Comprehensive Examination

Department of Physics and Astronomy Stony Brook University

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

General Instructions:

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

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

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

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

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

Classical Mechanics 1

Thin rod sliding

A thin uniform rod of length l and mass m is held upright against a wall. When it is released, it begins to slide down the wall and across the floor, forming an angle θ with the wall, as shown in Fig. 1. During this time, the rod moves horizontally while rotating about its center of mass. Assume the wall and the floor are frictionless.



Figure 1: A thin rod sliding against a wall and the floor.

- (a) (2pts) Explain in words what forces act on the rod to make it accelerate down and to the right.
- (b) (8pts) Compute the angle θ at the moment the rod stops touching the wall. Explain why the horizontal center of mass velocity of the rod, v_x , reaches a maximum at this moment.
- (c) (2pts) What is v_x at the moment the rod stops touching the wall?
- (d) (8pts) What is the rod's center of mass velocity when it hits the floor? Give your answer as a vector $\mathbf{v} = (v_x, v_y)$.

Solution

A thin uniform rod of length l and mass m is held upright against a wall. When it is released, it begins to slide down the wall and across the floor, forming an angle θ with the wall, as shown in Fig. 1. During this time, the rod moves horizontally while rotating about its center of mass.

Assume the wall and the floor are frictionless.

(a) **[2pts]** Explain in words what forces act on the rod to make it accelerate down and to the right.

Gravity makes the rod accelerate down. The normal force from the wall causes it to accelerate to the right.

(b) **[8pts]** Compute the angle θ at the moment the rod stops touching the wall. Explain why the horizontal center of mass velocity of the rod reaches a maximum at this moment.

The rod accelerates to the right because of the normal force. When it stops touching the wall, there is no normal force and hence no acceleration to the right. Thus, the center of mass velocity reaches a maximum at the moment the rod stops touching the wall.

To find the angle θ at this moment, we will use energy conservation to solve for v_x as a function of θ ; the rod stops touching the wall when v_x has a maximum, as explained above.

The potential energy is given by:

$$P.E. = \frac{1}{2}mgl\cos\theta,\tag{1}$$

while the kinetic energy has both translational and rotational parts:

$$K.E. = \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2,$$
(2)

where $v = \frac{1}{2}l\dot{\theta}$ is the center of mass velocity, $I = \frac{1}{12}ml^2$ is the moment of inertia, and $\omega = \dot{\theta}$ is the rotational frequency, so that the kinetic energy can be rewritten in terms of m, l and θ as:

$$K.E. = \frac{1}{8}ml^2\dot{\theta}^2 + \frac{1}{24}ml^2\dot{\theta}^2 = \frac{1}{6}ml^2\dot{\theta}^2$$
(3)

Conservation of energy implies:

$$\frac{1}{2}mgl = \frac{1}{2}mgl\cos\theta + \frac{1}{6}ml^2\dot{\theta}^2\tag{4}$$

Since we are trying to solve for the maximum in v_x , it is useful to solve for $v = \frac{1}{2}l\theta$, i.e.,

$$\frac{1}{2}mgl(1-\cos\theta) = \frac{2}{3}mv^2 \Rightarrow v = \sqrt{\frac{3}{4}gl(1-\cos\theta)}$$
(5)

Thus,

$$v_x = v\cos\theta = \sqrt{\frac{3}{4}gl\left(1 - \cos\theta\right)}\cos\theta \tag{6}$$

The maximum in v_x occurs when $\dot{v}_x = 0$; taking the derivative of (6) yields:

$$\dot{v}_x = \sqrt{\frac{3gl}{4}} \left[\frac{\sin\theta}{2\sqrt{1-\cos\theta}} \cos\theta - \sqrt{1-\cos\theta} \sin\theta \right]$$
(7)

Thus $\dot{v}_x = 0$ when the quantity in brackets vanishes, i.e., when $\cos \theta = \frac{2}{3}$.

(c) [2pts] What is v_x at the moment the rod stops touching the wall? From Eq. (6) and the result of part (b), at the moment the rod stops touching the wall,

$$v_x = \frac{1}{3}\sqrt{gl} \tag{8}$$

(d) [8pts] What is the rod's center of mass velocity when it hits the floor? Give your answer as a vector $\mathbf{v} = (v_x, v_y)$.

Conservation of energy dictates

$$\frac{1}{2}mgl(1-\cos\theta) = \frac{1}{2}m(v_x^2+v_y^2) + \frac{1}{24}ml^2\dot{\theta}^2,$$
(9)

following Eqs. (1) and (2). Now consider the center-of-mass velocity components. After the rod detaches from the wall, it no longer experiences a normal force from the wall. Hence, v_x continues to take the value in Eq. (8) after the rod detaches from the wall. However, v_y depends on θ by

$$v_y = \dot{y} = \frac{d}{dt} \left[\frac{l}{2} \cos \theta \right] = -\frac{l}{2} \dot{\theta} \sin \theta \tag{10}$$

Plugging the expressions for v_x and v_y from Eqs. (8) and (10) into Eq. (9) yields:

$$\frac{1}{2}mgl(1-\cos\theta) = \frac{1}{18}mgl + \frac{1}{8}ml^2\dot{\theta}^2\sin^2\theta + \frac{1}{24}ml^2\dot{\theta}^2$$
(11)

after the rod detaches from the wall.

At the moment the rod hits the ground, $\theta = \pi/2$. Thus, Eq. (11) simplifies to:

$$\frac{1}{2}mgl = \frac{1}{18}mgl + \frac{1}{6}ml^2\dot{\theta}^2,$$
(12)

from which it follows:

$$\dot{\theta} = \sqrt{\frac{8g}{3l}} \tag{13}$$

at the moment the rod hits the floor.

Thus, from Eqs. (8) and (10), the center-of-mass velocity vector at the moment the rod hits the floor is

$$\mathbf{v} = \left(\frac{1}{3}\sqrt{gl}, -\sqrt{\frac{2}{3}gl}\right) \tag{14}$$

Discussion: We have assumed that the tip of the rod never leaves the floor. We should check that this is the case by finding the normal force. Newton's equation of motion in the y direction reads

$$-mg + F_N = ma_y, \tag{15}$$

$$= -m\frac{l}{2}\left[\ddot{\theta}\sin\theta + \dot{\theta}^2\cos\theta\right],\qquad(16)$$

$$\Rightarrow -m\frac{l}{2}\ddot{\theta}\,,\tag{17}$$

where in the last step we assumed $\theta = \pi/2$. The torque equation $\tau = I\alpha$ applied around the center of mass gives

$$F_N \sin \theta \frac{l}{2} = \frac{1}{12} m l^2 \ddot{\theta} \,. \tag{18}$$

Using these equations we can solve for F_N , eliminating $\ddot{\theta}$. The result at $\theta \to \pi/2$ is

$$F_N = \frac{mg}{4} \tag{19}$$

Since this is positive, the tip of the rod never leaves the bottom of the floor.

Classical Mechanics 2

Bead on a rotating wire

A bead of mass m in the earths gravitational field slides without friction along a thin rod of negligible mass inclined at an angle θ (see figure). The rod is forced to rotate with a constant angular velocity Ω about the vertical axis. Below, $\ell(t)$ notates the bead's displacement along the wire measured from the axis of rotation.



- (a) (3 points) Using $\ell(t)$ as a generalized coordinate, determine the Lagrangian of the system and find the equation of motion for the bead.
- (b) (4 points) From the equation of motion show that the bead is in equilibrium at a constant position $\ell(t) = \ell_0 \equiv g \cos \theta / (\Omega \sin \theta)^2$ and interpret ℓ_0 using Newton's second law, $\mathbf{F} = m\mathbf{a}$.
- (c) (5 points) Discuss the stability of this equilibrium point against small displacements along the wire by solving for the deviation $\eta(t) \equiv \ell(t) \ell_0$. Assume that at t = 0 the bead has $\dot{\ell}(t) = 0$ and initial deviation η_0 .
- (d) (8 points) We will now consider a general solution $\ell(t)$ and analyze the forces of constraint.
 - i. Find the external torque required to keep the rod rotating with angular velocity Ω around the z axis in terms of $\ell(t)$ and its derivatives. *Hint:* $\dot{\ell}$ and $\ddot{\ell}$ parameterize the velocity and acceleration in the co-rotating frame. What is the corresponding acceleration in the lab frame?
 - ii. Show how the required torque is determined by the inertial forces (such as the centripetal force) in the co-rotating frame.

Solution:

(a) Writing

$$x = \ell(t)\sin\theta\cos(\Omega t), \qquad (1a)$$

$$y = \ell(t) \sin \theta \sin(\Omega t)$$
, (1b)

$$z = \ell(t) \cos \theta \,, \tag{1c}$$

we find

$$v^2 = \dot{\ell}^2 + \Omega^2 \ell^2 \sin^2 \theta \,. \tag{2}$$

So the Lagrangian is

$$L = \frac{1}{2}m\left(\dot{\ell}^2 + \Omega^2 \ell^2 \sin^2 \theta\right) - mg\ell \cos \theta \,, \tag{3}$$

$$=\frac{1}{2}m\dot{\ell}^{2} - V_{\rm eff}(\ell) \,. \tag{4}$$

where

$$V_{\text{eff}}(\ell) = -\frac{1}{2}m\Omega^2\ell^2\sin^2\theta + mg\ell\cos\theta \,.$$

(b) The potential takes the form

$$\frac{V_{\text{eff}}}{m\Omega^2 \sin^2 \theta} = -\frac{1}{2}\ell^2 + \ell\ell_0 \,, \tag{5}$$

where $\ell_0 = g \cos \theta / \Omega^2 \sin^2 \theta$.

The potential is plotted in Fig. 1 and has a maximum at $\ell = \ell_0$. The equation of motion is

$$m\tilde{\ell} = m\Omega^2 \sin^2 \theta \left(\ell - \ell_0\right) \,, \tag{6}$$

showing that the acceleration is zero at $\ell = \ell_0$. But since the potential is a maximum, and not a minimum, this is an unstable equilibrium as we will analyze next.

In the Newtonian formalism, the "equilibrium" point happens when the acceleration of gravity along the wire $g \cos \theta$ exactly equals the component of the centripetal acceleration along the wire. The centripetal acceleration is $a_{\text{cent}} = \Omega^2 r_{\perp} = \Omega^2 \ell \sin \theta$ (see Fig. 2) and the component along the wire is $a_{\text{cent}} \sin \theta = \Omega^2 \ell \sin^2 \theta$. Thus equating the two accelerations and solving for ℓ , we have condition $\ell = g \cos \theta / \Omega^2 \sin^2 \theta$.

(c) The equation of motion for eta takes the form

$$\ddot{\eta} = \Omega^2 \sin^2 \theta \eta \,, \tag{7}$$

with general solution

$$\eta = \eta_0 \cosh(\Omega \sin \theta t) + \dot{\eta}_0 \sinh(\Omega \sin \theta t) \,. \tag{8}$$

In the current case we have $\dot{\eta}_0 = 0$ and so

$$\eta(t) = \eta_0 \cosh(\Omega \sin \theta t) \,. \tag{9}$$



Figure 1: The effective potential given in Eq. (5)

(d) The first pick a co-rotating set of basis vectors e_1 , e_2 (into the page) and e_3 , as shown in Fig. 2. The position r, the velocity v_r and acceleration a_r in the rotating frame are directed along the rod

$$\boldsymbol{r} = \ell(t)\hat{\boldsymbol{r}},\tag{10}$$

$$\boldsymbol{v}_r = \dot{\ell}(t)\hat{\boldsymbol{r}} \,, \tag{11}$$

$$\boldsymbol{a}_r = \ddot{\boldsymbol{\ell}}(t)\hat{\boldsymbol{r}} \,. \tag{12}$$

The lab frame velocity and acceleration are

$$\boldsymbol{v}(t) = \boldsymbol{v}_r + \boldsymbol{\Omega} \times \boldsymbol{r} \,, \tag{13}$$

$$\boldsymbol{a}(t) = \boldsymbol{a}_r + 2\boldsymbol{\Omega} \times \boldsymbol{v}_r + \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r}) \,. \tag{14}$$

The centripetal acceleration $\boldsymbol{a}_{\text{cent}} = \boldsymbol{\Omega} \times (\boldsymbol{\Omega} \times \boldsymbol{r})$ points toward the center (see figure), while the Coriolis acceleration $\boldsymbol{a}_{\text{cor}} = 2\boldsymbol{\Omega} \times \boldsymbol{v}_r$ is into the page (see figure). The forces on the bead cause the acceleration

$$\boldsymbol{F}_{N} - mg\hat{\boldsymbol{z}} = m\boldsymbol{a} = m\boldsymbol{a}_{r} + m\boldsymbol{a}_{cor} + m\boldsymbol{a}_{cent}$$
(15)

So the normal force is

$$\boldsymbol{F}_N = m\boldsymbol{a}_r + m\boldsymbol{a}_{\rm cor} + m\boldsymbol{a}_{\rm cent} + mg\hat{\boldsymbol{z}} \tag{16}$$

From the picture it is clear that the the only torque on the bead in the z direction is from the normal force causing Coriolis acceleration. The relevant normal force is

$$m\boldsymbol{a}_{\rm cor} = 2m\Omega\ell\sin\theta\,\boldsymbol{e}_2\tag{17}$$

The torque in the z-direction due to this normal force is

$$\tau^{z} \hat{\boldsymbol{z}} = \boldsymbol{r}_{\perp} \times (m \boldsymbol{a}_{\rm cor}), \qquad (18)$$

$$= \ell \sin \theta (2m\Omega \ell \sin \theta) \,\hat{\boldsymbol{z}} \,, \tag{19}$$

$$= 2m\Omega\sin^2\theta\ell\ell\,.\tag{20}$$



Figure 2: The centripetal and Coriolis accelerations in the system. The basis vectors e_1, e_2, e_3 are corotating with the rod and are shown in the figure.

Alternate solution: Another way to proceed is to evaluate

$$\frac{dL_z}{dt} = m\frac{d}{dt}(x\dot{y} - y\dot{x}) = m\frac{d}{dt}(\Omega\ell^2\sin^2\theta) = 2m\Omega\ell\dot{\ell}\sin^2\theta$$
(21)

with x and y given by Eq. 1. The interpretation in terms of the Coriolis force is given above.

Classical Mechanics 3

A driven set of oscillators

A particle of mass m and is attached to a spring of spring constant k. At t = 0 an external time-dependent force $F(t) = F_0 e^{-\alpha t}$ is applied and the particle is displaced in the horizontal direction. Assume that the system is at rest before the force acts, and neglect friction and gravity.



(a) (6 points) Find the displacement, x(t), at late times, long after the force has decayed.

Now consider two masses, $m_1 = 2m$ and $m_2 = m$, suspended in a uniform gravitational field g by identical massless springs with spring constant k. Assume that only vertical motion occurs, and let z_1 and z_2 denote the vertical displacement of the masses from their equilibrium positions, increasing in the downward direction as shown. As in the previous part, at t = 0 an external time-dependent force $F(t) = F_0 \exp(-\alpha t)$ is applied to the lower mass, with F > 0 indicating a downward vertical force. Again assume that the system is initially at rest in its equilibrium configuration before the force acts.



- (b) (7 points) Construct the Lagrangian for the system without the force and find the normal modes and frequencies.
- (c) (7 points) Now include the external force and determine the oscillations of $z_1(t)$ and $z_2(t)$ long after the force has decayed.

Solution:

(a) The solution is expressed using the retarded green function

$$x(t) = \int_0^t dt' G_R(t - t') \frac{F_0}{m} e^{-\alpha t'}$$
(1)

with $G_R(\tau) = \theta(\tau) \sin(\omega_0 \tau) / \omega_0$. Writing out relevant factor, $\sin(\omega_0(t - t'))$:

$$\sin(\omega_0(t-t')) = \sin(\omega_0 t)\cos(\omega_0 t') - \cos(\omega_0 t)\sin(\omega_0 t'), \qquad (2)$$

we find for $t \gg \alpha^{-1}$

$$x(t) = \frac{F_0}{m\omega_0} \sin(\omega_0 t) \int_0^\infty \cos(\omega_0 t') e^{-\alpha t'} dt' - \frac{F_0}{m\omega_0} \cos(\omega_0 t) \int_0^\infty \sin(\omega_0 t') e^{-\alpha t'} dt'$$
(3)

The two integrals in this expression, I_1 and I_2 , are easily done

$$I = I_1 + iI_2 = \int_0^\infty dt' e^{(i\omega - \alpha)t'}, \qquad (4)$$

$$=\frac{1}{\alpha - i\omega},\tag{5}$$

$$=\frac{\alpha+i\omega}{\omega^2+\alpha^2}\,,\tag{6}$$

leading to

$$x(t) = \frac{F_0}{m\omega_0} \left[\frac{\alpha}{\omega_0^2 + \alpha^2} \sin(\omega_0 t) - \frac{\omega_0}{\omega_0^2 + \alpha^2} \cos(\omega_0 t) \right] \,. \tag{7}$$

(b) The Lagrangian of the system without the force is

$$L_0 = \frac{1}{2}(2m)\dot{z}_1^2 + \frac{1}{2}m\dot{z}_2^2 - \frac{1}{2}kz_1^2 - \frac{1}{2}k(z_2 - z_1)^2, \qquad (8)$$

while the force term adds the following driving term

$$L_F = F(t)z_2. (9)$$

Differentiation of $L = L_0 + L_F$ yields the equations of motion

$$\begin{pmatrix} 2m & 0\\ 0 & m \end{pmatrix} \begin{pmatrix} \ddot{z}_1\\ \ddot{z}_2 \end{pmatrix} = \begin{pmatrix} 2k & -k\\ -k & k \end{pmatrix} \begin{pmatrix} z_1\\ z_2 \end{pmatrix} + \begin{pmatrix} 0\\ F(t) \end{pmatrix} .$$
(10)

Let us look for the normal modes $(z_1, z_2) = (u_1, u_2)e^{-i\omega t}$ where (u_1, u_2) is a constant eigenvector. We find the eigenvectors of satisfy the generalized eigenvalue problem

$$-\omega^{2}\underbrace{\begin{pmatrix} 2m & 0\\ 0 & m \end{pmatrix}}_{\equiv \mathcal{M}} \begin{pmatrix} u_{1}\\ u_{2} \end{pmatrix} = \underbrace{\begin{pmatrix} 2k & -k\\ -k & k \end{pmatrix}}_{\equiv \mathcal{K}} \begin{pmatrix} u_{1}\\ u_{2} \end{pmatrix} .$$
(11)

The generalized eigenvalue problem is of the form (with $\lambda = -\omega^2$)

$$\mathcal{K}\vec{E} = \lambda \,\mathcal{M}\vec{E} \,. \tag{12}$$

with a positive definite mass matrix \mathcal{M} acting as a weight. Setting the characteristic polynomial det $(\mathcal{K} - \lambda \mathcal{M})$ to zero

$$(2k - \lambda 2m)(k - \lambda m) - k^2 = 0, \qquad (13)$$

we solve for the eigen-frequencies

$$\omega_{\pm}^2 = \frac{k}{2m} (2 \pm \sqrt{2}) \,. \tag{14}$$

The corresponding eigenmodes are

$$\vec{E}_{\pm} = \begin{pmatrix} \pm \sqrt{2} \\ 2 \end{pmatrix} \,. \tag{15}$$

We note that the vectors are orthogonal with the mass matrix \mathcal{M} acting as a weight:

$$\vec{E}_{+}^{T}\mathcal{M}\vec{E}_{-} = 0.$$
⁽¹⁶⁾

.

(c) The solution is expanded in terms of the eigen-basis basis

$$\begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix} = z_+(t)\vec{E}_+ + z_-(t)\vec{E}_- \,.$$
 (17)

Substituting this form into the equations of motion we have

$$\left(\ddot{z}_{+} + \omega_{+}^{2} z_{+}\right) \vec{E}_{+} + \left(\ddot{z}_{-} + \omega_{-}^{2} z_{-}\right) \vec{E}_{-} = \mathcal{M}^{-1} \begin{pmatrix} 0\\F(t) \end{pmatrix}.$$
(18)

The force is decomposed into eigen vectors

$$\mathcal{M}^{-1}\begin{pmatrix}0\\F(t)\end{pmatrix} = \begin{pmatrix}0\\\frac{F(t)}{m}\end{pmatrix} = \frac{F(t)}{4m}\vec{E}_{+} + \frac{F(t)}{4m}\vec{E}_{-},\qquad(19)$$

and the equations to be solved are

$$\ddot{z}_{+} + \omega_{+}^{2} z_{+} = \frac{F(t)}{4m} , \qquad (20a)$$

$$\ddot{z}_{-} + \omega_{-}^2 z_{-} = \frac{F(t)}{4m} \,. \tag{20b}$$

These equations are solved directly by comparison with part (a):

$$z_{\pm}(t) = \frac{F_0}{4m\omega_{\pm}} \left[\frac{\alpha}{\omega_{\pm}^2 + \alpha^2} \sin(\omega_{\pm}t) - \frac{\omega_{\pm}}{\omega_{\pm}^2 + \alpha^2} \cos(\omega_{\pm}t) \right].$$
(21)

Electromagnetism 1

Waves in the Earth's atmosphere

We consider the atmosphere of the Earth as a neutral and dilute plasma of uniform density, consisting of classical non-interacting dissociated electrons and stationary ions. The atmosphere is permeated by the Earth's static and uniform magnetic field in the z-direction, $\mathbf{B}_E = B_E \hat{\mathbf{z}}$. We want to find out how radio waves propagate in the Earth's atmosphere. For this purpose, consider circularly polarized radio waves propagating in the z-direction:

$$\mathbf{E}_{\pm} = E_0 \left(\hat{\mathbf{x}} \pm i \hat{\mathbf{y}} \right) e^{-i\omega t + ikz} \,. \tag{1}$$

The magnetic field of the wave is substantially weaker than the Earth's magnetic field B_E .

1. (6 points) For an electron of charge -e and mass m, write and solve the classical evolution equations for the steady state oscillations $\delta \mathbf{r}_{\pm}(t)$ of the electron around its mean position $\mathbf{r} = (x, y, z)$, in the fields of the Earth and a radio wave of specified circular polarization, \pm . Assume that the electron is at rest on average. Express your solution in terms of the Earth's Larmor frequency¹, $\omega_B = eB_E/mc$.

Hint: Neglect the magnetic field of the wave in comparison to the Earth's, and look for a steady state displacement of the form $\delta \mathbf{r}(t) = \mathbf{r}_{\perp} e^{-i\omega t + ikz}$ where \mathbf{r}_{\perp} lies in the xy plane.

- 2. (6 points) For both polarizations of the radio waves, derive the frequency-dependent dielectric constant ε_{\pm} and the polarization P_{\pm} of the plasma. Assume the electron density is N per unit volume, with plasma frequency² $\omega_p^2 = 4\pi N e^2/m$.
- 3. (6 points) When the frequency of the wave ω is much smaller than the ω_B and ω_p , derive the phase and group velocities, v_p^{\pm} and v_q^{\pm} , for both polarizations of radio waves. Do both polarizations propagate? Explain.
- 4. (2 points) In the Earth's atmosphere $\omega_B \approx \omega_p \approx 10^7$ Hz. Consider two propagating signals of frequency $\omega_1 \simeq 10^5$ Hz and $\omega_2 \simeq 2 \times 10^5$ Hz, emitted simultaneously from New York. Estimate the difference in their arrival times in Shanghai. Assume that New York and Shanghai are on opposite sides of the Earth, and that the Earth's curvature guides the waves around the Earth in a circle of radius $R_E \approx 6 \times 10^8$ cm.

¹We are using Gaussian units. In SI units, $\omega_B = eB/m$. ²We are using Gaussian units. In SI units, $\omega_p^2 = Ne^2/m\epsilon_0$.

Solution

a. The motion of the ionized electron is given by

$$m\ddot{\mathbf{x}} = -\frac{e}{c}\dot{\mathbf{x}} \times \mathbf{B}_E - eE_0(\hat{\mathbf{x}} \pm i\hat{\mathbf{y}})e^{-i\omega t + ikz}.$$
(2)

For a weak magnetic field, the steady state solution is driven by the polarized wave, so we seek a solution of (2) of the form

$$\mathbf{x}_{\pm} = \underline{\mathbf{x}} + A^{\pm} (\hat{\mathbf{x}} \pm i \hat{\mathbf{y}}) e^{-i\omega t + ik\underline{z}} , \qquad (3)$$

with A the amplitude, and $\underline{\mathbf{x}} = (\underline{x}, \underline{y}, \underline{z})$ the average 3-position of the ionized electron. Inserting (3) into (2) yields the amplitude

$$A^{\pm} = \frac{eE_0}{m\omega(\omega \mp \omega_B)} \,. \tag{4}$$

b. The polarization carried by the displaced ionized electron in the plasma is

$$\mathbf{P}_{\pm} = -Ne(\mathbf{x}_{\pm} - \underline{\mathbf{x}}) = -\frac{Ne^2}{m\omega(\omega \mp \omega_B)} \mathbf{E} = \chi_E^{\pm} \mathbf{E} \,, \tag{5}$$

and the corresponding dielectric constant is

$$\epsilon^{\pm} = 1 + 4\pi \chi_E^{\pm} = 1 - \frac{\omega_p^2}{\omega(\omega \mp \omega_B)} \,. \tag{6}$$

c. For radio waves with $\omega \ll \omega_B \approx \omega_p$

$$\epsilon^{\pm} \approx \pm \frac{\omega_p^2}{\omega \omega_B} \,, \tag{7}$$

which clearly shows that only the left-handed (+) radio wave propagates. The right-handed one (-) does not. The phase velocity is

$$v_{\varphi}^{+} = \frac{\omega}{k} = \frac{c}{n} = \frac{c}{\sqrt{\epsilon^{+}}} = \frac{c}{\omega_{p}}\sqrt{\omega\omega_{B}}, \qquad (8)$$

and

$$k(\omega) = \frac{\omega}{v_{\varphi}^{+}(\omega)} \,. \tag{9}$$

The group velocity is

$$v_g = \frac{d\omega}{dk} = \left(\frac{dk}{d\omega}\right)^{-1} = \frac{2c}{\omega_p}\sqrt{\omega\omega_B} = 2v_{\varphi}^+, \qquad (10)$$

after using $k(\omega)$ from (9). Higher frequencies travel faster.

d. For waves with $\omega \approx 10^5$ Hz and $\omega_p \approx \omega_B \approx 10^7$ Hz, $v_{\varphi}^+ \approx c/10$. The time difference is

$$\Delta t = \frac{\pi R_E}{v_{g1}} - \frac{\pi R_E}{v_{g2}} = \frac{\pi R_E}{2c} \frac{\omega_p}{\sqrt{\omega_B}} \left(\frac{1}{\sqrt{\omega_1}} - \frac{1}{\sqrt{\omega_2}}\right),\tag{11}$$

$$=\frac{\pi R_E}{2c} \frac{\omega_p}{\sqrt{\omega_B \omega_1}} \left(1 - \sqrt{\frac{\omega_1}{\omega_2}}\right),\tag{12}$$

with specifically

$$\Delta t \approx \frac{\pi (6 \cdot 10^8 \,\mathrm{cm})}{2(3 \cdot 10^{10} \mathrm{cm/s})} \frac{10^7}{\sqrt{10^7 \times 10^5}} (1 - \frac{1}{\sqrt{2}}) \approx 0.1 \,\mathrm{s} \,.$$
(13)

Electromagnetism 2

Potential above a surface



The xy plane has no net charge, and is held at a specified electrostatic potential V(x, y), as shown above.

- (a) (4 points) Determine the electrostatic potential, $\phi(x, y, z)$, for z > 0 for the specific case $V(x, y) = V_0 \cos(\kappa x)$.
- (b) (4 points) Now consider a general boundary potential V(x, y). Determine $\phi(x, y, z)$ for z > 0 in terms of the Fourier transform of V(x, y)

$$\hat{V}(\boldsymbol{q}) \equiv \int d^2 \boldsymbol{r} \, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \, V(\boldsymbol{r}) \,. \tag{1}$$

Here the boldface symbols \boldsymbol{r} and \boldsymbol{q} denote the two dimensional vectors, i.e. $\boldsymbol{r} = (x, y)$ and $\boldsymbol{q} = (q_x, q_y)$, and the Fourier transform of a two dimensional function $f(\boldsymbol{r})$ is notated $\hat{f}(\boldsymbol{q})$.

Now consider an infinite surface Σ with no net charge dividing space into two pieces. Σ is a small distortion of the xy plane, and is parameterized by z = H(x, y) as shown in the figure above. The electrostatic scalar potential ϕ is specified to have the value V(x, y) at the point (x, y, H(x, y)) on the surface.

(c) (2 points) By assuming that H(x, y) is small, show that $\phi(x, y, z)$ satisfies the effective boundary condition on the surface z = 0

$$\phi(x,y,0) + \left. \frac{\partial \phi(x,y,z)}{\partial z} \right|_{z=0} H(x,y) = V(x,y) \,. \tag{2}$$

(d) (6 points) Consider a specific case $V(x, y) = V_0 \cos(\kappa_1 x)$ and $H(x, y) = H_0 \cos(\kappa_2 x)$, determine the effective boundary condition $\phi(x, y, 0)$ to first order in H, and then determine the potential $\phi(x, y, z)$ above the surface. What is the leading behavior at large z when κ_1 is nearly κ_2 ? Explain.

Hint: You may find the trigonometric identities helpful here

$$\cos(\theta_1)\cos(\theta_2) = \frac{1}{2}\cos(\theta_1 + \theta_2) + \frac{1}{2}\cos(\theta_1 - \theta_2), \qquad (3)$$

$$\sin(\theta_1)\cos(\theta_2) = \frac{1}{2}\sin(\theta_1 + \theta_2) + \frac{1}{2}\sin(\theta_1 - \theta_2).$$
(4)

(e) (4 points) Now consider a general $V(\mathbf{r})$ and $H(\mathbf{r})$. To first order in H, find the solution for the electrostatic potential $\phi(x, y, z)$ for z > 0 in terms of integrals over the Fourier transforms $\hat{V}(\mathbf{q})$ and $\hat{H}(\mathbf{q})$.

Hint: You may use the convolution theorem without proof:

$$\int d^2 \boldsymbol{r} \, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \, f(\boldsymbol{r}) \, g(\boldsymbol{r}) = \int \frac{d^2 \boldsymbol{k}}{(2\pi)^2} \, \hat{f}(\boldsymbol{k}) \, \hat{g}(\boldsymbol{q}-\boldsymbol{k}) \,. \tag{5}$$

Solution:

Note: To simplify the notation when confusion can not arise, we indicate Fourier transform of a function $f(\mathbf{r})$ is by its argument, i.e. we write $f(\mathbf{q})$ and $f(\mathbf{k})$ instead of $\hat{f}(\mathbf{q})$ and $\hat{f}(\mathbf{k})$ to indicate the Fourier transform.

(a) For the specific boundary condition $V(\mathbf{r}) = V_0 \cos(\kappa x)$, we are to solve the Laplace equation

$$-\left(\frac{\partial^2 \phi}{\partial z^2} + \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) = 0.$$
(6)

The equation separates in Cartesian coordinates. Guessing a solution of the form $Z(z)cos(\kappa x)$ we substitute and solve for Z(z)

$$Z(z) = Ae^{-\kappa z} + Be^{+\kappa z}.$$

Rejecting the growing exponential we set B = 0, and choosing A so that the boundary condition $Z(0) = V_0$ is reproduced, we have finally:

$$\phi(\mathbf{r}, z) = V_0 \cos(\kappa x) e^{-\kappa z} \,. \tag{7}$$

(b) We have the Laplace equation

$$-\left(\frac{\partial^2 \phi}{\partial z^2} + \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) = 0, \qquad (8)$$

and Fourier transform in the x and y directions yielding

$$-\phi''(z, q) + q^2 \phi(z, q) = 0.$$
(9)

Here $q^2 = q_x^2 + q_y^2 = |\mathbf{q}|^2$ the prime's denote z derivatives. The solution is

$$\phi(z, \boldsymbol{q}) = A(\boldsymbol{q})e^{-qz} + B(\boldsymbol{q})e^{qz}.$$
(10)

The growing exponential is discarded on physical grounds. In order to match the boundary conditions at z = 0 we must have $A(\mathbf{q}) = V(\mathbf{q})$ leading to

$$\phi(\mathbf{r}, z) = \int \frac{d^2 \mathbf{q}}{(2\pi)^2} e^{i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{q}) e^{-qz} \,. \tag{11}$$

(c) We have by Taylor series

$$\phi(x, y, H(x, y)) = \phi_0(x, y) + \phi'_0(x, y)H(x, y), \qquad (12)$$

where we use the abbreviations

$$\phi_0(x,y) \equiv \phi(x,y,z)|_{z=0} , \qquad \phi_0'(x,y) \equiv \left. \frac{\partial \phi(x,y,z)}{\partial z} \right|_{z=0} . \tag{13}$$

The boundary condition is $\phi(x, y, H(x, y)) = V(x, y)$ leading to the stated result

$$\phi_0(x,y) + \phi'_0(x,y)H(x,y) = V(x,y).$$
(14)

(d) Since at leading order $\phi(x, y, z) \simeq V_0 \cos(\kappa_1 x) e^{-\kappa_1 x}$, we have $\phi'_0(x, y) \simeq -\kappa_1 V_0 \cos(\kappa_1 x)$. So the mixed term in the boundary conditions is approximately

$$\phi_0'(x,y)H_0\cos(\kappa_2 x) \simeq -V_0\kappa_1 H_0\cos(\kappa_2 x)\cos(\kappa_1 x), \qquad (15)$$

$$= -V_0\kappa_1 H_0 \left[\frac{1}{2}\cos(\kappa_S x) + \frac{1}{2}\cos(\Delta\kappa x)\right] . \tag{16}$$

Here for later use we have defined the sum and difference in the wavenumbers

$$\kappa_S \equiv \kappa_1 + \kappa_2, \qquad \Delta \kappa = \kappa_1 - \kappa_2$$

Thus the modified boundary condition is

$$\phi_0(x,y) = V_0 \cos(\kappa_1 x) + V_0 \kappa_1 H_0 \left[\frac{1}{2} \cos(\kappa_S x) + \frac{1}{2} \cos(\Delta \kappa x)\right] \,. \tag{17}$$

Part (b) worked out the solution for a boundary condition $\propto \cos(\kappa x)$ for any κ . Using the superposition principle, we can write the solution now as a sum of such solutions, since the boundary condition is a sum of such cosines:

$$\phi(x, y, z) = V_0 \cos(\kappa_1 x) e^{-\kappa z} + V_0 \left(\kappa_1 H_0\right) \left[\frac{1}{2} \cos(\kappa_S x) e^{-\kappa_S z} + \frac{1}{2} \cos(\Delta \kappa x) e^{-|\Delta \kappa| z}\right] .$$
(18)

Thus we see that at large z and small $|\Delta \kappa|$ we have

$$\phi(x, y, z) \simeq \frac{1}{2} V_0\left(\kappa_1 H_0\right) \cos(\Delta \kappa x) e^{-|\Delta \kappa| z} \,. \tag{19}$$

(e) Expressing Eq. 12 in Fourier space we have the boundary condition

$$\phi_0(\boldsymbol{q}) + \int \frac{d^2 \boldsymbol{k}}{(2\pi)^2} \phi_0'(\boldsymbol{k}) H(\boldsymbol{q} - \boldsymbol{k}) = V(\boldsymbol{q}) \,. \tag{20}$$

The solution for $\phi(\boldsymbol{q}, z)$ is the same as before

$$\phi(\boldsymbol{q}, z) = A(\boldsymbol{q})e^{-qz}, \qquad (21)$$

$$\phi'(\boldsymbol{q}, z) = -qA(\boldsymbol{q})e^{-qz}, \qquad (22)$$

but the boundary conditions have changed. Motivated by the zeroth order solution in part (a), we write

$$A(\boldsymbol{q}) = V(\boldsymbol{q}) + \delta A(\boldsymbol{q}) \,. \tag{23}$$

Here $\delta A(\mathbf{q})$ is of order *H*. Setting up an expansion scheme, we have the approximation we have to first order in *H*

$$\int \frac{d^2 \boldsymbol{k}}{(2\pi)^2} \phi_0'(\boldsymbol{k}) H(\boldsymbol{q} - \boldsymbol{k}) \simeq -\int \frac{d^2 \boldsymbol{k}}{(2\pi)^2} k V(\boldsymbol{k}) H(\boldsymbol{q} - \boldsymbol{k}).$$
(24)

Substituting Eq. 23 into the boundary conditions and using Eq. 24, we have

$$\delta A(\boldsymbol{q}) \simeq \int \frac{d^2 \boldsymbol{k}}{(2\pi)^2} \, k V(\boldsymbol{k}) H(\boldsymbol{q} - \boldsymbol{k}) \,, \tag{25}$$

leading to our final somewhat formal result:

$$\phi(x, y, z) = \int \frac{d^2q}{(2\pi)^2} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} (V(\boldsymbol{q}) + \delta A(\boldsymbol{q})) e^{-qz} \,.$$
(26)

Discussion: To verify consistency with part (d) we not that the Fourier transforms of $V(\mathbf{r})$ and $H(\mathbf{r})$ are

$$V(\boldsymbol{k}) = \frac{V_0}{2} (2\pi)^2 \left[\delta(\boldsymbol{k} - \kappa_1 \boldsymbol{e}_x) + \delta(\boldsymbol{k} + \kappa_1 \boldsymbol{e}_x) \right] , \qquad (27)$$

$$H(\boldsymbol{q}) = \frac{V_0}{2} (2\pi)^2 \left[\delta(\boldsymbol{q} - \kappa_2 \boldsymbol{e}_x) + \delta(\boldsymbol{q} + \kappa_2 \boldsymbol{e}_x) \right] .$$
⁽²⁸⁾

Then substituting these results into Eq. (25) we find

$$\delta A(\boldsymbol{q}) = \frac{1}{4} V_0 \left(\kappa_1 H_0\right) (2\pi)^2 \left[\delta(\boldsymbol{q} - \kappa_S \boldsymbol{e}_x) + \delta(\boldsymbol{q} + \kappa_S \boldsymbol{e}_x) + \delta(\boldsymbol{q} - \Delta \kappa \boldsymbol{e}_x) + \delta(\boldsymbol{q} + \Delta \kappa \boldsymbol{e}_x)\right] .$$
⁽²⁹⁾

Finally substituting $\delta A(q)$ into Eq. (26) we find Eq. (18).

Electromagnetism 3

A moving mirror

A mirror moves relativistically with velocity v in the lab frame with position z = vt. A linearly polarized plane wave of light, with amplitude E_I and wavenumber k, i.e.

$$\boldsymbol{E}_{I}(t,z) = E_{I}\cos(k(z-ct))\,\hat{\boldsymbol{x}}\,,\tag{1}$$

is normally incident upon the mirror and is reflected. The goal of the problem is to analyze the reflected light.



- (a) (4 points) Determine the incident electric field in the frame of the mirror. Explicitly show the dependence on the coordinates (t', x', y', z') in the transformed frame. What is the frequency of the incident light in this frame?
- (b) (7 points) Write down the reflected wave in the *mirror* frame, explicitly indicating the dependence on the transformed coordinates (t', x', y', z'). Then determine the amplitude and frequency of reflected electric field in the *lab* frame.
- (c) (5 points) Determine the time-averaged force per area on the mirror by the light.
- (d) (4 points) Now work entirely in the lab frame and *do not* use Lorentz transformations. The solution to the left of the mirror can be written³

$$\boldsymbol{E}(t,z) = E_I e^{i(kz-\omega t)} \,\hat{\boldsymbol{x}} + E_R e^{i(-k_R z - \omega_R t)} \,\hat{\boldsymbol{x}}$$
(2)

where E_R , k_R and ω_R are the reflected amplitude, wavenumber, and frequency, respectively. Determine the amplitude and frequency of the reflected light.

Hint: Impose the boundary condition that the Lorentz force, $\mathbf{F} \propto \mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}$, on the surface of the moving mirror is zero for all times.

³The physical electric field is the real part of this complex expression.

Solution

Notation: E_I , E_R are positive and denote the magnitude of the *x* component of the electric field for the incident and reflected waves, respectively. Similarly, B_I and B_R are the magnitude *y* components of the magnetic fields. The incident and reflected waves have $\omega = ck$, and the *E* and *B* fields have equal magnitude. \vec{E} and \vec{B} denote the vector amplitudes of the sinusoidal waves:

$$\boldsymbol{E}_{I}(t,z) = \vec{E}_{I}\cos(kz - \omega t) = E_{I}\cos(kz - \omega t)\hat{\boldsymbol{x}}$$
(3)

$$\boldsymbol{B}_{I}(t,z) = \vec{B}_{I}\cos(kz - \omega t) = E_{I}\cos(kz - \omega t)\hat{\boldsymbol{y}}.$$
(4)

The reflected wave, which is left moving and involves $\cos(-k_R z - \omega_R t)$, takes the form

$$\boldsymbol{E}_{R}(t,z) = \vec{E}_{R}\cos(-k_{R}z - \omega_{R}t) = -E_{R}\cos(-k_{R}z - \omega_{R}t)\hat{\boldsymbol{x}}, \qquad (5)$$

$$\boldsymbol{B}_{R}(t,z) = \vec{B}_{R}\cos(-k_{R}z - \omega_{R}t) = E_{R}\cos(-k_{R}z - \omega_{R}t)\hat{\boldsymbol{y}}, \qquad (6)$$

where we have anticipated that the reflected wave is inverted, $\vec{E}_R = -E_R \hat{x}$.

(a) Using the Lorentz transformation rules

$$\underline{\boldsymbol{E}}_{\perp} = \gamma \boldsymbol{E}_{\perp} + \gamma \boldsymbol{\beta} \times \boldsymbol{B}_{\perp} \,, \tag{7}$$

$$\underline{B}_{\perp} = \gamma B_{\perp} - \gamma \beta \times B_{\perp} , \qquad (8)$$

we can determine the electric and magnetic fields in the mirror frame. Using $\boldsymbol{\beta} \times \boldsymbol{B} \propto E_I \beta \hat{\boldsymbol{z}} \times \hat{\boldsymbol{y}} = -E_I \beta \hat{\boldsymbol{x}}$, we find

$$\underline{\vec{E}}_{I} = (E_{I}\gamma - \gamma\beta E_{I})\,\hat{\boldsymbol{x}}\,,\tag{9}$$

or

$$\underline{E}_{I} = \sqrt{\frac{1-\beta}{1+\beta}} E_{I} \,. \tag{10}$$

The coordinates also transform. The lightlike wave number four vector is $K^{\mu} = (\omega/c, k) = (k, k)$, and the argument of the cosine, $K_{\mu}X^{\mu}$, is Lorentz invariant:

$$K_{\mu}X^{\mu} = \underline{K}_{\mu}\underline{X}^{\mu} \,. \tag{11}$$

The transformation of K_{μ} reads⁴

$$\underline{K}_{\nu} = K_{\mu} (\Lambda^{-1})^{\mu}_{\nu} , \qquad (12)$$

 \mathbf{SO}

$$\begin{pmatrix} -\underline{\omega}/c & \underline{k} \end{pmatrix} = \begin{pmatrix} -k & k \end{pmatrix} \begin{pmatrix} \gamma & \gamma\beta \\ \gamma\beta & \gamma \end{pmatrix}$$
(13)

⁴The metric here is $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$.

leading to

$$\underline{\omega}/c = \underline{k} = \sqrt{\frac{1-\beta}{1+\beta}}k.$$
(14)

This is the relativistic Doppler shift of the frequency.

The full wave is

$$\underline{\boldsymbol{E}}_{I} = \underline{\boldsymbol{E}}_{I} \cos(\underline{\boldsymbol{k}}\underline{\boldsymbol{z}} - \underline{\omega}\underline{\boldsymbol{t}})\hat{\boldsymbol{x}}$$
(15)

(b) In the mirror frame the incident wave is inverted under reflection, while the frequency is the same:

$$\vec{E}_R = -\underline{E}_I \hat{x}$$
 and $\underline{\omega}_R / c = \underline{k}_R = \underline{\omega} / c = \underline{k}.$

The magnetic field is not inverted $\underline{\vec{B}}_R = \underline{B}_I \hat{y}$. Summarizing

$$\underline{\boldsymbol{E}}_{R} = -\underline{\boldsymbol{E}}_{I}\cos(-\underline{\boldsymbol{k}}\underline{\boldsymbol{z}}-\underline{\boldsymbol{\omega}}\underline{\boldsymbol{t}})\hat{\boldsymbol{x}}, \qquad (16)$$

where we note that the argument of the cosine involves $-\underline{kz}$ since the reflected wave is left moving. Transforming back to the lab frame we repeat the analysis of part (a), but we have several different signs:

$$\beta \to -\underline{\beta} \qquad k \to -\underline{k} \qquad E \to -\underline{E}.$$
 (17)

The wave number of the reflected wave is

$$(\underline{K}_R)_{\mu} = (-\underline{\omega}_R/c, -\underline{k}_R).$$
(18)

Transforming $(K_R)_{\mu}$ to the lab frame we have

$$\begin{pmatrix} -\omega_R/c & -k_R \end{pmatrix} = \begin{pmatrix} -\underline{k}, -\underline{k} \end{pmatrix} \cdot \begin{pmatrix} \gamma & -\gamma\beta \\ -\gamma\beta & \gamma \end{pmatrix} = -\sqrt{\frac{1-\beta}{1+\beta}\underline{k}} \begin{pmatrix} 1 & 1 \end{pmatrix},$$
 (19)

i.e.

$$\omega_R = \frac{1-\beta}{1+\beta} \, ck \,. \tag{20}$$

For the electric field amplitude we make a boost with $-\beta = -\beta \hat{z}$

$$\boldsymbol{E}_{R} = \underline{\boldsymbol{E}}_{R} + \gamma(-\boldsymbol{\beta}) \times \underline{\boldsymbol{B}}_{R} \,. \tag{21}$$

So in terms of the amplitudes:

$$\vec{E}_R = -E_R \hat{\boldsymbol{x}} = \hat{\boldsymbol{x}} \left(-\gamma \underline{E}_R + \gamma \beta \underline{E}_R \right) , \qquad (22)$$

$$= -\hat{\boldsymbol{x}}\sqrt{\frac{1-\beta}{1+\beta}\underline{E}_R},\qquad(23)$$

$$= -\hat{\boldsymbol{x}}\frac{1-\beta}{1+\beta}E_I.$$
(24)

The full solution is

$$\boldsymbol{E}_{R} = -\hat{\boldsymbol{x}} \frac{1-\beta}{1+\beta} E_{I} \cos(-k_{R}(z+ct)) \,. \tag{25}$$

where $k_R = ((1 - \beta)/(1 + \beta))k$.

(c) It is simplest to use the photon picture. Here the incoming density of photons is

$$n = \frac{\frac{1}{2}E_I^2}{\hbar ck_I} \tag{26}$$

The relative velocity of the light and the mirror is $v_{rel} = (c - v)$, and so the flux of photons is

$$\Phi \equiv \frac{1}{A} \frac{dN_{\gamma}}{dt} = nv_{\rm rel} = \frac{\frac{1}{2}E_I^2}{\hbar k_I} (1 - \beta)$$
(27)

Each photon strikes the mirror with momentum $\hbar k_I \hat{z}$ and departs with momentum $-\hbar k_R \hat{z}$; the momentum transfer in the z direction is (using Eq. (20))

$$\Delta p^{z} = \hbar k_{I} \left(1 + \frac{1 - \beta}{1 + \beta} \right) = \frac{2}{1 + \beta} \hbar k_{I}$$
(28)

So the force per area (i.e. the momentum transfer per area per time) is

$$\frac{F^z}{A} = \Phi \Delta p^z = 2\left(\frac{1-\beta}{1+\beta}\right) \frac{1}{2}E_I^2 \tag{29}$$

Two alternate solutions are presented below. The first is simple, and involves working in the rest frame. The second is completely classical and works entirely in the lab frame.

(d) We have for the incident wave

$$\mathbf{F}_I \propto \mathbf{E}_I + \frac{\mathbf{v}}{c} \times \mathbf{B}_I = (1 - \beta) E_I \cos(k(z - ct)) \hat{\mathbf{x}}$$
 (30)

For the reflected wave

$$\boldsymbol{F}_R \propto \boldsymbol{E}_R + \frac{\boldsymbol{v}}{c} \times \boldsymbol{B}_R = -(1+\beta)E_R\cos(k_R(z+ct))\hat{\boldsymbol{x}}$$
 (31)

Requiring that the force be zero at z = vt for all times:

$$\boldsymbol{F}_I + \boldsymbol{F}_R = 0, \qquad (32)$$

yields

$$E_R = \frac{(1-\beta)}{(1+\beta)} E_I \qquad k_R = \left(\frac{v-c}{v+c}\right) k, \qquad (33)$$

in agreement with the previous parts.

Discussion: Two alternative solution to part (c) are given below.

Alternate Solution 1: One strategy is to work in the rest frame of the mirror where the incoming light is simply reflected. In a (proper) time τ and surface area A, a volume of light $\mathcal{V} = Ac\tau$ is reflected. The momentum per volume in the incoming light is

$$\left\langle \underline{\boldsymbol{g}}_{I} \right\rangle = \frac{1}{2c} \underline{\vec{E}}_{I} \times \underline{\vec{B}}_{I} = \frac{1}{2c} \left(\frac{1-\beta}{1+\beta} \right) E_{I}^{2}$$
(34)

So the momentum *transfer* to the mirror

$$\Delta \underline{P}^{z} = 2\mathcal{V}\left\langle \underline{\boldsymbol{g}}_{I} \right\rangle = (A\tau) \, 2\left(\frac{1-\beta}{1+\beta}\right) \left(\frac{1}{2}E_{I}^{2}\right) \,, \tag{35}$$

The energy transfer in the mirror frame is zero, $\Delta \underline{P}^0 = 0$. Transforming $\Delta \underline{P}^{\mu}$ to the lab frame

$$\begin{pmatrix} \Delta P^0 \\ \Delta P^z \end{pmatrix} = \begin{pmatrix} \gamma & \gamma\beta \\ \gamma\beta & \gamma \end{pmatrix} \begin{pmatrix} 0 \\ \Delta \underline{P}^z \end{pmatrix}, \tag{36}$$

we find

$$\Delta P^{z} = \gamma(A\tau) \, 2\left(\frac{1-\beta}{1+\beta}\right) \frac{1}{2} E_{I}^{2} \,. \tag{37}$$

Since $\gamma \tau = t$, the force per area (or the momentum per area per time) is:

$$\frac{F^z}{A} = 2\left(\frac{1-\beta}{1+\beta}\right) \frac{1}{2}E_I^2,\tag{38}$$

in agreement with part (c).

Alternate Solution 2: It is a rewarding exercise to work entirely in the lab frame and with classical electrodynamics to reproduce part (c). The momentum entering the mirror is

$$\Delta P^z = \frac{1}{c} \int d\Sigma_\mu T^{\mu z} \,, \tag{39}$$

where $d\Sigma_{\mu}$ is the spacetime surface of the mirror. The spacetime surface of the mirror is spanned by three vectors

$$d\ell_1^{\mu} = dx \,(0, 1, 0, 0) \tag{40}$$

$$d\ell_2^{\rho} = dy \,(0, 0, 1, 0) \tag{41}$$

$$d\ell_3^{\sigma} = cdt \left(1, 0, 0, \beta\right) \tag{42}$$

leading to the surface element (see figure)

$$d\Sigma_{\mu} = \epsilon_{\mu\nu\rho\sigma} \, d\ell_1^{\nu} \, d\ell_2^{\rho} \, d\ell_3^{\sigma} = dA \, cdt \, \left(-\beta, 0, 0, 1\right) \,, \tag{43}$$

where we used $\epsilon_{3120} = -\epsilon_{0123} = 1$.

Integrating over the surface, we have

$$\Delta P^{z} = At \left\langle -\beta T^{0z} + T^{zz} \right\rangle \,, \tag{44}$$

where the angular brackets denote the time average over the sinusoidal fields. The components of the energy momentum tensor are

$$T^{0z} = (\boldsymbol{E} \times \boldsymbol{B})^z \,, \tag{45}$$

$$T^{zz} = \left(-E^{z}E^{z} + \frac{1}{2}E^{2}\delta^{zz}\right) + \left(-B^{z}B^{z} + \frac{1}{2}B^{2}\delta^{zz}\right).$$
(46)



Figure 1: World line of mirror. We are indicating the t and z components only.

On the mirror's surface the amplitude of the electric and magnetic fields are:

$$\vec{E} = \left[E_I - \left(\frac{1-\beta}{1+\beta}\right) E_I \right] \hat{\boldsymbol{x}} = \beta \left(\frac{2}{1+\beta}\right) E_I \hat{\boldsymbol{x}}, \tag{47}$$

$$\vec{B} = \left[B_I + \left(\frac{1-\beta}{1+\beta}\right)B_I\right]\hat{\boldsymbol{y}} = \left(\frac{2}{1+\beta}\right)E_I\hat{\boldsymbol{y}}.$$
(48)

We note that $E = \beta B$ on the surface of the mirror, reflecting the boundary condition $E + \beta \times B = 0$. Performing the time averages we find

$$\langle -\beta T^{0z} \rangle = -\beta^2 \left(\frac{1}{2} B^2 \right), \qquad \langle T^{zz} \rangle = \frac{1}{2} (\beta^2 + 1) \left(\frac{1}{2} B^2 \right).$$
 (49)

Assembling the ingredients, we obtain finally

$$\frac{\Delta P^z}{At} = \frac{1}{2} (1 - \beta^2) \left(\frac{1}{2}B^2\right) = 2 \left(\frac{1 - \beta}{1 + \beta}\right) \left(\frac{1}{2}E_I^2\right) \,, \tag{50}$$

in agreement with part (c).

Quantum Mechanics 1

Diatomic molecule in an electric field

In the presence of a uniform and static external electric field \vec{E} , a homonuclear diatomic molecule (i.e., formed by two identical atoms) experiences an interaction described by the Hamiltonian

$$H_{\alpha} = -\frac{1}{2}\alpha E^2 \cos^2\theta,$$

where α is the average polarizability of the molecule, and θ is the angle between the external field and the molecular axis, as shown in the Figure. Describe the molecule as a linear rigid



Figure 1: Homonuclear molecule in an external electric field. The molecule is assumed to behave as a linear rigid rotor, and θ is the angle between the external field and the molecular axis.

rotor, and assume that the two atoms in the molecule are completely identical, with the total electron spin and nuclear spin of each atom equal to zero.

(a) (2 pts) In the rotational motion, the molecule rotates around its center-of-mass O. Treating the molecule as two point masses M distance d apart, express the Hamiltonian H_{rot} of this motion in terms of the angular momentum L of the molecule and its moment of inertia I (in the absence of the electric field).

(b) (4 *pts*) What are the energy eigenvalues of H_{rot} and rotational energy levels of the molecule?

(c) (4 pts) Write down explicitly all of the wavefunctions of the lowest and first excited energy levels as functions of the angles θ and ϕ of the spherical coordinate system with the center O. (Helpful formulas are given below.)

(d) (4 pts) Calculate the first-order correction to the rotational energies of states in part (c) due to the perturbation H_{α} .

(e) (4 pts) Calculate the second-order correction to the energy of the rotational ground state due to H_{α} . [*Hint:* The relevant properties of the matrix elements can be deduced directly from the properties of the spherical harmonics $Y_l^m(\theta, \phi)$, in particular, $Y_2^0(\theta, \phi)$.]

(f) (2 pts) Taking M = 16 amu, d = 0.12 nm, and $\alpha = 1.74 \times 10^{-40} \text{ m}^2\text{C/V}$, calculate the electric field strength which would make the first-order correction to the energy difference

between the ground and the first excited state of the molecule with m = 0 the same as the difference between their zero-order rotational energies.

A possibly useful expression:

$$Y_l^m(\theta,\phi) = \frac{1}{2^l l!} \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} (1-x^2)^{|m|/2} e^{im\phi} \frac{d^{l+|m|}}{dx^{l+|m|}} (x^2-1)^l \Big|_{x=\cos\theta}.$$
 (1)

Solution

(a) As usual, the Hamiltonian can be derived using the classical mechanics. In the coordinate system with the origin at the center of mass, the two point masses have opposite linear velocities of the same magnitude v, and the molecule rotates around O. In terms of v, kinetic energy of this motion is $E_{rot} = Mv^2$, while the angular momentum around O is L = Mvd. In terms of the moment of inertia of the molecule relative to O, $I = Md^2/2$, the energy can be expressed through the angular momentum as $E_{rot} = L^2/(2I)$. Thus,

$$H_{rot} = \frac{L^2}{2I} \,.$$

(b) In quantum mechanics, the values of the orbital angular momentum are characterized by an integer l, and the energy eigenvalues of H_{rot} follow directly from the known eigenvalues of the L^2 operator:

$$E_l = \frac{\hbar^2 l(l+1)}{2I}, \quad l = 0, 1, 2, \dots$$

Not all of these eigenvalues, however, correspond to the actual rotational energies of the diatomic molecule. Identical atoms with zero spin are bosons, and the wavefunctions of the molecule should be symmetric with respect to the interchange of the two atoms. If one characterizes orientation of the molecule with the unit vector \hat{r} pointing along the molecular axis from O towards the first atom, interchange of the two atoms corresponds to the inversion: $\hat{r} \rightarrow -\hat{r}$. It is knows that the momentum eigenstates are eigenstates of the inversion, with eigenvalues $(-1)^l$, i.e., states with even l are symmetric and states with odd l antisymmetric under inversion. This means that only the energies E_l with even l,

$$l = 0, 2, 4, \dots$$

give the actual rotational energy levels for the molecule in this problem.

(c) The eigenstates of the angular momentum, and therefore of H_{rot} , are the spherical harmonics $Y_l^m(\theta, \phi)$. From the formula given in the problem (Eq. 1), one gets directly:

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}}, \quad Y_2^0(\theta,\phi) = \sqrt{\frac{5}{16\pi}} \left(3\cos^2\theta - 1 \right),$$
$$Y_2^{\pm 1}(\theta,\phi) = \sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta \ e^{\pm i\phi}, \quad Y_2^{\pm 2}(\theta,\phi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta \ e^{\pm 2i\phi}$$

(d) Using the standard formula of the stationary perturbation theory, one sees that the first-order correction to the rotational states Y_l^m is given in general by the following integral:

$$\delta E_{lm}^{(1)} = -\frac{\alpha E^2}{2} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin \theta \cos^2 \theta \ |Y_l^m|^2.$$

The formulas for spherical harmonics re-derived in (c) give then explicitly:

$$\delta E_{00}^{(1)} = -\frac{\alpha E^2}{4} \int_{-1}^{1} dx x^2 = -\frac{\alpha E^2}{6}, \qquad \delta E_{20}^{(1)} = -\frac{5\alpha E^2}{16} \int_{-1}^{1} dx x^2 (3x^2 - 1)^2 = -\frac{11\alpha E^2}{42},$$

$$\delta E_{21}^{(1)} = -\frac{15\alpha E^2}{8} \int_{-1}^{1} dx x^4 (1-x^2) = -\frac{3\alpha E^2}{28}, \qquad \delta E_{22}^{(1)} = -\frac{15\alpha E^2}{32} \int_{-1}^{1} dx x^2 (1-x^2)^2 = -\frac{\alpha E^2}{28}$$

and expressions for the negative values of m are the same as for the corresponding positive ms.

(e) Since the Hamiltonian H_{α} is independent of the angle ϕ , it has non-vanishing matrix elements only between the states with the same m. Therefore, only the states with m = 0 contribute to the energy shift of the ground state l = 0, m = 0. From the general equation of the perturbation theory, we have then:

$$\delta E_{00}^{(2)} = \sum_{j=1}^{\infty} \frac{|\langle l=0, m=0 | H_{\alpha} | l=2j, m=0 \rangle|^2}{E_0 - E_{2j}}$$

Also, one can notice that the function $\cos^2 \theta$ that gives the θ -dependence of H_{α} can be expressed as a combination of two spherical harmonics, Y_2^0 and Y_0^0 . The fact that Y_0^0 is a constant and spherical harmonics are orthogonal, then means that only the matrix element with l = 2 is non-vanishing in the sum for $\delta E_{00}^{(2)}$. Thus,

$$\begin{split} \delta E_{00}^{(2)} &= -\frac{|\langle l=0,m=0|H_{\alpha}|l=2,m=0\rangle|^2}{E_2} = -\frac{I(\alpha E^2)^2}{12\hbar^2}H^2 \\ H &= \sqrt{\frac{5}{16}}\int_{-1}^1 dx x^2 (3x^2-1) = \sqrt{\frac{4}{45}} \,. \end{split}$$

Finally, the second-order correction to the energy of the rotational ground state is:

$$\delta E_{00}^{(2)} = -\frac{I(\alpha E^2)^2}{135\hbar^2} \,.$$

(f) The energy difference between the ground and the first excited rotational state of the molecule with l = 2 is $3\hbar^2/I = 6\hbar^2/(Md^2)$. For the given parameters, this is roughly 1.7×10^{-22} J. On the other hand, as we have seen above, the electric field causes a shift of each of the rotational states, and the energy difference between the ground state and the l = 2, m = 0 is changed by In particular, the ground rotational state experiences a shift given by

$$\Delta E = \alpha E^2 (\frac{11}{42} - \frac{1}{6}) = \frac{2}{21} \alpha E^2.$$

This energy becomes equal to the rotational energy difference estimated above for an electric field of 3.2×10^9 V/m.

Quantum Mechanics 2

3D spherical potential well

A quantum particle of mass m moves in a 3D attractive potential V(r) with the following dependence on the distance r to the center O of a spherical coordinate system:

$$V(r) = \begin{cases} -U, & r < a, \\ 0, & r > a. \end{cases}$$

The particle has vanishing angular momentum, l = 0, relative to O, and negative energy -E, with E > 0.

(a) (3 pts) What is the dependence of the particle wavefunction $\psi(\vec{r})$ on the angular coordinates θ and ϕ of the spherical coordinate system with the center O? Write down the radial part of the stationary Schrödinger equation that governs the evolution of the radial part $\psi(r)$ of the particle wavefunction.

(b) (3 pts) Write down the general form of the wavefunction $\psi(r)$ that satisfies the Schrödinger equation inside and outside of the potential well, and satisfies the appropriate boundary conditions at r = 0 and $r \to \infty$. Next, write down the boundary condition this wavefunction should satisfy at r = a.

(c) (4 pts) Transform the relations from part (b) to obtain the equation that determines the energies of the bound states in the well. Analyze this equation to find the value of the potential strength U at which the first bound state appears in the well.

Now, consider particles with positive energy $E = \hbar^2 k^2 / (2m)$ incident from afar on the same potential V(r) and scattered by it. Assume that the energy is small, $E \to 0$.

(d) (2 pts) Argue qualitatively (in no more than one or two sentences) why the "s-wave" scattering with l = 0 dominates the scattering process at small energies E. Write down an explicit condition on E that ensures the validity of this "low-energy" approximation.

(e) (6 pts) What is the form of the l = 0 part of the wavefunction of the scattered particles outside of the potential well, at r > a? Match this wavefunction with that inside the well to calculate the s-wave scattering phase shift δ_0 and the corresponding total scattering crosssection σ_0 .

(f) (2 pts) At what values of the potential strength U the cross-section σ_0 becomes infinitely large? Provide a very brief physical reason for this behavior.

Solution

(a) The states with vanishing angular momentum, l = 0, are spherically symmetric, and the particle wavefunction $\psi(\vec{r})$ is independent of the angular coordinates θ and ϕ , i.e., reduces to the function $\psi(r)$ of the radial coordinate r only. The stationary Schrödinger equation for this function has the standard form

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + V(r)\psi = -E\psi(r)\,.$$

_

Introducing an auxiliary function u(r) by the relation $\psi(r) = u(r)/r$, one reduces this equation to the 1D Schrödinger equation:

$$-\frac{\hbar^2}{2m}u'' + V(r)u = -Eu(r).$$

(b) In a bound state, both $\psi(r)$ and u(r) should vanish at $r \to \infty$. To keep $\psi(r)$ sufficiently well-behaved at r = 0, the function u(r) should also vanish at r = 0. With these boundary conditions, the usual solutions of the 1D Schrödinger equation for u(r) give for $\psi(r)$ inside and outside the well:

$$\psi(r) = \frac{1}{r} \begin{cases} A\sin(qr), & r < a, \\ Be^{-\kappa r}, & r > a. \end{cases}$$

Here A and B are some constants, and the wavevectors q and κ are determined by energies U and E:

$$q^2 = \frac{2m(U-E)}{\hbar^2}, \quad \kappa^2 = \frac{2mE}{\hbar^2}$$

At r = a, both the wavefunction and its derivative should be continuous, i.e.:

$$A\sin(qa) = Be^{-\kappa a}, \quad qA\cos(qa) = -\kappa Be^{-\kappa a}$$

(c) Dividing the last two equations from part (b) one by another, and taking into account the relation between q and κ , one gets the condition that determines the energies of the stationary bound states:

$$-q\cot(qa) = \kappa = \sqrt{(2mU/\hbar^2) - q^2}.$$

As a function of \underline{q} , for $\underline{q} > 0$, the right-hand-side of this equation describes a quarter of a circle of radius $\sqrt{2mU/\hbar^2}$ with the center at the origin. The left-hand-side reaches minimum -1/a at q = 0 and increases with q, reaching value zero for the first time at $q = \pi/2a$. This means that for small U's, solution of this equation starts being possible only if U is sufficiently large, so that the two curves go through the same point on the q axis (so that $\kappa = 0$):

$$\sqrt{2mU/\hbar^2} = \pi/2a$$
 .

Thus, to have a bound state in a 3D spherical potential well of radius a, the depth U of the well should be sufficiently large:

$$U \ge \frac{\pi^2 \hbar^2}{8ma^2} \,.$$

(d) At low energies E of the incident particles, the wavelength of the particle wavefunction is very large in comparison to the size of the potential well, i.e., the scattering potential looks like a point. This means that it scatters uniformly in all directions, the situation that corresponds to particles having zero angular momentum relative to that point. More quantitatively, this approximation can be expressed as a condition on the wavevector k: $ka \ll 1$.

(e) For the l = 0 scattering, the Schrödinger equation and its solution inside the well are the same as above. In the scattering problem, however, the particles move from and back to infinity, and the solution of the Schrödinger equation outside of the well takes the form different from that for a bound state: $u(r) \propto \sin(kr + \delta_0)$ for r > a, where δ_0 is the phase shift of the s-wave scattering. Thus, the l = 0 part of the wavefunction of the scattered particles is:

$$\psi(r) = \frac{1}{r} \begin{cases} A\sin(qr), & r < a, \\ B\sin(kr + \delta_0), & r > a. \end{cases}$$

Imposing, as above, the conditions that $\psi(r)$ and its derivative are continuous at r = a, one gets the equation for δ_0 :

$$q\cot qa = k\cot(ka + \delta_0).$$

For $E \to 0$, one can drop E from the definition of q, and also take into account that both the phase shift δ_0 and the product ka are small. Then it is legitimate to approximate $\cot x$ as 1/x for small argument, and equation for δ_0 immediately gives:

$$\delta_0 = k \frac{\tan qa - qa}{q}, \quad q = (2mU)^{1/2}/\hbar.$$

From the known relation between the small scattering phase δ_0 and the cross-section σ_0 , one gets finally

$$\sigma_0 = 4\pi (\delta_0/k)^2 = 4\pi \frac{(\tan qa - qa)^2}{q^2}$$

(f) We see that σ_0 becomes infinitely large, when $qa = \pi(n + 1/2)$ with an integer n, i.e. for the potential strength

$$U_n = \frac{\pi^2 \hbar^2}{2ma^2} (n+1/2)^2, \quad n = 0, 1, 2, \dots$$

These divergencies of the low-energy cross-section σ_0 correspond to resonant scattering by the bound states with vanishing energies that appear in the well at these values of the potential strength U. One can check this explicitly by comparing the values U_n to those that follow from the equation for U obtained in part (c). As was shown there explicitly, U_0 is the depth of the potential well which has the first bound state with vanishing energy.

Quantum Mechanics 3

Coherent states of a 1D harmonic oscillator

A particle of mass m moves in a 1D harmonic oscillator potential with frequency ω . The raising a^{\dagger} and lowering a operators are $\sqrt{1/2\hbar m\omega}(m\omega \hat{x} \mp i\hat{p})$, where \hat{x} and \hat{p} are the operators of coordinate and momentum of the particle. As a reminder, the wavefunction of the ground state of the oscillator is $\psi_0(x) = (m\omega/\pi\hbar)^{1/4} \exp\{-(m\omega x^2/2\hbar)\}$, and the excited states are $\psi_n = (a^{\dagger})^n \psi_0/\sqrt{n!}$.

(a) (2 points) Calculate the commutator $[a, a^{\dagger}]$. Show that the Hamiltonian H can be written in terms of the operators a^{\dagger}, a .

(b) (2 points) Find the matrix elements $\langle l|\hat{x}|n\rangle$ and $\langle l|\hat{p}|n\rangle$ in the basis of the energy eigenstates $|n\rangle$ of the oscillator: $H|n\rangle = E_n|n\rangle$.

(c) (4 points) An eigenstate of the lowering operator: $a|\psi_{\alpha}\rangle = \alpha|\psi_{\alpha}\rangle$ is called a "coherent state of the oscillator". It is a state of minimum uncertainty of x and p. Since the operator a is not hermitian, the eigenvalues α are, in general, complex: $\alpha = re^{i\phi}$, where r and ϕ are real. Find the coherent state wavefunction $\psi_{\alpha}(x)$ in the coordinate representation. (No need to normalize it.)

(d) (4 points) Like any other state, a coherent state can be expanded in the complete basis of the energy eigenstates $\{|n\rangle\}$ as $|\psi_{\alpha}\rangle = \sum_{n} c_{n} |n\rangle$. Find the coefficients c_{n} such that $|\psi_{\alpha}\rangle$ is normalized.

(e) (4 points) Derive the time evolution of the state $|\psi_{\alpha}\rangle$ obtained in part (d) due to the free evolution of the harmonic oscillator driven by the Hamiltonian H, to obtain the time-dependent state $|\psi_{\alpha}\rangle(t)$. Show that $|\psi_{\alpha}\rangle(t)$ is a coherent state, and find the time-dependent eigenvalue $\alpha(t)$.

(f) (4 point) Calculate the time-dependent expectation value $\langle \psi_{\alpha} | \hat{x} | \psi_{\alpha} \rangle(t)$ of the particle coordinate and momentum $\langle \psi_{\alpha} | \hat{p} | \psi_{\alpha} \rangle(t)$ in a coherent state. Next, calculate $\langle \psi_{\alpha} | \hat{x}^2 | \psi_{\alpha} \rangle(t)$ and $\langle \psi_{\alpha} | \hat{p}^2 | \psi_{\alpha} \rangle(t)$, and show that $| \psi_{\alpha} \rangle(t)$ is a minimum uncertainty state.

Solution

(a) From the expressions for the creation/annihilation operators a^{\dagger} , a and canonical commutation relations for \hat{x} and \hat{p} , one has directly:

$$a^{\dagger}a = \frac{1}{2\hbar m\omega}(m\omega\hat{x} - i\hat{p})(m\omega\hat{x} + i\hat{p}) = \frac{1}{\hbar\omega}\left(\frac{\hat{p}^{2}}{2m} + \frac{1}{2}m\omega^{2}\hat{x}^{2}\right) - \frac{1}{2},$$
$$aa^{\dagger} = \frac{1}{2\hbar m\omega}(m\omega\hat{x} + i\hat{p})(m\omega\hat{x} - i\hat{p}) = \frac{1}{\hbar\omega}\left(\frac{\hat{p}^{2}}{2m} + \frac{1}{2}m\omega^{2}\hat{x}^{2}\right) + \frac{1}{2}.$$

From these relations, we obtain, first, the commutation relation for a, a^{\dagger} :

$$[a, a^{\dagger}] = 1 \,,$$

and, secondly, expression for the Hamiltonian in terms of these operators:

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 = \hbar\omega \left(a^{\dagger}a + \frac{1}{2}\right) \,.$$

(b) Inverting the expressions for a^{\dagger}, a , we get

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

and from known action of the creation/annihilation operators on the oscillator energy eigenstates:

$$a^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a|n\rangle = \sqrt{n}|n-1\rangle,$$

we get the matrix elements of the coordinate and momentum operators in the basis of energy eigenstates:

$$\langle l|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle l|a+a^{\dagger}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n}\delta_{l,n-1} + \sqrt{n+1}\delta_{l,n+1}\right).$$

Similarly,

$$\langle l|\hat{p}|n\rangle = -i\sqrt{\frac{\hbar m\omega}{2}}\langle l|a-a^{\dagger}|n\rangle = -i\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n}\delta_{l,n-1} - \sqrt{n+1}\delta_{l,n+1}\right).$$

(c) In coordinate representation, equation for $\psi_{\alpha}(x)$ takes the form:

$$\sqrt{\frac{1}{2\hbar m\omega}} \left(\hbar \frac{d}{dx} + m\omega x\right) \psi_{\alpha}(x) = \alpha \psi_{\alpha}(x) \,,$$

i.e.

$$\frac{d\psi_{\alpha}(x)}{dx} = \left(\sqrt{\frac{2m\omega}{\hbar}}\alpha - \frac{m\omega}{\hbar}x\right)\psi_{\alpha}(x)\,.$$

Integrating this equation directly, one gets:

$$\psi_{\alpha}(x) = C \exp\{-\frac{m\omega}{2\hbar}x^2 + \sqrt{\frac{2m\omega}{\hbar}}\alpha x\}.$$

For completeness, we mention that the simplest way to normalize this Gaussian wavefunction is to notice that the term linear in x shifts the position of the Gaussian peak by some distance \bar{x} , as one can see by rewriting this expression for $\psi_{\alpha}(x)$ as follows

$$\psi_{\alpha}(x) = C' \exp\{-\frac{m\omega}{2\hbar}(x-\bar{x})^2 + i\sqrt{\frac{2m\omega}{\hbar}}\Im(\alpha)x\}, \quad \bar{x} = \sqrt{\frac{2\hbar}{m\omega}}\Re(\alpha) = \sqrt{\frac{2\hbar}{m\omega}}r\cos\phi.$$

In this form, it is immediate that the normalization constant C' is the same as of the unshifted Gaussian, which is the ground state $\psi_0(x)$ of the oscillator. Normalization of $\psi_0(x)$ is given in the problem, and we have for the properly normalized $\psi_{\alpha}(x)$

$$\psi_{\alpha}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\{-\frac{m\omega}{2\hbar}(x-\bar{x})^2 + i\sqrt{\frac{2m\omega}{\hbar}}\Im(\alpha)x\}.$$

(d) Expansion coefficients c_n of $|\psi_{\alpha}\rangle$ in the basis $\{|n\rangle\}$ of the energy eigenstates are given, as usual, as $\langle n|\psi_{\alpha}\rangle$. This expression can be evaluated directly using equation for $|n\rangle$ given in the problem, $|n\rangle = (a^{\dagger})^n |0\rangle / \sqrt{n!}$ and the fact that follows directly from the definitions for the creation/annihilation operators: $(a^{\dagger})^{\dagger} = a$. With these relations, one has:

$$c_n = \langle n | \psi_{\alpha} \rangle = \frac{1}{\sqrt{n!}} \langle 0 | a^n | \psi_{\alpha} \rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0 | \psi_{\alpha} \rangle .$$

Unknown constant in this equation, $\langle 0|\psi_{\alpha}\rangle$, can be determined from the normalization condition of the coefficients c_n :

$$\sum_{n=0}^{\infty} |c_n|^2 = \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} |\langle 0|\psi_{\alpha}\rangle|^2 = |\langle 0|\psi_{\alpha}\rangle|^2 e^{|\alpha|^2} = 1.$$

This means that

$$|\langle 0|\psi_{\alpha}\rangle| = e^{-|\alpha|^2/2},$$

and up to inessential overall phase factor,

$$c_n = \frac{\alpha^n}{\sqrt{n!}} e^{-|\alpha|^2/2}$$

(e) As known for an arbitrary system with the time-independent Hamiltonian H characterized by the energy eigenstates $|n\rangle$ and the corresponding energy eigenvalues E_n , the time dependence of the state $|n\rangle$ is given by the time-dependent phase factor $\exp(-iE_nt/\hbar)$. This means that an arbitrary state $|\psi\rangle = \sum_n c_n |n\rangle$ evolves in time as $|\psi\rangle(t) = \sum_n c_n |n\rangle \exp(-iE_nt/\hbar)$, i.e., the state $|\psi\rangle(t)$ is the solution of the time-dependent Schrödinger equation with the Hamiltonian H and initial condition $|\psi\rangle(t=0) = |\psi\rangle$. For the coherent state $|\psi_{\alpha}\rangle$ of a Harmonic oscillator, this mean that the time evolution of $|\psi_{\alpha}\rangle$ is

$$|\psi_{\alpha}\rangle(t) = \sum_{n} c_{n} |n\rangle \exp(-iE_{n}t/\hbar),$$

with the coefficients c_n obtained in part (d). Accounting for the energy eigenvalues E_n of the harmonic oscillator, the time-dependent state $|\psi_{\alpha}\rangle(t)$ is expressed as

$$|\psi_{\alpha}\rangle(t) = \sum_{n=0}^{\infty} c_n |n\rangle e^{-i\omega(n+1/2)t} = e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} e^{-|\alpha|^2/2}.$$

One sees directly that up to an irrelevant overall phase factor $e^{-i\omega t/2}$ this is a coherent state, the same as $|\psi_{\alpha}\rangle$ but with the time-dependent eigenvalue

$$\alpha(t) = \alpha e^{-i\omega t}.$$

(f) Coordinate and momentum expectation values in a coherent state are calculated directly:

$$\langle \psi_{\alpha} | \hat{x} | \psi_{\alpha} \rangle(t) = \sqrt{\frac{\hbar}{2m\omega}} \langle \psi_{\alpha} | a + a^{\dagger} \rangle | \psi_{\alpha} \rangle(t) = \sqrt{\frac{\hbar}{2m\omega}} (\alpha(t) + [\alpha(t)]^{*}) = \sqrt{\frac{2\hbar}{m\omega}} r \cos(\omega t - \phi) ,$$

$$\langle \psi_{\alpha} | \hat{p} | \psi_{\alpha} \rangle(t) = i \sqrt{\frac{\hbar m \omega}{2}} ([\alpha(t)]^{*} - \alpha(t)) = -\sqrt{2\hbar m \omega} r \sin(\omega t - \phi) .$$

For the squares, we have:

$$\hat{x}^2 = \frac{\hbar}{2m\omega} [a^2 + aa^{\dagger} + a^{\dagger}a + (a^{\dagger})^2] = \frac{\hbar}{2m\omega} [a^2 + 2a^{\dagger}a + (a^{\dagger})^2 + 1].$$
$$\hat{p}^2 = \frac{\hbar m\omega}{2} [aa^{\dagger} + a^{\dagger}a - a^2 - (a^{\dagger})^2] = \frac{\hbar m\omega}{2} [2a^{\dagger}a + 1 - a^2 - (a^{\dagger})^2].$$

From these expressions:

$$\begin{split} \langle \psi_{\alpha} | \hat{x}^{2} | \psi_{\alpha} \rangle(t) &= \frac{\hbar}{2m\omega} [(\alpha(t))^{2} + 2|\alpha(t)|^{2} + ([\alpha(t)]^{*})^{2} + 1] = \frac{\hbar}{2m\omega} [1 + \alpha^{2} e^{-i2\omega t} + [\alpha^{*}]^{2} e^{i2\omega t} + 2|\alpha|^{2}] \\ &= \frac{\hbar}{2m\omega} [1 + 4r^{2} \cos^{2}(\omega t - \phi)] \,. \\ \langle \psi_{\alpha} | \hat{p}^{2} | \psi_{\alpha} \rangle(t) &= \frac{\hbar m\omega}{2} [2|\alpha(t)|^{2} + 1 - ([\alpha(t)]^{*})^{2} - (\alpha(t))^{2}] = \frac{\hbar m\omega}{2} [1 + [\alpha^{*}]^{2} - e^{i2\omega t} + 2|\alpha|^{2} - \alpha^{2} e^{-i2\omega t}] \\ &= \frac{\hbar m\omega}{2} [1 + 4r^{2} \sin^{2}(\omega t - \phi)] \,. \end{split}$$

Finally, the standard deviations are:

$$\sigma_x^2 = \langle \psi_\alpha | \hat{x}^2 | \psi_\alpha \rangle(t) - [\langle \psi_\alpha | \hat{x} | \psi_\alpha \rangle(t)]^2 = \frac{\hbar}{2m\omega} ,$$

$$\sigma_p^2 = \langle \psi_\alpha | \hat{p}^2 | \psi_\alpha \rangle(t) - [\langle \psi_\alpha | \hat{p} | \psi_\alpha \rangle(t)]^2 = \frac{\hbar m\omega}{2} ,$$

and we see that a coherent state is indeed a minimum uncertainty state:

$$\sigma_x \sigma_p = \frac{\hbar}{2}$$

Statistical Mechanics 1

The first molecule

Approximately 300,000 years after the Big Bang, the first atoms and molecules were formed in the so-called "recombination era". HeH⁺ is a singly ionized molecule consisting of helium and hydrogen atoms and is widely believed to be the first molecule ever formed. We will explore the formation of the first molecule using equilibrium statistical mechanics.

Consider the plasma in the recombination era to be a neutral gas at temperature T consisting of free electrons, protons, and fully ionized helium⁵ He²⁺, and their bound states: H, He, and He⁺. The components of the plasma are at low densities and high temperatures, and may be treated as classical ideal gasses; you may neglect the electrostatic interactions between the components. The total proton density (H and H⁺) is n_0 , with $n_0 = 10^4$ cm⁻³ numerically. The total helium density (He⁺⁺, He⁺ and He) is n_1 , with $n_1 \simeq n_0/12$. To approximate the partition functions of the bound-states and their chemical potentials, only include the ground state electronic configuration in the sum over states. The table below gives the binding energies of these configurations and their degeneracies, which arise from the spins of the electrons and nuclei.

State	Degeneracy	Binding energy
Η	4	$\varepsilon_{\rm H} \equiv -13.6 {\rm eV}$
He^+	2	$\varepsilon_{\rm He^+} \equiv -54.4 {\rm eV}$
He	1	$\varepsilon_{\rm He} \equiv -81.0 {\rm eV}$

- (a) (2 points) Compute the chemical potentials of free electrons μ_e and protons μ_p as a function of the temperature and the corresponding densities n_e and n_p
- (b) (2 points) Compute the chemical potentials of H, He⁺, and He as a function of the temperature, and the corresponding densities n_H , n_{He^+} , and n_{He} and binding energies.
- (c) (2 points) Determine the equilibrium constants K_1 , K_2 and K_3 (defined below) as a function of temperature for the following reactions:

$$K_{1}(T) \equiv \frac{n_{\mathrm{H}}}{n_{e} n_{p}} \qquad p + e^{-} \iff \mathrm{H}$$

$$K_{2}(T) \equiv \frac{n_{\mathrm{He}^{+}}}{n_{e} n_{\mathrm{He}^{2+}}} \qquad \mathrm{He}^{2+} + e^{-} \iff \mathrm{He}^{+}$$

$$K_{3}(T) \equiv \frac{n_{\mathrm{He}}}{n_{e}^{2} n_{\mathrm{He}^{2+}}} \qquad \mathrm{He}^{2+} + 2e^{-} \iff \mathrm{He}^{-}$$

Is $K_i(T)$ a function of the chemical potentials of parts (a) and (b)? Explain.

(d) (6 points)

⁵The He²⁺ nucleus is also known as an alpha particle. It has zero spin, consists of two protons and two neutrons, and has a mass of $m_{\rm He^{2+}} \approx 4m_{\rm H} \approx 4m_p$ where m_p is the proton mass.

- (i) Find a set equations for the density of the electrons, protons, and ionized helium (He^{2+}) as function of temperature and n_0 and n_1 .
- (ii) In the limit where the ionized helium concentration is negligible, solve these equations for the fraction of unbound protons $x_p \equiv n_p/n_0$ as a function of temperature and n_0 .
- (iii) The equilibrium constants (normalized by n_0) found in part (b) are given in the table below to the nearest factor of 10:

Temperature
$$n_0K_1$$
 n_0K_2 $n_0^2K_3$ 3000 K10^610^{75}10^{102}

With the same approximations as (ii), determine the ratios of abundances at T = 3000 K by filling in the table below to within a factor of ten:

- (e) (5 points) Compute the chemical potential of the He⁺H molecule in terms of its density $n_{\text{He}^+\text{H}}$ and its binding energy $\Delta \varepsilon_{\text{He}^+\text{H}}$, where $\Delta \varepsilon_{\text{He}^+\text{H}}$ is measured relative to the unbound He⁺ and H states. Treat the molecule as a classical rigid rotor with bond length *a* and neglect radial vibrations.
- (f) (3 points) Find the equilibrium constant for the following reaction

$$K_4(T) \equiv \frac{n_{\rm He^+H}}{n_{\rm H} n_{\rm He^+}} \qquad \qquad {\rm He^+ + H \Longleftrightarrow He^+H} \,.$$

When the binding energy is $\Delta \varepsilon_{\text{He}^+\text{H}} = -2.0 \text{ eV}$, and the bond length $a = 8 \times 10^{-11} \text{m}$, the equilibrium constant is $n_H K_4 = n_{\text{He}^+\text{H}}/n_{\text{He}^+} \simeq 10^{-17}$ at a temperature of T = 3000 K, and the formation of the first molecule is strongly disfavored. Explain why this is the case physically, although the Boltzmann factor $\exp(-\Delta \varepsilon_{\text{He}^+\text{H}}/k_B T) \simeq 2000$ would suggest that this ratio should be almost unity.

You may find the following numbers useful:

$$m_e \approx 9.11 \cdot 10^{-31} \text{ kg} \approx 5.11 \cdot 10^5 \text{ eV}/c^2$$
,
 $m_p \approx 1.67 \cdot 10^{-27} \text{ kg} \approx 9.38 \cdot 10^8 \text{ eV}/c^2$,
 $1 \text{ eV}/k_B \approx 1.15 \cdot 10^4 \text{ K}$.

Solution

(a) Using grand-canonical ensemble for ideal gas,

$$\mu = T \log \frac{\lambda^3 n}{g}, \qquad (1)$$

where $\lambda = \sqrt{\frac{2\pi\hbar^2}{mT}}$ is the thermal wavelength and g is the internal degeneracy (e.g., spin degeneracy $g_S = 2S + 1$). For fermions e^- and p+, $g = g_S = 2$. Below we will write this result in the following convenient form

$$n = \frac{g}{\lambda^3} e^{\mu/T} \,. \tag{2}$$

(b) If the chemical potentials are essentially energies and can be deined with respect to arbitrary "energy baselines". It may be convenient to use the same "baseline" for different gases, so that the chemical (binding) energies are included automatically in the equilibrium equations. In this case, the chemical potentials are

$$\begin{split} \mu_e &= T \log \left(\frac{1}{2} n_e \lambda_e^3 \right) \,, \\ \mu_p &= \mu_{\mathrm{H}^+} = T \log \left(\frac{1}{2} n_p \lambda_p^3 \right) \,, \\ \mu_{\mathrm{H}} &= T \log \left(\frac{1}{4} n_{\mathrm{H}} \lambda_p^3 \right) + \varepsilon_{\mathrm{H}} \,, \\ \mu_{\mathrm{He}} &= T \log \left(n_{\mathrm{He}} \lambda_{\mathrm{He}}^3 \right) + \varepsilon_{\mathrm{He}} \,, \\ \mu_{\mathrm{He}^+} &= T \log \left(\frac{1}{2} n_{\mathrm{He}^+} \lambda_{\mathrm{He}}^3 \right) + \varepsilon_{\mathrm{He}^+} \,, \\ \mu_{\mathrm{He}^{2+}} &= T \log \left(n_{\mathrm{He}^{2+}} \lambda_{\mathrm{He}}^3 \right) + \varepsilon_{\mathrm{He}^{2+}} \,. \end{split}$$

Discussion: The He atom has no internal degeneracy (g = 1): the nucleus (α -particle) has no spin, and the electron spins add up to zero. Similarly, the He²⁺ ion has g = 1. However, He⁺ ion has g = 2 due to the single electron spin. The degeneracy of the proton H⁺ is g = 2 and of the hydrogen H g = 4 due to spins of the proton and the electron (we neglect the hyperfine splitting between ortho- and para-hydrogen).

(c) Using the equilibrium condition $\sum_{i \in in} \mu_i = \sum_{j \in out} \mu_j$ (the binding energies are already taken into account above)

$$K_{1} = \frac{n_{\rm H}}{n_{e} n_{p}} = \lambda_{e}^{3} e^{-\Delta \varepsilon^{\rm H}/T} ,$$

$$K_{2} = \frac{n_{\rm He^{+}}}{n_{e} n_{\rm He^{2+}}} = \lambda_{e}^{3} e^{-\Delta \varepsilon_{2}^{\rm He}/T} ,$$

$$K_{3} = \frac{n_{\rm He}}{n_{e}^{2} n_{\rm He^{2+}}} = \frac{1}{4} \lambda_{e}^{6} e^{-\Delta \varepsilon_{1+2}^{\rm He}/T}$$

The equilibrium constants are just a function of temperature.

Discussion: Evaluting these three constants numerically at the temperatures T = 3000 K and T = 10000 K to the nearest power of 10 we find

Temperature	$n_0 K_1$	$n_0 K_2$	$n_0^2 K_3$
$3000\mathrm{K}$	10^{6}	10^{74}	10^{101}

The wide range of chemical constants is due to the exponents such as $\exp(-\varepsilon_{\text{He}}/T)$, nd the enormous phase space, $n_0 \lambda_e^3$.

(d)

(i) The equations to be solved are: charged neutrality

$$-n_e + n_p + n_{\mathrm{He}^+} + 2n_{\mathrm{He}^{2+}} = 0; \qquad (3)$$

conservation of proton number

$$n_{\rm H^+} + n_H = n_0 \tag{4}$$

and conservation of helium number

$$n_{\rm He^{2+}} + n_{\rm He^{+}} + n_{\rm He} = n_1 \tag{5}$$

(ii) When the ionized helium fraction is negligible we have

$$n_e \simeq n_p \tag{6}$$

Writing $n_H = n_e n_p K_1 \simeq n_p^2 K_1$ and diving through by n_0 we have

$$x_p + x_p^2 n_0 K_1 = 1, (7)$$

where $x_p = n_p/n_0$. Solving the quadratic equation we have

$$x_p = \frac{1}{2n_0 K_1} \left[-1 + \sqrt{1 + 4n_0 K_1} \right] \,. \tag{8}$$

When $n_0 K_1 \gg 1$, dynamics strongly favors the bound state, and we have

$$x_p \simeq \frac{1}{\sqrt{n_0 K_1}} \,. \tag{9}$$

In the opposite limit $n_0 K_1 \ll 1$, the dynamics disfavors the bound states, and we have

$$x_p \simeq 1 - n_0 K_1$$
. (10)

(iii) For large $n_0 K_1$

$$x_p = \frac{1}{\sqrt{n_0 K_1}} \simeq 10^{-3} \tag{11}$$

The hydrogen fraction is $x_H = n_H/n_0 = 1 - x_p \simeq 1$.

Let y, y_+ , and y_{2+} denote the fraction of un-ionized, singly ionized, and double ionized helium. For the helium budget we have

$$y_{2+} + y_+ + y = 1. (12)$$

Using the equilbrium constants we have

$$y_{2+} + y_{2+}x_p(n_0K_2) + y_{2+}(x_p^2n_0^2K_3) = 1$$
(13)

In the low temperature case the last term dominates

$$y_{2+} \simeq \frac{1}{x_p^2 n_0^2 K_3} \simeq 10^{-95}$$
 (14)

and

$$y_{+} = y_{2+} x_p(n_0 K_2) \simeq 10^{-24} \tag{15}$$

and finally

$$y \simeq 1 \tag{16}$$

Summarizing in tabular form, the ratios are

(e) The total masss is $m_{\text{He}^+\text{H}} = 5m_p$, and the center of mass at a distance a/5 from the He nucleus. The moment of inertia around the helium nucleus is $m_p a^2$, while around the center of mass is

$$I = m_p a^2 - 5m_p (a/5)^2 = \frac{4}{5}m_p a^2.$$
(17)

To simplify the notation in the rest of this item we will drop the He^+H label. The rotational partition function

$$Z_{\rm rot} = \sum_{\ell} (2\ell+1) \exp(-\hbar^2 \ell (\ell+1)/2IT) \simeq \int_0^\infty d\ell \, 2\ell \, e^{-\hbar^2 \ell^2/2IT} = \frac{2IT}{\hbar^2} \tag{18}$$

The full partition function is

$$Z = \frac{1}{N!} Z_{\rm trans}^N Z_{\rm rot}^N \tag{19}$$

So the free energy has

$$F = -T\log Z \tag{20}$$

$$= NT \log(n\lambda^3/e) - NT \log\left(2IT/\hbar^2\right) + N\epsilon_0$$
(21)

Here the ϵ_0 takes into account the binding energy. It is only important when comparing the bound state to other states. Differentiation gives

$$\mu = \frac{\partial F}{\partial N} = T \log(n\lambda^3) - T \log\left(2IT/\hbar^2\right) + \epsilon_0.$$
(22)

In the next item we will express this equation in the following form

$$n = \frac{1}{\lambda^3} e^{-\epsilon_0/T + \mu/T} \left(\frac{2IT}{\hbar^2}\right) \,. \tag{23}$$

(f) Using

$$n_{\rm H} = \frac{g_{\rm H}}{\lambda_{\rm H}^3} e^{(\mu_{\rm H} - \varepsilon_{\rm H})T} \,, \tag{24}$$

$$n_{\mathrm{He}^{+}} = \frac{g_{\mathrm{He}^{+}}}{\lambda_{\mathrm{He}^{+}}^{3}} e^{(\mu_{\mathrm{He}^{+}} - \varepsilon_{\mathrm{He}^{+}})/T}, \qquad (25)$$

the equilibrium constant reads

$$\frac{n_{\rm He^+H}}{n_{\rm He^+}n_{\rm H}} = \frac{1}{g_{\rm He^+}g_{\rm H}} \frac{\lambda_{\rm H}^3 \lambda_{\rm He^+}^3}{\lambda_{\rm He^+H}^3} \left(\frac{2IT}{\hbar^2}\right) e^{-\Delta\varepsilon_{\rm He^+H}/T},$$
(26)

where $\Delta \varepsilon_{\mathrm{He^+H}} = -\epsilon_0 + \varepsilon_{\mathrm{H}} + \varepsilon_{\mathrm{He^+}}$. Grouping the terms

$$n_0 K_4 = \left(\frac{n_0 \lambda_{\rm H}^3}{g_{\rm H}}\right) \frac{1}{g_{\rm He^+}} \left(\frac{5}{4}\right)^{3/2} e^{-\Delta \varepsilon_{\rm He^+H}/T} \left(\frac{2IT}{\hbar^2}\right) \tag{27}$$

$$\sim \left(\frac{n_0 \lambda_{\rm H}^3}{g_{\rm H}}\right) e^{-\Delta \varepsilon_{\rm He^+H}/T} \left(\frac{2IT}{\hbar^2}\right) ,$$
 (28)

Evaluating it numerically we have

$$n_0 K_4 \simeq 8 \times 10^{-18}$$
. (29)

Qualitatively this means that only a very small fraction of ionized helium is bound up as a molecule. The reason for this is phase space or entropy, or more precisely free energy. Heuristically, each hydrogen occupies a volume $v_0 \simeq 1/n_0$. The increase in entropy associated with producing a hydrogen by breaking up the He⁺H molecule is

$$e^{S_{\text{trans}}} \sim \frac{v_0}{\lambda_H^3}$$
 (30)

The phase space lost by breaking up the diatomic molecule is the rotational phase space of the diatomic:

$$e^{S_{\rm rot}} \sim \frac{2IT}{\hbar^2}$$
 (31)

The prefactor in the equilibrium constant reflects the difference

$$e^{S_{\rm rot}-S_{\rm trans}} \sim n_0 \lambda^3 \frac{2IT}{\hbar^2},$$
(32)

and competes with the Boltzmann factor.

Statistical Mechanics 2

Weakly doped semiconductor

Consider a semiconductor with a valence and a conduction bands, in which the energy depends on the momentum as

$$\varepsilon_V(p) = -\frac{p^2}{2m_V}, \quad \varepsilon_C(p) = \frac{p^2}{2m_C} + \Delta$$

where Δ is the band gap. Interactions between electrons can be neglected. At T > 0, some electrons in the valence band may be excited and "jump" into the conductance band leaving behind a "hole" in the otherwise filled band. Such a hole can be treated as particle with the energy $\varepsilon_h = -\varepsilon_e$, where ε_e is the unfilled energy level.



- (a) [2pt] Write the Fermi-Dirac distribution for holes $f_h(\varepsilon_h)$ if they are in equilibrium with electrons that have chemical potential μ_e .
- (b) [2pt] Under what conditions can one treat electrons in the conductance band and holes in the valence band as Boltzmann gases?
- (c) [5pt] Use the condition in (b) to compute the densities of electrons n_e and holes n_h .

The semiconductor is slightly doped, so that at zero temperature the valence band is completely filled and the conductance band contains a small density of electrons n_0 . However, at normal ("room") temperature the densities of holes and electrons are much larger $n_{e,h} \gg$ $(n_e - n_h) = n_0$.

- (d) [5pt] Calculate the density of holes and electrons and find the electron chemical potential μ_e as a function of "room" temperature T.
- (e) [6pt] Compute the thermoelectric coefficient of the semiconductor, i.e. the e.m.f. induced by a temperature gradient $\mathcal{E}_T = S\Delta T$. It is sufficient to compute the result to the first order in $O(n_0/n_{e,h}) \ll 1$.

Hint: a difference in temperature leads to a difference in electron chemical potential. The latter would induce diffusion current unless electric potential is applied to compensate the difference $\Delta \varphi = \Delta \mu_e \approx \frac{d\mu_e}{dT} \Delta T$.

Solution: Weakly doped semiconductor

(a) Since the hole is defined as absense of an electron, the probability to find a particular state filled by a hole is complementary to that of an electron, so

$$f_h(\varepsilon_h) = \left(1 - f_e(\varepsilon_e)\right)_{\varepsilon_e = -\varepsilon_h} = 1 - \frac{1}{e^{(-\varepsilon_h - \mu_e)/T} + 1} = \frac{1}{e^{(+\varepsilon_h + \mu_e)/T} + 1},$$
(1)

so that the chemical potential of holes $\mu_h = -\mu_e$ is opposite to that of electrons; however, we will only use μ_e below to avoid configuion.

(b) In the Boltzmann-gas approximation, one neglects quantum statistics effects by dropping the "+1" in the denominator of the Fermi-Dirac distribution. In order for this to be valid, the exponential must be much larger than 1 and thus

$$(\varepsilon_{e} - \mu_{e}) \ge (\Delta - \mu_{e}) \gg T, \qquad f_{e}(\varepsilon_{e}) \approx e^{\frac{\mu_{e} - \varepsilon_{C}}{T}} = e^{\frac{\mu_{e} - \varepsilon_{C}(p_{e})}{T}} = \exp\left[\frac{1}{T}\left(\mu_{e} - \Delta - \frac{p_{e}^{2}}{2m_{C}}\right)\right]$$
(2)
$$(\varepsilon_{h} + \mu_{e}) \ge \mu_{e} \gg T, \qquad f_{h}(\varepsilon_{h}) \approx e^{\frac{-\mu_{e} - \varepsilon_{h}}{T}} = e^{\frac{-\mu_{e} + \varepsilon_{V}(p_{h})}{T}} = \exp\left[\frac{1}{T}\left(-\mu_{e} - \frac{p_{h}^{2}}{2m_{V}}\right)\right]$$
(3)

for electrons and holes, respectively. In the equation above, we used $\varepsilon_e = \varepsilon_C(p_e)$ and $\varepsilon_h = -\varepsilon_V(p_h) = +\frac{p_h^2}{2m_V}$.

(c) To find the energy distribution of the electron/hole density, one needs to complement the Fermi-Dirac statistics with the density of energy levels, which is determined by the phase space $\propto (d^3x d^3p)$ and the spin degeneracy $g_S = 2$,

$$d\Gamma = g_S \frac{d^3 x d^3 p}{(2\pi\hbar)^3} \,. \tag{4}$$

In uniform space one can replace $d^3x = dV$ and find the spatial density as

$$n = g_S \int \frac{d^3p}{(2\pi\hbar)^3} f(\varepsilon(p)) \tag{5}$$

The integration over momenta must be performed so that the energies $\varepsilon(p)$ correspond to the appropriate bands. For the electrons,

$$n_e = g_S \int \frac{d^3 p}{(2\pi\hbar)^3} \exp\left[\frac{\mu_e - \Delta - p^2/(2m_C)}{T}\right] = g_S \lambda_C^{-3} e^{(\mu_e - \Delta)/T}$$
(6)

where $\lambda_C = \sqrt{\frac{2\pi\hbar^2}{m_C T}}$ is the thermal wavelength in the conductance band. Analogously, for the holes,

$$n_h = g_S \int \frac{d^3 p}{(2\pi\hbar)^3} \exp\left[\frac{-\mu_e - p^2/(2m_V)}{T}\right] = g_S \lambda_V^{-3} e^{-\mu_e/T}$$
(7)

where $\lambda_V = \sqrt{\frac{2\pi\hbar^2}{m_V T}}$ is the thermal wavelength in the valence band.

(d) Both densities are determined by the electron chemical potential μ_e in equilibrium. It is easy to see that these densities are constrained by

$$n_e n_h = g_S^2 (\lambda_C \lambda_V)^{-3} e^{-\Delta/T} = n_X^2(T)$$
(8)

because the chemical potential cancels in the product above. Together with the equation for the total carrier density $n_e - n_h = n_0$, we have two equations to determine n_e and n_h . Solving the quadratic equation following from

$$n_e - \frac{n_X^2(T)}{n_e} = n_0$$
(9)

we obtain

$$n_e = \frac{1}{2} \left(\sqrt{4n_X^2(T) + n_0^2} + n_0^2 \right), \tag{10}$$

$$n_h = n_e - n_0 = \frac{1}{2} \left(\sqrt{4n_X^2(T) + n_0^2} - n_0 \right).$$
(11)

The chemical potential is easily found from one of the expressions above, e.g.,

$$\mu_e(T) = -T \log \frac{n_h \lambda_V^3}{g_S} = -T \log \frac{\lambda_V^3 (\sqrt{4n_X^2(T) + n_0^2} - n_0)}{2g_S} \,. \tag{12}$$

The condition $n_e \gg n_0$ can be satisfied only if $n_X \gg n_0$, which one can use to simplify the expression for the chemical potential. Keeping the leading n_0/n_X terms only, one obtains

$$\mu_e(T) \approx -T \log \frac{\lambda_V^3 \left(n_X(T) - n_0/2 \right)}{g_S}$$

$$\approx -T \log \left(\frac{\lambda_V}{\lambda_C} \right)^3 + \frac{\Delta}{2} - T \frac{n_0}{2n_X(T)}$$

$$= \frac{3}{2} T \log \frac{m_V}{m_C} + \frac{\Delta}{2} - T \frac{n_0}{2n_X(T)}$$
(13)

(e) The thermoelectric coefficient is

$$S = \frac{d\mu_e}{dT} \approx \frac{3}{2} \log \frac{m_V}{m_C} - \frac{n_0}{2n_X} + T \frac{n_0}{2n_X^2} \frac{dn_X(T)}{dT}$$
(14)

Using the expression for $n_X(T)$, one can find

$$\frac{dn_X(T)}{dT} = \frac{d}{dT} \left[g_S \left(\frac{m_V m_C}{4\pi^2 \hbar^2} \right)^{3/4} T^{3/2} e^{-\frac{\Delta}{2T}} \right] = \left(\frac{3}{2T} + \frac{\Delta}{2T^2} \right) n_X \tag{15}$$

and finally

$$S = \frac{3}{2}\log\frac{m_V}{m_C} + \frac{n_0}{2n_X}\left(\frac{1}{2} + \frac{\Delta}{2T}\right) \tag{16}$$

Statistical Mechanics 3

Gas in a vessel with attractive walls

Consider a classical ideal gas in a cubic vessel $L \times L \times L$. Each wall attracts gas molecules with a narrow "potential well" $d \ll L$ (see the figure). This attraction creates a spectrum of wall-bound states: for example, the energy states each of the walls perpendicular to the \hat{x} axis are

$$E_{B(x)} = -\varepsilon + \frac{p_y^2 + p_z^2}{2m} \,,$$



where ε is the binding energy, and $p_{y,z}$ is the momentum of motion tangential to the wall, which is not affected by the interaction. The interaction has negligible effect on unbound molecules, and they can move freely within the rest of the vessel volume.

(1)

- (a) [5pt] Calculate the chemical potentials of the gas molecules bound to the walls and free molecules in the box volume from their surface n_b and volume n_f densities, respectively. Show that the chemical potential of the bound molecules depends only on the total area of the vessel walls.
- (b) [5pt] Assuming that the total number of molecules is $N = N_b + N_f$, find the numbers of bound and free molecules as functions of temperature.
- (c) [2pt] Now consider an elastic balloon of radius R filled with N molecules of ideal gas. The balloon walls have constant surface tension σ . Neglecting the wall attraction for now, find the radius of the balloon in vacuum. *Hint:* the surface tension creates pressure $p = 2\sigma/R$ inside the balloon.
- (d) [4pt] How will the wall-bound molecules affect the surface tension of the balloon walls? Calculate contribution $\Delta \sigma_b = \sigma' \sigma$ resulting from their kinetic motion.
- (e) [4pt] Imagine that the wall attractive potential can be "switched" on and off. How will the balloon radius change, all else being equal? Assume that the change in the radius is small and the temperature is constant.

Solution

(a) The bound and unbound molecules can be considered separate gases for the purpose of computing their partition functions:

$$Z_N(T, V, A) = Z_{N_f}^f(T, V) \cdot \sum_{N_{b(1)} + \dots + N_{b(6)} = N_b} \prod_i Z_{N_{b(i)}}^b(T, A_i)$$
(2)

where $V = L^3$ is the vessel volume and $A_i = L^2$ are the areas of the vessel walls. The bound molecules can be distributed in any way between the six walls as long as their total number is equal to N_b . Let's first compute the partition function of the free molecules Z^f , which describes the ordinary ideal gas,

$$Z_{N_f} = \frac{1}{N_f!} Z_{1p}^{(3D)}, \qquad Z_{1p}^{(3D)} = \int \frac{d^3 x d^3 p}{(2\pi\hbar)^3} e^{-\frac{\vec{p}^2}{2mT}} = \frac{V}{\lambda_T^3}$$
(3)

where the $1/N_f!$ is the Boltzmann factor and $\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mT}}$ is the thermal wavelength. For molecules bound to one wall, the calculation is very similar except that one integrates over two dimensions tangent to the wall and the molecular energy is shifted by $(-\varepsilon)$:

$$Z_{N_{b(i)}} = \frac{1}{N_{b(i)}!} Z_{1p}^{(2D)}, \qquad Z_{1p}^{(2D)} = \int \frac{d^2 x d^2 p}{(2\pi\hbar)^2} e^{-\frac{1}{T} \left(\frac{\vec{p}^2}{2m} - \varepsilon\right)} = \frac{A_i}{\lambda_T^2} e^{\varepsilon/T}$$
(4)

with the same thermal wavelength. The Boltzmann factors $1/N_{b(i)}$ are particularly important to show that it is the total area that defines $Z_{N_b}^b$:

$$Z_{N_b}^b = \sum_{N_{b(1)} + \dots + N_{b(6)} = N_b} \prod \frac{1}{N_{b(1)}! \cdots N_{b(6)}!} A_1^{N_{b(1)}} \cdots A_6^{N_{b(6)}} = \frac{1}{N_b!} (A_1 + \dots + A_6)^{N_b} = \frac{1}{N_b!} A_1^{N_b}$$
(5)

which results from the multinomial (generalization of Newton's binomial) formula.

(b) One way to find the equilibrium between the bound and unbound portions of the gas is to use the minimum of the total Gibbs potential. An equivalent way is to equate their chemical potentials. To find the chemical potential, let's compute the grand canonical partition function of the free molecules, and deduce the chemical potential corresponding to their density N_f/V :

$$Z_{G}^{f}(T, V, \mu_{f}) = \sum_{N_{f}} e^{\frac{\mu_{f}N_{f}}{T}} Z_{N_{f}}^{f} = \sum_{N_{f}} e^{\frac{\mu_{f}N_{f}}{T}} \cdot \frac{1}{N_{f}!} \left(V\lambda_{T}^{-3} \right)^{N_{f}} = \exp\left[e^{\mu_{f}/T} V\lambda_{T}^{-3} \right], \quad (6)$$

$$\Omega^{f}(T, V, \mu_{f}) = -T \log Z_{G}^{f}(T, V, \mu_{f}) = -T e^{\mu_{f}/T} V \lambda_{T}^{-3},$$
(7)

$$N_f = -\left(\frac{\partial Z_G^f}{\partial \mu_f}\right)_{T,V} = e^{\mu_f/T} V \lambda_T^{-3} \quad \Leftrightarrow \quad \mu_f = T \log \frac{N_f \lambda_T^3}{V} \,. \tag{8}$$

In complete analogy, the grand canonical partition function, the density, and the number chemical potential of the bound molecules are

$$Z_B^b(T, A) = \sum_{N_b} e^{\frac{\mu_b N_b}{T}} Z_{N_b}^b = \sum_{N_b} e^{\frac{\mu_b N_b}{T}} \cdot \frac{1}{N_b!} \left(A\lambda_T^{-2} e^{\varepsilon/T}\right)^{N_b} = \exp\left[e^{(\mu_b + \varepsilon)/T} A\lambda_T^{-2}\right], \quad (9)$$

$$\Omega^{b}(T, A, \mu_{b}) = -T \log Z_{G}^{b}(T, V, \mu_{b}) = -T e^{\mu_{b}/T} A \lambda_{T}^{-2}, \qquad (10)$$

$$N_f = -\left(\frac{\partial Z_G^b}{\partial \mu_b}\right)_{T,A} = e^{\mu_b/T} A \lambda_T^{-2} \quad \Leftrightarrow \quad \mu_b = T \log \frac{N_b \lambda_T^2}{A} - \varepsilon \,. \tag{11}$$

The equilibrium between the bound and the unbound portions of the gas implies that their chemical potentials are the same,

$$\mu_f = \mu_b \qquad \Longrightarrow \qquad \frac{N_f}{N_b} = \frac{V}{A\lambda_T} e^{-\varepsilon/T}$$
(12)

and at $T \to 0$ all the molecules will be bound.

(c) For a regular gas (free from walls), the pressure is $p = \frac{NT}{V}$, so the equilibrium requires that

$$\frac{2\sigma}{R} = \frac{NT}{(4\pi/3)R^3} \qquad \Longrightarrow \qquad R_0 = \sqrt{\frac{3NT}{8\pi\sigma}} \tag{13}$$

(d) Now, if some portion of the gas is bound, it results in less pressure pushing against the balloon walls,

$$p = \frac{N_f}{V}T\tag{14}$$

Where N_f is the number of free molecules. In addition, the surface tension is reduced by "surface pressure" of the bound gas⁶,

$$\Delta \sigma_b = -\frac{N_b T}{A} \,. \tag{15}$$

(e) The mechanical equilibrium implies

$$\frac{2(\sigma + \Delta \sigma_b)}{R} = \frac{2(\sigma - N_b T / (4\pi R^2))}{R} = p_f = \frac{N_f T}{(4\pi/3)R^3}$$
$$\Leftrightarrow \frac{2\sigma}{R} = \frac{3T}{4\pi R^3} \left(N_f + \frac{2}{3}N_b \right) = \frac{3NT}{4\pi R^3} \left(1 - \frac{N_b}{3N} \right)$$
$$\Leftrightarrow R = \sqrt{\frac{3NT}{8\pi\sigma} \left(1 - \frac{N_b}{3N} \right)} \approx R_0 \left(1 - \frac{N_b}{6N} \right)$$
(16)

so the radius will decrease. For the radius change to be small, the total number of molecules must be $N \approx N_f \gg N_b$; using also $R \approx R_0$, we get

$$\frac{N_b}{N} \approx \frac{N_b}{N_f} = A\lambda_T / V e^{\varepsilon/T} \approx \frac{3\lambda_T}{R_0} e^{\varepsilon/T}$$
(17)

⁶Both formulas (14,15) can be deduced from their grand potentials $\Omega_f = -pV$ and $\Omega_b = \Delta \sigma_b A$.

and finally

$$R \approx R_0 - \frac{1}{6}R_0 \cdot \frac{3\lambda_T}{R_0}e^{\varepsilon/T} = R_0 - \frac{1}{2}\lambda_T e^{\varepsilon/T}.$$
(18)