Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

Fall 2024 (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.

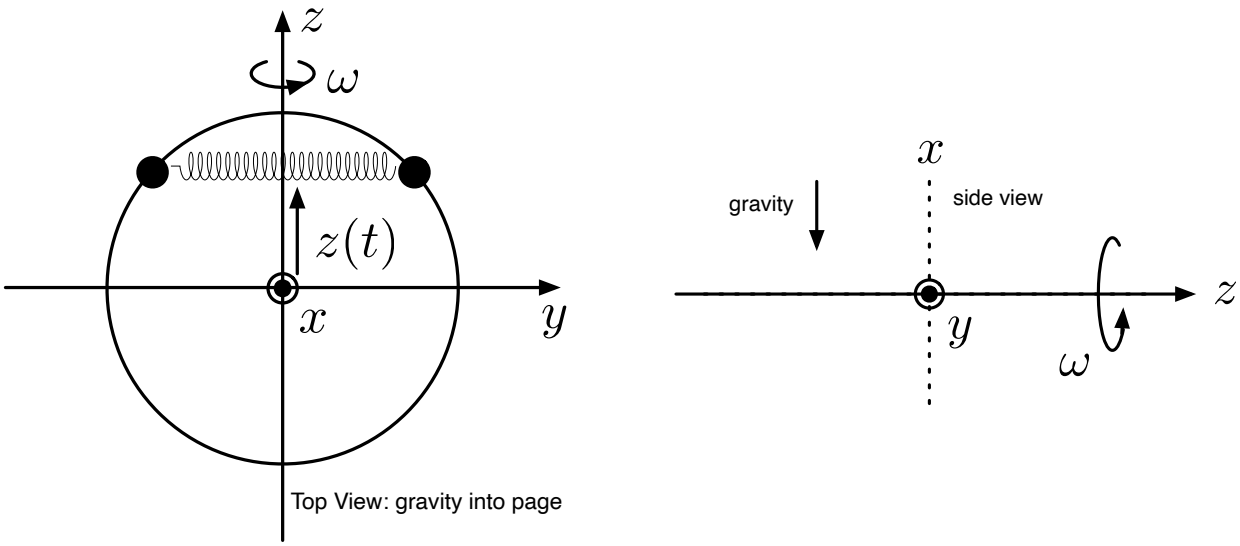
Write your ID number (not your name!) on each exam booklet.

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

Two beads on a rotating circle tied by a spring

Consider two particles of equal mass m tied by a massless spring on a circle of radius R in the yz-plane. The spring constant is k and the length of the spring at rest is 2ℓ with $\ell < R$. The beads slide on the circle without friction. The circle rotates about the z-axis with uniform circular velocity ω, as illustrated in the figure below. Gravity acts in the x-direction.

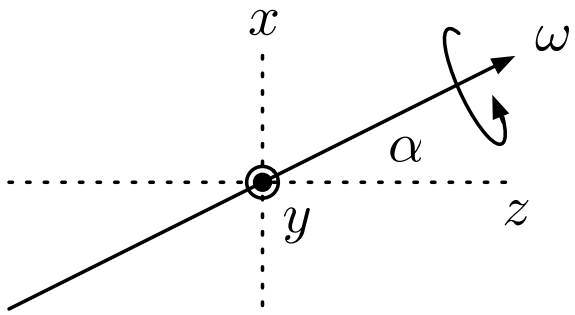


(a) (5 points) Use $z(t)$ as a generalized coordinate and derive the Lagrangian for this system.

(b) (5 points) Use the Lagrangian to derive the equilibrium position(s) as a function of frequency, $z_0(\omega)$. Determine the conditions when these position(s) are stable.

(c) (5 points) Determine the frequencies of small oscillations about the stable equilibrium points.

(d) (5 points) The axis of rotation is turned by a small angle α about the y-axis (see below). Determine how the stable equilibria of part (b) are shifted by α. Which of the equilibrium positions represent local and global equilibria respectively?



Solution

a. Since the CM is on the z-axis, there is no effect of gravity which is acting along the x-axis. With this in mind, the Lagrangian in cylindrical coordinates is

$$\mathcal{L} = m(\dot{r}^2 + r^2\dot{\phi}^2 + \dot{z}^2) - 2k(r-l)^2 \tag{1}$$

with $r^2 = R^2 - z^2$ and constant circular velocity $\dot{\phi} = \omega$. Substituting these values give

$$\mathcal{L} = \frac{1}{2}\mu\dot{z}^2 - V(z) \tag{2}$$

with

$$\mu = 2m(1 - z^2/R^2) \qquad\qquad V(z) = 2k(\sqrt{R^2 - z^2} - l)^2 - m\omega^2(R^2 - z^2) \tag{3}$$

b. At equilibrium $dV/dz = 0$

$$\frac{dV}{dz} = 4klz\left(\frac{1}{\sqrt{R^2 - z^2}} - \frac{1}{r(\omega)}\right) = 0 \qquad\qquad r(\omega) = \frac{2kl}{2k - m\omega^2} \tag{4}$$

which amounts to three real roots

$$z(\omega) = 0, \pm\sqrt{R^2 - r^2(\omega)} \tag{5}$$

If $r(\omega) > R$ or $r(\omega) < 0$ there is only a single equilibrium point $z(\omega) = 0$. The critical velocity is fixed by the condition $r(\omega_c) = R$. For $\omega < \omega_c$ there are three equilibrium points, whereas for $\omega > \omega_c$ there is only one.

Their stability follows from

$$V''(z) = \frac{d^2V}{dz^2} = 4kl\left(\frac{R^2}{(R^2 - z^2)^{\frac{3}{2}}} - \frac{1}{r(\omega)}\right) \tag{6}$$

which is symmetric under $z \to -z$. It follows that $V''(0) < 0$ (for $\omega < \omega_c$) is unstable, but $V''(0) > 0$ (for $\omega > \omega_c$) is stable. The equilibrium points $z(\pm\sqrt{R^2 - r^2(\omega)})$ for $\omega < \omega_c$ are stable.

d. Around the equilibrium points, the effective spring constant is

$$\begin{aligned} k_E(\omega) =& 4kl\left(\frac{1}{R} - \frac{1}{r(\omega)}\right) \qquad\qquad z(\omega) = 0 \qquad \omega > \omega_c \\ k_E(\omega) =& 4kl\left(\frac{R^2}{r^3(\omega)} - \frac{1}{r(\omega)}\right) \qquad z(\omega) = \pm\sqrt{R^2 - r^2(\omega)} \qquad \omega < \omega_c \end{aligned} \tag{7}$$

The angular frequencies of small oscillations are given by $\sqrt{k_E(\omega)/\mu}$.

c. If the axis of rotation is tillted by an angle α, then the potential $V(z)$ acquires a contribution from gravity

$$\tilde{V}(z) = V(z) + 2mgz\sin\alpha \tag{8}$$

which we can recast in dimensionless form

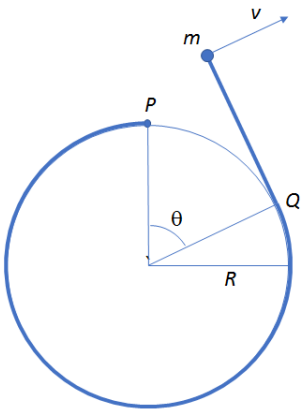
$$\frac{\tilde{V}(z)}{2kR^2} = \left(\sqrt{1-\frac{z^2}{R^2}} - \frac{r(\omega)}{R}\right)^2 - \left(1-\frac{r(\omega)}{R}\right)\left(\frac{\omega}{\omega_c}\right)^2\left(1-\frac{z^2}{R^2}\right) + \frac{mgz\sin\alpha}{kR^2} \tag{9}$$

Gravity breaks $z \to -z$ symmetry. When $\omega < \omega_c$, $\tilde{V}(z)$ has a global minimum (old negative root) and a local minimum (old positive root). When $\omega > \omega_c$ there is only one global minimum (old null root).

Classical Mechanics 2

Unwinding a cord from a cylinder

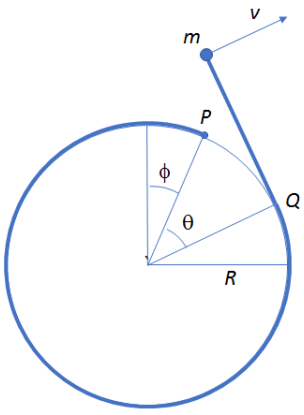
A point particle of mass m is attached to a massless thin cord whose other end is wound around a fixed cylinder of radius R in two spatial dimensions. (There are no external forces and no gravity in this problem.) Initially the cord is snugly and completely wound around the cylinder so that the mass touches the cylinder at point P as shown below. At $t = 0$ an impulse directed radially outward gives the mass an initial velocity of magnitude v_0. This starts the unwinding of the cord from the cylinder. Point Q, also shown below, is the instantaneous contact point between the cord and the cylinder.



(a) (5 points) Find the Lagrangian and equation of motion in terms of the generalized coordinate θ as a function of time, satisfying the initial conditions.

(b) (3 points) Using the solution of (a), find the angular momentum of the mass about the center of the cylinder. Is angular momentum conserved? Explain. Is the energy conserved? Explain.

Now consider a new situation in which the cylinder is hollow and of mass M and can spin freely around its axis as the cord and cylinder unwind. The new angle ϕ measures the position of P (the place where the mass was at rest) with respect to the vertical axis as shown below.



(c) (6 points) Write down the Lagrangian in terms of the generalized coordinates θ and ϕ. Identify two conserved quantities and express them as functions of θ and ϕ.

(d) (6 points) Solve for $\theta(t)$. Which way does the cylinder spin? Explain.

Solution

(a) One can write a Lagrangian using Cartesian coordinates and express it as a function of θ. However, noticing that the length of the unwound string is $R\theta$ and it unwinds with angular velocity $\dot{\theta}$ we can immediately write a Lagrangian, which is just a kinetic energy in this case

$$\mathcal{L} = \frac{1}{2} m R^2 \theta^2 \dot{\theta}^2 \tag{1}$$

The equation of motion is then:

$$\frac{d}{dt}(\theta^2 \dot{\theta}) - \dot{\theta}^2 \theta = 0 \tag{2}$$

or

$$\theta^2 \ddot{\theta} + \dot{\theta}^2 \theta = 0 \tag{3}$$

for $\theta \neq 0$, this is

$$\frac{d}{dt}(\dot{\theta}\theta) = \frac{1}{2}\frac{d^2}{dt^2}(\theta^2) = 0 \tag{4}$$

The solution is simply $\theta^2 = At + B$. From the initial condition $\theta(0) = 0$ and

$$\mathcal{L}(0) = \frac{1}{2} m v_0^2 \tag{5}$$

i.e., $\theta(0)\dot{\theta}(0) = v_0/R$, we get $B = 0$ and $A = 2v_0/R$. Hence:

$$\theta = \sqrt{2v_0 t/R} \tag{6}$$

(b) The angular momentum L about the center of the cylinder is given by:

$$L = m\vec{r} \times \vec{v} = mR\theta v_0 \hat{z} = mR\sqrt{2v_0 t/R}\hat{z} \tag{7}$$

The angular momentum is not conserved because there is a torque from the cord connected to the cylinder. The energy is conserved because the tension of the cord is always perpendicular to the velocity of the mass.

$$E = \mathcal{L} = \frac{1}{2} m v_0^2 \tag{8}$$

(c) Here again we use the fact that the cord is always perpendicular to the radius of the cylinder at the point of contact. Consider the velocity of the mass in relation with point Q and the (orthogonal) velocity of the cord at point Q, we can write the Lagrangian in the form

$$\mathcal{L} = \frac{1}{2} m R^2 \dot{\phi}^2 + \frac{1}{2} m R^2 \theta^2 (\dot{\phi} + \dot{\theta})^2 + \frac{1}{2} M R^2 \dot{\phi}^2 \tag{9}$$

From this equation, we can immediately obtain the integrals of motion. An angular momentum which is now conserved is

$$L = \frac{d\mathcal{L}}{d\dot{\phi}} \tag{10}$$

This is initially zero, and since the initial impulse does not give the system any angular momentum, it will be zero for all time. So we have

$$(m+M)\dot{\phi} + m\theta^2(\dot{\phi}+\dot{\theta}) = 0 \tag{11}$$

Energy is also conserved:

$$\frac{1}{2}(m+M)R^2\dot{\phi}^2 + \frac{1}{2}mR^2\theta^2(\dot{\phi}+\dot{\theta})^2 = \frac{1}{2}mv_0^2 \tag{12}$$

(d) From equation (11) we can express $\dot{\phi}$ in terms of θ and $\dot{\theta}$:

$$\dot{\phi} = -\frac{\dot{\theta}\theta^2}{\theta^2+1+(M/m)} \tag{13}$$

Substituting this into (12) we have:

$$(1+\frac{M}{m})\frac{\dot{\theta}^2\theta^4}{[\theta^2+1+(M/m)]^2} + \theta^2[\dot{\theta} - \frac{\dot{\theta}\theta^2}{\theta^2+1+(M/m)}]^2 = \frac{v_0^2}{R^2} \tag{14}$$

After some algebra this becomes:

$$\frac{\dot{\theta}^2\theta^2}{\theta^2+1+(M/m)} = \frac{v_0^2}{R^2[1+(M/m)]} \tag{15}$$

hence

$$\frac{\dot{\theta}\theta}{\sqrt{\theta^2+1+(M/m)}} = \sqrt{\frac{v_0^2}{R^2[1+(M/m)]}} \tag{16}$$

Integrating this equation results in

$$\sqrt{\theta^2+1+(M/m)} = \sqrt{\frac{v_0^2}{R^2[1+(M/m)]}}t + C \tag{17}$$

Therefore:

$$\theta^2 = \frac{v_0^2t^2}{R^2[1+(M/m)]} + 2\sqrt{\frac{v_0^2}{R^2[1+(M/m)]}}Ct + C^2 - 1 - (M/m) \tag{18}$$

With the initial condition $\theta(0) = 0$, we get $C^2 = 1+(M/m)$, so

$$\theta = \sqrt{\frac{v_0^2t^2}{R^2[1+(M/m)]} + \frac{2v_0t}{R}} \tag{19}$$

For $M/m \to \infty$ (i.e., a fixed cylinder), this result reduces to that obtained in (6). It is obvious from angular momentum conservation that the cylinder would spin in the opposite direction from that of the unwinding cord. Indeed, from (13) we see that $\dot{\theta}$ and $\dot{\phi}$ have opposite signs.

Classical Mechanics 3

Physics in discretized maps

Consider a one-dimensional physical system with canonical coordinates (q, p) evolving according to Hamilton's equations of motion.

(a) (3 points) Show that the phase space area is preserved by the time evolution.

Now consider a model for the evolution of a chaotic physical system evolving in phase space in discrete time steps, $t = 0$, Δ, 2Δ, ... Let (q_n, p_n) denote the canonical cooridnates after n steps of the evolution. In each time step the canonical coordinates are updated according to the following non-linear map:

$$q_{n+1} = 1 - q_n^2 + p_n \tag{1}$$
$$p_{n+1} = q_n \tag{2}$$

(b) (3 points) Show that the map is area preserving.

(c) (2 points) Find the fixed points of the map.

(d) (6 points) Find the Lyapunov exponents of the map near the fixed points of map[1]. What constraint does part (b) place on these exponents? Explain.

(e) (6 points) Find the directions of the stable and unstable lines (or manifolds) near the fixed points. Draw a schematic picture of these lines in the (q, p) plane, indicating the stable and unstable directions. Based on the behavior near the fixed points, sketch a flow diagram in phase space for the system's time evolution[2].

[1] The Lyapunov exponent is the rate of exponential growth (or decay) of a perturbation $(\delta q(t), \delta p(t))$ asymptotically close to the fixed points under iterations of the map.

[2] i.e. sketch the streamlines in the (q, p) plane for how the points evolve in phase space

Solution

(a) Do this infinitesimally. Then the absolute value of the Jacobian is one.

(b) Put $q_{n+1} = q_n$ and $p_{n+1} = p_n$. This gives (1,1) and (-1,-1).

(c) Follows from the eigenvalues of the linearized map at the fixed point, $q_k = q^* + \delta q_k$, $p_k = p^* + \delta p_k$. This gives

$$\begin{pmatrix} \delta q_{n+1} \\ \delta p_{n+1} \end{pmatrix} = \begin{pmatrix} -2q^* & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \delta q_n \\ \delta p_n \end{pmatrix} \tag{3}$$

The secular equation is $\lambda^2 + 2q^*\lambda - 1 = 0$. This gives eigenvalues $\sqrt{2} - q^*$ and $-\sqrt{2} - q^*$, which are the Lyapunovs at the fixed point. Because the map is area preserving, the absolute value their product is equal to one (not that $q^* = \pm 1$).

(d) They are given by the eigenvectors of the linearized map at the fixed point. The eigenvector for eigenvalues $\sqrt{2} - q^*$ and $-\sqrt{2} - q^*$ are given by

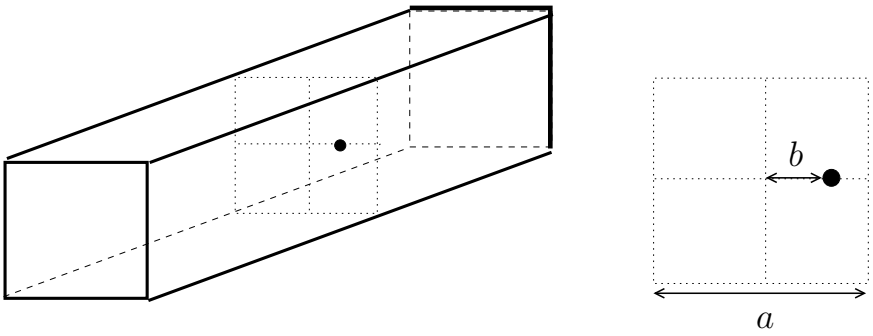
$$\begin{pmatrix} 1 \\ \sqrt{2} + q^* \end{pmatrix} \qquad \begin{pmatrix} \\ -\sqrt{2} + q^* \end{pmatrix} \tag{4}$$

respectively.

Electromagnetism 1

A charge in a rectangular tube

A point charge is placed in an infinitely long grounded rectangular tube as shown below. The sides of the square cross section of the tube have length a.



(a) (5 points) Show that the solutions to the *homogeneous* Laplace equation (i.e. without the extra point charge) are linear combinations of functions of the form

$$\Phi(k_x z)\,\Phi(k_y y)\,e^{\pm\kappa_z z} \qquad \text{where} \qquad \Phi(u) = \Big\{\cos(u) \text{ or } \sin(u) \tag{1}$$

for specific values of k_x, k_y and κ_z. Determine the allowed the values of k_x, k_y and κ_z and their associated functions.

(b) (8 points) Now consider a point charge displaced from the center of the tube by a distance b in the x direction (see above). Use a series expansion in terms of the solutions of part (a) to determine the potential from the point charge described.

(c) (7 points) Far from the charge, $z \gg a$, determine the surface charge density and the force per area on the walls of the rectangular tube.

Solution

(a) The Laplace equation is

$$-\nabla^2\varphi = 0 \tag{2}$$

Separating variables with $\varphi = X(x)Y(y)Z(z)$ we must have

$$-\frac{d^2X}{dx^2} = k_x^2 X \tag{3a}$$

$$-\frac{d^2Y}{dy^2} = k_y^2 Y \tag{3b}$$

$$-\frac{d^2Z}{dz^2} = k_z^2 Z \tag{3c}$$

In order to satisfy Eq. (2), the separation constants satisfy

$$k_x^2 + k_y^2 + k_z^2 = 0 \tag{4}$$

and thus

$$\frac{d^2Z}{dz^2} = \kappa^2 Z \qquad \text{with} \qquad \kappa = \sqrt{k_x^2 + k_y^2} \tag{5}$$

The solutions to Eq. (3a) may be either sin or cos

$$X(x) = \Phi(k_x x)\,, \tag{6}$$

with k_x at this point still arbitrary. In order to satisfy the boundary conditions $X(\pm a/2) = 0$, we require for the cos functions that

$$k_x a/2 = (n + \tfrac{1}{2})\pi\,. \tag{7}$$

Similarly, for the sin functions

$$k_x a/2 = n\pi\,. \tag{8}$$

Thus, the general form is

$$X_n(x) = \Phi_n(k_n x) \qquad n = 0, 1, \ldots \tag{9}$$

with $k_n = (n+1)\pi/a$ and

$$\Phi_n(u) = \begin{cases} \cos(u) & \text{n even} \\ \sin(u) & \text{n odd} \end{cases}\,. \tag{10}$$

The $Y(y)$ direction follows by analogy

$$Y_m(y) \qquad \Phi_m(k_m x) \qquad m = 0, 1, \ldots \tag{11}$$

with $k_m = (m+1)\pi/a$ The solutions to the z direction are

$$Z(z) = e^{\pm\kappa z} \qquad \kappa = \sqrt{k_n^2 + k_m^2} \tag{12}$$

(b) For the potential at $\boldsymbol{r}$ due to a point charge at $\boldsymbol{r}_o = (b, 0, 0)$, we expand the potential as

$$\phi(\boldsymbol{r}; \boldsymbol{r}_o) = \left(\frac{2}{a}\right)^2 \sum_{n,m=0}^{\infty,\infty} X_n(x) X_n(b)\, Y_m(y) Y_m(0)\, g_{n,m}(z) \tag{13}$$

and substitute into the Poisson equation

$$-\nabla^2 \varphi(\boldsymbol{r}; \boldsymbol{r}_o) = q\delta(x-b)\delta(y)\delta(z)\,. \tag{14}$$

The leading factors $(2/a)^2$ arise from the fact that we have not normalized the eigenfunctions X and Y

$$\int_{-a/2}^{a/2} dx\, X_n(x) X_{n'}(x) = \frac{a}{2}\,\delta_{n,n'} \tag{15}$$

$$\int_{-a/2}^{a/2} dy\, Y_m(y) Y_{m'}(y) = \frac{a}{2}\,\delta_{m,m'} \tag{16}$$

If $g_{n,m}(z)$ satisfies

$$\left(k_n^2 + k_m^2 - \frac{\partial^2}{\partial z^2}\right) g_{n,m}(z) = q\delta(z)\,, \tag{17}$$

then using the completeness relation

$$\frac{2}{a}\sum_n X_n(x) X_n(x_o) = \delta(x - x_o) \tag{18}$$

$$\frac{2}{a}\sum_m Y_m(x) Y_m(x_o) = \delta(y - y_o) \tag{19}$$

it is not difficult to show that Eq. (14) is satisfied.

The solution to Eq. (17) is

$$g_{n,m}(z) = \begin{cases} Ae^{-\kappa_{n,m} z} & z > 0 \\ Ae^{\kappa_{n,m} z} & z < 0 \end{cases} \tag{20}$$

Integrating across the δ-fcn in Eq. (17) we have

$$-\left.\frac{dg}{dz}\right|_{z=0^+} + \left.\frac{dg}{dz}\right|_{0^-} = q \tag{21}$$

With this requirement $A = \frac{q}{2\kappa_{n,m}}$ and

$$\phi(\boldsymbol{r}; \boldsymbol{r}_o) = \frac{4q}{a^2} \sum_{n,m=0}^{\infty,\infty} X_n(x) X_n(b)\, Y_m(y) Y_m(0) \frac{e^{-\kappa_{n,m}|z|}}{2\kappa_{n,m}} \tag{22}$$

(c) At asymptotic distances the terms with the smallest $\kappa_{n,m}$ dominate the sum. We then have only the contribution from $n = m = 0$ mode, and

$$\kappa_{0,0} = \sqrt{2}\pi/a\,. \tag{23}$$

The potential reads

$$\phi(\boldsymbol{r};\boldsymbol{r}_o) \simeq \frac{4q}{a^2}\cos(\pi x/a)\cos(\pi b/a)\,\cos(\pi y/a)\frac{e^{-\kappa_{0,0}|z|}}{2\kappa_{0,0}} \tag{24}$$

or

$$\phi(\boldsymbol{r};\boldsymbol{r}_o) \simeq \frac{\sqrt{2}q}{\pi a} cos(\pi x/a)\cos(\pi b/a)\,\cos(\pi y/a) e^{-\sqrt{2}\pi|z|/a} \tag{25}$$

Let us calculate the charge density on the bottom plate

$$\sigma = \boldsymbol{n}\cdot\boldsymbol{E} = -\partial_y\phi|_{y=-a/2}\,, \tag{26}$$

$$= -\frac{\sqrt{2}q}{a^2}\cos(\pi x/a)\cos(\pi b/a)\,e^{-\sqrt{2}\pi|z|/a}\,. \tag{27}$$

Finally, the force per area on the bottom plate is

$$\frac{F^y}{A} = \frac{\sigma^2}{2}\,, \tag{28}$$

$$= \frac{q^2}{a^4}\cos^2(\pi x/a)\cos^2(\pi b/a)\,e^{-2\sqrt{2}\pi|z|/a}\,. \tag{29}$$

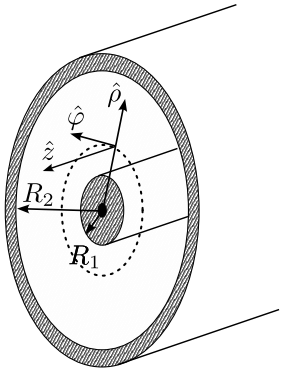
The direction of the force is into the tube. The other walls of the tube have the same force per area.

Electromagnetism 2

Coaxial transmission line

Consider a radio-frequency wave propagating in a long and straight coaxial cable. The cable consists of two concentric cylindrical conductors of inner and outer radii R_1 and R_2 respectively. The space between the conductors is vacuum.

The conductors carry currents in opposite directions along the cable ($\pm\hat{z}$) and have opposite local charge densities, so the electromagnetic fields are contained between the conductors. Assume the conductors have negligible resistance.



(a) (4pt) Use the Mawell equations to show that the coaxial cable supports wave solutions:

$$\boldsymbol{E}(t,\vec{r},z) = \vec{E}(\vec{r})\, e^{ikz-i\omega t}\,,$$
$$\boldsymbol{B}(t,\vec{r},z) = \vec{B}(\vec{r})\, e^{ikz-i\omega t}\,.$$

Here $\vec{r} = (x, y)$ is a transverse position vector. $\vec{E}(\vec{r})$ and $\vec{B}(\vec{r})$ are time independent transverse vector fields, e.g. $\vec{E}(\vec{r}) = (E_x(\vec{r}), E_y(\vec{r}))$. Show that:

(i) $\vec{E}$ and $\vec{B}$ satisfy the equations of electro and magneto-statics respectively.

(ii) The waves propagate at the speed of light with $\vec{E}$ orthogonal to $\vec{B}$.

(b) (3pt) Calculate the capacitance $C_0 = \Delta C/\Delta x$ per unit of length of the coaxial cable assuming that the charge densities are constant and uniform (e.g., if the wavelength is very long).

(c) (3pt) Now calculate the inductance $L_0 = \Delta L/\Delta x$ per unit length under the same assumptions as (b).

The complex impendance $Z(z,\omega)$ at position z along the cable is defined as the ratio between the voltage and the current for a sinusoidal frequency ω

$$Z(z,\omega) \equiv \frac{V(z,\omega)}{I(z,\omega)}\,. \tag{1}$$

Here $V(z,\omega)e^{-i\omega t}$ is the voltage drop from the inner to the outer radius, and $I(z,\omega)e^{-i\omega t}$ is the current in the z direction on the inner conductor. In general, the electromagnetic fields in the cable are a superposition of right and left moving waves with frequency ω.

(d) (5pt) For a right moving wave (and not a superposition), determine the impedance Z_0 and estimate Z_0 numerically in Ohms for a typical coaxial cable ($R_2/R_1 \approx 5$).

(e) (5pt) Now consider a superposition of waves travelling in a transmission line of length ℓ. The line is connected to a load (e.g. an antenna) located at the end of the line, $z = 0$. If the impedance at the load is purely real $Z(0, \omega) = R$, then:

(i) Find the impedance at the start of the transmission line.

(ii) For a specific value of load impedance Z_{match}, the impedance at the start of the line will remain real for any length ℓ. Determine Z_{match}. Explain why having $Z(0, \omega) = Z_{\text{match}}$ is desirable from a engineering perspective.

Solution

(a) The Maxwell's equations without currents and charges (inside the cable) applied to the transverse fields yield the following:

$$\begin{aligned}(\vec{\nabla}\times\vec{E})_z = \partial_x E_y - \partial_y E_x = -\frac{\partial B_z}{\partial t} = 0\,,\\ \vec{\nabla}\cdot\vec{E} = \partial_x E_x + \partial_y E_y = 0\,,\\ (\vec{\nabla}\times\vec{B})_z = \partial_x B_y - \partial_y B_x = \frac{1}{c^2}\frac{\partial E_z}{\partial t} = 0\,,\\ \vec{\nabla}\cdot\vec{B} = \partial_x B_x + \partial_y B_y = 0\,,\end{aligned}$$

These two equations show that the two-dimensional fields (E_x, E_y) and (B_x, B_y) have zero divergence and curl, i.e., satisfy electro- and magnetostatic equations in vacuum. They can only be nonzero if there are charges and currents on the boundary (inner and/or outer conductors).

Further, the relation between k and ω can be found from the other components of, e.g., $\vec{\nabla}\times\vec{B}$,

$$\begin{aligned}\vec{\nabla}\times(\vec{\nabla}\times\vec{B}) &= \vec{\nabla}\times(-ikB_y, ikB_x, 0)e^{ikz-i\omega t} = (k^2B_x, k^2B_y, 0)e^{ikz-i\omega t}\\ &= -\frac{1}{c^2}\frac{\partial^2}{\partial t^2}(B_x, B_y, 0)e^{ikz-i\omega t} = \frac{\omega^2}{c^2}(B_x, B_y, 0)e^{ikz-i\omega t}\end{aligned}$$

so that the phase velocity $\omega/k = c$ is the speed of light in vacuum. Finally, the electric and magnetic fields are orthogonal since

$$\begin{aligned}\vec{\nabla}\times\vec{E} &= -\frac{\partial}{\partial t}\vec{B}\\ ik(-E_y, E_x, 0)e^{ikz-i\omega t} &= i\omega(B_x, B_y, 0)e^{ikz-i\omega t}\end{aligned}$$

or $E_y = -cB_x$, $E_x = cB_y$ and $\vec{E}\perp\vec{B}$.

(b) [3pt]

The capacitance per unit length is easily calculated from the axial-symmetric electrostatic fields between two cylinders of length Δx carrying charges $\pm\lambda\Delta x$, where λ is the linear charge density. From the Gauss theorem, the electric field is radial (fringe effects are neglected)

$$\vec{E}(r) = \frac{\lambda}{2\pi\epsilon r}\hat{r} \tag{2}$$

so that the voltage is

$$V = \int_{R_1}^{R_2} dr\, E_r(r) = \frac{\lambda}{2\pi\varepsilon}\log\frac{R_2}{R_1} \tag{3}$$

and the capacitance *per unit length* is

$$C_0 = \frac{\Delta C}{\Delta x} = \frac{\lambda\Delta x/V}{\Delta x} = \frac{2\pi\varepsilon}{\log\frac{R_2}{R_1}} \tag{4}$$

Note that the electric field is radial.

(c) [3pt]

One can compute the inductance, e.g., from the energy stored in the magnetic fields between the conductors (there are no fields outside of the larger cylinder). If the conductors carry currents $\pm I$, the magnetic field is tangential (along $\hat{\varphi}$) and from the Green's theorem are

$$\vec{B} = \frac{\mu I}{2\pi r}\hat{\varphi} \tag{5}$$

and their energy per unit length is

$$\frac{\Delta E_m}{\Delta x} = \int_{R_1}^{R_2} 2\pi r\, dr\, \frac{1}{2\mu}[\vec{B}(r)]^2 = \frac{\mu I^2}{4\pi}\log\frac{R_2}{R_1} \tag{6}$$

Therefore, the inductance can be easily found from the relation $\Delta E_m = \frac{1}{2}\Delta L I^2$, and the inductance *per unit length* is

$$L_0 = \frac{\Delta L}{\Delta x} = \frac{\Delta E_m/(I^2/2)}{\Delta x} = \frac{\mu}{2\pi}\log\frac{R_2}{R_1} \tag{7}$$

Note that the magnetic field is tangential (along vector $\hat{\varphi}$).

(d) [5pt]

Finding the impedance of a cable requires connecting the voltage between the conductors to the current on the surface. Since the electric field $E_\rho \propto 1/\rho$, the voltage is

$$V = \int E_\rho(R_1)\int d\rho\frac{R_1}{\rho} = R_1 E_\rho(R_1)\log\frac{R_2}{R_1} \tag{8}$$

where $E_\rho(R_1)$ is the radial electric field near the inner conductor. The total current at the central conductor is

$$I = 2\pi R_1 K_1 = \frac{2\pi}{\mu_0}R_1 B_\varphi(R_1) \tag{9}$$

where K_1 is the surface current on the inner conductor and $B_\varphi(R_1)$ is the magnetic field created by it. Finally, using the relation $E_\rho = cB_\varphi$ between the electric and magnetic fields in the EM wave propagating in the positive $\hat{z}$ direction,

$$Z_0 = \frac{V}{I} = \frac{R_1 E_\rho(R_1)\log(R_2/R_1)}{\frac{2\pi}{\mu_0}R_1 B_\varphi(R_1)} = \frac{\mu_0 c}{2\pi}\log\frac{R_2}{R_1}\,. \tag{10}$$

Plugging in the numbers,

$$Z_0 \approx 96.6\,\Omega\,. \tag{11}$$

Note that the actual coaxial cable will have smaller impedance due to dielectric material, not vacuum, filling the space between the conductors.

(d) [5pt]

In case there are two waves propagating in opposite directions, if their voltages add with the same sign (convention choice), then their currents must add with the opposite signs:

$$Z(z) = \frac{V_R(z)+V_L(z)}{I_R(z)-I_L(z)} = \frac{V_R(0)e^{ikz}+V_L(0)e^{-ikz}}{I_R(0)e^{ikz}-I_L(0)e^{-ikz}}\,, \tag{12}$$

and the impedance depends on the position along the cable z as well as the ratio $S = V_L(0)/V_R(0)$ of the left- and right-moving wave amplitudes. These waves can be thought of as the reflected and the incident waves (or vice-versa), respectively. Also, for each of the waves we have $V_L(z)/I_L(z) = V_R(z)/I_R(z) = Z_0$, so that

$$Z(z) = Z_0 \frac{1 + Se^{-2ikz}}{1 - Se^{-2ikz}} \,. \tag{13}$$

Note that $Z(0) = R$ because it is the load at the end of the cable, from which we can find the reflection coefficient S,

$$R = Z(0) = Z_0 \frac{1+S}{1-S} \quad \Longleftrightarrow \quad S = \frac{R/Z_0 - 1}{R/Z_0 + 1} \tag{14}$$

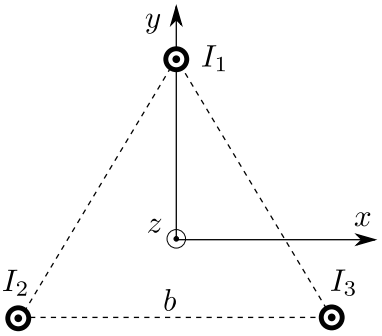
and the impedance at the other end of the cable is

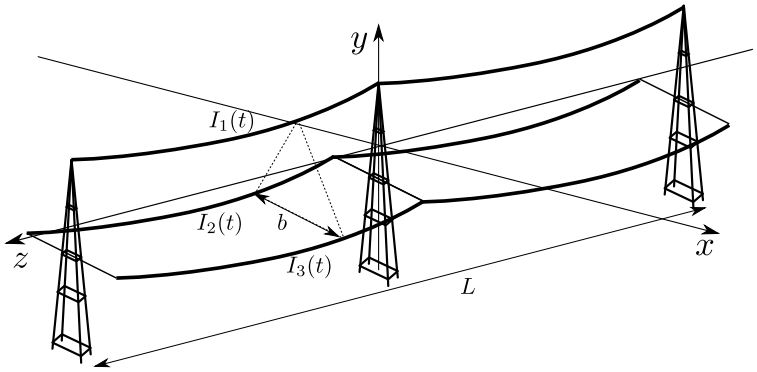
$$Z(l) = Z_0 \frac{R\cos(kl) + iZ_0 \sin(kL)}{Z_0 \cos(kl) + iR\sin(kl)} \tag{15}$$

which is real only if $R = Z_0 = Z_{match}$, leading to zero ($S = 0$) reflection. Such condition is desirable because all the radiowave power is transmitted to the load.

Electromagnetism 3

Three-phase transmission line





Three wires are arranged in an equilateral triangle with side $b = 10$ m as shown in the picture, forming a three-phase alternating-current (AC) power line of length $L = 5$ km. The voltages and currents in the wires are

$$\begin{aligned} I_1(t) &= I_0 \cos(\omega t)\,, & V_1(t) &= V_0 \cos(\omega t)\,, \\ I_2(t) &= I_0 \cos(\omega t - \frac{2\pi}{3})\,, & V_2(t) &= V_0 \cos(\omega t - \frac{2\pi}{3})\,, \\ I_3(t) &= I_0 \cos(\omega t - \frac{4\pi}{3})\,, & V_3(t) &= V_0 \cos(\omega t - \frac{4\pi}{3})\,, \end{aligned} \tag{1}$$

(note that $I_1 + I_2 + I_3 = 0$, $V_1 + V_2 + V_3 = 0$) where I_0 is the amplitude of the current and $\omega = 2\pi\nu$, $\nu = 60$ Hz, is the frequency. Each wire in the transmission line has $V_{rms} = 110$ kV r.m.s. voltage and the total transmitted power is $P = 10$ MW. Assume that the wires are straight (no sagging) and there is no absorption or reflection from the ground and the atmosphere. Some useful formulas are given below.

(a) [1pt] Find the amplitude of the currents I_0.

(b) [5pt] Show that these currents create a magnetic dipole vector rotating in the (xy) plane,

$$\vec{m}(t) = m_0\big[\hat{x}\cos(\omega t + \phi) + \hat{y}\sin(\omega t + \phi)\big]\,, \tag{2}$$

and find its amplitude m_0 (in $[\mathrm{A}\cdot\mathrm{m}^2]$) and phase ϕ.

(c) [4pt] Calculate the electric field $\vec{E}(x, y, z)$ far from the transmission line, but still short compared to λ, i.e. $b, L \ll |x|, |y|, |z| \ll \lambda = c/\nu$.

Now we will study radiated electromagnetic fields at distances $r \gg L$, $r \gg \lambda = c/\nu$.

(d) [2pt] How do the radiated fields E and B depend on the distance r and frequency ω?

(e) [4pt] What is the polarization (direction of $\vec{E}$, $\vec{B}$) at points on $\hat{x}$ axis ? $\hat{y}$ axis? $\hat{z}$ axis?

(f) [4pt] Find the total power radiated from this transmission line.

Vacuum permittivity : $\varepsilon_0 = 8.85 \cdot 10^{-12}\,\mathrm{F/m}$, magnetic constant : $\mu_0 = 4\pi \cdot 10^{-7}\,\mathrm{H/m}$.
Power emitted by a linear oscillating magnetic dipole $\vec{m}(t) = (m_0 \hat{z}) \cos(\omega t)$: $\frac{d\langle P \rangle}{d\Omega} = \frac{\mu_0 m_0^2 \omega^4 \sin^2\theta}{32\pi^2 c^3}$.

Solution

(a) [1pt] The total transmitted power is evenly divided between the wires, so each is carrying $P/3 \approx 3.33$ MW. For the AC current, the power is given by the product of r.m.s voltage and current carried by the wire (assuming no phase shift), so the amplitudes are

$$I_0 = \sqrt{2} I_{rms} = \frac{\sqrt{2} P}{3 V_{rms}} \approx 42.9\, A. \tag{3}$$

(b) [5pt] The three currents add up to zero at any moment, but they are not in the same plane. However, they can be thought of as a superposition of three closed-loop currents, each comprised by one of the wires and by the "return current" flowing in the opposite direction in the center of the triangle. These return currents will cancel each other because $I_1(t) + I_2(t) + I_3(t) = 0$ at any moment. The area of each loop is $A = bL/\sqrt{3}$. Using the right-hand rule and reading the directions off the figure,

$$\begin{aligned} \vec{m}_1 &= A I_1(t)\big(+ \hat{x}\big) \\ \vec{m}_2 &= A I_2(t)\big(-\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\big) \\ \vec{m}_3 &= A I_3(t)\big(-\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}\big) \end{aligned} \tag{4}$$

Adding these contributions, and using trigonometric identities (or vector diagrams),

$$\begin{aligned} \vec{m} &= \vec{m}_1 + \vec{m}_2 + \vec{m}_3 \\ &= A\left(I_1 - \frac{1}{2} I_2 - \frac{1}{2} I_3\right)\hat{x} + A\,\frac{\sqrt{3}}{2}\big(I_2 - I_3\big)\hat{y} \\ &= \frac{3}{2} A I_0\big(\cos(\omega t)\hat{x} + \cos(\omega t - \frac{\pi}{2})\hat{y}\big) \\ &= \frac{\sqrt{3}}{2} bL I_0\big(\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y}\big) \end{aligned} \tag{5}$$

and thus $m_0 = \frac{\sqrt{3}}{2} bL I_0$ and $\phi = 0$.

(c) [4pt] The electric field can be calculated from the vector potential of the magnetic dipole, which in the near zone can be treated as static:

$$\vec{A}(r,t) = \frac{\mu_0 \vec{m}(t) \times \hat{r}}{4\pi r^2} \tag{6}$$

so that the electric field is

$$\vec{E}(r,t) = -\frac{\partial \vec{A}}{\partial t} = \frac{\mu_0 m_0 \omega}{4\pi r^2}\big[\sin(\omega t)\hat{x} - \cos(\omega t)\hat{y}\big] \times \hat{r}\ . \tag{7}$$

(d) [2pt] Electromagnetic fields radiated by a compact sources have to fall off inversely proportional to the distance, so that the Poynting vector satisfies the inverse-square law: $|E|, |B| \propto \frac{1}{r}$. Also, their amplitude must increase $\propto \omega^2$. No proof was required for this question.

(e) [4pt] The rotating dipole is a superposition of two magnetic dipoles linearly oscillating along $\hat{x}$ and $\hat{y}$ axes, respectively. They do not radiate fields only along $\hat{x}$ and $\hat{y}$ axes, respectively. In other directions, their radiated magnetic fields will be aligned with their dipole orientation ($\hat{x}$ and $\hat{y}$, respectively), while their radiated electric fields will be transverse both to the dipole orientation and the radial direction. Combining together,

- $\hat{x}$ axis : only $\hat{y}$ dipole radiates an EM wave polarized linearly in the $\hat{z}$ direction ($E_z \neq 0$, $B_y \neq 0$)
- $\hat{y}$ axis : only $\hat{x}$ dipole radiates an EM wave polarized linearly in the $\hat{z}$ direction ($E_z \neq 0$, $B_x \neq 0$)
- $\hat{z}$ axis : both $\hat{x}$, $\hat{y}$ dipoles radiate but with a $\frac{\pi}{2}$ phase shift; the EM wave is circularly polarized in the $\hat{x}\hat{y}$ plane ($E_{x,y} \neq 0$, $B_{x,y} \neq 0$).

(f) [4pt] The total radiated power will be twice the total power radiated by a linear dipole. Integrating the provided expression over the solid angle,

$$P_{tot} = 2\int d\Omega \frac{\mu_0 m_0^2 \omega^4 \sin^2\theta}{32\pi^2 c^3} = \frac{\mu_0 m_0^2 \omega^4}{8\pi c^3}\int d\cos\theta \sin^2\theta = \frac{\mu_0 m_0^2 \omega^4}{6\pi c^3}\,. = \frac{\mu_0 b^2 L^2 I_0^2 \omega^4}{8\pi c^3}\,. \quad (8)$$

Substituting the numbers,

$$P_{tot} \approx 1.72 \cdot 10^{-10}\,\mathrm{W}\,. \quad (9)$$

Of course, the real losses in a real AC powerline are much higher due to absorbtion of the EM energy in the near zone as well as wire resistance.

Quantum Mechanics 1

Two electron atoms

The wave function of two electron atoms, *e.g.* He, Mg, Ca, *etc.*, are not the same as for one-electron atoms, *e.g.* H, Na, K, *etc.* The single-electron wave functions in the Coulomb field of the nucleus are labeled by $|nlms\rangle$. Here $n = 1, 2, \ldots$ is the principal quantum number labeling the single-particle energy, ℓ and m label the magnitude and z-component of the electron's orbital angular momentum, and finally $s = \pm$ labels the z-component of its spin.

In two electron atoms, the states are labeled by quantum numbers indicating the total orbital angular momentum by (L, M) and the total spin by (S, S_z).

(a) (3 points) For an independent (or non-interacting) electron approximation, write down the ground state wave function of the He atom in terms of tensor products of single-particle states $|n_1\ell_1 m_1 s_1\rangle \otimes |n_2\ell_2 m_2 s_2\rangle$. What are the quantum numbers (n_1, n_2, L, M, S, S_z) of the ground state?

(b) (3 points) For such an independent electron approximation with one electron in the first excited energy level, list the possible states and their the quantum numbers (n_1, n_2, L, M, S, S_z). What is the total number of states with one electron in the first excited energy level?

(c) (3 points) For the first excited states of part (b) write the wave-functions using tensor products of single-particle states $|n_1\ell_1 m_1 s_1\rangle \otimes |n_2\ell_2 m_2 s_2\rangle$.

(d) (6 points) The Coulomb interaction between the atomic electrons partly removes the degeneracies of part (b). Consider how the exchange symmetry of the electrons affects the interaction energy and qualitatively sketch an energy level diagram of the He atom (an example is shown below). In your diagram include the states corresponding to parts (a) and (b) .

   (i) For each energy level indicate the quantum numbers (L, S) and their degeneracy.

   (ii) For each level, explain why you chose the energy to be higher or lower relative to the other energy levels in the diagram.

(e) (5 points) Indicate the allowed optical transitions on the energy level diagram of part (c).

   (i) For each allowed transition write down a matrix element squared which is proportional to the transition rate between the energy levels.

   (ii) For each forbidden transition explain (with formulas) why the relevant matrix element vanishes.

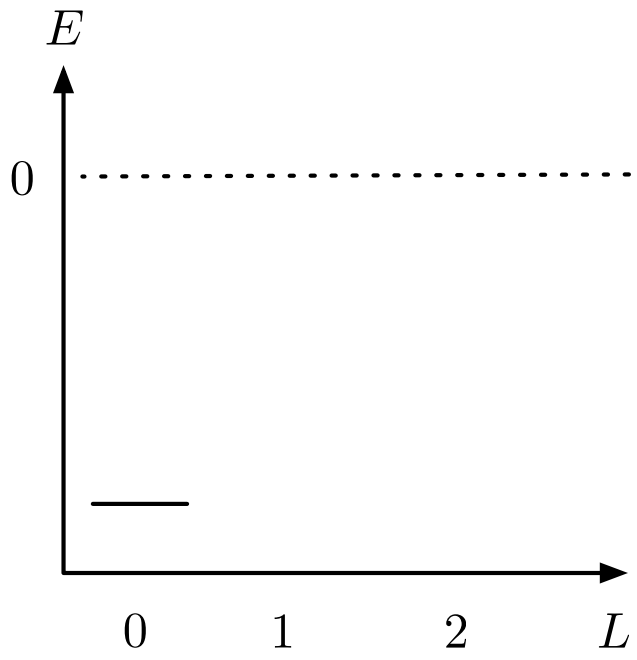


Figure 1: An energy level diagram showing energy on the y-axis and total orbital angular momentum on the x-axis. Fill in the remaining levels.

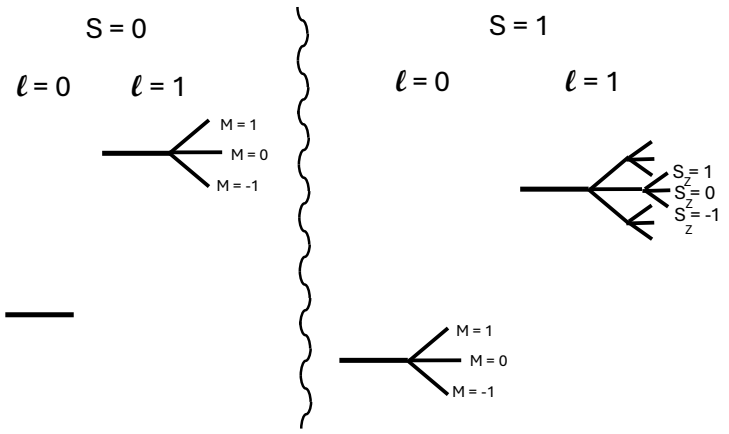
Solution:

(a) The single electron quantum numbers are $|n, \ell, m_\ell, s, m_s\rangle$ so when each of two electrons knows nothing about the other one, the wave function is denoted as $|n_1, \ell_1, m_{\ell,1}, s_1, m_{s,1}\rangle \otimes |n_2, \ell_2, m_{\ell,2}, s_2, m_{s,2}\rangle$. For the ground state with two non-interacting electrons this becomes $|n, L, M_\ell, S, M_s\rangle = |1, 0, 0, 0, 0\rangle$ since the values for m_s must have opposite signs. However, if there is truly zero interaction, meaning they're totally independent, this condition on the m_s values vanishes so S can be 0 or 1 and for $S = 1$, M_s can be -1, 0, 1.

(b) For one electron having $n = 2$ (it doesn't matter which one but we'll choose #2), the condition on s, m_s vanishes because the n-values are different. So S can be 0 or 1 as above. Moreover, for $n = 2$ it's possible to have $\ell = 1$ (or, of course, 0) so there are 4 possible arrangements. These are $|n_1, \ell_1, m_{\ell,1}, s_1, m_{s,1}\rangle \otimes |n_2, \ell_2, m_{\ell,2}, s_2, m_{s,2}\rangle$. For $\ell_1 = 0 = \ell_2$ and $s_1 = 0 = s_2$ both M and S_z are zero so there's only one state. But if $\ell_2 = 1 (\ell_1$ can only be 0 because $n_1 = 1$) there are three values for M. Similarly for $s_2 = 1$. If both ℓ_2 and s_2 are equal 1, there are three values for each M and S_z so there are 9 ways these can be arranged. The total number of possible arrangements is 16.

(c) Now for $\ell_2 = 0, s_2 = 0$, the wave functions is $|1, 0, 0, 0, 0\rangle \otimes |2, 0, 0, 0, 0\rangle$, and for simplicity we'll always write the $n = 1$ electron's ket as $A \equiv |1, 0, 0, 0, 0\rangle$. Thus for $\ell_2 = 1, s_2 = 0$ we have $\{A \otimes |2, 1, -1, 0, 0\rangle,\ A \otimes |2, 1, 0, 0, 0\rangle,\ A \otimes |2, 1, 1, 0, 0\rangle\}$ making 3 more. Similarly for s_2, s_z we have $|2, 0, 0, 1, \pm 1 or 0\rangle$, making 3 more so we have 7 in all. Now, with both ℓ_2 and s_2 both = 1, there are 3 x 3 possible arrangements of M and S_z making 9 more, and 9+7=16 as in part (b) above.

(d) Figure (not to sc



(e) There are no transitions that cross the wiggly line. This is because the transition matrix element $\langle n', L', M', S, m_s | e\vec{\mathcal{E}} \cdot \vec{r} | n, L, M, S, m_s\rangle$ has no spin dependence so spin can't change. Said another way, singlet $\leftrightarrow$ triplet transitions are forbidden. On each side, all $\Delta\ell = \pm 1$ transitions are allowed but no $\Delta\ell = 0$ transitions. If the spin-orbit interactions had been included in this problem, there would be a different basis set and different selection rules.

Quantum Mechanics 2

Spin Hamiltonian

Consider the following spin Hamiltonian

$$H = -DS_z^2 - \varepsilon(S_x^2 - S_y^2)\,,$$

where $S_{x,y,z}$ are conventional spin operators.

a) (5 points) For the total spin $S = 1$ find exact eigenenergies of the above Hamiltonian.

b) (5 points) For general spin $S > 1$ and $\varepsilon = 0$ find the eigenenergies and eigenstates of the Hamiltonian. What is the degeneracy of the ground state for $D > 0$?

c) (5 points) Using perturbation theory in ε, compute the first non-vanishing correction to the ground state energy found in b).

d) (5 points) Notice that in a) for $D > 0$ and ε small the ground state degeneracy was lifted in the first order in ε. In what order in ε you expect the lifting of degeneracy of the ground state for an arbitrary $S > 1$?

Hint: you can use the following matrix elements of spin operators in the eigenbasis of S_z

$$\langle m|S_z|m\rangle = \hbar m\,, \qquad \langle m+1|S_+|m\rangle = \hbar\sqrt{S(S+1) - m(m+1)}\,,$$

where $S_+ = S_x + iS_y$ and $m = -S, -S+1, \ldots, S$.

Solution:

a) We find

$$H = -DS_z^2 - \frac{\varepsilon}{2}(S_+^2 + S_-^2)$$

and

$$\langle m+2|S_+^2|m\rangle = \hbar^2\sqrt{S(S+1)-m(m+1)}\sqrt{S(S+1)-(m+1)(m+2)}$$

For $S = 1$ the Hamiltonian becomes explicitly in the basis $|-1\rangle, |0\rangle, |1\rangle$

$$H = -\hbar^2 \begin{pmatrix} D & 0 & \varepsilon \\ 0 & 0 & 0 \\ \varepsilon & 0 & D \end{pmatrix}.$$

Its eigenenergies are

$$E = \hbar^2(-D-\varepsilon, -D+\varepsilon, 0)$$

b) We have

$$E_m = -\hbar^2 D m^2\,, \qquad m = -S, -S+1, \dots S$$

corresponding to the eigenstates of S_z denoted as $|m\rangle$. The ground state $E = -\hbar^2 DS^2$ is twofold degenerate for $D > 0$ and the eigenestate is given by any superposition of $|-S\rangle$ and $|S\rangle$.

c) The perturbation V does not have a non-vanishing matrix element between two ground states $|-S\rangle$ and $|S\rangle$ and no diagonal elements in the $|m\rangle$ basis. Therefore, we can compute the correction in the second order of non-degenerate perturbation theory. Let us consider one of the ground states $|-S\rangle$.

$$\begin{aligned} E_{-S}^{(2)} &= \sum_{m\neq -S} \frac{\left|\langle m|V|-S\rangle\right|^2}{E_{-S}^{(0)} - E_m^{(0)}} = \frac{\left|\langle -S+2|V|-S\rangle\right|^2}{E_{-S}^{(0)} - E_{-S+2}^{(0)}} = \left(\frac{\varepsilon}{2}\right)^2 \frac{\left|\langle -S+2|S_+^2|-S\rangle\right|^2}{E_{-S}^{(0)} - E_{-S+2}^{(0)}} \\ &= \hbar^2\left(\frac{\varepsilon}{2}\right)^2 \frac{[(S(S+1)-S(S-1))(S(S+1)-(S-1)(S-2)]}{-DS^2 - D(-S+2)^2} \\ &= -\hbar^2 \frac{\varepsilon^2}{2D} S \frac{1-\frac{1}{2S}}{1-\frac{1}{S}} \end{aligned} \tag{1}$$

or

$$E_{-S} \approx -\hbar^2 DS^2 - \hbar^2 \frac{\varepsilon^2}{2D} S \frac{1-\frac{1}{2S}}{1-\frac{1}{S}}\,. \tag{2}$$

The correction to the energy E_S is identical and the degeneracy of the ground state is still twofold within this order of perturbation theory.

d) It is clear that the perturbation V has only matrix elements between states separated by two, i.e. between $|m\rangle$ and $|m+2\rangle$. The number of steps between ground states is $2S$.

If S is integer, the matrix element of the perturbation $\langle S|V^S|-S\rangle \neq 0$ and degenerate perturbation theory will lift the degeneracy in the order ε^S.

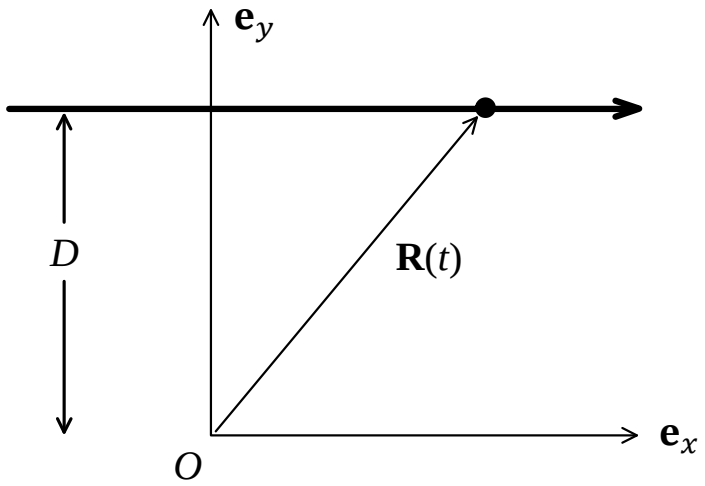
If S is half-integer, the subspace $|-S\rangle, |-S+2\rangle, \ldots, |S-1\rangle$ is not coupled by the perturbation with the other half of the states. In this case, the twofold degeneracy of the ground state is exact and is not lifted by the perturbation neither perturbatively nor nonperturbatively.

The latter statement also follows from the Kramers theorem for half-integer spin.

Quantum Mechanics 3

Coulomb excitation

The nucleus of a hydrogen atom is fixed at the origin O of a coordinate system. A heavy point-particle of charge Ze, whose motion we treat classically, is projected with speed V along the trajectory $\mathbf{R}(t) = Vt\,\mathbf{e}_x + D\,\mathbf{e}_y$, as shown in the figure, where $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ are basis vectors for a Cartesian coordinate system. The point of closest approach of the heavy particle to the hydrogen atom's nucleus occurs at time $t = 0$, at which time the distance between the heavy particle and the nucleus is D.



(a) (2 points) The electron orbiting the atom's nucleus has charge $-e$ and position $\mathbf{r}$. State the operator $\hat{H}_1(t)$ that describes the Coulomb interaction at time t between the heavy particle and the electron. Give your answer in terms of Z, e, $\mathbf{R}(t)$, the electron position operator $\hat{\mathbf{r}}$, and any other necessary factors.

(b) (6 points) Regard the heavy particle as creating a time-dependent perturbation of the hydrogen atom. By starting with the time-dependent Schrödinger equation, derive a formula for the first-order probability, $P_{n\to m}$, that if the electron is in the atomic eigenstate $|n\rangle$ (which has energy eigenvalue ϵ_n) at time T_0 then it will be found in an orthogonal eigenstate $|m\rangle$ (which has energy eigenvalue ϵ_m) at the later time T_1. At this stage, you should not attempt to evaluate any integrals.

(c) (6 points) By assuming that D^2 is large compared with the mean square radius of the atomic eigenstates $|n\rangle$ and $|m\rangle$ (which justifies a Taylor expansion of the Coulomb interaction), show that the leading-order contribution to $P_{n\to m}$ takes the form

$$P_{n\to m} \approx C_1 \left| \int_{T_0}^{T_1} dt\, \frac{(C_2\,t)\,x_{mn} + y_{mn}}{\left[(C_3\,t)^2 + 1\right]^{3/2}}\, \exp\left(i\omega_{mn}t\right) \right|^2 ,$$

and specify the requisite constants C_1, C_2 and C_3. Note the definitions $\hbar\omega_{mn} \equiv \epsilon_m - \epsilon_n$, $x_{mn} \equiv \langle m|\hat{x}|n\rangle$ and $y_{mn} \equiv \langle m|\hat{y}|n\rangle$, and that $\hat{x}$ and $\hat{y}$ are Cartesian components of $\hat{\mathbf{r}}$.

(d) (6 points) Now introduce the characteristic time-scale $\tau \equiv D/V$ and focus on the situation in which $T_0 \ll -\tau$ and $T_1 \gg \tau$. For the eigenstates in question, consider the limit where $|\omega_{mn}\tau| \ll 1$.

(i) What is the physical meaning of the condition $|\omega_{mn}\tau| \ll 1$? Explain.

(ii) Show that in this limit $P_{n\to m} \approx C_4 \, |\langle m|\hat{y}|n\rangle|^2$ for a suitable constant C_4 that you should specify.

Solution: Coulomb excitation.

a) The Coulomb interaction operator $\hat{H}_1(t)$ is given by:

$$\hat{H}_1(t) = -\frac{Ze^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{R}(t) - \hat{\mathbf{r}}|}\,.$$

b) Start with the time-dependent Schrödinger equation,

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = [\hat{H}_0 + \hat{H}_1(t)]|\psi(t)\rangle,$$

where $\hat{H}_0$ is the (time-independent) atomic Hamiltonian and $\hat{H}_1(t)$ is the time-dependent perturbation due to the heavy charged particle. The (complete, orthonormal) set of atomic eigenstates $\{|n\rangle\}$ and eigenvalues $\{\epsilon_n\}$ obey the time-independent Schrödinger equation $\hat{H}_0|n\rangle = \epsilon_n|n\rangle$. Introduce the interaction picture:

$$|\psi(t)\rangle \to |\tilde{\psi}(t)\rangle \equiv \exp\left(i\hat{H}_0 t/\hbar\right)|\psi(t)\rangle\,.$$

Then, straightforward algebra shows that the time-dependent Schrödinger equation becomes:

$$i\hbar\frac{d}{dt}|\tilde{\psi}(t)\rangle = \exp\left(i\hat{H}_0 t/\hbar\right)\hat{H}_1(t)\exp\left(-i\hat{H}_0 t/\hbar\right)|\tilde{\psi}(t)\rangle,$$

where the operator on the right-hand side is the interaction-picture version of the time-dependent perturbation due to the heavy charged particle. Now integrate term-by-term from time T_0 to time T_1 to obtain:

$$|\tilde{\psi}(T_1)\rangle = |\tilde{\psi}(T_0)\rangle + \frac{1}{i\hbar}\int_{T_0}^{T_1} dt\,\exp\left(i\hat{H}_0 t/\hbar\right)\hat{H}_1(t)\exp\left(-i\hat{H}_0 t/\hbar\right)|\tilde{\psi}(t)\rangle\,.$$

Then iterate once, truncate at first order in $\hat{H}_1$, and apply the initial condition $|\tilde{\psi}(T_0)\rangle = |n\rangle$ or $|\tilde{\psi}(T_0)\rangle = \exp\left(i\hat{H}_0 t/\hbar\right)|n\rangle = \exp\left(i\epsilon_n t/\hbar\right)|n\rangle$ to obtain:

$$|\tilde{\psi}(T_1)\rangle \approx \mathrm{e}^{i\epsilon_n T_0/\hbar}|n\rangle + \frac{1}{i\hbar}\int_{T_0}^{T_1} dt\,\exp\left(i\hat{H}_0 t/\hbar\right)\hat{H}_1(t)\exp\left(-i\hat{H}_0 t/\hbar\right)\exp\left(i\epsilon_n t/\hbar\right)|n\rangle\,.$$

Reverting to the Schrödinger picture we obtain:

$$\begin{aligned}|\psi(T_1)\rangle &= \mathrm{e}^{-i\hat{H}_0 T_1/\hbar}|\tilde{\psi}(T_1)\rangle \\ &\approx \mathrm{e}^{-i\epsilon_n(T_1-T_0)/\hbar}|n\rangle + \frac{1}{i\hbar}\int_{T_0}^{T_1} dt\,\mathrm{e}^{i\hat{H}_0(t-T_0)/\hbar}\hat{H}_1(t)\mathrm{e}^{-i\hat{H}_0(t-T_0)/\hbar}|n\rangle\,.\end{aligned}$$

Now compute the *amplitude* $\langle m|\psi(T_1)\rangle$ to be in an eigenstate $|m\rangle$ of $\hat{H}_0$ at time T_1, dropping the zeroth-order term using the the orthogonality of $|m\rangle$ to the initial state $|n\rangle$:

$$\begin{aligned}\langle m|\psi(T_1)\rangle &\approx \frac{1}{i\hbar}\int_{T_0}^{T_1} dt\,\mathrm{e}^{i\epsilon_m(t-T_0)/\hbar}\,\langle m|\hat{H}_1(t)|n\rangle\,\mathrm{e}^{-i\epsilon_n(t-T_0)/\hbar} \\ &= \frac{1}{i\hbar}\mathrm{e}^{-i(\epsilon_m-\epsilon_n)T_0/\hbar}\int_{T_0}^{T_1} dt\,\langle m|\hat{H}_1(t)|n\rangle\mathrm{e}^{i(\epsilon_m-\epsilon_n)t/\hbar}\,.\end{aligned}$$

Then the *probability* $P_{n\to m}$ to be in an eigenstate $|m\rangle$ of $\hat{H}_0$ orthogonal to $|n\rangle$ at time T_1 is given by:

$$P_{n\to m} = |\langle m|\psi(T_1)\rangle|^2 \approx \frac{1}{\hbar^2}\left|\int_{T_0}^{T_1} dt\,\langle m|\hat{H}_1(t)|n\rangle \exp\Big(i(E_m-E_n)t/\hbar\Big)\right|^2 .$$

Inserting the particular form of the time-dependent perturbation due to the Coulomb interaction with the heavy charged particle gives:

$$P_{n\to m} \approx \frac{1}{\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2\left|\int_{T_0}^{T_1} dt\,\langle m|\,|\mathbf{R}(t)-\hat{\mathbf{r}}|^{-1}\,|n\rangle \exp\Big(i(E_m-E_n)t/\hbar\Big)\right|^2 .$$

c) Now Taylor-expand the Coulomb interaction, in effect assuming that the position operator $\hat{\mathbf{r}}$ is small:

$$|\mathbf{R}(t)-\hat{\mathbf{r}}|^{-1} = \big(|\mathbf{R}(t)-\hat{\mathbf{r}}|^2\big)^{-1/2} \approx \Big(|\mathbf{R}(t)|2 - 2\hat{\mathbf{r}}\cdot\mathbf{R}(t)\Big)^{-1/2} \approx \frac{1}{|\mathbf{R}(t)|} + \frac{\hat{\mathbf{r}}\cdot\mathbf{R}(t)}{|\mathbf{R}(t)|^3}\,.$$

The necessary matrix elements then become (using the orthogonality of $|m\rangle$ and $|n\rangle$):

$$\langle m||\mathbf{R}(t)-\hat{\mathbf{r}}|^{-1}|n\rangle \approx \langle m|\left(\frac{1}{|\mathbf{R}(t)|} + \frac{\hat{\mathbf{r}}\cdot\mathbf{R}(t)}{|\mathbf{R}(t)|^3}\right)|n\rangle \approx \frac{\langle m|n\rangle}{|\mathbf{R}(t)|}(=0) + \frac{\langle m|\hat{\mathbf{r}}|n\rangle\cdot\mathbf{R}(t)}{|\mathbf{R}(t)|^3}\,.$$

Next, we insert the specific form of the trajectory of the heavy particle, *i.e.*, $\mathbf{R}(t) = Vt\mathbf{e}_x + D\mathbf{e}_y$, to obtain:

$$\langle m||\mathbf{R}(t)-\hat{\mathbf{r}}|^{-1}|n\rangle \approx \frac{Vtx_{mn}+Dy_{mn}}{\big[(Vt)^2+D^2\big]^{3/2}} = \frac{1}{D^2}\frac{(Vt/D)x_{mn}+y_{mn}}{\big[(Vt/D)^2+1\big]^{3/2}}\,,$$

where $x_{mn} \equiv \langle m|\hat{x}|m\rangle$ and $y_{mn} \equiv \langle m|\hat{y}|m\rangle$ are matrix elements of the Cartesian components $\hat{x}$ and $\hat{y}$ of the position operator $\hat{\mathbf{r}}$. Using these matrix elements, the probability $P_{n\to m}$ becomes:

$$\begin{aligned} P_{n\to m} &\approx \frac{1}{\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2\left|\frac{1}{D^2}\int_{T_0}^{T_1} dt\,\frac{(Vt/D)x_{mn}+y_{mn}}{\big[(Vt/D)^2+1\big]^{3/2}}\,\mathrm{e}^{i\omega_{mn}t}\right|^2 \\ &= C_1\left|\int_{T_0}^{T_1} dt\,\frac{(C_2t)x_{mn}+y_{mn}}{\big[(C_3t)^2+1\big]^{3/2}}\,\mathrm{e}^{i\omega_{mn}t}\right|^2, \\ \text{where}\quad C_1 &\equiv \frac{1}{\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\frac{1}{D^2}\right)^2, \quad C_2 \equiv V/D, \quad \text{and} \quad C_3 \equiv V/D\,. \end{aligned}$$

d-i) The condition $|\omega_{mn}\tau| \ll 1$ means that for the atomic states in question, namely $|n\rangle$ and $|m\rangle$, the energies are close, compared with the uncertainty energy $\hbar/(D/V)$ associated with the time D/V it takes for the heavy particle to pass the atom.

d-ii) We may set the integration limits T_0 and T_1 respectively to $-\infty$ and ∞ and drop the phase factor $\mathrm{e}^{i\omega_{mn}t}$. Then the term associated with the matrix element x_{mn} vanishes (by the oddness in time of the integrand), leaving the one remaining contribution:

$$P_{n\to m} \approx C_1\,|y_{mn}|^2\left|\int_{\infty}^{\infty} dt\,\frac{1}{\big[(C_3t)^2+1\big]^{3/2}}\right|^2 .$$

To evaluate the remaining integral, make the substitution $t \to \theta$ such that $C_3\, t = \tan\theta$. Then the transition probability becomes:

$$P_{n\to m} \approx \frac{C_1}{C_3^2}\,|y_{mn}|^2 \left| \int_{-\pi/2}^{\pi/2} d\theta\, \frac{\sec^2\theta}{\left[\tan^2\theta + 1\right]^{3/2}} \right|^2 = \frac{C_1}{C_3^2}\,|y_{mn}|^2 \left| \int_{-\pi/2}^{\pi/2} d\theta \cos\theta \right|^2 = \frac{4C_1}{C_3^2}\,|y_{mn}|^2 \,.$$

Thus, we have $P_{n\to m} \approx C_4\,|y_{mn}|^2$, where:

$$C_4 = 4\,C_1/C_3^2 = 4\left(\frac{Ze^2}{4\pi\epsilon_0 D}\frac{1}{\hbar V}\right)^2 \,.$$

Statistical Mechanics 1

Condensation in a deformed trap

Consider a gas of N non-interacting bosons of mass m and temperature T in an isotropic harmonic trapping potential:

$$V(x, y, z) = \frac{m\Omega^2}{2}(x^2 + y^2 + z^2)\,. \tag{1}$$

Some integrals are given below.

(a) (4 points) Show that the density of single-particle states $g(\varepsilon)\,\mathrm{d}\varepsilon$ (i.e. the number of single-particle states with energy between ε and $\varepsilon + \mathrm{d}\varepsilon$) is

$$g(\varepsilon)\mathrm{d}\varepsilon = \frac{\varepsilon^2 \mathrm{d}\varepsilon}{2(\hbar\Omega)^3} \tag{2}$$

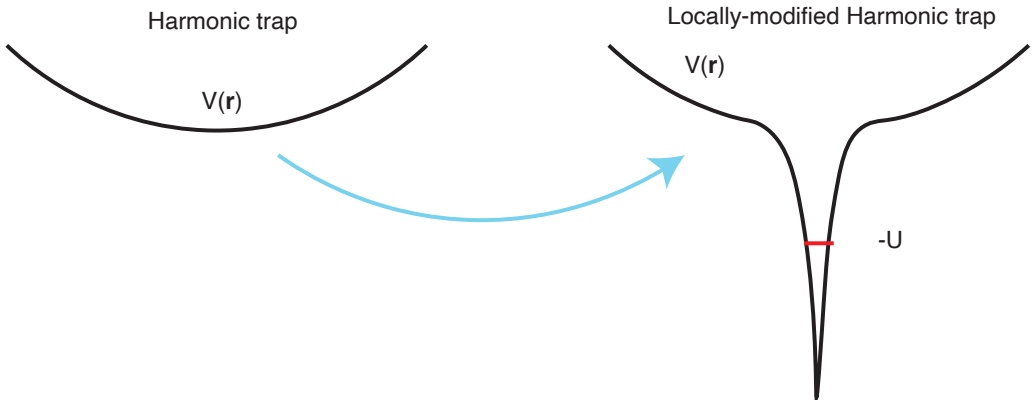
Assume that the energy ε is large compared to the $\hbar\Omega$.

(b) (4 points) The gas will experience condensation and macroscopic occupation of the ground state of the trap at T_c, representing the critical temperature for Bose-Einstein condensation. Calculate T_c.

(c) (4 points) Calculate the condensation fraction (the number of bosons in the condensed phase versus the total number of bosons) at a given temperature T.

(d) (4 points) Calculate the entropy per particle of the gas for $T < T_c$.

(e) (4 points) The trap potential is adiabatically modified as shown below. At some point the new dip in the potential contains a single bound state of energy $-U$. Calculate the new critical temperature.



Integrals:

The following integrals may be useful

$$g_\nu(z) \equiv \frac{1}{\Gamma(\nu)} \int \frac{x^{\nu-1} \mathrm{d}x}{z^{-1}e^x - 1} \tag{3}$$

- Here $\Gamma(\nu)$ is the gamma function

$$\Gamma(\nu) \equiv \int_0^\infty \mathrm{d}x\, x^{\nu-1} e^{-x} \tag{4}$$

The Γ-function has the reccurrence relation $\Gamma(\nu+1) = \nu\Gamma(\nu)$ and the special values

$$\Gamma(1) = 1 \qquad \Gamma(\tfrac{1}{2}) = \sqrt{\pi} \tag{5}$$

- The $g_\nu(z)$ function has the Taylor series

$$g_\nu(z) \simeq z + \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} + \frac{z^4}{4^\nu} \dots \tag{6}$$

- The value at $z = 1$ is given by the Riemann zeta function $\zeta(\nu)$

$$g_\nu(1) = \sum_{n=1}^{\infty} \frac{1}{n^\nu} \equiv \zeta(\nu) \qquad \nu > 1 \tag{7}$$

Special values of the zeta function are

$$\begin{gathered} \zeta(2) = \frac{\pi^2}{6} \simeq 1.64493 \quad \zeta(4) = \frac{\pi^4}{90} \simeq 1.08232 \quad \zeta(6) = \frac{\pi^6}{945} \simeq 1.01734 \\ \zeta(\tfrac{3}{2}) \simeq 2.6123 \qquad \zeta(\tfrac{5}{2}) \simeq 1.34149 \quad \zeta(\tfrac{7}{2}) \simeq 1.12673 \end{gathered} \tag{8}$$

and finally

$$\zeta(3) \simeq 1.20206 \quad \zeta(5) = 1.03693 \quad \zeta(7) \simeq 1.00835 \tag{9}$$

Solution

(a) The single particle energy is

$$\epsilon = \hbar\Omega(n_x + n_y + n_z + \frac{3}{2}) \simeq \hbar\Omega(n_x + n_y + n_z)\,. \tag{10}$$

The number of states *less than* ϵ is $\Sigma(\epsilon)$:

$$\Sigma(\epsilon) = \int_0^{\epsilon} g(\epsilon')\mathrm{d}\epsilon' = \int_0^{\epsilon/\hbar\Omega} dn_x \int_0^{n_x} dn_y \int_0^{n_y} dn_z = \frac{1}{6}\frac{\epsilon^3}{(\hbar\Omega)^3} \tag{11}$$

Differentiating with respect to ϵ produces the result.

(b) he critical temperature T_c is found when $N_T(z = 1, T_c) = N$ where

$$N_T(z, T_c) = \int_0^{\infty} \frac{g(\epsilon)d\epsilon}{z^{-1}e^{\beta\epsilon} - 1}. \tag{12}$$

Taking into account the density of states from (a), we find

$$N = \frac{\zeta(3)}{\beta_c^3(\hbar\Omega)^3}, \tag{13}$$

and

$$k_B T_c = \hbar\Omega \frac{N^{1/3}}{\zeta(3)^{1/3}} \tag{14}$$

(c) Below the critical temperature, the number of bosons in an excited state is given by

$$N_{ex} = N_T(1, T) = \int_0^{\infty} \frac{g(\epsilon)d\epsilon}{e^{\beta\epsilon} - 1} = \frac{\zeta(3)}{\beta^3(\hbar\Omega)^3}, \tag{15}$$

and comparing this wit Eq.(4), we find

$$N_{ex} = N\left(\frac{T}{T_c}\right)^3 \tag{16}$$

(d) The total energy of the gas in a BEC phase is

$$E = \int_0^{\infty} \frac{\epsilon g(\epsilon)d\epsilon}{e^{\beta\epsilon} - 1} = \frac{\pi^4}{30\beta^4(\hbar\Omega)^3}, \tag{17}$$

and the specific heat is given by

$$C_v = \frac{\partial E}{\partial T} = 4\frac{E}{T}. \tag{18}$$

On the other hand $C_v = T\frac{\partial S}{\partial T}$, and hence

$$S = \frac{4}{3}\frac{E}{T} \tag{19}$$

(e) In this case $\epsilon_0 = -U$, so the fugacity at the critical point is $z = e^{-\beta U}$, and the condition for the BEC reads as

$$N_T(e^{-\beta U}, T_c) = \left(\frac{k_B T_c}{\hbar\Omega}\right)^3 g_3(e^{-U/k_B T_c}) = N. \tag{20}$$

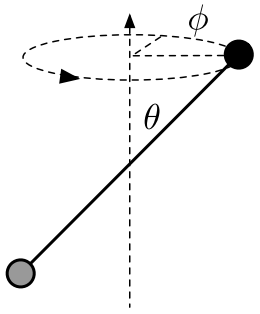
Statistical Mechanics 2

Classical Thermodynamics of Diatomic Molecules

Consider an ideal gas in contact with a reservoir at temperature T consisting of N diatomic molecules, consisting of two non-identical atoms of similar mass. The total mass of the molecule is M and the moment of inertia I. The Langrangian of an individual molecule is thus

$$L = \frac{1}{2} M \dot{\boldsymbol{R}}_0^2 + \frac{1}{2} I \dot{\theta}^2 + \frac{1}{2} I \sin^2\theta \, \dot{\phi}^2 \tag{1}$$

Here $\boldsymbol{R}_0$ is the position of the center of mass and θ and ϕ are the angular coordinates of the rotation (shown below).



(a) (8 points)

(i) Determine the classical Hamiltonian for a single molecule.

(ii) Determine the classical rotational partition function by integrating over the appropriate phase space. Determine the corresponding rotational contribution to the free energy, energy, and entropy of the gas.

(b) (8 points) Next treat the rotations of the molecule quantum mechanically as opposed to classically.

(a) Determine the quantum rotational partition function of the diatomic molecule.

(b) Approximately evaluate the sum over rotational states with using the Euler-Maclurin formula:

$$\sum_{i=m}^{n} f(i) \simeq \int_m^n dx f(x) + \frac{f(n) + f(m)}{2} + \mathcal{O}(f'(n)) \tag{2}$$

What is the condition on the temperature, so that replacing the sum by an integral is approximately valid?

(c) Find the first quantum correction to the classical result for the energy of the diatomic gas.

(c) (2 points) Now suppose the molecule has a small permanent electric dipole moment $\boldsymbol{d}$, directed along the axis of the molecule (see above). This adds an interaction term to the classical Hamiltonian in the presence of an electric field

$$\Delta U = -\boldsymbol{d} \cdot \boldsymbol{E}. \tag{3}$$

Here $\boldsymbol{E} = E\,\hat{\mathrm{z}}$ is uniform external field, which can be considered weak. As a function of the applied field, determine the electrical polarization of the gas, defined as $\boldsymbol{P} \equiv N \langle \boldsymbol{d} \rangle$.

(d) (2 points) If the electric field is slowly increased from zero to $E_{\max}$, how much heat flows into or out of the gas. Give a qualitative explanation for the sign of the heat flow.

Soluton

(a) The Hamiltonian is

$$H = \frac{\boldsymbol{P}_0^2}{2m} + \left(\frac{p_\theta^2}{2I} + \frac{p_\phi^2}{2I \sin^2\theta} \right) = H_{\rm trans} + H_{\rm rot} \tag{4}$$

The partition function is

$$Z = \frac{Z_1^N}{N!} \qquad Z_1 = \int \frac{d^3R_0 d^3P_0}{(2\pi\hbar)^3} \int \frac{d\theta dp_\theta}{(2\pi\hbar)} \int \frac{d\phi dp_\phi}{(2\pi\hbar)} e^{-\beta H} = Z_{\rm 1trans} Z_{\rm 1rot} \,. \tag{5}$$

The single particle rotational partition function is just the last piece

$$Z_{\rm 1rot} = \int \frac{d\theta dp_\theta}{(2\pi\hbar)} \int \frac{d\phi dp_\phi}{(2\pi\hbar)} e^{-\beta H_{\rm rot}} \,, \tag{6}$$

where the $H_{\rm rot}$ is the part that depends on θ and ϕ. Minus free energy (by T) is $\ln Z$:

$$-\frac{F}{T} = \ln Z = \ln(Z_{\rm 1trans}^N/N!) + N \ln Z_{\rm 1rot} \simeq N \ln(Z_{\rm 1trans}/N) + N \ln Z_{\rm 1rot} \tag{7}$$

The first term is the translational free energy and the rotational contribution is the last term. The rotational free energy per particle is

$$F_{\rm 1rot} = -T \ln Z_{\rm 1rot} \tag{8}$$

Performing the integrals and p_θ and p_ϕ using the results for Gaussian integrals

$$\int_{-\infty}^{\infty} e^{-x^2/2\sigma^2} = \sqrt{2\pi\sigma^2} \,, \tag{9}$$

we find

$$Z_{\rm 1rot} = \frac{1}{(2\pi\hbar)^2} \int d\theta d\phi \, \sqrt{2\pi IT} \sqrt{2\pi I \sin^2\theta T} = \frac{IT}{\hbar^2} \int \sin\theta {\rm d}\theta = \frac{2IT}{\hbar^2} \tag{10}$$

In the last part of this probelem the integral over θ is modified. Then we can evaluate the contribution to the rotational free energy from a single particle

$$F_{\rm 1rot} = = -T \ln \left(\frac{2IT}{\hbar^2} \right) \,. \tag{11}$$

For N particles, you can just multiply by N as the free energy is extensive and the particles are independent.

The mean rotational energy of one particle is given by

$$\langle \epsilon_{\rm rot} \rangle = -\frac{\partial \ln Z_{\rm 1rot}}{\partial \beta} = T \tag{12}$$

For N particles, just multiply by N.

Differentiating we find the rotational entropy from a single particle

$$S_{1\text{rot}} = -\left(\frac{\partial F_{1\text{rot}}}{\partial T}\right), \tag{13}$$

$$= \ln Z_{1\text{rot}} + T\frac{\partial}{\partial T}\ln Z(T), \tag{14}$$

$$= \ln\left(\frac{2IT}{\hbar^2}\right) + 1. \tag{15}$$

Again for N particles, you can just multiply by N.

(b) If we treat the rotations quantum mechanically

$$Z_{1\text{rot}} = \sum_{\ell,m} e^{-\beta\epsilon_\ell} = \sum_{\ell}(2\ell+1)e^{-\beta\hbar^2\ell(\ell+1)/2I}, \tag{16}$$

where the energy levels of a rigid rotor are

$$\epsilon_\ell = \frac{\ell(\ell+1)\hbar^2}{2I}. \tag{17}$$

Using the required summation formula

$$Z_{1\text{rot}} = \left[\int_0^\infty (2\ell+1)e^{-\beta\hbar^2\ell(\ell+1)/2I}\right] + \frac{1}{2} \tag{18}$$

$$= -\frac{2Ie^{-\beta\ell(\ell+1)}}{\hbar^2\beta}\bigg|_0^\infty + \frac{1}{2} \tag{19}$$

$$= \frac{2I}{\beta\hbar^2} + \frac{1}{2} \tag{20}$$

Then using for large a, $\log(a+b) \simeq \ln(a) + b/a$,

$$\ln Z_{\text{rot}} \simeq \log\left(\frac{2I}{\beta\hbar^2} + \frac{1}{2}\right) = \log\left(\frac{2I}{\beta\hbar^2}\right) + \frac{\beta\hbar^2}{4I} \tag{21}$$

Then evaluating the shift we find

$$\langle\epsilon_{\text{rot}}\rangle = -\frac{\partial \ln Z}{\partial\beta} \simeq T - \frac{\hbar^2}{4I}. \tag{22}$$

The classical approximation is valid when the spacing between energy levels is small compared to T. For this to be valid we need

$$T \gg \frac{\hbar^2}{2I}, \tag{23}$$

i.e. the correction to ϵ_{rot} of part (a) should be small.

(c) The integral over θ in part (a), $\int \sin\theta \mathrm{d}\theta = 2$ is replaced with

$$Z_\theta = \int \sin\theta \mathrm{d}\theta \, e^{\beta dE \cos\theta} \tag{24}$$

stemming from the additional interaction Hamiltonian, $H_\theta = -dE\cos\theta$. This partition function describes the orientation θ of the molecule and all other coordinates can be ignored.

We expanded Z_θ to quadratic order in the electric field and use that

$$\left\langle \cos^2\theta \right\rangle = \frac{1}{3}\,, \tag{25}$$

to find

$$Z_\theta(E) \simeq 2(1 + \frac{(\beta dE)^2}{6}) \qquad \ln Z_\theta(E) \simeq \text{const} + \frac{(\beta dE)^2}{6}\,. \tag{26}$$

The polarization is related to the mean energy

$$\langle \epsilon_\theta(E) \rangle = -\langle d_z \rangle E\,. \tag{27}$$

So computing the mean energy

$$\langle \epsilon_\theta(E) \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{(dE)^2}{3T}\,. \tag{28}$$

The polarization is thus

$$P_z(E) = \frac{N}{3T} d^2 E\,. \tag{29}$$

(d) Then

$$\Delta U = Q_{\text{in}} + W\,. \tag{30}$$

We have the change in energy per particle

$$\Delta U = \langle \epsilon_\theta \rangle = -\frac{1}{3T}(dE_{\max})^2\,. \tag{31}$$

The work done per particle is

$$W = -\int_0^{E_{\max}} d_z(E)\mathrm{d}E = -\frac{1}{6T}(dE_{\max})^2\,, \tag{32}$$

and then

$$Q_{\text{in}} = -\frac{(dE_{\max})^2}{6T}\,. \tag{33}$$

Qualitatively the entropy goes down as the molecule becomes increasingly locked towards the pole of the sphere, rather than fully exploring the angular phase space. Thus the heat flow $Q_{\text{in}} = T\Delta S$ is negative.

Discussion: We offer two ultimately equivalent ways to solve this problem.

(i) The work done on the gas is the change in its free energy at constant temperature:

$$W = \Delta F = -T(\ln Z_\theta(E_{\max}) - \ln Z_\theta(0)) = -\frac{(dE)^2}{6T}\,. \tag{34}$$

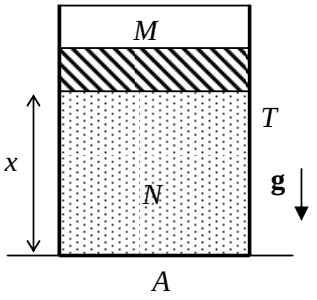
Then $Q = T\Delta S = \Delta U - \Delta F = -(dE_{\max})^2/6T$, reproducing the same result.

(ii) By computing $T\Delta S = -T\partial\Delta F/\partial T = -(dE_{\max})^2/6T$ we find the same result.

Statistical Mechanics 3

Brownian motion of a Cylinder

A vertical cylinder with the walls kept at a constant temperature T, is closed with a heavy piston of mass M, as shown in the Figure, and contains $N \gg 1$ atoms of an ideal monatomic gas. All other notations in the Figure are self-explanatory.



Neglecting external (atmospheric) pressure and the friction between the piston and the cylinder's walls, calculate:

(a) *(2 pts)* Equilibrium position x_0 of the piston.

(b) *(4 pts)* Frequency ω_0 of small oscillations of the piston around the equilibrium position assuming that the gas maintains the temperature T during the oscillations.

(c) *(4 pts)* R.m.s. value Δx of thermal fluctuations of the piston's position under the isothermal assumption as in part (b).

(d) *(5 pts)* If the piston moves with a small but finite velocity u, reflection of the gas atoms from it produces the friction force $F = -\eta u$ acting on the piston. Find the friction coefficient η. (*Hint:* An atom of mass m with the x-component v_x of velocity that approaches the slow-moving heavy piston, changes the piston momentum by $\Delta p = 2m(v_x - u)$ upon reflection. Average this result over the Maxwell distribution.)

(e) *(5 pts)* As derived in previous parts, the piston moves as a damped harmonic oscillator. In equilibrium at finite temperature T, in addition to the "usual" forces discussed above, collisions with individual atoms create a random time-dependent force $f(t)$ on the piston with zero average. The force is δ-correlated in time in the relevant low-frequency range:

$$\langle f(t) \rangle = 0\,, \qquad \langle f(t) f(t') \rangle = K\delta(t - t')\,.$$

Solve the corresponding equation of motion of the piston in Fourier components. Convert back to the time domain to find the r.m.s. value Δx of fluctuations of the piston's position in terms of the magnitude K of the random force. Comparing to Δx found in part (c) establish the "fluctuation-dissipation" relation between K and the friction coefficient η.

Solution

(a) In equilibrium, from the ideal gas equation

$$Mg = k_B T N/x_0\,, \quad \text{i.e.,} \quad x_0 = k_B T N/Mg\,.$$

(b) The oscillation frequency depends on the gas compressibility

$$\omega_0 = (\kappa/M)^{1/2}\,, \quad \kappa = -\frac{dF}{dx} = -\frac{\partial P}{\partial V}A^2\,.$$

Under the isothermal conditions,

$$-\frac{\partial P}{\partial V} = \frac{P}{V} = \frac{Mg}{A^2 x_0}\,, \quad \text{i.e.,} \quad \kappa = \frac{Mg}{x_0}\,,$$

and

$$\omega_0 = (g/x_0)^{1/2} = (M/k_B T N)^{1/2} g\,.$$

(c) The simplest way to find the magnitude of fluctuations of the piston position is to take into account that for small fluctuations the piston is effectively a harmonic oscillator with frequency ω_0 and spring constant κ. We know that in equilibrium at temperature T the average potential and kinetic energies of the oscillator are both equal to $k_B T/2$. Thus,

$$\frac{\kappa(\Delta x)^2}{2} = \frac{k_B T}{2}\,,$$

i.e.,

$$\Delta x = \Big(\frac{k_B T}{\kappa}\Big)^{1/2} = \frac{k_B T\sqrt{N}}{Mg} = x_0/\sqrt{N}\,.$$

and we see that, as usual for thermodynamical systems, fluctuations are smaller than the average values by the factor $\sqrt{N}$.

(d) The total force F produced on the piston can be written as the sum of the forces $F(v_x)$ produced by atoms moving towards the piston with the component of velocity v_x:

$$F = \int_0^\infty dv_x F(v_x)\,.$$

Note that one integrates only over the positive values of v_x because only those atoms move towards the piston, not away from it, as the atoms with $v_x < 0$. The force $F(v_x)$ is the change of piston momentum due to collisions over some small time interval Δt:

$$F(v_x) = \frac{\Delta p C}{\Delta t}\,, \qquad \Delta p = 2m(v_x - u)\,,$$

where Δp is momentum change in one collision, and C is the number of collisions for atoms moving with v_x:

$$C = nA\rho(v_x)v_x\Delta t\,,$$

where n is the total gas concentration, $v_x\Delta t$ is the length of the interval of coordinate x from which the atoms with v_x reach the piston during an arbitrary time interval of duration Δt, and $\rho(v_x)$ is the Maxwell distribution which gives the fraction of the atoms with v_x out of the total n:

$$\rho(v_x) = \Big(\frac{\lambda}{\pi}\Big)^{1/2} e^{-\lambda v_x^2}, \qquad \lambda \equiv \frac{m}{2k_BT}\,.$$

Since the quantities we need to average depend only on the x-component of velocity, we can keep in mind only that part of the Maxwell distribution.

Collecting everything and evaluating the standard simple integrals, we have:

$$F = 2mnA\int_0^\infty dv_x(v_x-u)v_x\rho(v_x) = nk_BTA - unA\Big(\frac{2mk_BT}{\pi}\Big)^{1/2}.$$

The first term here is the usual static pressure of an ideal gas, whereas the second term describes the dissipative force with the friction coefficient

$$\eta = \frac{N}{x_0}\Big(\frac{2mk_BT}{\pi}\Big)^{1/2} = Mg\Big(\frac{2m}{\pi k_BT}\Big)^{1/2}.$$

(e) Equation of motion of the damped harmonic oscillator has the usual from in the frequency domain:

$$-\omega^2 x - i\nu\omega x + \omega_0^2 x = \frac{f(\omega)}{M}\,, \qquad \nu \equiv \eta/M\,,$$

where $f(\omega)$ is the Fourier transform of the random time-dependent force on the oscillator:

$$f(\omega) = \int dt f(t)e^{-i\omega t}\,, \quad \langle f(\omega)f(\omega')\rangle = 2\pi K\delta(\omega+\omega')\,,$$

where the last relation follows directly from the force correlator in the time domain. Immediate solution of the equation of motion gives:

$$x(\omega) = \frac{f(\omega)}{(-\omega^2 - i\nu\omega + \omega_0^2)M}$$

we find the magnitude of the fluctuations of x:

$$\langle x^2(t)\rangle = \frac{1}{4\pi^2}\int d\omega\langle x(\omega)x(\omega')\rangle e^{i(\omega+\omega')t} = \frac{K}{2\pi}\int \frac{d\omega}{|\omega^2 + i\nu\omega - \omega_0^2|^2}\,.$$

Evaluating this integral with the residue theorem, one gets:

$$\langle x^2\rangle = \frac{K}{2\nu M^2\omega_0^2} = \frac{K}{2\eta M\omega_0^2}\,.$$

Comparing this expression for coordinate fluctuations to the equilibrium result obtained in part (c) one gets the following fundamental relation between the magnitude of the random "Brownian" force and the friction coefficient:

$$K = 2k_BT\eta\,.$$