vec{E}_r &= E_{0r} \hat{x} e^{-ikz - i\omega t} & \vec{B}_r &= -\frac{k}{\omega} E_{0r} \hat{y} e^{-ikz - i\omega t} \\ \vec{E}_t &= E_{0t} \hat{x} e^{ik_2 z - i\omega t} & \vec{B}_t &= \frac{k_2}{\omega} E_{0t} \hat{y} e^{ik_2 z - i\omega t} \end{aligned}$$

can be matched as

$$\begin{aligned} E_{0i} + E_{0r} &= E_{0t} \\ \frac{k}{\omega} E_{0i} - \frac{k}{\omega} E_{0r} &= \frac{k_2}{\omega} E_{0t} \end{aligned}$$

where $k = \omega/c$ and $k_2 = k\sqrt{1 - \omega_p^2/\omega^2}$ is the wave number in the plasma. Solving the above equations yields

$$E_{0t} = \frac{2}{1 + k_2/k} E_{0i}, \quad E_{0r} = \frac{1 - k_2/k}{k_2/k + 1} E_{0i},$$

and the reflection coefficient

$$R(\omega) = \left| \frac{E_{0r}}{E_{0i}} \right|^2 = \left| \frac{1 - \sqrt{1 - \omega_p^2/\omega^2}}{1 + \sqrt{1 - \omega_p^2/\omega^2}} \right|^2$$

For small frequencies at and below ω_p , the reflection is complete $R(\omega \leq \omega_p) = 1$. For large frequencies, expanding in ω_p/ω yields

$$R(\omega \gg \omega_p) \approx \left(\frac{\omega_p}{2\omega} \right)^4$$

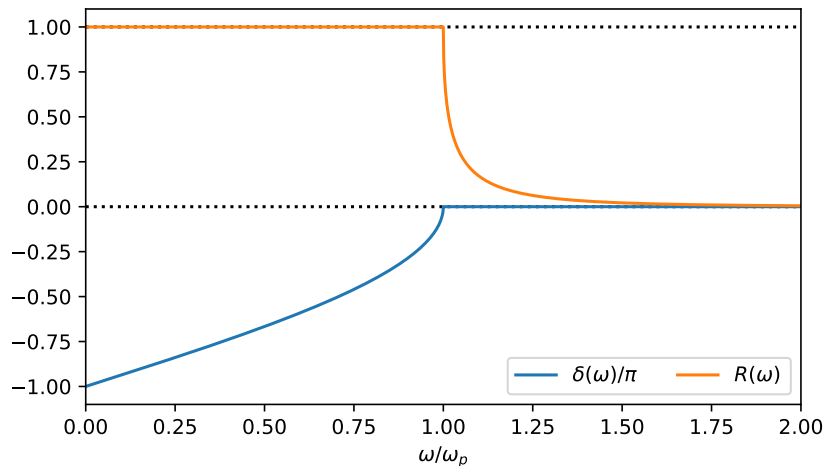
(e) The relations from the previous part hold also for $\omega < \omega_p$ but now the wave number $k_2 = i\sqrt{\omega_p^2/\omega^2 - 1}$ is complex, and the sign is chosen such that the wave amplitude decays exponentially with z . Using the relation between the amplitudes on the boundary, the phase shift can be determined as

$$\delta(\omega) = \arg \frac{E_{0r}}{E_{0i}} = \arg \frac{1 - i\sqrt{\omega_p^2/\omega^2 - 1}}{1 + i\sqrt{\omega_p^2/\omega^2 - 1}} = -2 \arctan \sqrt{\omega_p^2/\omega^2 - 1}$$

Taking the interesting limits, we get

$$\delta(\omega \rightarrow 0) \rightarrow -\pi, \quad \delta(\omega \rightarrow \omega_p) \rightarrow 0.$$

Both $R(\omega)$ and $\delta(\omega)$ are sketched below. As long as the limits were shown correctly, the sketches counted for the full score. It is also instructive to observe that $R = 1$ (full reflection) for $\omega < \omega_p$ and $\delta = 0$ (\vec{E}_i and \vec{E}_r co-aligned) for $\omega > \omega_p$.



QUANTUM MECHANICS 1

Interaction representation and rotating-wave approximation

For many quantum systems, a Hamiltonian H can be separated into $H_0 + V$, where H_0 is the main non-interacting (“free”) Hamiltonian and perturbation V describes interaction. To simplify the time evolution of the usual Schrödinger wave function $|\psi^S\rangle$

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

the so-called interaction-representation wave function $|\psi^I(t)\rangle$ is defined that evolves only due to the perturbation V :

$$i\hbar \frac{d}{dt} |\psi^I(t)\rangle = V_I(t) |\psi^I(t)\rangle, \quad \text{where } V_I(t) \equiv e^{iH_0 t/\hbar} V(t) e^{-iH_0 t/\hbar}, \quad (1)$$

and at the reference time $t = 0$ matches the Schrödinger wave function $|\psi^I(0)\rangle = |\psi^S(0)\rangle$.

(a)[3pt] What is the relation between the wavefunctions $|\psi^I(t)\rangle$ and $|\psi^S(t)\rangle$?

(b)[3pt] Suppose a two-state atom interacts with a classical field that oscillates with frequency ω and drives transition between the two atom states. Such atom can be described by the following Hamiltonian

$$H = H_0 + V(t), \quad H_0 = \frac{\hbar\omega_s}{2} \sigma_z, \quad V(t) = g\sigma_x \cos(\omega t),$$

where $\sigma_{x,y,z}$ denote the usual Pauli matrices. Use Eq. (1) to derive the explicit form of the field term $V_I(t)$ in the interaction representation. Does $V_I(t)$ commute with $V_I(t')$ if $t' \neq t$?

Now assume that the frequencies ω_s and ω are much larger than all the other frequencies in the evolution of $|\psi^I(t)\rangle$, specifically g/\hbar and the “detuning” $\Delta \equiv (\omega - \omega_s)$. In this case, one can make the so-called “rotating wave” approximation by neglecting all the terms in the evolution equation that oscillate with large frequencies on the order of ω_s and ω , and keep only the terms with small frequencies g/\hbar and Δ .

(c)[3pt] Write down the evolution equation for $|\psi^I(t)\rangle$ using $V_I(t)$ obtained above and simplify it using this rotating-wave approximation.

(d)[4pt] The interaction term $V_I(t)$ in the rotating wave approximation derived above is in general time-dependent. Perform a unitary transformation $K(t)$ on $|\psi^I(t)\rangle$ so that the evolution of $K|\psi^I(t)\rangle \equiv |\chi(t)\rangle$ is governed by time-independent term V'_I , $i\hbar \frac{\partial}{\partial t} |\chi(t)\rangle = V'_I |\chi(t)\rangle$, and find V'_I .

(e)[5pt] In this form, the time evolution of the state of the atom

$$|\chi(t)\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$$

can be found explicitly, e.g., by evaluating the time evolution operator $U(t) = e^{-iV_I t/\hbar}$. Find $a(t)$ and $b(t)$ with an arbitrary initial condition $a(0) = a_0$ and $b(0) = b_0$.

(f)[2pt] Simplify expression obtained in (e) to the situation when the atom is initially in the ground state, $b_0 = 1$, to find the probability $p_0(t)$ that it remains in the ground state at later times t . (Note that the transformations between the different forms of the atom wavefunctions, $|\psi^S(t)\rangle$, $|\psi^I(t)\rangle$, and $|\chi(t)\rangle$, do not affect the occupation probabilities of the atomic states.)

You may find useful the standard relation

$$e^{i(\vec{\sigma} \cdot \hat{n})A} = \cos A + i(\vec{\sigma} \cdot \hat{n}) \sin A$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\hat{n} = (n_x, n_y, n_z)$ is an arbitrary unit vector, $n_x^2 + n_y^2 + n_z^2 = 1$.

Solution

(a) Since $|\psi^I(t)\rangle$ is defined to evolve only due to the perturbation V , to obtain $|\psi^I(t)\rangle$ explicitly, one needs to remove from $|\psi^S(t)\rangle$ the evolution due to the free part H_0 of the Hamiltonian. This means that

$$|\psi^I(t)\rangle \equiv e^{iH_0t/\hbar}|\psi^S(t)\rangle.$$

One can check by direct substitution that $|\psi^I(t)\rangle$ defined in this way indeed satisfies the evolution equation (1).

(b) Using the form of the operators H_0 and $V(t)$ for the atom, and multiplying directly the corresponding two-by-two matrices, we get

$$V_I(t) = e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar} = \exp\left\{i\frac{\omega_s t}{2}\sigma_z\right\}g\sigma_x \cos(\omega t) \exp\left\{-i\frac{\omega_s t}{2}\sigma_z\right\} = g \cos(\omega t) \begin{pmatrix} 0, & e^{i\omega_s t} \\ e^{-i\omega_s t}, & 0 \end{pmatrix}.$$

This gives the following evolution equation for $|\psi^I(t)\rangle$:

$$i\hbar \frac{d}{dt}|\psi^I(t)\rangle = g \cos(\omega t) \begin{pmatrix} 0, & e^{i\omega_s t} \\ e^{-i\omega_s t}, & 0 \end{pmatrix} |\psi^I(t)\rangle.$$

This expression also shows that the operator $V_I(t)$ in general does not commute with $V_I(t')$ for $t' \neq t$.

(c) Analyzing obtained evolution equation for $|\psi^I(t)\rangle$ we see that it contains the terms oscillating as functions of time t with large frequency $\omega + \omega_s$, and the terms oscillating with small frequency $\omega - \omega_s \equiv \Delta$. Omitting the large-frequency terms we get:

$$i\hbar \frac{d}{dt}|\psi^I(t)\rangle = V_I(t)|\psi^I(t)\rangle = \frac{g}{2} \begin{pmatrix} 0, & e^{i(\omega_s - \omega)t} \\ e^{-i(\omega_s - \omega)t}, & 0 \end{pmatrix} |\psi^I(t)\rangle = \frac{g}{2} \begin{pmatrix} 0, & e^{-i\Delta t} \\ e^{i\Delta t}, & 0 \end{pmatrix} |\psi^I(t)\rangle.$$

(d) The matrix elements of the operator $V_I(t)$ in the “rotating wave” approximation derived above oscillate as functions of time t with frequencies $\pm\Delta$. From the form of this time dependence shows that it can be removed by the following unitary transformation K of the state $|\psi^I(t)\rangle$:

$$|\chi(t)\rangle = K|\psi^I(t)\rangle, \quad K = \exp\left\{i\frac{\Delta t}{2}\sigma_z\right\}.$$

Using these equations, one sees directly that $|\chi(t)\rangle$ satisfies the following evolution equation:

$$i\hbar \frac{d}{dt}|\chi(t)\rangle = -\frac{\hbar\Delta}{2}\sigma_z|\chi(t)\rangle + KV_I(t)K^\dagger|\chi(t)\rangle = V'_I|\chi(t)\rangle, \quad \text{where } V'_I = -\frac{\hbar\Delta}{2}\sigma_z + \frac{g}{2}\sigma_x.$$

(e) Evolution equation for $|\chi(t)\rangle$ with the time-independent V_I can be solved immediately in the standard general form:

$$|\chi(t)\rangle = U(t)|\chi(0)\rangle \quad U(t) = e^{-iV_I t/\hbar}.$$

Using the properties of the Pauli σ matrices, we get the following expression for the evolution operator $U(t)$:

$$U(t) = e^{-iV_1 t/\hbar} = \exp\left\{i\frac{(\hbar\Delta\sigma_z - g\sigma_x)t}{2\hbar}\right\} = \cos(\Omega t/2) + i\frac{\Delta\sigma_z - (g/\hbar)\sigma_x}{\Omega} \sin(\Omega t/2), \quad \Omega \equiv [\Delta^2 + (g/\hbar)^2]^{1/2}.$$

From this, we get the time-dependent amplitudes of the state $|\chi(t)\rangle$:

$$a(t) = [\cos(\Omega t/2) + i\frac{\Delta}{\Omega} \sin(\Omega t/2)]a_0 - i\frac{g}{\hbar\Omega} \sin(\Omega t/2)b_0,$$

$$b(t) = [\cos(\Omega t/2) - i\frac{\Delta}{\Omega} \sin(\Omega t/2)]b_0 - i\frac{g}{\hbar\Omega} \sin(\Omega t/2)a_0.$$

(f) If the atom is initially in the ground state, $a_0 = 0$, $b_0 = 1$, the obtained amplitudes give the following probability for the atom to stay in the initial state:

$$p_0(t) = |b(t)|^2 = \cos^2(\Omega t/2) + \frac{\Delta^2}{\Omega^2} \sin^2(\Omega t/2) = 1 - \frac{\Delta^2}{\Omega^2} \sin^2(\Omega t/2) = 1 - p_1(t),$$

where $p_1(t) = \frac{\Delta^2}{\Omega^2} \sin^2(\Omega t/2)$ is the probability of the transition from the initial state

QUANTUM MECHANICS 2

Cyclic Permutation Protocol

Consider a system of two qubits (two-level systems) defined by the standard basis of states $\{|\uparrow\uparrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\downarrow\rangle\}$. The system has the following Hamiltonian:

$$H_{12} = J \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2,$$

where $\boldsymbol{\sigma}_1 = (\sigma_1^x, \sigma_1^y, \sigma_1^z)$ is the triplet of Pauli matrices acting on the first qubit, and $\boldsymbol{\sigma}_2$ is the corresponding triplet acting on the second qubit.

(a)[3pt] Determine how the operators $(1 + \sigma_1^z \sigma_2^z)/2$ and $(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)/2$ act on the states of the standard basis of the system. For the second operator, it can be convenient to express it through the “raising and lowering” operators $\sigma^\pm = (\sigma^x \pm i\sigma^y)/2$.

(b)[3pt] From the results of part (a) show that the action of the **swap** operator

$$P_{12} = (1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)/2, \tag{1}$$

can be viewed as exchanging the states of qubits 1 and 2 in an arbitrary product state $|\alpha\rangle_1 \otimes |\beta\rangle_2$ of the two-qubit system.

(c)[5pt] Denote the unitary evolution operator of the two-qubit system by

$$S_{12}(t) = e^{-\frac{i}{\hbar} H_{12} t}. \tag{2}$$

Consider an arbitrary initial product state $|\alpha\rangle_1 \otimes |\beta\rangle_2$. Find a value of the evolution time $t = T$ such that

$$S_{12}(T) \left(|\alpha\rangle_1 \otimes |\beta\rangle_2 \right) = e^{i\gamma} |\beta\rangle_1 \otimes |\alpha\rangle_2, \tag{3}$$

i.e., the evolution swaps the states of the two qubits up to a “global” phase γ . What is γ ?

(d)[5pt] Now consider a system of three qubits. Let us denote by C_{123} the operator that performs a cyclic permutation of the qubit states, meaning that for any product state

$$C_{123} \left(|\alpha\rangle_1 \otimes |\beta\rangle_2 \otimes |\gamma\rangle_3 \right) = |\beta\rangle_1 \otimes |\gamma\rangle_2 \otimes |\alpha\rangle_3. \tag{4}$$

Determine the eigenvalues and eigenvectors of the operator C_{123} .

(e)[4pt] Assume that the system evolves under a time-dependent Hamiltonian

$$H(t) = J_1(t) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + J_2(t) \boldsymbol{\sigma}_2 \cdot \boldsymbol{\sigma}_3 + J_3(t) \boldsymbol{\sigma}_3 \cdot \boldsymbol{\sigma}_1, \tag{5}$$

where the time-dependent parameters $J_j(t)$, $j = 1, 2, 3$, can be arbitrarily controlled. Provide an example of a quantum protocol (specific choices of the functions $J_j(t)$) such that the time evolution of the three-qubit system over a time \tilde{T} implements the cyclic permutation operator C_{123} up to some phase γ' .

Solution

(a) Since the σ^z matrix is diagonal in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis, direct evaluation shows that the operator $(1 + \sigma_1^z \sigma_2^z)/2$ equals 1, when the two qubits are in the same states, i.e., in the subspace $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, and 0 - in the $\{|\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle\}$ subspace.

Next, expressing the σ^x and σ^y matrices through σ^+ and σ^- ,

$$\sigma^x = \sigma^+ + \sigma^-, \quad \sigma^y = i(\sigma^- - \sigma^+),$$

we see that

$$(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)/2 = \sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+.$$

This equation shown immediately that the operator $(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)/2$ equals 0 in the subspace $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, and exchanges the two basis states in the $\{|\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle\}$ subspace:

$$(1/2)(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)|\downarrow\uparrow\rangle = |\uparrow\downarrow\rangle, \quad (1/2)(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y)|\uparrow\downarrow\rangle = |\downarrow\uparrow\rangle.$$

(b) For the product states of the two qubits, exchange of the basis states in the $\{|\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle\}$ subspace is equivalent to the exchange of the amplitudes of the two states. Therefore, the properties of the product operators derived in part(a) mean that the operator P_{12} [which is the sum of the two operators considered in (a)]:

$$P_{12} = \frac{1}{2} (\mathbb{I} + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2), \quad (6)$$

where \mathbb{I} is the identity operator on the two-qubit Hilbert space, acts as the **swap operator**, which exchanges the states of qubits 1 and 2:

$$P_{12}(|\alpha\rangle_1 \otimes |\beta\rangle_2) = |\beta\rangle_1 \otimes |\alpha\rangle_2. \quad (7)$$

(c) From the definition of the swap operator we see that

$$\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = 2P_{12} - \mathbb{I},$$

and therefore the Hamiltonian of the two-qubit system can be written as

$$H_{12} = J \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = J(2P_{12} - \mathbb{I}).$$

The corresponding evolution operator then becomes

$$S_{12}(t) = e^{-\frac{i}{\hbar} H_{12} t} = e^{-\frac{i}{\hbar} J(2P_{12} - \mathbb{I}) t} = e^{\frac{iJt}{\hbar}} e^{-\frac{2iJt}{\hbar} P_{12}}, \quad (8)$$

where we used that \mathbb{I} and P_{12} commute.

As can be checked directly, P_{12} satisfies the condition $P_{12}^2 = \mathbb{I}$. This makes it possible to expand the exponential like this:

$$e^{-\frac{2iJt}{\hbar}P_{12}} = \cos\left(\frac{2Jt}{\hbar}\right)\mathbb{I} - i\sin\left(\frac{2Jt}{\hbar}\right)P_{12}. \quad (9)$$

Thus,

$$S_{12}(t) = e^{\frac{iJt}{\hbar}} \left(\cos\left(\frac{2Jt}{\hbar}\right)\mathbb{I} - i\sin\left(\frac{2Jt}{\hbar}\right)P_{12} \right). \quad (10)$$

We now demand that

$$S_{12}(T) = P_{12} \quad (\text{up to a global phase}), \quad (11)$$

and see that this happens if

$$\cos\left(\frac{2JT}{\hbar}\right) = 0, \quad \sin\left(\frac{2JT}{\hbar}\right) = 1,$$

which is achieved when

$$\frac{2JT}{\hbar} = \frac{\pi}{2} \quad \Rightarrow \quad T = \frac{\pi\hbar}{4J}. \quad (12)$$

Thus, the required time is

$$\boxed{T = \frac{\pi\hbar}{4J}}, \quad (13)$$

and at this time, the global phase is:

$$\gamma = \frac{JT}{\hbar} - \frac{\pi}{2} = -\frac{\pi}{4}. \quad (14)$$

(d) Now consider a system of three qubits. The cyclic permutation operator C_{123} :

$$C_{123}\left(|\alpha\rangle_1 \otimes |\beta\rangle_2 \otimes |\gamma\rangle_3\right) = |\alpha\rangle_3 \otimes |\beta\rangle_1 \otimes |\gamma\rangle_2. \quad (15)$$

cyclically shifts the amplitudes u_j of a quantum state

$$|\Psi\rangle = u_1|\alpha\rangle_1 \otimes |\beta\rangle_2 \otimes |\gamma\rangle_3 + u_2|\gamma\rangle_1 \otimes |\alpha\rangle_2 \otimes |\beta\rangle_3 + u_3|\beta\rangle_1 \otimes |\gamma\rangle_2 \otimes |\alpha\rangle_3.$$

so that $(u_1, u_2, u_3) \xrightarrow{C_{123}} (u_2, u_3, u_1)$. This means that for a state to be the eigenstate of C_{123} with eigenvalue λ , the amplitudes need to satisfy the condition $u_j = \lambda u_{j-1}$, i.e. one has:

$$u_j \propto \lambda^j, \quad \lambda^3 = 1.$$

These conditions show that there are three eigenvalues of C_{123} :

$$\lambda_k = e^{i2\pi k/3}, \quad k = 0, 1, 2,$$

with the corresponding eigenstates given by the normalized amplitudes described above

$$u_j^{(k)} = \frac{1}{\sqrt{3}}(\lambda_k)^j.$$

(e) As usual, the cyclic permutation C_{123} can be represented as a sequence of pairwise permutations, i.e., swap operators:

$$C_{123} = P_{23}P_{12}, \tag{16}$$

where P_{12} swaps qubits 1 and 2, and P_{23} swaps qubits 2 and 3.

Indeed, acting sequentially:

- P_{12} exchanges qubits 1 and 2: $|\alpha\rangle_1 \otimes |\beta\rangle_2 \otimes |\gamma\rangle_3 \rightarrow |\beta\rangle_1 \otimes |\alpha\rangle_2 \otimes |\gamma\rangle_3$,
- then P_{23} exchanges qubits 2 and 3: $|\beta\rangle_1 \otimes |\alpha\rangle_2 \otimes |\gamma\rangle_3 \rightarrow |\beta\rangle_1 \otimes |\gamma\rangle_2 \otimes |\alpha\rangle_3$.

Renaming qubits as $1 \rightarrow 3$, $2 \rightarrow 1$, $3 \rightarrow 2$, this is precisely the cyclic permutation desired.

If one takes into account the results of part (c), this representation of the cyclic permutation operator C_{123} means that this operator can be implemented if one applies two consecutive pulses to the 3-qubit system:

- switching on $J_1(t)$ from 0 to constant J_1 and back to 0 for the time interval $\pi\hbar/4J_1$ to exchanges qubits 1 and 2;
- switching on $J_2(t)$ from 0 to constant J_2 and back to 0 for the time interval $\pi\hbar/4J_2$ to exchanges qubits 2 and 3.

QUANTUM MECHANICS 3

Heating in Optical Lattices due to Laser Intensity Noise

Consider an atom of mass M trapped in a one-dimensional optical lattice potential given by

$$V(x) = V_0 \sin^2(kx),$$

where V_0 is the lattice depth, and $k = 2\pi/\lambda$ is the wave number of the trapping laser of wavelength λ . We will study atom states localized around just one minimum of the potential (say $x = 0$) using harmonic oscillator approximation.

(a)[2pt] Expand the lattice potential around the equilibrium position $x = 0$ up to the second order in x . Find the harmonic oscillator frequency ω_{trap} in terms of V_0 , k , and M .

(b)[6pt] Suppose now that the lattice depth fluctuates with time as

$$V_0(t) = V_0[1 + \epsilon(t)],$$

where $\epsilon(t)$ is a small dimensionless noise term with zero mean, $\langle \epsilon(t) \rangle = 0$. Within the first-order perturbation theory, explain why the noise term $V(t) \propto \epsilon(t)$ can induce transitions only between harmonic oscillator levels different by two quanta, $n \rightarrow n \pm 2$. Calculate the respective matrix elements $\langle n + 2 | V(t) | n \rangle$.

Hint: One possible way to do this is to express the perturbation term using ladder operators.

(c)[6pt] Using first-order time-dependent perturbation theory, write an expression for the transition rate $\Gamma_{n \rightarrow n \pm 2}$ (transition probability per unit time) between harmonic oscillator levels induced by such fluctuations. Further, assuming that t is much larger than the *correlation time* of the noise τ_ϵ , express your answer in terms of the power spectral density

$$\langle \epsilon(t)\epsilon(t') \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} S_\epsilon(\omega) e^{-i\omega(t-t')} d\omega,$$

and show that the transition probabilities depend only on its value at frequency $\omega = 2\omega_{\text{trap}}$.

Hint: express the transition probability in terms of the noise autocorrelation $\langle \epsilon(t)\epsilon(t + \tau) \rangle$ and assume that it falls off rapidly with increasing $|\tau| > \tau_\epsilon$.

(d)[6pt] Using the transition rates derived in (c), find the resulting expression for the rate of change of the atom's average energy $\langle E(t) \rangle$. Show that such noise leads to exponential heating (the energy to grow exponentially with time).

Assume that initially the atom occupies level n with probability P_n and has average energy $\langle E \rangle = \sum_n \hbar\omega_{\text{trap}} n P_n = \hbar\omega_{\text{trap}} \langle n \rangle$. Express the rate of the average energy change $d\langle E \rangle/dt$ using the transition probabilities computed above.

Solution

(a) For small displacements $|kx| \ll 1$ expand $\sin(kx) \simeq kx$:

$$V(x) \simeq V_0 k^2 x^2 = \frac{1}{2} M \omega_{\text{trap}}^2 x^2, \quad \Longrightarrow \quad \boxed{\omega_{\text{trap}} = \sqrt{\frac{2V_0 k^2}{M}}}.$$

(b) Intensity noise is described by a real, zero-mean process $\epsilon(t)$:

$$V(t) = \frac{1}{2} M \omega_{\text{trap}}^2 x^2 \epsilon(t) = \frac{\hbar \omega_{\text{trap}}}{4} (a + a^\dagger)^2 \epsilon(t).$$

Because $(a + a^\dagger)^2 = a^2 + a^{\dagger 2} + 2n + 1$, only a^2 and $a^{\dagger 2}$ connect the states with $\Delta n = \pm 2$. From $\langle n+1 | a^\dagger | n \rangle = \langle n | a | n+1 \rangle = \sqrt{n+1}$, the respective matrix elements are

$$\langle n+2 | V(t) | n \rangle = \frac{1}{4} \hbar \omega_{\text{trap}} \langle n+2 | a^{\dagger 2} | n \rangle \epsilon(t) = \frac{1}{4} \hbar \omega_{\text{trap}} \sqrt{(n+1)(n+2)} \epsilon(t) \quad (1)$$

(c) Let \mathcal{T} be the total observation time. The first-order transition *probability* from $|n\rangle$ to $|n+2\rangle$ is

$$P_{n \rightarrow n+2}(\mathcal{T}) = \frac{1}{\hbar^2} \int_0^{\mathcal{T}} dt_1 \int_0^{\mathcal{T}} dt_2 \langle \langle n+2 | V(t_1) | n \rangle \langle n | V(t_2) | n+2 \rangle \rangle e^{i2\omega_{\text{trap}}(t_1-t_2)}.$$

Using $\langle n+2 | V(t) | n \rangle = \frac{\hbar \omega_{\text{trap}}}{4} \sqrt{(n+1)(n+2)} \epsilon(t)$ we pull out $\hbar^2 \omega_{\text{trap}}^2 (n+1)(n+2)/16$ and focus on the noise double integral

$$I(\mathcal{T}) \equiv \int_0^{\mathcal{T}} dt_1 \int_0^{\mathcal{T}} dt_2 \langle \epsilon(t_1) \epsilon(t_2) \rangle e^{i2\omega_{\text{trap}}(t_1-t_2)}.$$

Define the new variables

$$\tau = t_1 - t_2, \quad T = t_1 + t_2 \quad (\text{Jacobian } \frac{1}{2}).$$

The domain $0 \leq t_1, t_2 \leq \mathcal{T}$ maps to $-\mathcal{T} \leq \tau \leq \mathcal{T}$ and $|\tau| \leq T \leq 2\mathcal{T} - |\tau|$:

$$I(\mathcal{T}) = \frac{1}{2} \int_{-\mathcal{T}}^{\mathcal{T}} d\tau \int_{|\tau|}^{2\mathcal{T}-|\tau|} dT C_\epsilon(\tau) e^{i2\omega_{\text{trap}}\tau},$$

where $C_\epsilon(\tau) = \langle \epsilon(t) \epsilon(t+\tau) \rangle$ (stationarity). Executing the T -integration gives the triangular window $(\mathcal{T} - |\tau|)$:

$$I(\mathcal{T}) = \int_{-\mathcal{T}}^{\mathcal{T}} (\mathcal{T} - |\tau|) C_\epsilon(\tau) e^{i2\omega_{\text{trap}}\tau} d\tau.$$

If the noise correlation time $\tau_c \ll \mathcal{T}$:

$$I(\mathcal{T}) \approx \mathcal{T} \int_{-\infty}^{\infty} C_\epsilon(\tau) e^{i2\omega_{\text{trap}}\tau} d\tau = \mathcal{T} S_\epsilon(2\omega_{\text{trap}}),$$

using the two-sided PSD definition. Therefore

$$P_{n \rightarrow n+2}(\mathcal{T}) \approx \mathcal{T} \frac{\omega_{\text{trap}}^2}{16} (n+1)(n+2) S_\epsilon(2\omega_{\text{trap}}).$$

yielding the *rate*

$$\Gamma_{n \rightarrow n+2} = \frac{\omega_{\text{trap}}^2}{16} (n+1)(n+2) S_\epsilon(2\omega_{\text{trap}}).$$

Analogously, $\Gamma_{n \rightarrow n-2} = \frac{\omega_{\text{trap}}^2}{16} n(n-1) S_\epsilon(2\omega_{\text{trap}})$.

Note : Here we have assumed that \mathcal{T} is much shorter than the time-scale over which level populations vary significantly but much larger than the correlation time of the noise. This separation of time scales is fundamental to many stochastic processes (quantum or not) in physics.

(d) Each upward jump delivers an energy gain of $2\hbar\omega_{\text{trap}}$ while a downward jump removes the same amount. Weighting these increments by their respective rates gives the net energy flow:

$$\frac{d\langle E \rangle}{dt} = 2\hbar\omega_{\text{trap}} \sum_n \left[\Gamma_{n \rightarrow n+2} P_n - \Gamma_{n \rightarrow n-2} P_n \right].$$

Insert the explicit rates from part (c). Using $\sum_n P_n = 1$ and $\sum_n n P_n = \langle n \rangle$:

$$\frac{d\langle E \rangle}{dt} = \frac{\omega_{\text{trap}}^2}{4} S_\epsilon(2\omega_{\text{trap}}) \langle E \rangle.$$

Solving the differential equation gives the exponential heating law

$$\langle E(t) \rangle = \langle E(0) \rangle e^{\gamma t}, \quad \gamma = \frac{\omega_{\text{trap}}^2}{4} S_\epsilon(2\omega_{\text{trap}}).$$

Note : This trap-induced heating is common in all laser based traps for cold atoms. It can be used as a tool, for example to determine trap frequency by adding a perturbation, scanning its frequency and looking for loss peaks. For ultracold atoms, degenerate gases, atomic clocks and quantum computing, it is often crucial to heavily suppress laser intensity noise at $2\omega_{\text{trap}}$ by various techniques. Also, note that this entire calculation can actually be done classically using Ehrenfest's theorem.

STATISTICAL MECHANICS 1

Classical Ising model

Consider a system of N classical binary spins $S_i \in \{+1, -1\}$, where each spin interacts equally with every other spin. The Hamiltonian for this all-to-all interaction Ising model in the presence of an external magnetic field h is given by:

$$H = -\frac{J}{N} \sum_{i < j} S_i S_j - h \sum_{i=1}^N S_i. \quad (1)$$

The factor of $1/N$ in the interaction term ensures that the energy per particle remains finite as $N \rightarrow \infty$, which is crucial for a well-defined thermodynamic limit.

(a)[3pt] Calculate the number of states (statistical weight) that correspond to the total magnetization M .

(b)[3pt] Write an expression for the system's partition function in terms of summation over the values of M , the number of spins N , the inverse temperature $\beta = 1/(k_B T)$, and the spin interaction strength J .

(c)[4pt] Take the thermodynamic limit (N large) and express the partition function as an integral over the average magnetization $m = M/N$,

$$Z_N = \int_{-1}^1 dm e^{-N\beta f(m)} \quad (\text{find function } f(m)).$$

(d)[5pt] Derive the self-consistent equation for $m = M/N$ determining the most statistically probable state of the system.

(e)[5pt] For which temperature T at which magnetization m can spontaneously become nonzero, $m \neq 0$?

Hint: Stirling's approximation for large n gives $\ln n! \approx n \ln n - n$

Solution

(a) Introducing the total magnetization $M = \sum_{i=1}^N S_i$, we can rewrite the Hamiltonian. Note that $M^2 = (\sum_{i=1}^N S_i)^2 = \sum_{i=1}^N S_i^2 + 2 \sum_{i<j} S_i S_j = N + 2 \sum_{i<j} S_i S_j$. Thus, $\sum_{i<j} S_i S_j = \frac{1}{2}(M^2 - N)$. Substituting this into the Hamiltonian, we get:

$$H = -\frac{J}{2N}(M^2 - N) - hM = -\frac{J}{2N}M^2 + \frac{J}{2} - hM. \quad (2)$$

The total magnetization M can take values from $-N$ to N in steps of 2. Let $W(M, N)$ be the number of configurations with a total magnetization M . This is given by the number of ways to choose $(N + M)/2$ spins to be $+1$ (and the remaining $(N - M)/2$ to be -1):

$$W(M, N) = \binom{N}{(N+M)/2} = \frac{N!}{[(N+M)/2]![(N-M)/2]!}. \quad (3)$$

(b) The partition function Z_N at inverse temperature $\beta = 1/(k_B T)$ is the sum over all 2^N spin configurations:

$$Z_N = \sum_{\{S_i\}} e^{-\beta \mathcal{H}(\{S_i\})} = \sum_{\{S_i\}} \exp\left(\beta \left(\frac{J}{2N}M^2 - \frac{J}{2} + hM\right)\right). \quad (4)$$

Since the Hamiltonian depends only on the total magnetization M , we can group the terms by the value of M . The partition function can then be written as a sum over possible values of M :

$$Z_N = \sum_{M=-N, M \text{ both even or odd}}^N W(M, N) \exp\left(\beta \left(\frac{J}{2N}M^2 - \frac{J}{2} + hM\right)\right). \quad (5)$$

(c) Using the Stirling formula, we have

$$\ln W(M, N) \approx N \ln N - N - \left(\frac{N+M}{2} \ln \frac{N+M}{2} - \frac{N+M}{2}\right) - \left(\frac{N-M}{2} \ln \frac{N-M}{2} - \frac{N-M}{2}\right) \quad (6)$$

and

$$\ln W(M, N) \approx N \ln 2 - \frac{N+M}{2} \ln \left(\frac{1+m}{2}\right) - \frac{N-M}{2} \ln \left(\frac{1-m}{2}\right), \quad (7)$$

where $m = M/N$ is the magnetization per spin.

Together with the exponent in the Boltzmann factor

$$-\beta H(M) = -\beta \left(-\frac{J}{2N} M^2 + \frac{J}{2} - hM \right) = \frac{\beta J}{2} m^2 N - \frac{\beta J}{2} + \beta h m N. \quad (8)$$

The partition function is

$$Z_N = \int_{-1}^1 dm e^{-N\beta f(m)}, \quad (9)$$

where

$$\beta f(m) = -\ln 2 + \frac{1+m}{2} \ln \left(\frac{1+m}{2} \right) + \frac{1-m}{2} \ln \left(\frac{1-m}{2} \right) - \frac{\beta J}{2} m^2 - \beta h m. \quad (10)$$

(d) To obtain the highest Boltzmann weight, we maximize the function (divided by N):

$$g(m) \equiv -\beta f(m) = \ln 2 - \frac{1+m}{2} \ln \left(\frac{1+m}{2} \right) - \frac{1-m}{2} \ln \left(\frac{1-m}{2} \right) + \frac{\beta J}{2} m^2 + \beta h m. \quad (11)$$

We find the maximum by setting the derivative with respect to m to zero:

$$\frac{dg}{dm} = 0. \quad (12)$$

This gives

$$\begin{aligned} \frac{1}{2} \ln \left(\frac{1-m}{1+m} \right) + \beta J m + \beta h &= 0, \\ \ln \left(\frac{1-m}{1+m} \right) &= -2\beta(Jm + h), \\ \frac{1-m}{1+m} &= e^{-2\beta(Jm+h)}. \end{aligned} \quad (13)$$

Alternatively, by considering the derivative of $\ln W(M, N) - \beta H(M)$ directly with respect to M and setting it to zero, and then taking the limit $N \rightarrow \infty$, we arrive at the same self-consistent equation for the magnetization per spin m :

$$m = \tanh(\beta(Jm + h)). \quad (14)$$

The solution m^* gives the m of the configuration with highest Boltzmann weight.

This state gives the dominant contribution to the statistical sum since the statistical probability quickly diminishes away from that point, increasingly so in the thermodynamic limit ($N \rightarrow \infty$). It is used in the so-called saddle-point approximation, in which the entire sum is approximated by this largest contribution which maximizes the product of the number of configurations $W(M, N)$ and the Boltzmann factor $\exp(-\beta H)$ is maximized. Equivalently, we can maximize $\ln W(M, N) - \beta H(M)$.

(e) For a non-zero spontaneous magnetization ($h = 0$, $m^* \neq 0$), the self-consistent equation becomes:

$$m = \tanh(\beta J m). \quad (15)$$

For small m , we can use the Taylor expansion of $\tanh(x) \approx x - \frac{x^3}{3} + \dots$:

$$\begin{aligned} m &\approx \beta J m - \frac{(\beta J m)^3}{3}, \\ m(1 - \beta J + \frac{(\beta J)^3 m^2}{3}) &\approx 0. \end{aligned} \quad (16)$$

A non-zero solution ($m \neq 0$) exists when:

$$1 - \beta J < 0 \implies \beta J > 1 \implies \frac{J}{k_B T} > 1 \implies T < J/k_B. \quad (17)$$

The temperature $T_c = J/k_B$ marks the critical temperature for this mean-field model.

STATISTICAL MECHANICS 2

Chemical equilibrium

A long cylindrical tube of length L and radius $R \ll L$ is held vertically under the influence of earth's gravity with acceleration g . The tube is first completely evacuated and then filled with isotopically pure ^{40}Ar gas to a pressure of roughly 10^{-8} Pa which equilibrates with the walls of the tube. The tube is held at a constant temperature of 300 K. The argon atoms can adsorb onto binding sites on the tube walls, with density of \mathcal{N} sites per unit area, with binding energy $(-\epsilon)$ compared to a zero kinetic energy state in the adjacent gas. For this problem, we will neglect motion of the surface-bound Ar atoms.

(a)[6pt] Calculate the z -dependent density of Ar atoms $\rho_{\text{Ar}}(z)$ relative to the equilibrated density at the bottom of the tube $\rho_{\text{Ar}}(z = 0)$.

(b)[6pt] Calculate the fraction of surface binding sites occupied as a function of z . Again express your answer in terms of the equilibrated gas density at the bottom of the tube $\rho_{\text{Ar}}(z = 0)$.

After the Ar has equilibrated with the walls of the tube, a small amount of isotopically pure fluorine gas $^{19}\text{F}_2$ (molecular mass ≈ 38) is introduced into the tube, with density much less than the argon density. The fluorine can also adsorb onto the walls with binding energy $-\epsilon$ and also react with Ar to form ArF molecules via the reaction



(c)[8pt] Derive an expression for $\rho_{\text{ArF}}(z)$ in terms of the new equilibrated densities of Ar and F_2 at the bottom of the tube $\rho_{\text{Ar}}(z = 0)$ and $\rho_{\text{F}_2}(z = 0)$.

Solution

We can first determine if we are in the classical ideal gas limit using the information given. If an ideal gas, the number density is related to the pressure via $\rho = p/k_B T$, which for 300 K and 10^{-6} Pa gives a number density of $\rho = 2.4 \times 10^{12} \text{ m}^{-3}$. The thermal de Broglie wavelength for Ar at 300 K is

$$\lambda_{\text{Ar}} = \frac{h}{\sqrt{2\pi m_{\text{Ar}} k_B T}} \approx 1.6 \times 10^{-11} \text{ m}, \quad (2)$$

so the quantum degeneracy parameter $\rho \lambda_{\text{Ar}}^3 \approx 10^{-20}$ and we are very much in the classical limit. One can also just reason this out without calculating by knowing that atmospheric pressure is roughly 10^5 Pa such that 10^{-8} Pa corresponds to ultrahigh vacuum and a very dilute gas.

(a) There are several ways to get $\rho(z)$. Here are a few.

Method 1: Include gravitational potential into constant chemical potential.

The chemical potential of an ideal gas in the absence of an external potential is given by $\mu = k_B T \ln(\rho \lambda^3)$. The gravitational potential $m_{\text{Ar}} g z$ will add to this. The total chemical potential throughout the gas must be constant such that

$$\begin{aligned} \mu_{\text{Ar}} &= k_B T \ln(\rho_{\text{Ar}}(0) \lambda_{\text{Ar}}^3) = k_B T \ln(\rho_{\text{Ar}}(z) \lambda_{\text{Ar}}^3) + m_{\text{Ar}} g z \\ \Rightarrow \ln\left(\frac{\rho_{\text{Ar}}(z)}{\rho_{\text{Ar}}(0)}\right) &= -\beta m_{\text{Ar}} g z \\ \boxed{\rho_{\text{Ar}}(z) = \rho_{\text{Ar}}(0) e^{-\beta m_{\text{Ar}} g z}}, \end{aligned} \quad (3)$$

with $\beta = 1/k_B T$.

Method 2: Reduced distribution function

The Hamiltonian for the system is

$$\mathcal{H} = \sum_{i=1}^N \frac{p_i^2}{2m} + mg \sum_{i=1}^N z_i. \quad (4)$$

The full distribution function for all the particles is proportional to $\exp[-\beta \mathcal{H}(r^N, p^N)]$. The z -dependent density $\rho(z)$, a reduced distribution function, can be related to full distribution

via partial integration, viz.

$$\begin{aligned}
\pi R^2 \int_0^L dz_1 \rho(z_1) &= N \times 1 \\
&= N \frac{\int dr^N \int dp^N e^{-\beta \mathcal{H}}}{\int dr^N \int dp^N e^{-\beta \mathcal{H}}} \\
&= N \left(\frac{1}{\int_0^L dz_1 e^{-\beta m g z_1}} \right) \int_0^L dz_1 e^{-m g z_1} \\
&\Rightarrow \rho(z) = (\text{const.}) e^{-\beta m g z} \\
&\Rightarrow \boxed{\rho_{\text{Ar}}(z) = \rho_{\text{Ar}}(z=0) e^{-\beta m_{\text{Ar}} g z}} .
\end{aligned} \tag{5}$$

Note that one can also derive this formula for $\rho(z)$ from the condition of hydrostatic equilibrium $-\nabla p + \rho \mathbf{g} = 0$ and the ideal gas law. However, in this case of ultrahigh vacuum the mean free path of the Ar atoms is very large, on the order of 10^6 m. In principle the idea of hydrostatic equilibrium can still be valid if the (unstated) dimensions of the container are much larger than the mean free path, but the container would have to be very large for this to make sense. Since the problem says to use a constant gravitational acceleration g it is implicit that the dimensions of the container are much smaller than the radius of the earth ($\sim 10^7$ m), and thus also much smaller than the mean free path. In this “molecular flow regime,” common to high vacuum systems, the Ar atoms are not colliding with each other and only collide with the chamber walls, such that the fluid mechanics concept of hydrostatic equilibrium is nonsensical.

(b) At any position z , the problem can be solved considering each binding site as a grand canonical system in equilibrium with the gas with chemical potential $\mu(z)$. There are only two states for the binding site, occupied with $n = 1$ and total energy $\varepsilon(z)$, and empty with $n = 0$ and energy 0. The grand partition function is then

$$\Xi = \sum_v e^{-\beta(E_v - \mu n_v)} = 1 + e^{-\beta[\varepsilon(z) - \mu(z)]} . \tag{6}$$

The coverage fraction is then just given by the probability of occupancy

$$\begin{aligned}
\Theta(z) = p_1(z) &= \frac{e^{-\beta[\varepsilon(z) - \mu(z)]}}{\Xi} \\
\Rightarrow \Theta(z) &= \frac{1}{e^{\beta[\varepsilon(z) - \mu(z)]} + 1} .
\end{aligned} \tag{7}$$

The subtlety of the problem comes in how to think about the z -dependence of the bound-state energy and the chemical potential. If one thinks about the problem globally, over the whole tube, then it is natural to take the gas chemical potential as a constant $\mu(z) = \mu(0) =$

$k_B T \ln [\rho_{\text{Ar}}(0)\lambda_{\text{Ar}}^3]$, but then we must consider that a binding site at elevation z has $m_{\text{Ar}}gz$ higher energy than a binding site at $z = 0$, such that $\varepsilon(z) = -\epsilon + m_{\text{Ar}}gz$ and

$$\Theta(z) = \frac{\rho_{\text{Ar}}(0)\lambda_{\text{Ar}}^3}{e^{\beta[-\epsilon+m_{\text{Ar}}gz]} + \rho_{\text{Ar}}(0)\lambda_{\text{Ar}}^3} \quad (8)$$

If one instead thinks locally, one can consider binding sites with energy $\varepsilon = -\epsilon$ at a height z to be in chemical equilibrium with the local gas at the same gravitational potential. The local gas density $\rho_{\text{Ar}}(z) = \rho_{\text{Ar}}(0) \exp[-\beta m_{\text{Ar}}gz]$ and local chemical potential is $\mu(z) = k_B T \ln [\rho_{\text{Ar}}(z)\lambda_{\text{Ar}}^3]$. Inserting these parameters into equation (7) gives the same result as (8).

(c) c) The law of mass action for gas-phase reactions is

$$\prod_{i=1}^r \rho_i^{\nu_i} = \prod_{i=1}^r \left(\frac{q_i}{V} \right)^{\nu_i} = K(T) , \quad (9)$$

where r is the number of species, the q_i are the single-molecule partition functions, the ν_i are the reaction coefficients, and V is the container volume. Critically, the equilibrium constant K only depends on temperature, so it is independent of z . Taking the reaction coefficients to be positive for the reactants (species on right-hand side of equation (1)) and negative for the products (species on the left-hand side of equation (1)), we have

$$\frac{\rho_{\text{Ar}}^2 \rho_{\text{F}_2}}{\rho_{\text{ArF}}^2} = K_0 . \quad (10)$$

Regardless of how much F_2 sticks to the walls, we still must have chemical equilibrium throughout the gas, such that the F_2 density will also have the z dependence

$$\rho_{\text{F}_2}(z) = \rho_{\text{F}_2}(0) e^{-\beta m_{\text{F}_2}gz} , \quad (11)$$

and combining (10) and (11), we arrive at the result

$$\rho_{\text{ArF}} = \frac{1}{\sqrt{K_0}} \rho_{\text{Ar}}(0) [\rho_{\text{F}_2}(0)]^{1/2} \exp \left[-\beta \left(m_{\text{Ar}} + \frac{m_{\text{F}_2}}{2} \right) gz \right] \quad (12)$$

One can also use the opposite sign convention for the reaction coefficients, in which case $K_0 \rightarrow 1/K_0$.

STATISTICAL MECHANICS 3

Canonical and grand-canonical ensemble for a system of fermions with an energy gap

This problem discusses the subtleties of the thermodynamic limit in systems with an energy gap, which manifest themselves experimentally, e.g., through “parity effects” in superconductors.

Consider a system of two degenerate energy levels, one with energy 0 and the other with energy $\Delta > 0$. Each level is N_0 -fold degenerate. The system is in equilibrium at temperature T and is occupied by N non-interacting and effectively spinless fermions.

(a)[4pt] Assume that both N s are large, $N, N_0 \gg 1$ so that the system can be described within the grand canonical ensemble characterized by the chemical potential μ and concentration of particles in the system, $n = N/N_0$. Write down the equation that determines μ . Solve this equation in the case $N = N_0$, and find explicitly μ and the occupation probabilities f and g of the upper and lower energy levels, respectively. Simplify the expression for f at low temperatures $T \ll \Delta$.

(b)[4pt] Take $N > N_0$. Find μ from the equation obtained in part (a) in the low-temperature limit, $T \ll \Delta$.

(c)[4pt] Rederive the result from part (b) in a simpler fashion, using the thermodynamic definition of the chemical potential μ and calculating directly the entropy of the fermions in the upper energy level.

(d)[6pt] From now on, take $N = N_0$. Describe the system using the canonical ensemble. Write down the partition function and evaluate it to find the occupation probabilities f and g in the two limits:

(1) thermodynamic limit $N \rightarrow \infty$, while keeping temperature constant;

(2) low-temperature limit $T \rightarrow 0$, assuming N large but constant.

Hint: You might need to use Stirling's approximation $N! \simeq (N/e)^N$, for $N \gg 1$.

(e)[2pt] Compare the results for f at low temperatures obtained in the grand-canonical ensemble [part (a)] and canonical ensemble [part (d2)]. Derive the condition of applicability of the grand canonical ensemble to the system with fixed number of particles N .

Solution

(a) In the grand canonical ensemble, for the system considered, the self-consistency condition for μ is:

$$N = \frac{N_0}{e^{-\mu/k_B T} + 1} + \frac{N_0}{e^{(\Delta-\mu)/k_B T} + 1}.$$

Introducing $z = e^{-\mu/k_B T}$ one can transform this relation into a quadratic equation for z :

$$(z + 1)(\lambda z + 1) = \frac{1}{n}(2 + (1 + \lambda)z),$$

and

$$\lambda z^2 + (1 + \lambda)\frac{n-1}{n}z - \frac{2-n}{n} = 0,$$

where $\lambda \equiv e^{\Delta/k_B T}$. Since $z > 0$, one should keep only the plus sign in the quadratic equation formula:

$$z = -b + \left(b^2 + \frac{2-n}{n\lambda}\right)^{1/2}, \quad b \equiv \frac{1 + \lambda}{2\lambda} \frac{n-1}{n}.$$

This relation determines μ for any concentration n . For $n = 1$ ($N = N_0$) it gives:

$$z = 1/\sqrt{\lambda} \Rightarrow e^{-\mu/k_B T} = e^{-\Delta/2k_B T}, \quad \text{i.e.,} \quad \mu = \Delta/2.$$

With this value of the chemical potential, the occupation probabilities f and g of the upper and lower energy levels are:

$$f = \frac{1}{e^{\Delta/2k_B T} + 1}, \quad g = \frac{1}{1 + e^{-\Delta/2k_B T}}.$$

At low temperatures $T \ll \Delta$ the expression for f simplifies to

$$f = e^{-\Delta/2k_B T}.$$

(b) For $N > N_0$, $n > 1$ and the factor b in the equation for μ derived in part (a) is positive. In this case, one can use Taylor expansion of the square root in this equation to the first order in small factor $1/\lambda$ to obtain:

$$\begin{aligned} z &= -b + b\left(1 + \frac{2-n}{2b^2n\lambda}\right) = \frac{2-n}{2bn\lambda} = \frac{2-n}{(1+\lambda)(n-1)} \\ &\simeq \frac{1}{\lambda} \frac{2-n}{n-1}. \end{aligned}$$

This gives for μ :

$$\mu = -k_B T \ln z = \Delta - k_B T \ln \frac{2-n}{n-1}.$$

The first term in this equation has a direct physics sense. For $N > N_0$ and low temperatures, the added particles with dominant probability go only into the upper level with energy Δ , since the lower level is completely filled.

(c) The second term in the equation for μ also has a direct physics sense. The standard thermodynamic definition of the chemical potential is:

$$\mu = \left(\frac{\partial F}{\partial N} \right)_T = \left(\frac{\partial(U - TS)}{\partial N} \right)_T = \left(\frac{\partial(\Delta M - TS(M))}{\partial M} \right)_T,$$

where M is the number of particles in the upper level, and we used the notion that up to the exponentially small corrections, for $N > N_0$ and $T \ll \Delta$, the added particles go into the upper energy level. The entropy $S(M)$ of M particles in this level is determined by the number of distinct ways in which the particles can be distributed over the N_0 degenerate states:

$$S(M) = k_B \ln \frac{N_0!}{M!(N_0 - M)!}.$$

From this,

$$\frac{\partial S(M)}{\partial M} = S(M + 1) - S(M) = k_B \ln \frac{N_0 - M}{M},$$

and we obtain for the chemical potential:

$$\mu = \Delta - k_B T \ln \frac{N_0 - M}{M}$$

Since the lower level is completely filled, $M = N - N_0$, and we see that this expression indeed coincides with the equation for μ obtained in (b).

(d) In the canonical ensemble, the total energy of the system is $E_M = M\Delta$, and therefore the partition function Z , can be expressed in terms of the number M of the particles in the upper energy level. Counting the number of way of taking M particles from the lower N levels and distributing them over the upper N levels, one finds

$$Z = \sum_{M=0}^N \left[\frac{N!}{M!(N - M)!} \right]^2 e^{-M\Delta/k_B T}.$$

(1) To find the occupation probabilities in the thermodynamic limit $N \rightarrow \infty$, we notice that the sum over M in Z is dominated by the largest term, which can be found by using Stirling's approximation for the factorials in the sum. In this way, one finds that the largest term corresponds to

$$M = \frac{N}{e^{\Delta/2k_B T} + 1},$$

i.e.,

$$f = M/N = \frac{1}{e^{\Delta/2k_B T} + 1}, \quad g = (N - M)/N = \frac{1}{1 + e^{-\Delta/2k_B T}},$$

in agreement with the results of the grand canonical ensemble.

(2) In the low-temperature limit $T \rightarrow 0$, however, the partition function Z is dominated by the first two terms in the sum over M :

$$Z \simeq 1 + N e^{-\Delta/k_B T},$$

so that

$$f = e^{-\Delta/k_B T}, \quad g = 1 - e^{-\Delta/k_B T}.$$

We see that first, as should be, in the thermodynamic limit, the occupation probabilities are independent of the ensemble used. There are the same in the canonical and grand canonical ensembles. In the low-temperature limit, however, the occupation probabilities are different from the ones in the grand canonical ensemble even for very large N s.

(e) Comparing the low-temperature results for f in part (a) (and, equivalently, in the thermodynamic limit (d1) of the canonical ensemble) we see that for the system with fixed number of particles N , the grand canonical ensemble with its Fermi distribution can be used to describe the occupation probabilities only at not-too-low temperatures, when the number of excited particles is large:

$$N e^{-\Delta/k_B T} \gg 1, \quad \text{i.e.,} \quad k_B T \gg \Delta / \ln N.$$

Although formally this condition is satisfied in the thermodynamic limit $N \rightarrow \infty$ for all temperatures, logarithm is a very slow function, and the regime of the small number of excitations can be important experimentally, e.g., in samples of superconductors which are “macroscopic” in all other respects.