Comprehensive Examination

Department of Physics and Astronomy Stony Brook University

January 2018 (in 4 separate parts: CM, EM, QM, SM)

General Instructions:

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

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

Some of the problems may cover multiple pages. Use one exam book for each problem, and label it carefully with the problem topic and number and your ID number.

Write your ID number (not your name!) on the 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

The conical and the inverted pendulum.

A massive homogeneous bar of length l and total mass M is attached to the ceiling and forced to rotate around a vertical axis with constant angular velocity ω . The point where the bar is attached to the ceiling does not move, so the bar can only swing in a vertical plane that rotates uniformly. The angle between the bar and the vertical axis of rotation is θ .

- 1. Derive the equation of motion of θ for arbitrary (not only small) values of θ . (4 points)
- 2. At what rotation rate ω_c does the stationary solution $\theta_0 = 0$ become unstable? (4 points)
- 3. For $\omega > \omega_c$ there is a stable solution with constant $\theta_0 > 0$. What is the frequency of small oscillations about this solution? (4 points)

Now consider the same pendulum, but upside down (called the upsidedown pendulum, or the inverted pendulum, or the Kapitza pendulum). The bottom of the pendulum is forced to move vertically with periodic motion $A\cos(\gamma t)$. We consider now motion in a fixed vertical plane, rather than a rotating plane. The angle θ measures how far the bar deviates from the vertical position. We consider the case that $A \ll l$, but the frequency may become large. For given $A \ll l$ there is a critical value γ_{crit} of the frequency such that for frequencies larger than γ_{crit} the bar does not fall down but stays in upright position.

4. Derive the following equation of motion for small values of θ

$$\theta'' + (p + q \cos z)\theta = 0; \quad p = -\frac{3}{2}\frac{g}{l\gamma^2}; \quad q = \frac{3}{2}\frac{A}{l}.$$

Here $z = \gamma t$ and θ' denotes $\frac{d\theta}{dz}$. (4 points)

5. It can be shown that at $\gamma = \gamma_{crit}$ the function $\theta(z)$ is periodic or antiperiodic in z with period 2π . What is the value of γ_{crit} ? (4 points)

Hint: expand p and θ into a power series of q.



Solution

1. The kinetic and potential energy of a segment of length Δx of the bar which is a distance x away from the top of the bar are given by

$$T(x)\Delta x = \frac{1}{2} \left(\frac{M}{l}\Delta x\right) \left[(x\dot{\theta})^2 + (x\sin\theta)^2 \omega^2 \right]$$
$$V(x)\Delta x = -\left(\frac{M}{l}\Delta x\right) g(x\cos\theta) \,.$$

Then $L = \int_0^l [T(x) - V(x)] dx$ is given by¹

$$L = \frac{1}{6}Ml^2\dot{\theta}^2 + \frac{1}{6}Ml^2\sin^2\theta\omega^2 + \frac{1}{2}Mlg\cos\theta.$$

The equation of motion is thus

$$\frac{1}{3}Ml^2\ddot{\theta} - \frac{1}{3}Ml^2\sin\theta\cos\theta\omega^2 + \frac{1}{2}Mlg\sin\theta = 0.$$

2. For small oscillations about $\theta_0 = 0$ the equation of motion becomes

$$\frac{1}{3}Ml^2\ddot{\theta} - \frac{1}{3}Ml^2\omega^2\theta + \frac{1}{2}Mlg\theta = 0$$

Hence the critical value of ω where instability about $\theta_0 = 0$ sets in is

$$\omega_c^2 = \frac{3}{2} \frac{g}{l} \cdot$$

- 3. For sufficiently large (how large will be determined) ω there is a stationary point at $\theta_0 > 0$. The equation for θ_0 follows from the equation of motion by substituting $\ddot{\theta} = 0$.
 - $-\frac{1}{3}Ml^2\sin\theta_0\cos\theta_0\omega^2 + \frac{1}{2}Mlg\sin\theta_0 = 0 \quad \Rightarrow \quad \cos\theta_0 = \frac{3}{2}\frac{g}{l\omega^2} \cdot$

The frequency Ω of small oscillations $\theta - \theta_0 = \eta$ about θ_0 follows from the equation of motion by substituting $\ddot{\eta} = -\Omega^2 \eta$, expanding about θ_0 , and substituting the value of $\cos \theta_0$

$$0 = -\frac{1}{3}Ml^2\Omega^2 - \frac{1}{3}Ml^2\left(\cos^2\theta_0 - \sin^2\theta_0\right)\omega^2 + \frac{1}{2}Mlg\cos\theta_0$$

= $-\frac{1}{3}Ml^2\Omega^2 - \frac{1}{3}Ml^2\left[2\left(\frac{3}{2}\frac{g}{l\omega^2}\right)^2 - 1\right]\omega^2 + \frac{1}{2}Mlg\frac{3}{2}\frac{g}{l\omega^2}\cdot$

Hence

$$\frac{1}{3}Ml^{2}\Omega^{2} = -\frac{3}{2}\frac{Mg^{2}}{\omega^{2}} + \frac{1}{3}Ml^{2}\omega^{2} + \frac{3}{4}\frac{Mg^{2}}{\omega^{2}}$$
$$= -\frac{3}{4}\frac{Mg^{2}}{\omega^{2}} + \frac{1}{3}Ml^{2}\omega^{2}$$
$$\Omega^{2} = \omega^{2} - \frac{9}{4}\frac{g^{2}}{l^{2}\omega^{2}} = \omega^{2}\left[1 - \left(\frac{\omega_{c}}{\omega}\right)^{4}\right]$$

Hence for $\omega > \omega_c$ stability holds, but the frequency of small oscillations about $\theta_0 > 0$ is smaller than the frequency with which the pendulum rotates about the vertical axis.

¹Even for $\dot{\theta} = 0$ the kinetic energy is not $\frac{1}{2}Mv_{cm}^2$ (which gives $\frac{1}{8}Ml^2\sin^2\theta\omega^2$), but

$$\frac{1}{2}\left(\frac{M}{l}\right)\int_0^\ell (x\sin\theta)^2\omega^2 dx = \frac{1}{6}Ml^2\sin^2\theta\omega^2.$$

The difference $(\frac{1}{24}M\ell^2\sin^2\theta\omega^2)$ is due to a rotation of the bar about the vertical axis, $\frac{1}{2}I_{\rm cm}\sin^2\theta\omega^2$.

4. Consider a small segment of the bar of length Δx which is a distance x away from the bottom of the bar. Let $\overline{x}(t)$ and $\overline{z}(t)$ and denote its cartesian coordinates in the lab frame. The figure in the problem statement shows that

$$\overline{z}(t) = A\cos(\gamma t) + x\cos\theta,$$

$$\overline{x}(t) = -x\sin\theta,$$

and thus

$$\dot{\overline{x}}^2 + \dot{\overline{z}}^2 = \left[(x\dot{\theta})^2 + 2A\gamma x\dot{\theta}\sin(\gamma t)\sin\theta + A^2\gamma^2\sin^2(\gamma t) \right].$$

The kinetic and potential energy of the segment are given by

$$T(x)\Delta x = \frac{1}{2} \left(\frac{M}{l}\Delta x\right) \left[(x\dot{\theta})^2 + 2A\gamma x\dot{\theta}\sin(\gamma t)\sin\theta + A^2\gamma^2\sin^2(\gamma t) \right]$$
$$V(x)\Delta x = \left(\frac{M}{l}\Delta x\right) g \left[x\cos\theta + A\cos(\gamma t) \right].$$

Then $L = \int_0^l [T(x) - V(x)] dx$ is given by (ignoring total derivatives and θ -independent terms)

$$L = \frac{1}{6}Ml^2\dot{\theta}^2 + \frac{1}{2}MAl\gamma^2\cos(\gamma t)\cos\theta - \frac{1}{2}Mlg\cos\theta.$$

The equation of motion is thus

$$\frac{1}{3}Ml^2\ddot{\theta} + \left(\frac{1}{2}MAl\gamma^2\cos(\gamma t) - \frac{1}{2}Mlg\right)\sin\theta = 0.$$

For small oscillations about $\theta_0 = 0$ the equation of motion becomes (transforming $t \rightarrow z = \gamma t$)

$$\theta'' + \left(\frac{3A}{2l}\cos z - \frac{3g}{2l\gamma^2}\right)\theta = 0$$

$$\Rightarrow \theta'' + \left(p + q\cos z\right)\theta = 0.$$

5. We consider a fixed A but various γ . So, the idea is to treat p and θ as functions of q, and to substitute a power expansion of p(q) and $\theta(z,q)$ into the equation of motion.

$$\theta(z,q) = \theta_0(z) + q\theta_1(z) + q^2\theta_2(z) + \cdots$$
$$p(q) = p_0 + qp_1 + q^2p_2 + \cdots$$

Because $\theta(z,q)$ is periodic or antiperiodic at the critical frequency², all $\theta_0(z), \theta_1(z), \theta_2(z), \cdots$ have to be periodic or antiperiodic. We get a hierarchy of relations.

$$\theta''(z,q) + (p(q) + q\cos z)\theta(z,q) = 0.$$

Order q^0 : $\theta_0''(z) + p_0\theta_0(z) = 0 \Rightarrow \theta_0(z) = \cos(\sqrt{p_0}z)$. (Anti)periodicity of $\theta_0(z)$ requires $p_0 = \frac{n^2}{4}$ for n = 0, 1, 2. We take the lowest value

$$\theta_0(z) = 1; \qquad p_0 = 0.$$

²As shown for example in Landau-Lifshitz volume 1 Mechanics, section 27, the solution for θ is of the form $(\mu^1)^{z/2\pi}\Pi_1 + (\mu^2)^{z/2\pi}\Pi_2$, where $\Pi_i(z) = \Pi_i(z + 2\pi)$ and $\mu^1\mu^2 = 1$. Either μ^1 and μ^2 are real (instability) or they are phases $(|\mu^1| = |\mu^2| = 1$, stability). At the critical point, the phases become real, and this occurs if $\mu^1 = \mu^2 = +1$ (periodicity) or $\mu^1 = \mu^2 = -1$ (antiperiodicity).

Order q¹: $\theta_1''(z) + p_1\theta_0(z) + p_0\theta_1(z) + (\cos z)\theta_0 = 0 \Rightarrow \theta_1''(z) + p_1 + \cos z = 0$. The solution is $\theta_1 = a_1 + b_1z + \frac{1}{2}p_1z^2 + \cos z$. (Anti)periodicity requires $b_1 = p_1 = 0$. Hence

$$\theta_1(z) = a_1 + \cos z; \qquad p_1 = 0.$$

Order q²: $\theta_2''(z) + p_2\theta_0(z) + p_1\theta_1(z) + p_0\theta_2(z) + (\cos z)\theta_1 = 0 \Rightarrow \theta_2''(z) + p_2 + \cos z(a_1 + \cos z) = 0$. We use $\cos z \cos z = \frac{1}{2}(1 + \cos(2z))$. Then (anti)periodicity requires that $p_2 + \frac{1}{2} = 0$. This is the crucial relation. It implies that

$$p(q) = -\frac{1}{2}q^2 + \cdots.$$

Substituting $p = -\frac{3}{2} \frac{g}{l\gamma^2}$, and $q = \frac{3}{2} \frac{A}{l}$ we find

$$\gamma_{crit}^2 = \frac{4gl}{3A^2}$$

For example, if A = 1cm and l = 30cm, one finds ($\gamma = 2\pi\nu$) for the critical frequency ν_{crit}

$$\nu_{crit} = \frac{1}{2\pi} \sqrt{\frac{4 \cdot 10^3 \cdot 30}{3}} \simeq 32 \,\mathrm{Hz}.$$

Classical Mechanics 2

Nonlinear oscillations

Consider a weakly-nonlinear oscillator: a particle of mass m moving in the potential

$$U(x) = m\omega_0^2 \left[\frac{x^2}{2} - \lambda \frac{x^3}{3}\right],$$

which in the absence of nonlinearity ($\lambda = 0$) performs harmonic oscillations of frequency ω_0 :

$$x^{(0)}(t) = a\cos\omega_0 t\,.\tag{1}$$

- (a) (3 points) Determine the correction $x^{(1)}(t)$ of first order in λ to the unperturbed oscillations in eq. (1) using direct (or "naive") perturbation theory.
- (b) (6 points) Do the same for the second order correction $x^{(2)}(t)$.
- (c) (7 points) Find the correction $x^{(1)}(t) + x^{(2)}(t)$ up to second order in λ using secular perturbation theory, where the "zeroth-order" oscillations are represented by $x^{(0)}(t) = a \cos \omega t$. Determine the oscillation frequency ω to order λ^2 .
- (d) (4 points) Compare the time ranges of validity of the direct and secular perturbation theories using the solutions from parts (a) and (b), and (c), respectively.

Solution

(a) The equation of motion satisfied by the oscillator is:

$$\ddot{x} + \omega_0^2 x = \lambda \omega_0^2 x^2 \,.$$

For the unperturbed solution $x^{(0)}(t) = a \cos \omega_0 t$, the first-order correction $x^{(1)}(t)$ should satisfy the equation

$$\ddot{x}^{(1)} + \omega_0^2 x^{(1)} = \lambda \omega_0^2 [x^{(0)}]^2 = \frac{\lambda \omega_0^2 a^2}{2} [1 + \cos 2\omega_0 t].$$

The solution of this equation determines $x^{(1)}(t)$:

$$x^{(1)}(t) = \frac{\lambda a^2}{2} \left[1 - \frac{1}{3} \cos 2\omega_0 t \right].$$

(b) Iterating further, and keeping only the terms of the required second order in λ on the right-hand-side of the equation of motion, we get similarly the equation for the second-order correction $x^{(2)}(t)$:

$$\ddot{x}^{(2)} + \omega_0^2 x^{(2)} = 2\lambda \omega_0^2 x^{(0)} x^{(1)} = \frac{\lambda^2 \omega_0^2 a^3}{6} \left[5\cos\omega_0 t - \cos 3\omega_0 t \right].$$

As for all other terms in the perturbative expansion of x, the term $x^{(2)}(t)$ is given by the particular solution of this differential equation. The presence of the "resonant" terms of frequency ω_0 on the right-hand-side of this equation leads to a term linear in time:

$$x^{(2)}(t) = \frac{\lambda^2 a^3}{12} \left[5\omega_0 t \sin \omega_0 t + \frac{1}{4} \cos 3\omega_0 t \right].$$

(c) In the asymptotic perturbation theory, one takes into account explicitly that the oscillation frequency ω is affected by the nonlinearity, and, in addition to the expansion for the coordinate x:

$$x(t) = x^{(0)}(t) + x^{(1)}(t) + x^{(2)}(t) + \dots, \quad x^{(0)}(t) = a \cos \omega t,$$

can also be directly expanded in the perturbation series in λ :

$$\omega = \omega_0 + \omega^{(1)} + \omega^{(2)} + \dots$$

The terms of the expansion for ω are then defined through the condition that there are no resonant contributions in each order of the overall perturbation-theory expansion of the equations of motion. Explicitly, the first order terms in the expansion of the equation of motion are

$$\frac{\omega_0^2}{\omega^2}\ddot{x}^{(1)} + \omega_0^2 x^{(1)} = \lambda \omega_0^2 [x^{(0)}]^2 - \frac{2\omega_0 \omega^{(1)}}{\omega^2} \ddot{x}^{(0)} = \lambda \omega_0^2 a^2 \cos^2 \omega t + 2\omega_0 \omega^{(1)} a \cos \omega t \,,$$

and give

$$x^{(1)}(t) = \frac{\lambda a^2}{2} \left[1 - \frac{1}{3} \cos 2\omega t \right], \quad \omega^{(1)} = 0.$$

The second-order part of the equations of motion is:

$$\frac{\omega_0^2}{\omega^2} \ddot{x}^{(2)} + \omega_0^2 x^{(2)} = 2\lambda \omega_0^2 x^{(0)} x^{(1)} - \frac{2\omega_0 \omega^{(2)}}{\omega^2} \ddot{x}^{(0)} = \lambda^2 \omega_0^2 a^3 \cos \omega t \left(1 - \frac{1}{3} \cos 2\omega t\right) + 2\omega_0 \omega^{(2)} a \cos \omega t \,,$$

and gives:

$$x^{(2)}(t) = \frac{\lambda^2 a^3}{48} \cos 3\omega t$$
, $\omega^{(2)} = -\frac{5\lambda^2 a^2 \omega_0}{12}$.

(d) The usual condition of the validity of the perturbation expansion is that the perturbative corrections remain small in comparison with the zero-order term. For the asymptotic perturbation theory, this condition does not involve time and limits only the oscillation amplitude:

$\lambda a \ll 1$,

whereas the direct perturbation theory is only valid in the limited time interval, because of the resonant terms:

$\lambda^2 a^2 \omega_0 t \ll 1 \, .$

Classical Mechanics 3

The three body problem.

Consider the three body problem of the Earth–Sun system together with a satellite of negligible mass. The masses are $m_1, m_2 \gg m_3$. We work in the approximation that the orbit of the Earth around the Sun is circular. Let the Earth–Sun motion take place in the (x, y) plane, and let the center of mass coordinates of the Earth–Sun system be at the origin (see below).

$$\begin{array}{c} m_1 \vec{r_1} + m_2 \vec{r_2} = 0 \\ \vec{r} = \vec{r_1} - \vec{r_2} \end{array} \right\} \quad \begin{array}{c} \vec{r_1} = \frac{m_2}{m} \vec{r} \\ \vec{r_2} = -\frac{m_1}{m} \vec{r} \end{array} \right\} \quad m \equiv m_1 + m_2 \,.$$

The goal of this problem is to determine the five *Lagrangian points*, which are the (corotating) positions of the satellite which are stationary with respect to the rotating Earth-Sun coordinate system.

Using a complex notation the Earth-Sun separation, $\vec{r} = (x, y)$ can be replaced by z = x+iy where $z = a e^{i\omega t}$, $a \equiv \text{Earth-Sun distance}$, $\omega = \frac{2\pi}{T}$, T = 1 year. We have $\omega^2 = \frac{G(m_1+m_2)}{a^3}$. Assume that the third body also moves in the (x, y) plane (see below). Using the moving frame provided by z(t) and iz(t), the position of the third body can be written as:

$$z_{3}(t) = x_{3}(t) + iy_{3}(t) = \alpha(t)z(t) + \beta(t)iz(t) \equiv \zeta(t)z(t)$$

with real α and β .



- 1. Write the equations of motion for $z_3(t)$ and for $\zeta(t)$. (4 points)
- 2. Show that the condition that the satellite remains at rest with respect to the Earth–Sun system is:

$$\zeta - \frac{m_1}{m} \frac{\zeta - \frac{m_2}{m}}{|\zeta - \frac{m_2}{m}|^3} - \frac{m_2}{m} \frac{\zeta + \frac{m_1}{m}}{|\zeta + \frac{m_1}{m}|^3} = 0.$$
(2 points) (1)

3. Show that solutions to Eq. (1) with $\text{Im}\zeta \neq 0$, satisfy:

$$\frac{1}{|\zeta - m_2/m|^3} - \frac{1}{|\zeta + m_1/m|^3} = 0.$$
(3 points)

Reinserting this result in Eq. (1) yields

$$1 = \frac{1}{|\zeta - m_2/m|^3} \, \cdot \,$$

- 4. Show that Earth, Sun, and equilibrium point form an equilateral triangle of side a, and there are two possibilities, ahead or behind the Earth. These are the Lagrangian points L_4, L_5 . (3 points)
- 5. Look now for solutions of (1) with $\text{Im}\zeta = 0$, *i.e.*, along the Earth–Sun axis. By plotting (1) show that there are three solution: L_1, L_2, L_3 . (4 points)



6. Give a qualitative argument of why we should expect L_1, L_2, L_3 . (4 points)

Solution

We assume that m_2 (Sun) and m_1 (Earth) are on a circular orbit. We also provide that if a is the distance Earth–Sun, the period of revolution T (year) is given by:

$$T = 2\pi \left(\frac{a^3}{G(m_1 + m_2)}\right)^{1/2}$$

Then

$$\omega = \frac{2\pi}{T} = \left(\frac{G(m_1 + m_2)}{a^3}\right)^{1/2}$$

Choose (x, y) to be the plane where the motion takes place, and choose the origin at the centre of mass:

$$m_1 \vec{r_1} + m_2 \vec{r_2} = 0$$

Letting $\vec{r} = \vec{r_1} - \vec{r_2}$ we can easily show that

$$\vec{r_1} = \frac{m_2}{m}\vec{r}$$
, $\vec{r_2} = -\frac{m_1}{m}\vec{r}$, $m \equiv m_1 + m_2$.

Since $\vec{r_1}, \vec{r_2}$ are two-dimensional vectors, we can write them in terms of complex variables

$$z_i = x_i + iy_i, \qquad \vec{r}_i \cdot \vec{r}_j = \operatorname{Re} z_i \cdot \bar{z}_j$$

1. Adding a third body with mass m_3 in the same plane with $m_3 \ll m_1, m_2$, the equations of motion following from Newton's laws are

$$\ddot{\vec{r}}_3 = -\frac{Gm_1}{|\vec{r}_{13}|^3}\vec{r}_{31} - \frac{Gm_2}{|\vec{r}_{23}|^3}\vec{r}_{32} \,, \quad \vec{r}_{ij} \equiv \vec{r}_i - \vec{r}_j \,.$$

Using complex variables again:

$$\ddot{z}_3 = -\frac{Gm_1}{|z_{31}|^3} z_{31} - \frac{Gm_2}{|z_{32}|^3} z_{32} \,.$$

We go to the frame moving with the Earth–Sun system, *i.e.*, where they are at rest. If z(t) = x + iy, $(x, y) = \vec{r}$ the vector pointing from the Sun to the Earth, we know that

$$z(t) = a \exp i\omega t$$

because by assumption the orbit is circular. Then

$$z_1 = \frac{m_2}{m} z$$
, $z_2 = -\frac{m_1}{m} z$.

The vectors z(t) and iz(t) are orthogonal (notice that in components z(t) = (x, y), iz(t) = (-y, x)), hence we write z_3 in this basis:

$$z_3 = \alpha(t)z(t) + \beta(t)iz(t) = (\alpha + i\beta)z \equiv \zeta(t)z.$$

In this basis we write the equations of motion:

$$\frac{d^2}{dt^2}(\zeta z) = (\ddot{\zeta} + 2i\omega\dot{\zeta} - \omega^2\zeta)z = -\frac{Gm_1}{|\zeta - m_2/m|^3 a^3} \left(\zeta - \frac{m_2}{m}\right)z - \frac{Gm_2}{|\zeta + m_1/m|^3 a^3} \left(\zeta + \frac{m_1}{m}\right)z$$

where we used $\dot{z} = i\omega z$, $\ddot{z} = -\omega^2 z$. Dividing by z and moving $\omega^2 \zeta$ to the RHS, we have:

$$\ddot{\zeta} + 2i\omega\dot{\zeta} = \omega^2\zeta - \frac{Gm_1}{|\zeta - m_2/m|^3 a^3} \left(\zeta - \frac{m_2}{m}\right) - \frac{Gm_2}{|\zeta + m_1/m|^3 a^3} \left(\zeta + \frac{m_1}{m}\right)$$

2. The Lagrangian points are those places at rest relative to the Sun and Earth, hence we need to find solutions to:

$$\ddot{\zeta}=\dot{\zeta}=0$$

namely:

$$\omega^2 \zeta - \frac{Gm_1}{a^3} \frac{\zeta - \frac{m_2}{m}}{|\zeta - \frac{m_2}{m}|^3} - \frac{Gm_2}{a^3} \frac{\zeta + \frac{m_1}{m}}{|\zeta + \frac{m_1}{m}|^3} = 0$$

Using $\omega^2 = \frac{G(m_1+m_2)}{a^3}$, we simplify the equation:

$$\left|\zeta - \frac{m_1}{m} \frac{\zeta - \frac{m_2}{m}}{|\zeta - \frac{m_2}{m}|^3} - \frac{m_2}{m} \frac{\zeta + \frac{m_1}{m}}{|\zeta + \frac{m_1}{m}|^3} = 0.\right|$$
(2)

3. Look at the drawing. Equation (2) represents the cancellation of the centrifugal force on m_3 by the gravitational attraction of m_1, m_2 . We look for this force to vanish along ζ and along the orthogonal direction, $i\zeta$.



We first look for solutions to (2) with ζ not collinear with $m_1, m_2, i.e., \text{Im}\zeta \neq 0$. The condition that the forces vanish orthogonal to ζ , implies that we multiply (2) by $i\bar{\zeta}$ and take the real part (scalar product), this yields:

$$\frac{1}{|\zeta - {}^{m_2}\!/\!m|^3} - \frac{1}{|\zeta + {}^{m_1}\!/\!m|^3} = 0$$

Hence the equilibrium points are equidistant from m_1, m_2 . Using this condition in (2) yields:

$$1 = \frac{1}{|\zeta - m_2/m|^3} \, \cdot \,$$

Thus (m_1, m_2, m_3) form an equilateral triangle. In the CM frame the positions of L_4, L_5 are then:

$$\zeta_{4,5}:\left(\frac{1}{2}-\frac{m_2}{m},\frac{\sqrt{3}}{2}\right), \quad \left(\frac{1}{2}-\frac{m_2}{m},-\frac{\sqrt{3}}{2}\right).$$

4. Finally consider equilibrium positions on the Earth–Sun axis. Let $\alpha = \frac{m_1}{m}, \beta = \frac{m_2}{m}$



 $m = m_1 + m_2$, then we are looking for solutions of:

$$\zeta - \alpha \frac{\zeta - \beta}{|\zeta - \beta|^3} - \beta \frac{\zeta + \alpha}{|\zeta + \alpha|^3} = 0, \qquad \zeta \text{ real}$$

It is easy to plot the LHS as a function of ζ



showing that there are 3 collinear solutions.

5. The qualitative reason why L_1, L_2, L_3 exist is as follows. If m_2 is the Sun and m_3 is closer to m_2 than the Earth, then m_3 would go around the Sun faster than the Earth. However, if we include the Earth's attraction on m_3 , it cancels part of the Sun's, and hence there is an intermediate point L_1 , where the angular velocity is the same as the Earth. Similar arguments apply to L_2, L_3 but now it is the addition of Earth's attraction that makes m_3 at L_2, L_3 move faster. Thus L_2 and L_3 lie just outside the orbit of the earth, while L_1 lies just inside this orbit. (The distance of L_1 and L_2 from the earth is about 1.5 million kilometers.)

Electromagnetism 1

A neutral metallic sphere at rest and in motion

A small neutral metallic sphere of infinite conductivity and radius a (diameter 2a) is separated by a transverse distance $R \gg a$ from an infinitely long wire of negligible thickness, vanishing conductivity, and charge per length λ (see below).



(a) (6 points) Calculate the force between the metallic sphere and the wire. (Hint: recall that the induced electric dipole moment of a sphere in a constant electric field is $\boldsymbol{p} = 4\pi a^3 \boldsymbol{E}_0$.) Explain the direction of the force physically, and estimate error associated with the dipole approximation.

Now consider a different problem. A small neutral metallic sphere of radius a (diameter 2a) of infinite conductivity moves (non-relativistically) with velocity v along the wire. The sphere is separated by a transverse distance R from a neutral wire carrying a current I_0 in the same direction.



- (b) (5 points) There is a force between the wire and the sphere. Without using a Lorentz transformation, qualitatively explain the origin of this force in the lab frame and estimate its magnitude.
- (c) (6 points) Using a Lorentz transformation, determine the electric and magnetic fields in the frame of the sphere. What charges are responsible for the electric field in this frame? Show quantitatively that these charges give the required electric field.
- (d) (3 points) Compute the force on the metallic sphere in the sphere's frame and compare the result with part (a) and the estimate in part (b).

Solution

(a) The electric field from the line of charge is in the radial direction ρ

$$E_{\rho} = \frac{\lambda}{2\pi\rho} \,. \tag{1}$$

This electric field induces a dipole moment on the sphere, and then the induced dipole is in a spatially dependent electric field and experiences a force:

$$F_i = p_\ell \partial_i E^\ell = p_\ell \partial^\ell E_i \,. \tag{2}$$

In the current case the dipole moment is proportional to \boldsymbol{E}

$$\boldsymbol{p} = \alpha \boldsymbol{E} \quad \text{with} \quad \alpha = 4\pi a^3,$$
 (3)

and thus we evaluate the force at $x = \rho = R$ (see coordinates in Fig. 1)

$$F_x|_{x=R} = \frac{\alpha}{2}\partial_x E^2 = -\left(\frac{\lambda}{2\pi}\right)^2 \frac{8\pi a^3}{R^3}.$$
(4)

The force is clearly attractive as should be the case from the physical picture given in Fig. 1. There will be corrections to this calculation of order a/R stemming from higher terms in the multipole expansion



Figure 1: Induced charges on a sphere in the presence of a charged wire.

(b) The charge carriers in the moving conducting sphere experience a magnetic force due to the magnetic field of the wire:

$$B_{\phi} = \frac{I_0}{2\pi c\rho}, \qquad F_B \sim q \frac{v}{c} B.$$
(5)



Figure 2: The magnetic force F_B on positive charges in the sphere is directed towards the wire.

The charges inside the sphere separate and are transported to the surface of the sphere. The positive charge accumulates closer to the wire, and the negative charge accumulates farther from the wire – see Fig. 2.

This process continues until the force inside the sphere due to the induced electric field balances the magnetic force. We may estimate the magnitude of the charge separation as follows:

$$qE \sim \frac{qQ_{\rm ind}}{4\pi a^2} \sim q\frac{v}{c}B\,. \tag{6}$$

So we estimate that the induced charge is

$$Q_{\rm ind} \sim a^2 \frac{v}{c} B$$
 (7)

The force on the sphere in the x-direction may then estimated as the sum of magnetic forces from the top set of charges (the negatives) and the bottom set of charges (the positives)

$$F_x \sim \left(F_x^- + F_x^+\right) \sim Q_{\rm ind} \frac{v}{c} B(R+a) - Q_{\rm ind} \frac{v}{c} B(R) \sim Q_{\rm ind} \frac{v}{c} B'(R)a.$$
(8)

Thus, the force is attractive

$$F_x \sim a^3 \left(\frac{v}{c}\right)^2 B(R)B'(R) \sim -a^3 \left(\frac{v}{c}\right)^2 \left(\frac{I_0}{c}\right)^2 \frac{1}{R^3}.$$
(9)

(c) When we make a boost in the β direction³ the fields transform as

$$\underline{E}_{\parallel} = E_{\parallel} , \qquad (10)$$

$$\underline{B}_{\parallel} = B_{\parallel} , \qquad (11)$$

$$\underline{\boldsymbol{E}}_{\perp} = \gamma \boldsymbol{E}_{\perp} + \gamma \boldsymbol{\beta} \times \boldsymbol{B}_{\perp} \,, \tag{12}$$

$$\underline{\boldsymbol{B}}_{\perp} = \gamma \boldsymbol{B}_{\perp} - \gamma \boldsymbol{\beta} \times \boldsymbol{E}_{\perp} \,. \tag{13}$$

³Our conventions are such that a particle at rest in a frame \mathcal{O} moves with velocity $-\beta$ in frame $\underline{\mathcal{O}}$ after a Lorentz boost by β

We may limit ourselves to a non-relativistic approximation where⁴

$$\underline{\boldsymbol{E}}_{\perp} \simeq \boldsymbol{\boldsymbol{E}}_{\perp} + \boldsymbol{\beta} \times \boldsymbol{\boldsymbol{B}}_{\perp} \,, \tag{14}$$

$$\underline{B}_{\perp} \simeq B_{\perp} - \beta \times E_{\perp} \,. \tag{15}$$

More explicitly for $\boldsymbol{B} = \frac{I_0}{2\pi cR} \hat{\boldsymbol{y}}$ and $\boldsymbol{\beta} = \beta \hat{\boldsymbol{z}}$ (see coordinates in Fig. 1) we find

$$\underline{E}^x = -\frac{v}{c} \frac{I_0}{2\pi cR} \tag{16}$$

$$\underline{B}^y = \frac{I_0}{2\pi cR} \,. \tag{17}$$

The electric field is produced by the charges in the wire. If in the original frame the charge density is $\rho = 0$ and the current density is $j = I_0/A_{\perp}$, so that the four current density is $J^{\mu}/c = (0, j/c)$, then the transformed four current density is

$$\begin{pmatrix} \underline{\rho} \\ \underline{j/c} \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta \\ -\gamma\beta & \gamma \end{pmatrix} \begin{pmatrix} 0 \\ j/c \end{pmatrix} .$$
(18)

With the non-relativistic approximation we have

$$\underline{\lambda} \simeq -\frac{I_0}{c} \left(\frac{v}{c}\right) \,, \tag{19}$$

$$\underline{I}_0 \simeq I_0 \,. \tag{20}$$

Clearly this charge density yields results consistent with Eq. (16)

$$\underline{\underline{E}}^{x} = \frac{\underline{\lambda}}{2\pi R} = -\frac{I_{0}}{2\pi c R} \left(\frac{\underline{v}}{c}\right) , \qquad (21)$$

(d) The calculation is the same as part (a) with the replacement

$$\lambda \to -\frac{I_0}{c} \frac{v}{c} \,. \tag{22}$$

The force is then

$$F_{\rho} = -\left(\frac{I_0}{2\pi c}\right)^2 \left(\frac{v}{c}\right)^2 \frac{8\pi a^3}{R^3}.$$
(23)

which agrees with the estimate of part (b).

⁴It is easy to remember these formulas – If a non-relativistic particle has velocity $\boldsymbol{\beta}$ and Lorentz force $\boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{\beta} \times \boldsymbol{B})$, then after a small boost by $\boldsymbol{\beta}$ its velocity is zero, but the force is unchanged $\boldsymbol{F} = q\underline{E}$.

Electromagnetism 2

Dispersion in collisionless plasmas with an external magnetic field

Model a cold non-relativistic collisionless plasma as a system of non-interacting classical electrons of uniform number density n_0 . The electrons have charge q and mass m and are initially at rest. The electrons sit in a stationary and uniform background of positive charges of charge density $+|q|n_0$, whose only role in this problem is to neutralize the overall charge of the system. In the presence of an external electromagnetic field the electrons begin to move according to the classical equation of motion

$$m\frac{d^2\boldsymbol{x}}{dt^2} = q(\boldsymbol{E}(t,\boldsymbol{x}) + \frac{\boldsymbol{v}}{c} \times \boldsymbol{B}(t,\boldsymbol{x})).$$
(1)

Consider an electromagnetic plane wave with electric field $\boldsymbol{E}(t, \boldsymbol{x}) = \boldsymbol{E}_0 e^{-i\omega t + i\boldsymbol{k}\cdot\boldsymbol{x}}$ propagating in the plasma. The amplitude \boldsymbol{E}_0 is sufficiently small that the plasma is only weakly perturbed.

(a) (3 points) Determine the current density $\mathbf{j}(t, \mathbf{x})$ induced by the plane wave. Express your results in terms of the plasma frequency $\omega_p^2 = \frac{q^2 n_0}{m}$.

Hint: Work to leading order in the amplitude of the external field E_0 , so that an electron's position is constant up to small corrections proportional to E_0 , $\boldsymbol{x}(t) = \boldsymbol{x}_0 + \delta \boldsymbol{x}(t, \boldsymbol{x}_0)$.

- (b) (3 points) Determine the induced charge density $\rho(t, \boldsymbol{x})$. Show that \boldsymbol{E}_0 is transverse to \boldsymbol{k} for generic frequency ω .
- (c) (5 points) Determine the permittivity of the plasma, $\epsilon(\omega)$, as a function of frequency. Find a dispersion relation, $k(\omega)$, for the electromagnetic plane wave. For what range of frequencies will the plane wave propagate in the plasma? Explain.
- (d) (3 points) For $\omega \gg \omega_p$, how much does the group velocity of the wave deviate from the vacuum speed of light?

Now place the plasma in a strong time independent and homogeneous magnetic field of magnitude \mathcal{B}_0 pointing in z direction. We will reanalyze the dispersion relation when the additional magnetic field is present. For circularly polarized waves with $\mathbf{k} = k\hat{\mathbf{z}}$ in the z direction, the the electric field take the form

$$\boldsymbol{E}_{\pm}(t,\boldsymbol{x}) = E_0 \boldsymbol{\epsilon}_{\pm} e^{-i\omega t + ikz}, \quad \text{with} \quad \boldsymbol{\epsilon}_{\pm} \equiv \frac{\boldsymbol{x} \pm i\boldsymbol{y}}{\sqrt{2}}.$$
(2)

(e) (2 points) Determine the current induced by the circularly polarized waves. Express your result in terms of the plasma frequency ω_p^2 and the cyclotron frequency⁵

⁵In SI units $\Omega_c = q \mathcal{B}_0/m$.

 $\Omega_c = q \mathcal{B}_0/mc.$

Hint: Assume that $\delta \boldsymbol{x}(t, \boldsymbol{x}_0)$ is proportional to $\boldsymbol{\epsilon}_{\pm}$ and work to leading order in the electric field.

(f) (4 points) Determine the dispersion relation $k_{\pm}(\omega)$ of circularly polarized plane waves in the presence of \mathcal{B}_0 . Describe qualitatively how linearly polarized light at high frequency $\omega \gg \omega_p$ would change upon traversing a region of weak magnetic field.

Solution

(a) The electron coordinate is peturbed from its equilibrium position harmonically:

$$\boldsymbol{x}(t) = \boldsymbol{x}_0 + \underbrace{\boldsymbol{x}_{\omega}(\boldsymbol{x}_0)e^{-i\omega t}}_{\equiv \delta \boldsymbol{x}(t, \boldsymbol{x}_0)}, \qquad (3)$$

where here and below we notate harmonic time dependence of the variables with a subscript, e.g.

$$\boldsymbol{E}(t,\boldsymbol{x}_0) = \boldsymbol{E}_{\omega}(\boldsymbol{x}_0)e^{-i\omega t}, \qquad \boldsymbol{E}_{\omega}(\boldsymbol{x}_0) \equiv \boldsymbol{E}_0e^{i\boldsymbol{k}\cdot\boldsymbol{x}_0}.$$
(4)

Substituting Eq. (3) into the Newtonian equations of motion and solving to first order E_0 and δx we find

$$-m\omega^2 \boldsymbol{x}_{\omega} e^{-i\omega t} = q \boldsymbol{E}_0 e^{i\boldsymbol{k}\cdot\boldsymbol{x}_0 - i\omega t}, \qquad (5)$$

yielding

$$\boldsymbol{x}_{\omega}(\boldsymbol{x}_{0}) = -\frac{q\boldsymbol{E}_{0}(\boldsymbol{x}_{0})}{m\omega^{2}}.$$
(6)

Thus the harmonic current at point \boldsymbol{x}_0 is

$$\boldsymbol{j}(t,\boldsymbol{x}_0) = q n_0 \boldsymbol{v}(t,\boldsymbol{x}_0) = -\frac{n_0 q^2}{m \omega^2} \left(-i\omega \boldsymbol{E}_{\omega}(\boldsymbol{x}_0) e^{-i\omega_t}\right),\tag{7}$$

$$= -\frac{\omega_p^2}{\omega^2} \left(-i\omega \boldsymbol{E}_{\omega}(\boldsymbol{x}_0) \, e^{-i\omega t} \right), \tag{8}$$

where we have defined the plasma frequency

$$\omega_p^2 \equiv \frac{n_0 q^2}{m} \,. \tag{9}$$

(b) Once the current is specified the continuity equation

$$\partial_t \rho(t, \boldsymbol{x}_0) + \nabla_{\boldsymbol{x}_0} \cdot \boldsymbol{j}(t, \boldsymbol{x}_0) = 0, \qquad (10)$$

determines the induced charge density

$$\rho_{\omega}(\boldsymbol{x}_{0}) = \frac{\boldsymbol{k} \cdot \boldsymbol{j}_{\omega}(\boldsymbol{x}_{0})}{\omega}, \qquad (11)$$

$$= \frac{\omega_p^2}{\omega^2} i \boldsymbol{k} \cdot \boldsymbol{E}_0 e^{i \boldsymbol{k} \cdot \boldsymbol{x}_0} \,. \tag{12}$$

The Gaus law gives

$$\nabla \cdot \boldsymbol{E}_{\omega}(\boldsymbol{x}_0) = \rho_{\omega}(\boldsymbol{x}_0), \qquad (13)$$

yielding

$$i\boldsymbol{k}\cdot\boldsymbol{E}_{0} = \frac{\omega_{p}^{2}}{\omega^{2}}i\boldsymbol{k}\cdot\boldsymbol{E}_{0}.$$
(14)

For generic frequency this equation requires that $\mathbf{k} \cdot \mathbf{E}_0 = 0$, i.e. \mathbf{E}_0 is transverse. For the specific frequency $\omega = \omega_p$, longtidunal modes, known as plasma oscillations, are possible. Except at this frequency, the induced charged density is zero.

(c) The frequency dependent dielectric susceptibility is defined through the linear constitutive equation

$$\boldsymbol{j}_{\omega}(\boldsymbol{x}_{0}) = -i\omega\chi(\omega)\boldsymbol{E}_{\omega}(\boldsymbol{x}_{0}), \qquad (15)$$

and thus comparing Eq. (15) and Eq. (7) we find

$$\epsilon(\omega) = 1 + \chi(\omega) \qquad \chi(\omega) = -\frac{\omega_p^2}{\omega^2}.$$
(16)

In terms of χ the density reads

$$\rho = -\chi(\omega)(i\boldsymbol{k}\cdot\boldsymbol{E}_{\omega}) \tag{17}$$

Given the linear constitutive relations and the Maxwell equations

$$\nabla \cdot \boldsymbol{E}_{\omega} = \rho_{\omega} \,, \tag{18}$$

$$+i\frac{\omega}{c}\boldsymbol{E}_{\omega}+\nabla\times\boldsymbol{B}_{\omega}=\frac{\boldsymbol{j}_{\omega}}{c}\,,\tag{19}$$

$$\nabla \cdot \boldsymbol{B}_{\omega} = 0, \qquad (20)$$

$$-i\frac{\omega}{c}\boldsymbol{B}_{\omega} + \nabla \times \boldsymbol{E}_{\omega} = 0, \qquad (21)$$

we deduce that

$$\frac{\omega^2}{c^2}\epsilon(\omega) - k^2 = 0.$$
(22)

Thus, there are nontrivial solutions for specific values of k:

$$k(\omega) = \frac{\omega}{c} \sqrt{1 - \frac{\omega_p^2}{\omega^2}}.$$
(23)

For frequencies less than the plasma frequency, k is imaginary and the plasma does not support travelling waves. For frequencies greater than ω_p travelling waves are supported.

(d) At large frequencies we have

$$k(\omega) \simeq \frac{\omega}{c} \left(1 - \frac{\omega_p^2}{2\omega^2}\right),$$
 (24)

and we may solve approximately for $\omega(k)$

$$\omega(k) \simeq ck \left(1 + \frac{\omega_p^2}{2(ck)^2} \right) \,. \tag{25}$$

Differentiating with respect to k we determine the group velocity

$$v_g = \frac{d\omega}{dk} \simeq c \left(1 - \frac{\omega_p^2}{2c^2k^2} \right) \,. \tag{26}$$

Notice that the phase velocity $\omega(k)/k$ is greater than the speed of light, while the group velocity is less than the speed of light as should be the case.

(e) Now we have a strong magnetic field in the z direction. Since the light is circularly polarized we try the suggested ansatz

• 1

$$\boldsymbol{x}(t,\boldsymbol{x}_0) = x_{\omega}(\boldsymbol{x}_0)e^{-i\omega t}\boldsymbol{\epsilon}_+ \,. \tag{27}$$

The velocity is

$$\boldsymbol{v}(t,\boldsymbol{x}_0) = -i\omega x_{\omega}(\boldsymbol{x}_0)e^{-i\omega}\boldsymbol{\epsilon}_+\,,\tag{28}$$

and $\boldsymbol{v} \times \boldsymbol{B}$ is proportional to

$$\boldsymbol{\epsilon}_{\pm} \times \hat{\boldsymbol{z}} = (\hat{\boldsymbol{x}} \pm i\hat{\boldsymbol{y}}) \times \hat{\boldsymbol{z}}, \qquad (29)$$

$$= (-\hat{\boldsymbol{y}} \pm i\hat{\boldsymbol{x}}), \qquad (30)$$

$$=\pm i\boldsymbol{\epsilon}_{\pm}.$$

Substituting this form into the Newtonian equations of motion

$$m\frac{d^2\boldsymbol{x}(t,\boldsymbol{x}_0)}{dt} = q\left(\boldsymbol{E}_0(t,\boldsymbol{x}_0) + \frac{\boldsymbol{v}(t,x)}{c} \times \boldsymbol{\mathcal{B}}_0 \hat{\boldsymbol{z}}\right), \qquad (32)$$

we find

$$-m\omega^2 x_\omega = qE_0 e^{ikz} \pm \omega \frac{q}{c} \mathcal{B}_0 x_\omega , \qquad (33)$$

Minor manipulations yield

$$x_{\omega} = -\frac{qE_0 e^{\imath k z}}{m\omega} \frac{1}{\omega \pm \Omega_c}, \qquad (34)$$

where $\Omega_c = q \mathcal{B}_0 / mc$ is the cyclotron frequency. The induced current is

$$\boldsymbol{j}_{\omega} = n_0 q(-i\omega x_{\omega})\boldsymbol{\epsilon}_{\pm} \,, \tag{35}$$

$$= \left[-\frac{\omega_p^2}{\omega(\omega \pm \Omega_c)} \right] \left(-i\omega E_0 e^{ikz} \boldsymbol{\epsilon}_{\pm} \right) \,. \tag{36}$$

(f) Following the logic of part (c) the required dispersion relation is

$$k_{\pm}(\omega) = \frac{\omega}{c} \left[1 - \frac{\omega_p^2}{\omega(\omega \pm \Omega_c)} \right]^{1/2} .$$
(37)

For a $\omega \gg \omega_p \sim \Omega_c$ we have

$$k_{\pm}(\omega) = \frac{\omega}{c} \left(1 - \frac{\omega_p^2}{2\omega^2} \pm \frac{\omega_p^2 \Omega_c}{2\omega^3} + \dots \right) , \qquad (38)$$

and thus to order k^{-2} inclusive the dispersion relation reads

$$\omega_{\pm}(\boldsymbol{k}) = ck \left(1 + \frac{\omega_p^2}{2(ck)^2} \mp \frac{\omega_p^2 \Omega_c}{2(ck)^3} + \dots \right) \,. \tag{39}$$

Because the eigen frequencies of right-handed and left handed waves are different by a small amount, after a period of time ΔT the two waves will accumulate a small phase difference $\sim \omega_p^2 \Omega_c/(ck)^2 \Delta T$. The linearly polarized light will appear to slowly precess in time as it traverses the medium.

Electromagnetism 3

A relativistic particle

A relativistic particle of charge Q moves with constant velocity v along the z axis, crossing the origin at time t = 0. A stationary observer sits at point \mathcal{O} with spatial coordinates (b, 0, 0)as shown below. The questions below ask for the fields in the rest frame of this observer, i.e. the lab frame.



- (a) (4 points) Determine the vector potential in the Lorenz gauge at an arbitrary point (\vec{r}_{\perp}, z) as a function of time. Here $\vec{r}_{\perp} = (x, y)$ denotes the coordinates transverse to the motion.
- (b) (4 points) Use part (a) to determine the electric and magnetic fields at \mathcal{O} as a function of time. Verify that

$$oldsymbol{B}(oldsymbol{r},t) \propto oldsymbol{v} imes oldsymbol{E}(oldsymbol{r},t)$$
 .

- (c) (2 points) Find the ratio $|\boldsymbol{B}(\boldsymbol{r},t)| / |\boldsymbol{E}(\boldsymbol{r},t)|$ at point \mathcal{O} as a function of time. When does this ratio reach a maximum?
- (d) (4 points) At time t the particle is a distance R(t) from the point \mathcal{O} (see above). Find the ratio of the magnitude the electric field to the corresponding Coulomb expectation, i.e. determine

$$u \equiv \frac{|\boldsymbol{E}(\boldsymbol{r},t)|}{Q/R^2(t)} \tag{1}$$

as function of time.

- (i) Sketch the ratio u versus time for $\gamma \gg 1$.
- (ii) For $\gamma \gg 1$, find the time t_C when the ratio u is of order unity. Show that t_C vanishes as $v/c \to 1$.

(e) (6 points) Now consider a annular area lying in the xy plane as shown below. The area has inner radius b_1 and and outer radius b_2 with $b_2 \gg b_1$. Calculate the electromagnetic energy that crosses the area as the particle passes from $z = -\infty$ to $z = +\infty$.

The following integral may be useful:

$$\int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^n} = \sqrt{\pi} \frac{\Gamma(-\frac{1}{2}+n)}{\Gamma(n)} \quad \text{with} \quad \Gamma(\frac{1}{2}) = \sqrt{\pi}$$
(2)

Solution

(a) In the particle frame the vector potential is

$$\underline{A}^{0}(\underline{x}) = \frac{Q}{4\pi\sqrt{\underline{r}_{\perp}^{2} + \underline{z}^{2}}}, \qquad \underline{A}^{i}(\underline{x}) = 0.$$
(3)

We boost to the "lab" frame using the Lorentz transformation:

$$A^{\mu}(x) = (\mathcal{L})^{\mu}{}_{\nu}\underline{A}^{\nu}(\underline{x}), \qquad (4)$$

$$x^{\mu} = (\mathcal{L})^{\mu}{}_{\nu}\underline{x}^{\nu} , \qquad (5)$$

$$\underline{x}^{\mu} = (\mathcal{L}^{-1})^{\mu}_{\ \nu} x^{\nu} , \qquad (6)$$

where

$$(\mathcal{L})^{\mu}{}_{\nu} = \begin{pmatrix} \gamma & 0 & 0 & \gamma\beta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \gamma\beta & 0 & 0 & \gamma \end{pmatrix}, \qquad (\mathcal{L}^{-1})^{\mu}{}_{\nu} = \begin{pmatrix} \gamma & 0 & 0 & -\gamma\beta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\gamma\beta & 0 & 0 & \gamma \end{pmatrix}.$$
(7)

Thus

$$A^{0}(x) = \gamma \underline{A}^{0} \tag{8}$$

$$=\frac{Q}{4\pi}\frac{\gamma}{\sqrt{\vec{r}_{\perp}^2+\gamma^2(z-vt)^2}}\tag{9}$$

$$A^{z}(x) = \gamma \beta \underline{A}^{0}, \qquad (10)$$

$$= \frac{Q}{4\pi} \frac{\gamma\beta}{\sqrt{\vec{r}_{\perp}^2 + \gamma^2 (z - vt)^2}},\tag{11}$$

where we used

$$\vec{\underline{r}}_{\perp} = \vec{r}_{\perp} \,, \tag{12}$$

$$\underline{z} = \gamma z - \gamma v t \,. \tag{13}$$

(b) Then, using a, b, c, \ldots to denote transverse coordinates (so that E^a denotes (E^x, E^y) and r^a_{\perp} denotes (x, y)), we evaluate the transverse electric field:

$$E^a = -\partial^a A^0, \qquad (14)$$

$$= \frac{Q}{4\pi} \frac{\gamma r_{\perp}^{a}}{(\vec{r}_{\perp}^{2} + \gamma^{2}(z - vt)^{2})^{3/2}},$$
(15)

Similarly for the longitudinal electric field (do this algebra and see a cancellation!) :

$$E^{z} = -\frac{1}{c}\partial_{t}A^{z} - \partial^{z}A^{0}, \qquad (16)$$

$$= \frac{Q}{4\pi} \frac{\gamma^3 (z - vt)}{(\vec{r}_{\perp}^2 + \gamma^2 (z - vt)^2)^{3/2}} \left(-\beta^2 + 1\right) , \qquad (17)$$

$$= \frac{Q}{4\pi} \frac{\gamma(z - vt)}{(\vec{r}_{\perp}^2 + \gamma^2 (z - vt)^2)^{3/2}}.$$
 (18)

In the second line, the first term in parentheses comes from the time derivative of A^z , while the second term comes from the spatial derivative of A^0 . Then, we evaluate the magnetic field $B^i = \epsilon^{ijk} \partial_j A_k$

$$B^a = \epsilon^{abz} \partial_b A_z \,, \tag{19}$$

$$=\epsilon^{abz}(\beta\partial_b A^0)\,,\tag{20}$$

$$=\epsilon^{abz}(-E_b\beta). \tag{21}$$

where we have used that $A^z = \beta A^0$ and Eq. (14). The longitudinal magnetic field is zero since $\epsilon^{ziz} = 0$

$$B^z = 0. (22)$$

Thus from Eq. (19), we find

$$\vec{B}_{\perp} = -\vec{E}_{\perp} \times \boldsymbol{\beta} \,, \tag{23}$$

with $\boldsymbol{\beta} = \beta \hat{\boldsymbol{z}}$. This can be written

$$\boldsymbol{B} = \boldsymbol{\beta} \times \boldsymbol{E} \,. \tag{24}$$

Finally, we specialize these expressions to their values at the specific point \mathcal{O} :

$$E^{x} = \frac{Q}{4\pi} \frac{\gamma b}{(b^{2} + \gamma^{2} (vt)^{2})^{3/2}},$$
(25)

$$E^{z} = \frac{Q}{4\pi} \frac{-\gamma vt}{(b^{2} + \gamma^{2}(vt)^{2})^{3/2}},$$
(26)

$$B^{y} = \frac{Q}{4\pi} \frac{\gamma \beta b}{(b^{2} + \gamma^{2} (vt)^{2})^{3/2}},$$
(27)

with all other components zero.

(c) The required ratio is

$$\frac{|\boldsymbol{B}|}{|\boldsymbol{E}|} = \frac{\beta b}{\sqrt{b^2 + (vt)^2}} \tag{28}$$

Clearly this ratio reaches a maximum of β at t = 0.

(d) Note that $R^2 = b^2 + (vt)^2$ so the required ratio is

$$u = \frac{|\mathbf{E}|}{Q^2/(4\pi R^2)} = \gamma \left(\frac{b^2 + (vt)^2}{b^2 + \gamma^2(vt)^2}\right)^{3/2}.$$
(29)

(i) To understand this quantity let us plot it versus $y \equiv (vt)/b$

$$u = \gamma \left(\frac{1+y^2}{1+\gamma^2 y^2}\right)^{3/2} \,. \tag{30}$$

A sketch of this quantity for $\gamma = 10$ is shown below.



(ii) For $\gamma \gg 1$ we may approximate Eq. (30)

$$u = \frac{1}{\gamma^2} \left(\frac{1+y^2}{y^2}\right)^{3/2} \,. \tag{31}$$

In order for u to be unity for $\gamma \gg 1$, we require $y \ll 1$ and we may replace $1 + y^2 \rightarrow 1$ in Eq. (31). Thus, in this limit

$$u \simeq \frac{1}{\gamma^2 y^3} \,, \tag{32}$$

and we find that u is unity when

$$y = \gamma^{-2/3}$$
, or $t_C = \frac{b}{c\gamma^{2/3}}$. (33)

(e) To estimate the energy transported across the detector we have to integrate the energy flux over time:

$$dU = \int_{b_1}^{b_2} 2\pi b db \int_{-\infty}^{\infty} S^z dt \,.$$
 (34)

The Poynting vector is

$$dtS^{z} = c(\mathbf{E} \times \mathbf{B})^{z}dt = \frac{Q^{2}\gamma}{16\pi^{2}b^{3}} \frac{(\gamma v dt/b)}{(1 + (\gamma v t/b)^{2})^{3}}.$$
(35)

Switching variables to $w \equiv \gamma v t/b$ we find

$$U = \int_{b_1}^{b_2} (2\pi b) db \; \frac{Q^2 \gamma}{16\pi^2 b^3} \int_{-\infty}^{\infty} \frac{dw}{(1+w^2)^3} \,. \tag{36}$$

The dimensionless w-integral gives a number of order unity, while the remaining b integration is dominated by the lower end, yielding our estimate:

$$U \sim \frac{Q^2 \gamma}{b_1} \,. \tag{37}$$

The leading factor Q^2/b is required by dimension. The factor of γ arises because the E and B fields are each of order $\sim \gamma Q/b^2$ at maximum. The Poynting vector is $S \propto c \gamma^2 Q^2/b^4$ at maximum. But, the duration of the pulse is only of order $\Delta t \sim b/(c\gamma)$. The area is of order $A \sim \pi b^2$. Thus the energy is of order $U \sim AS\Delta t$ as given in Eq. (37). The exact expression is

$$U = \frac{3}{128} \frac{\gamma Q^2}{b_1} = 0.29 \frac{\gamma Q^2}{4\pi b_1}.$$
(38)

Quantum Mechanics 1

A magnetic barrier

The purpose of this problem is to study charged particle scattering through a planar magnetic barrier. Consider a particle of mass m, charge -e moving in the xy plane through a magnetic strip of width d with $\mathbf{B} = B\hat{z}$ for $0 \leq x \leq d$ and zero elsewhere. Choose the gauge $A_y = Bx$. The particle is incident from x < 0 and moving perpendicular to the barrier along the x-direction.

a. (5 points) If we denote by k and k_T the incident and transmitted wave numbers, find the relationship between k and k_T .

b. (3 points) Under what condition k_T becomes imaginary? Give a classical justification for this condition.

c. (6 points) What is the direction of the transmitted probability flux? Identify the direction for which the condition in **b** is realized.

d. (6 points) Find the reflection and transmission coefficients for the case $d \rightarrow 0$ but Bd fixed. What are the corresponding probability fluxes?

Solution

a. We will choose the gauge $A_{x,y,z} = 0$ for x < 0 and $A_{x,z} = 0$ but $A_y = Bx$ for 0 < x < d for which $B_z = B$. Continuity requires $A_y = Bd$ for x > d. The motion is xy-planar so the Hamiltonian is

$$H = \frac{1}{2m} \left(p_x^2 + \left(p_y + \frac{e}{c} A_y \right)^2 \right) \tag{1}$$

The stationary states follow from

$$\frac{p_x^2}{2m}\varphi = E\varphi \qquad x < 0$$

$$\left(\frac{p_x^2}{2m} + \frac{e^2B^2x^2}{2mc^2}\right)\varphi = E\varphi \qquad 0 < x < d$$

$$\left(\frac{p_x^2}{2m} + \frac{e^2B^2d^2}{2mc^2}\right)\varphi = E\varphi \qquad x > d$$
(2)

The 1-dimensional scattering wave set up is

$$\varphi(x) = e^{ikx} + Re^{-ikx} \qquad x < 0$$

$$\varphi(x) = Te^{ik_T x} \qquad x > d \qquad (3)$$

Inserting (3) for x < 0 and x > d we obtain

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k_T^2}{2m} + \frac{e^2 B^2 d^2}{2mc^2}$$
(4)

which leads to

$$k_T = \left(k^2 - \frac{m^2 \omega^2 d^2}{\hbar^2}\right)^{\frac{1}{2}} \tag{5}$$

with the cyclotron frequency $\omega = eB/mc$.

b. k_T becomes imaginary for $m\omega d > \hbar k$. In this case, the transmitted wave is damped for x > d. Recall that a classical particle of velocity v in the strip undergoes a cyclotron motion of radius $R = v/\omega$. For R > d or $mv/\omega > md$ the classical particle bounces back. This is the condition for which k_T becomes imaginary since $mv \to \hbar k$.

c. The probability current for x > d is fixed by the transmitted wavefunction

$$j_x = \frac{1}{2m} \left(\varphi^* p_x \varphi + \varphi^* p_x^{\dagger} \varphi \right) = |T|^2 \frac{\hbar k_T}{m}$$

$$j_y = \frac{1}{2m} \left(\varphi^* \left(p_y + \frac{eBd}{c} \right) \varphi + \varphi^* \left(p_y + \frac{eBd}{c} \right)^{\dagger} \varphi \right) = |T|^2 \omega d$$
(6)

We now identify

$$\tan \theta = \frac{j_y}{j_x} = \frac{m\omega d}{\hbar k_T} \tag{7}$$

as the angle the probability current makes up with the x-direction. k_T turns complex when $k_T = 0$, for which $\theta = \pi/2$. This corresponds to a current probability along the y-direction.

d. In the double limit $d \to 0$ and Bd fixed, the vector potential is a step function, $A_y = 0$ for x < 0 and $A_y = Bd$ for x > 0. Matching at x = 0 gives

$$1 + R = T$$
$$ik(1 - R) = ik_T T$$
(8)

Specifically, we have

$$R = \frac{k - k_T}{k + k_T}$$
$$T = \frac{2k}{k + k_T}$$
(9)

The normalized probability fluxes are

$$\mathbf{P}_{\mathbf{R}} = \frac{k|R|^2}{k} = \left(\frac{k - k_T}{k + k_T}\right)^2$$
$$\mathbf{P}_{\mathbf{T}} = \frac{k_T|T|^2}{k} = \frac{4kk_T}{(k + k_T)^2}$$
(10)

Quantum Mechanics 2

Diatomic nitrogen

When two identical atoms join to make a molecule, their valence electrons combine to form covalent bonds, and the spins of their (identical) nuclei $\vec{I}_{1,2}$ combine to form a total nuclear spin \vec{I} . The states of the molecule at room temperature may be written as a direct product of an electronic, vibrational, rotational and nuclear-spin state

 $|\psi\rangle_{N_2} = |\psi^{(electronic)}\rangle|\psi^{(vibrational)}\rangle|\psi^{(rotational)}\rangle|\psi^{(nuclear\,spin)}\rangle.$

The lowest excitation energies of these degrees of freedom obey the following hierarchy

$$E_{electronic} \gg E_{vibrational} \gg E_{rotational} \gg E_{nuclear spin}.$$

Here we consider the nitrogen molecule N_2 with two identical ${}^{14}_7N$ nuclei, each with nuclear spin 1.

- (a) (i) State the electronic configuration (i.e. s, p, d etc.) for the ground state of the nitrogen atom and explain why the valence electrons are in different orbitals (or *m*-levels). (ii) Briefly explain the concept of covalent bonds. What is the number of covalent bonds in the N_2 molecule? (iii) Estimate the values of $E_{electronic}$ and $E_{vibrational}$, and show that $E_{electronic} \gg E_{vibrational}$. (6 points)
- (b) Write down the eigenfunctions and energy eigenvalues for the vibrations. What is the symmetry of the vibrational part of the wave function of the ground state under exchange of the two atoms? (2 points)
- (c) Write down the eigenfunctions and energy eigenvalues of the rigid rotator formed by the molecule. What is the symmetry of the rotational part of the wave function of the ground state under exchange of the two atoms? (2 points)
- (d) What are the possible values of the total nuclear spin angular momentum I of the molecule? Neglecting any contribution of the nuclear spin to the energy what is the degeneracy of each I? For each allowed value of the total nuclear spin I, write down the allowed z components (magnetic quantum numbers m_I). Deduce the symmetry of each state $|I, m_I\rangle$ upon interchanging the two nuclei. (4 points)
- (e) It can be shown that the electonic part of the wave function of N_2 is antisymmetric under interchange of the two atoms. Make a rough estimate of the lowest order rotational energies of the molecule and compare it with $k_B T$ at a temperature of 300 °K. Using this estimate, how much more or less likely are you to find an N_2 molecule in the first excited rotational state l = 1 than in the ground state l = 0? (6 points)

(a) The electronic assignment of each ¹⁴N atom is $1s^2, 2s^2, 2p^3$. The outer orbitals are $2p^3 = 2(p_x, p_y, p_z)$. No two electrons can be in the same orbital if one wants to minimize the Coulomb repulsion between the electrons.

There are 3 covalent bonds: one electron from each atom in the p_x orbital, another pair in the p_y orbital, and a third pair in the p_z orbital. A covalent bond occurs when the orbital parts of such pairs of electrons is symmetric. Then this pair of electrons can come close to each other, and when that pair sits between the two atomic nuclei, one gets strong binding.

The value of $E_{\text{electronic}}$ follows from the uncertainty relation $\Delta x \Delta p \sim \hbar$ where Δx is equal to the size of the whole molecule, $\Delta x \sim 10^{-8}$ cm, and then $E_{\text{electronic}} = p^2/2m_e \sim \hbar^2/m_e (\Delta x)^2 \sim 2$ eV.

The vibrational energies of the nuclei are a factor $\sqrt{m_e/m_N}$ smaller, since the Coulomb interaction between two nuclei, and one nucleus and one electron, is the same. Using that for a harmonic oscillator $\omega = \sqrt{k/m}$, we get $E_{\text{vibrational}}/E_{\text{electronic}} \sim \sqrt{m_e/m_N}$. So $E_{\text{vibrational}} \sim 1/170 \times 2 \text{ eV} \sim 1/80 \text{ eV}$, smaller than room temperature.

- (b) The vibrations form a harmonic oscillator. The energy eigenfunctions are (proportional to) the Hermite polynomials times a Gaussian, and the energy eigenvalues are $E_n = (n + 1/2)\hbar\omega$. The ground state is proportional to $e^{-\gamma(\Delta R)^2}$, and hence it is symmetric under exchange of the two atoms.
- (c) The rigid rotator has $H = \vec{L} \cdot \vec{L}/(IN)$ where IN is the inertial moment given by $IN = \mu R^2$ with $\mu = (1/2)M_N$ the reduced mass, and R the internuclear distance. The eigenfunctions are the $Y_L^M(\theta, \phi)$ and the energy eigenvalues are $\hbar^2 L(L+1)/IN$. The ground state is Y_0^0 , and therefore it is also symmetric under exchange of the two atoms.
- (d) The largest weight state in the I = 2 shell is $|2, 2\rangle$ which is necessarily of the form $|2, 2\rangle = |1, 1\rangle |1, 1\rangle$ and symmetric. It is easy to guess that the shell with $|1, 1\rangle$ is antisymmetric and that the shell with $|0, 0\rangle$ is symmetric. Indeed, for $|1, 1\rangle$ the only allowed linear combinations by parity (symmetric molecule) are

$$|1,1\rangle_{\pm} = \frac{1}{\sqrt{2}} (|1,1\rangle |1,0\rangle \pm |1,0\rangle |1,1\rangle)$$
 (11)

It is easily checked that the raising operator $(I^+ = I_1^+ + I_2^+) |1, 1\rangle_{-} = 0$, which selects the antisymmetric combination, as the symmetric one does not vanish.

(e) The values of $E_{\text{rotational}}$ are $\frac{1}{2}\hbar^2 L(L+1)/(\mu R^2)$ where L = 0, 1, 2, ... and $\mu = \frac{1}{2}m_N$ is the reduced mass of the two nuclei.From $R \sim 0.15$ nm and $m_N c^2 \sim 14 \times 1000$ MeV. For L = 1 one obtains $E \sim \frac{1}{3}10^{-15}$ ergs $\sim \frac{1}{5}10^{-3}$ eV. This is much smaller that the $kT = \frac{1}{40}$ eV of room temperature, so the Boltzmann factor for rotational states is essentially one.

If the total (orbital + spin) part of the electronic wave function is antisymmetric under interchange of the atoms, the product of the other parts has to be symmetric. The vibrational part is always symmetric, and since the ¹⁴N atoms satisfy Fermi-Dirac statistics (14+7=odd), the spin part of the nuclei must be symmetric/antisymmetric if the rotational part is symmetric/antisymmetric. So the states with L = 0 can only have I = 2 and I = 0 and the total number of such states is $d_1 = 1 \times (5+1) = 6$, while L = 1 states can only have I = 1 and $d_0 = 3 \times 3 = 9$. Hence P(L = 1)/P(L = 0) = 9/6. (If the electronic part of the wave function were symmetric, one would find for this ratio the value of 6.)

Quantum Mechanics 3

Two spins-1/2

Consider a two-component system which may be described by the net spin operator $\hat{\mathbf{S}} \equiv \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$, where $\hat{\mathbf{s}}_j \equiv (\hbar/2)\hat{\mathbf{\sigma}}$, with j = 1, 2, are the usual spin- $\frac{1}{2}$ vector-operators of its components. The interaction of the components is described by the Hamiltonian

$$\hat{H} = \left(\hbar \hat{I} - 2\hat{s}_1^z\right) \left(\hbar \hat{I} - 2\hat{s}_2^z\right),$$

where \hat{I} is the identity operator, and \hat{s}_j^z is the Cartesian component of the operator \hat{s}_j along a certain axis *z*.

A (2 points). Express ket-vectors of all simultaneous eigenstates of operators \hat{S}^2 and \hat{S}_z via the eigenkets $|\uparrow\rangle$ and $|\downarrow\rangle$ of the operators \hat{s}_j^z . Calculate the corresponding eigenvalues of the operators \hat{S}^2 and \hat{S}_z .

B (4 points). Are these eigenstates, considered in part A, the stationary states of this interacting system? (Prove your answer.)

C (2 points). Suppose that the initial state of the system at t = 0 is described by the ket-vector

$$|\alpha(0)\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}} \otimes \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}},$$

where each operand of the direct product describes the corresponding component of the system. Calculate $|\alpha(t)\rangle$.

* * *

Now consider the reduced density operator of the component 1, formed from the full density operator of the system by tracing out the degrees of freedom of the component 2:

$$\hat{\rho}_{1}(t) \equiv \sum_{2=\uparrow,\downarrow} \langle 2 | \otimes (|\alpha(t)\rangle \langle \alpha(t)|) \otimes |2\rangle.$$

D (4 points). Prove that in the z-basis, the reduced density matrix may be always expressed as

$$\rho_1(t) = \frac{1}{2} [1 + \mathbf{r}(t) \cdot \boldsymbol{\sigma}],$$

where $\sigma = {\sigma_x, \sigma_y, \sigma_z}$ is the vector of Pauli matrices, and $\mathbf{r}(t)$ is a time-dependent *c*-number vector.

E (6 points). For our system, with the initial state specified in C, calculate $\mathbf{r}(t)$, and sketch $r^2(t)$ as a function of time.

F (2 points). Calculate $1 - Tr(\rho_1^2)$ as a function of time, and give an interpretation of this measure. At what time are the system's components maximally entangled?

Solutions

A. One considers $s^- \equiv (s^x - is^y) = \hbar |\downarrow\rangle\langle\uparrow|$ and use total $S_{\text{tot}}^- = s_1^- + s_2^-$ to lower $|1,1\rangle$ to $|1,0\rangle$:

$$|1,0\rangle \propto S_{\text{tot}}^{-}|1,1\rangle = (s_{1}^{-} + s_{2}^{-})|\uparrow\rangle \otimes |\uparrow\rangle = \hbar|\downarrow\rangle \otimes |\uparrow\rangle + \hbar|\uparrow\rangle \otimes |\downarrow\rangle.$$
(1)

Normalizing it, we get $|1,0\rangle = (|\downarrow\rangle \otimes |\uparrow\rangle + |\uparrow\rangle \otimes |\downarrow\rangle)/\sqrt{2}$. One can check that Given $|1,1\rangle$, $|1,0\rangle$, and $|1,-1\rangle$, the remaining state is $|0,0\rangle = a|\uparrow\rangle \otimes \downarrow\rangle + b|\downarrow\rangle \otimes |\uparrow\rangle$. Requiring this to be orthogonal to the former three, one can solve for a and b and arrive at $|1,-1\rangle = (-|\downarrow\rangle \otimes |\uparrow\rangle + |\uparrow\rangle \otimes |\downarrow\rangle)/\sqrt{2}$. The problem is simple enough that one does not even need to use the formula $S^{-}|S,m\rangle = \sqrt{(S+m)(S-m+1)} \hbar |S,m-1\rangle$, though of course this will give the same answer.

B. Using the basis $\{|\uparrow,\uparrow\rangle,|\uparrow\rangle,\downarrow\rangle,|\downarrow,\uparrow\rangle,|\downarrow,\downarrow\rangle\}$, the Hamiltonian is diagonal with diagonal elements being (0,0,0,4), i.e.,

Thus we see that H is diagonal in the $|S_{tot}, S_z\rangle$ basis, and the spin states of part (a) are the stationary eigenstates of the Hamiltonian.

C. The evolution operator and evolved wave function read

$$U(t) = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & e^{-i4t} \end{pmatrix}, \quad |\psi(t)\rangle = (|\uparrow\rangle\otimes|\uparrow\rangle+|\uparrow\rangle\otimes|\downarrow\rangle+|\downarrow\rangle\otimes|\uparrow\rangle+e^{-4it}|\downarrow\rangle\otimes|\downarrow\rangle)/2.$$
(3)

D. The reduced density matrix is a hermitian 2×2 matrix. A complete basis for such matrices is $\sigma_x, \sigma_y, \sigma_z$ and the identity 1. Thus the reduced density matrix takes the form

$$\rho = c_0(t)\mathbb{1} + \mathbf{c}(t) \cdot \boldsymbol{\sigma} \tag{4}$$

where $\mathbf{c}(t)$ is a vector of three real numbers. In addition we must have $\text{Tr}[\rho] = 1$. Since the Pauli matrices are traceless and $\text{Tr}[\mathbb{1}] = 2$, we must have $c_0(t) = 1/2$. Thus the full density matrix must take form

$$\rho = \frac{1}{2} \left(\mathbb{1} + \mathbf{r}(t) \cdot \boldsymbol{\sigma} \right) \,. \tag{5}$$

where $\mathbf{r}(t)$ is a real three dimensional vector. The density matrix satisfies

$$\operatorname{Tr}[\rho^2] \leqslant 1 \tag{6}$$

with equality holding for a pure state. This restriction places a restriction on $\mathbf{r}(t)$.

$$Tr[\rho^{2}] = \frac{1}{2} \left(1 + |\boldsymbol{r}(t)|^{2} \right)$$
(7)

E. First note that $_2\langle \uparrow | \cdot |\psi(t) \rangle = (|\uparrow\rangle + |\downarrow\rangle)/2$, and $_2\langle \downarrow | \cdot |\psi(t) \rangle = (|\uparrow\rangle + e^{-4it} |\downarrow\rangle)/2$. Thus, we have

$$\rho_A(t) = \frac{1}{4} \begin{pmatrix} 1\\1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 1\\e^{-4it} \end{pmatrix} \begin{pmatrix} 1 & e^{4it} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & \frac{1+e^{4it}}{2} \\ \frac{1+e^{-4it}}{2} & 1 \end{pmatrix},$$
(8)

and find

$$\boldsymbol{r}(t) = (1 + \cos(4t), -\sin(4t), 0)/2, \qquad (9)$$

$$|\mathbf{r}(t)|^2 = (1 + \cos(4t))/2.$$
 (10)

F. The deviation from a pure state is quantified by

$$1 - \text{Tr}[\rho^2] = \frac{1}{2} \left(1 - |\boldsymbol{r}(t)|^2 \right)$$
(11)

which is zero for a pure state. $1 - |r(t)|^2 = (1 - \cos(4t))/2$ achieves minimum (or equivalently the entanglement of the two particles is maximum) at $t = (1 + 2n)\pi/4$, where n is an integer.

Statistical Mechanics 1

Fermi gas

Consider a gas of non-interacting fermions, with the Fermi energy much larger than the thermal energy: $\varepsilon_{\rm F} >> k_{\rm B}T$, in thermal equilibrium.¹ Under this condition:

A (6 points). Calculate the small deviation,

$$\alpha \equiv \mu(T) - E_{\rm F},$$

of the chemical potential μ of the gas from its zero-temperature value E_F , in terms of the coefficients g_0 and g' participating in the Taylor expansion of the density of states $g \equiv (dN/dE)/V$ near the Fermi surface:

 $g \approx g_0 + g'(E - E_F)$, for $E - E_F << E_F$,

where *E* is the energy of one particle.

B (3 points). Estimate g_0 , g' and α in terms of E_F and T.

C (6 points). Calculate the specific heat per unit particle,

$$C_V \equiv \left(\frac{\partial E}{\partial T}\right)_V \; ,$$

in terms of T and g_0 .

D (3 points). Estimate C_V in terms of E_F and T, and compare it with its value for the classical ideal gas.

E (2 points). Estimate the difference $C_P - C_V$, and compare it with its value for the classical ideal gas.

Hint: You may like to use the following integral: $\int_0^\infty \frac{x}{e^x + 1} dx = \frac{\pi^2}{12}.$

¹ This model is frequently used for the description of conduction electrons in metals, where the Coulomb field of electrons is substantially compensated by the virtually equal and opposite field of the nuclei.

Solution

We will use two expressions are of fundamental importance that relate the number of particles, N, and the energy of the system, E, to the density of states:

$$N = V \int_0^\infty g(\epsilon) n_F(\epsilon) \mathrm{d}\epsilon \tag{12}$$

$$E = V \int_0^\infty \epsilon g(\epsilon) n_F(\epsilon) \mathrm{d}\epsilon \tag{13}$$

Here V is the volume, E is the energy of the electron system and $g(\epsilon)$ is the density of states as a function of electron energy ϵ . The Fermi function is

$$n_F = \frac{1}{e^{\beta(E-\mu)} + 1} \tag{14}$$

where $\beta = 1/k_B T$ and μ is the chemical potential (k_B is the Boltzmann constant and T is the temperature). The Fermi energy is defined as the chemical potential at zero temperature: $\epsilon_F = \mu(T = 0)$. The chemical potential is determined by the condition that the number of particles N is independent of the temperature and therefore $dN/d\beta = 0$. The specific heat calculation will require the temperature derivative of the energy, $dE/d\beta = 0$. We can express these two quantities as

$$\frac{\mathrm{d}N}{\mathrm{d}\beta} = V \int_0^\infty g(\epsilon) \frac{\mathrm{d}n_F}{\mathrm{d}\beta} \mathrm{d}\epsilon \tag{15}$$

$$\frac{\mathrm{d}E}{\mathrm{d}\beta} = V \int_0^\infty \epsilon g(\epsilon) \frac{\mathrm{d}n_F}{\mathrm{d}\beta} \mathrm{d}\epsilon \tag{16}$$

We introduce the new integration variable $x = \beta(\epsilon - \mu)$. The derivative of the Fermi function can be expressed as

$$\frac{\mathrm{d}n_F}{\mathrm{d}\beta} = \frac{\mathrm{d}}{\mathrm{d}\beta} \frac{1}{e^x + 1} \frac{\mathrm{d}x}{\mathrm{d}\beta} = \frac{-e^x}{(e^x + 1)^2} \left(\frac{x}{\beta} - \beta \frac{\mathrm{d}\mu}{\mathrm{d}\beta}\right) \tag{17}$$

Let us look at $n'_F(x) = \frac{-e^x}{(e^x+1)^2}$. First, notice that the derivative of the $n_F = 1/(e^x+1)$ function with respect to x is indeed equal to n'_F . The $-n'_F$ function has some interesting properties. It has a maximum of $-n'_F = 1/4$ at x = 0; it has exponentially small values for |x| >> 1; it is an even function of x. In the new variable x the lower limit of integration is $-\mu/\beta$ and in the limit of low temperatures this quantity can be replaced by $-\infty$. The area under the curve (from $x = -\infty$ to $x = +\infty$) is $\int_{-\infty}^{\infty} (-n'_F) dx = 1$. Over the broad range of x values that we are dealing with in this problem, the $-n'_F$ function looks very much like the Dirac delta function, $\delta(x)$.

We use the Taylor expansion of the density of states around x = 0, $g = g(\epsilon = \mu) + (\epsilon - \mu) dg/d\epsilon$. Since we know that the temperature dependence of μ is weak, we can use the density of state values at $\mu = \epsilon_F$, $g = g_0 + (x/\beta)g'$. We get

$$\frac{\mathrm{d}N}{\mathrm{d}\beta} = V \int_{-\infty}^{\infty} \left(g_0 + \frac{x}{\beta} g' \right) \left(\frac{x}{\beta} - \beta \frac{\mathrm{d}\mu}{\mathrm{d}\beta} \right) n'_F \frac{\mathrm{d}x}{\beta} \tag{18}$$

$$\frac{\mathrm{d}E}{\mathrm{d}\beta} = V \int_{-\infty}^{\infty} \left(\frac{x}{\beta} + \mu\right) \left(g_0 + \frac{x}{\beta}g'\right) \left(\frac{x}{\beta} - \beta\frac{\mathrm{d}\mu}{\mathrm{d}\beta}\right) n'_F \frac{\mathrm{d}x}{\beta} \tag{19}$$

Note that here μ and $\beta(d\mu/d\beta)$ are constants, as far as the integration is concerned. We know that $dN/d\beta = 0$ and that can be used to simplify the energy derivative:

$$\frac{\mathrm{d}E}{\mathrm{d}\beta} = \frac{V}{\beta} \int_{-\infty}^{\infty} \frac{x}{\beta} \left(g_0 + \frac{x}{\beta} g' \right) \left(\frac{x}{\beta} - \beta \frac{\mathrm{d}\mu}{\mathrm{d}\beta} \right) n'_F \mathrm{d}x \tag{20}$$

because, according to Eq. 18, the other term (containing the factor μ) is exactly zero.

We have only 4 types of integrals to calculate: $\int n'_F dx$, $\int xn'_F dx$, $\int x^2n'_F dx$ and $\int x^3n'_F dx$. The first integral yields $\int_{-\infty}^{\infty} n'_F dx = -1$ (see above). The second and the fourth is zero, due to the symmetry of n'_F around x = 0. For the third integral we do a partial integration and use the result given in the help section:

$$\int_{-\infty}^{\infty} x^2 n'_F dx = 2 \int_0^{\infty} x^2 n'_F dx = -4 \int_0^{\infty} x n_F dx = -\frac{\pi^2}{3}$$
(21)

A. For the particle number we collect all non-zero terms and make the derivative equal to zero:

$$\frac{\beta}{V}\frac{\mathrm{d}N}{\mathrm{d}\beta} = 0 = g_0\beta\frac{\mathrm{d}\mu}{\mathrm{d}\beta} - g'\frac{\pi^2}{3}\frac{1}{\beta^2}$$
(22)

The chemical potential satisfies

$$g_0 \beta \frac{\mathrm{d}\mu}{\mathrm{d}\beta} = g' \frac{\pi^2}{3} \frac{1}{\beta^2} \tag{23}$$

We solve this differential equation with the boundary condition of $\mu(T=0) = \epsilon_F$

$$\mu = \epsilon_F - \frac{g'}{g_0} \frac{\pi^2}{6} \frac{1}{\beta^2} = \epsilon_F - \frac{g'}{g_0} \frac{\pi^2}{6} k_B^2 T^2$$
(24)

The last part of this expression is $\alpha(T)$.

B. To evaluate the order of magnitude of the temperature dependence, we can take $g'/g_0 \approx 1/\epsilon_F$ and we get $\mu = \epsilon_F \left[1 - a \left(\frac{k_B T}{\epsilon_F} \right)^2 \right]$, with the parameter *a* in the order of unity. We see that indeed, the temperature dependence of the chemical potential is weak, proportional to the square of the temperature. The chemical potential may increase or decrease with temperature, depending on the sign of the first derivative of the density of states. (If g' = 0, for example in the two-dimensional electron gas, the chemical potential is independent of the temperature in this approximation.)

C. For the specific heat calculation we have

$$\frac{1}{V}\frac{\mathrm{d}E}{\mathrm{d}\beta} = \frac{1}{\beta} \int_{-\infty}^{\infty} \frac{x^2}{\beta^2} \left(g_0 - g'\beta \frac{\mathrm{d}\mu}{\mathrm{d}\beta}\right) n'_F \mathrm{d}x \tag{25}$$

Here the first term is much larger than the second term, that has an $1/\beta^2$ temperature dependence, as seen from Eq. 23. Therefore

$$\frac{1}{V}\frac{\mathrm{d}E}{\mathrm{d}\beta} = \frac{g_0}{\beta} \int_{-\infty}^{\infty} \frac{x^2}{\beta^2} n'_F \mathrm{d}x = -\frac{\pi^2}{3} \frac{g_0}{\beta^3}$$
(26)

and

$$C_V = \frac{1}{V} \frac{\mathrm{d}E}{\mathrm{d}\beta} \frac{\mathrm{d}\beta}{\mathrm{d}T} = \frac{-\pi^2}{3} \frac{g_0}{\beta^3} \frac{-1}{k_B T^2} = \frac{\pi^2}{3} g_0 k_B^2 T$$
(27)

This is the well-known temperature-linear specific heat of metallic electrons.

D. Since $g_0 \approx 1/\epsilon_F$, we can express the specific heat as $C_V \propto k_B (k_B T/\epsilon_F)$. For a classical ideal gas the corresponding expression is $C_V = \frac{3}{2}k_B$, independent of temperature. The result shows that in a Fermi gas at low temperature $(k_B T \ll \epsilon_F)$ only a small fraction of particles participate in the thermal response.

E. First we will argue that at low temperatures the two specific heats are very close, $C_P \approx C_V$. In a most general way, $C = \Delta Q/\Delta T$, where ΔQ is the heat transfer needed to raise the temperature by ΔT . It follows that in most systems C_P is larger than C_V . As the temperature is increased, most systems have to expand in order to maintain a constant pressure. The work done by this expansion adds to the amount of heat transfer needed for raising the temperature, thus $C_P > C_V$.

However, in an ideal Fermi gas at low temperature the pressure has very little temperature dependence as it is dominated by the pressure created by the fast-moving Fermions that are pushed to high energy states by the Pauli principle. Therefore constant pressure is maintained without much expansion, and $C_P \approx C_V$.

In a more precise way, the difference between the two quantities can be expressed as $C_P - C_V = VT\alpha^2/\beta_T$, where $\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P$ is the thermal expansion coefficient at constant pressure and $\beta_T = -\frac{1}{V} \left(\frac{\partial V}{\partial P}\right)_T$ is the isothermal compressibility. For a Fermi gas at low temperature α rapidly approaches zero whereas the compressibility is constant, determined by the re-arrangement of electronic states as the Fermions are squeezed together.

As we have shown, the first-order approximation yields $C_V = Ak_B(k_BT/\epsilon_F)$, where A is a numerical constant of the order of unity. Due to the argument outlined above, in first order the formula for C_P will be exactly the same, $C_P = Ak_B(k_BT/\epsilon_F)$. The small difference between the two quantities will appear in the next non-vanishing term of the expansion.

To get the next non-vanishing term for C_V we refer back to Eq. 20. If we continue the Taylor expansion of the density of states to the quadratic term in x, and also include the the quadratic term in the expansion of the chemical potential, we get a more complex integral, but the symmetry properties of the $-n'_F$ function will help us to sort out the vanishing terms.

We conclude that the next non-vanishing term in the expression of the specific heat is cubic in T,

$$C_V = k_B \left[A \frac{k_B T}{\epsilon_F} + B \left(\frac{k_B T}{\epsilon_F} \right)^3 + \dots \right]$$
(28)

where B is a numerical constant of the order of unity.

The other specific heat will have a similar expansion, except for the numerical constant:

$$C_P = k_B \left[A \frac{k_B T}{\epsilon_F} + B' \left(\frac{k_B T}{\epsilon_F} \right)^3 + \dots \right]$$
(29)

The difference is

$$C_P - C_V \approx k_B (B' - B) \left(\frac{k_B T}{\epsilon_F}\right)^3$$
 (30)

or

$$\frac{C_P - C_V}{C_V} \approx D \left(\frac{k_B T}{\epsilon_F}\right)^2 \tag{31}$$

where D is a numerical constant of order of unity. ⁶

Compared to the classical gas, where $C_P - C_V = k_B$, in the Fermi gas the difference is much smaller, for the reasons outlined in the beginning of our discussions.

⁶Please note that the exact result for the ideal Fermi gas in 3 dimensions is $\frac{C_P - C_V}{C_V} = \frac{\pi^2}{3} \left(\frac{k_B T}{\epsilon_F}\right)^2 + O\left(\frac{k_B T}{\epsilon_F}\right)^4$

Statistical Mechanics 2

2D Debye model

Consider a 2D lattice of N >> 1 similar particles, of size $L_x \times L_y$. The particles are elastically coupled, and can vibrate near their equilibrium positions in 2 mutually perpendicular directions. Using the Debye approximation, with the sound speed *c*, for the dispersion law of the resulting elastic waves in the system:

A (2 points). Calculate the spectral density $g(\omega) \equiv dn/d\omega$ of the modes, and their maximum ("cut-off") frequency ω_D .

B (4 points). Derive the general expression for the statistical sum ("partition function") Z of the system.

C (2 points). Calculate approximate expressions for $\ln Z$ in the limits of high and low temperatures.

D (6 points). Calculate internal energy, specific heat and entropy of the system at high and low temperature limits. How do these results compare with those for the usual 3D phonon gas?

E (4 points). Calculate the average number n_l of phonons in the normal mode of frequency ω_l , and its statistical variance $\langle (n_l - \langle n_l \rangle)^2 \rangle$.

E (2 points). Calculate the total number of phonons in the system in the high-temperature and low-temperature limits.

Hint: Useful integrals:

$$\int_0^\infty x \ln(1 - e^{-x}) dx = -\zeta(3) \approx -1.202, \qquad \int_0^\infty \frac{x dx}{e^x - 1} = \Gamma(2)\zeta(2) = \frac{\pi^2}{6}$$

(where $\zeta(x)$ is the Riemann zeta function, and $\Gamma(x)$ is the gamma function).

Solution:

A)
$$k_x = \frac{n_x \pi}{L_x}, k_y = \frac{n_y \pi}{L_y}, \omega(n_x, n_y) = kc = \pi c \sqrt{\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}}$$

Number of modes between ω and $\omega + d\omega$ is $\frac{\pi}{2} \frac{\omega L_x L_y}{(\pi c)^2} d\omega = \frac{\omega A}{2\pi c^2} d\omega$.

$$g(\omega) = \frac{\omega A}{2\pi c^2}$$

Total number of phonon mode is 2N: $\int_{0}^{\omega_{D}} g(\omega) d\omega = \frac{\omega_{D}^{2} A}{4\pi c^{2}} = 2N$

So
$$\omega_D = 2\sqrt{\frac{2\pi N}{A}}c$$

B) The energy of the system is a summation of the all the quantum harmonic oscillator modes: $\sum_{i=1}^{2N} \hbar \omega_i \left(n_i + \frac{1}{2} \right), \text{ where } n_i = 0,1,2..$ $Z = \sum_{\{n_i\}} e^{-\beta \sum_{i=1}^{2N} \hbar \omega_i \left(n_i + \frac{1}{2} \right)} = \sum_{n_1} \sum_{n_2} \dots \sum_{n_{2N}} \prod_{i=1}^{2N} e^{-\beta \hbar \omega_i n_i} e^{-\frac{\beta \hbar \omega_i}{2}} = \prod_{i=1}^{2N} e^{-\beta \hbar \omega_i n_i} e^{-\beta \hbar \omega_i n_i}$

Note that:

$$\sum_{n} e^{-nx} = \frac{1}{1 - e^x}$$

So:
$$Z = \prod_{i=1}^{2N} \frac{e^{-\frac{\beta\hbar\omega_i}{2}}}{1 - e^{-\beta\hbar\omega_i}}$$
$$\ln Z = \sum_{i=1}^{2N} \ln \left(\frac{e^{-\frac{\beta\hbar\omega_i}{2}}}{1 - e^{-\beta\hbar\omega_i}}\right) = \sum_{i=1}^{2N} \left(-\frac{\beta\hbar\omega_i}{2} - \ln\left(1 - e^{-\beta\hbar\omega_i}\right)\right)$$

Approximate the spectral as being continuous:

$$\ln Z \approx \int_0^{\omega_D} g(\omega) \left[-\frac{\beta \hbar \omega}{2} - \ln \left(1 - e^{-\beta \hbar \omega} \right) \right] d\omega = -\int_0^{\omega_D} \frac{\omega A}{2\pi c^2} \frac{\beta \hbar \omega}{2} d\omega - \int_0^{\omega_D} \frac{\omega A}{2\pi c^2} \ln \left(1 - e^{-\beta \hbar \omega} \right) d\omega$$

$$\ln Z = -\frac{\beta \hbar A \omega_D^3}{12\pi c^2} - \int_0^{\omega_D} \frac{\omega A}{2\pi c^2} \ln \left(1 - e^{-\beta \hbar \omega}\right) d\omega$$

C) At very high T.
$$1 - e^{-\beta\hbar\omega} \approx \beta\hbar\omega$$
,

$$\int_{0}^{\omega_{D}} \frac{\omega L^{2}}{2\pi c^{2}} \ln(\beta\hbar\omega) d\omega = \frac{\omega_{D}^{2}A}{4\pi c^{2}} \left[\ln(\beta\hbar\omega_{D}) - \frac{1}{2} \right]$$

$$\ln Z = -\frac{\beta\hbar A \omega_{D}^{3}}{12\pi c^{2}} - \frac{\omega_{D}^{2}A}{4\pi c^{2}} \left[\ln(\beta\hbar\omega_{D}) - \frac{1}{2} \right] = \frac{\omega_{D}^{2}A}{4\pi c^{2}} \left[\frac{-\beta\hbar\omega_{D}}{3} - \ln(\beta\hbar\omega_{D}) - \frac{1}{2} \right]$$

$$= 2N \left[\frac{-\beta\hbar\omega_{D}}{3} - \ln(\beta\hbar\omega_{D}) - \frac{1}{2} \right]$$

At very low T,
$$\beta \hbar \omega_D$$
 is very large,

$$\int_0^{\omega_D} \frac{\omega A}{2\pi c^2} \ln\left(1 - e^{-\beta \hbar \omega}\right) d\omega = \frac{A}{2(\beta \hbar)^2 \pi c^2} \int_0^{\infty} x \ln\left(1 - e^{-x}\right) dx = \frac{-A}{2(\beta \hbar)^2 \pi c^2} \zeta(3)$$

$$\ln Z = -\frac{\beta \hbar A \omega_D^3}{12\pi c^2} + \frac{A}{2(\beta \hbar)^2 \pi c^2} \zeta(3) = -\frac{2\beta \hbar \omega_D}{3} + \frac{A}{2(\beta \hbar)^2 \pi c^2} \zeta(3)$$

D) **Hight T limit:**

$$\ln Z \approx \frac{\omega_D^2 A}{4\pi c^2} \left[\frac{-\beta \hbar \omega_D}{3} - \ln(\beta \hbar \omega_D) - \frac{1}{2} \right]$$
Internal energy: $U = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\omega_D^2 A}{4\pi c^2} \left[\frac{-\hbar \omega_D}{3} - \frac{1}{\beta} \right] = \frac{\hbar \omega_D^3 A}{12\pi c^2} + \frac{\omega_D^2 A}{4\pi c^2} k_B T = \frac{2N\hbar \omega_D}{3} + 2Nk_B T$
Specific heat: $C = 2Nk_B$

$$S = k_B \left(\ln Z - \beta \frac{\partial \ln Z}{\partial \beta} \right) = 2Nk_B \left[-\ln(\beta \hbar \omega_D) + \frac{1}{2} \right]$$

The results for U and C are very similar to the 3D case, except a change of modes from 3N to 2N.

Low T limit:
$$\ln Z = -\frac{\beta \hbar A \omega_D^3}{12\pi c^2} + \frac{A}{2(\beta \hbar)^2 \pi c^2} \zeta(3)$$

Internal energy: $U = -\frac{\partial \ln Z}{\partial \beta} = \frac{\hbar A \omega_D^3}{12\pi c^2} + \frac{A}{2\hbar^2 \pi c^2} \zeta(3) (k_B T)^3 = \frac{2N\hbar\omega_D}{3} + \frac{4\zeta(3)Nk_B T^3}{\theta_D^2}$
 $(\theta_D = \frac{\hbar\omega_D}{k_B})$
Specific heat: $\frac{12\zeta(3)Nk_B T^2}{\theta_D^2}$

$$S = k_B \left(\ln Z - \beta \frac{\partial \ln Z}{\partial \beta} \right) = k_B \frac{3A}{2(\hbar \beta)^2 \pi c^2} \zeta(3)$$

In 3D, the internal energy at low temperature increases following T^4 temperature dependence. Here in 2D the internal energy has a T^3 temperature dependence. Correspondingly the specific heat also has its power-law temperature dependence changing from T^3 in 3D to T^2 in 2D.

E) The average phonon number for mode *l* is:

$$\langle n_l \rangle = \frac{\sum_{\{n_l\}} n_l e^{-\beta \sum_{i=1}^{2N} \hbar \omega_i \left(n_i + \frac{1}{2}\right)}}{Z} = \frac{\sum_{\{n_l\}} \left(\frac{-1}{\hbar} \frac{\partial \varepsilon}{\partial \omega_l} - \frac{1}{2}\right) e^{-\beta \varepsilon}}{Z} = \frac{-1}{\beta \hbar} \frac{\partial \ln Z}{\partial \omega_l} - \frac{1}{2}$$

$$\text{Take: } \ln Z = \sum_{i=1}^{2N} \ln \left(\frac{e^{-\beta \hbar \omega_i}}{1 - e^{-\beta \hbar \omega_i}}\right) = \sum_{i=1}^{2N} \left(-\frac{\beta \hbar \omega_i}{2} - \ln \left(1 - e^{-\beta \hbar \omega_i}\right)\right)$$

$$\langle n_l \rangle = \frac{e^{-\beta \hbar \omega_l}}{1 - e^{-\beta \hbar \omega_l}} = \frac{1}{e^{\beta \hbar \omega_l} - 1}$$

$$\left\langle n_{l}^{2}\right\rangle =\frac{\sum\limits_{\left\langle n_{l}\right\rangle }^{}n_{l}^{2}e^{-\beta \sum\limits_{i=1}^{2N}\hbar \omega_{i}\left(n_{i}+\frac{1}{2}\right)}}{Z}$$

$$\frac{\partial^2 Z}{\partial \omega_l^2} = \sum_{\{n_l\}} \left[\beta \hbar \left(n_l + \frac{1}{2} \right) \right]^2 e^{-\beta \sum_{l=1}^{2N} \hbar \omega_l \left(n_l + \frac{1}{2} \right)}$$

$$\left\langle n_{l}^{2}\right\rangle = \frac{1}{\left(\beta\hbar\right)^{2}}\frac{\frac{\partial^{2}Z}{\partial\omega_{l}^{2}}}{Z} - \left\langle n_{l}\right\rangle - \frac{1}{4}$$

$$Z = \prod_{i=1}^{2N} \frac{e^{-\frac{\beta\hbar\omega_i}{2}}}{1 - e^{-\beta\hbar\omega_i}} = \prod_{i=1}^{2N} \frac{e^{\frac{\beta\hbar\omega_i}{2}}}{e^{\beta\hbar\omega_i} - 1}$$

$$\begin{split} \frac{\partial Z}{\partial \omega_{l}} &= \left[\frac{\beta\hbar}{2}e^{\frac{\beta\hbar\omega_{l}}{2}}}{e^{\beta\hbar\omega_{l}}-1} - \frac{\beta\hbar e^{\beta\hbar\omega_{l}}e^{\frac{\beta\hbar\omega_{l}}{2}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}}\right] \prod_{i=l}^{2N} \frac{e^{\frac{\beta\hbar\omega_{l}}{2}}}{e^{\beta\hbar\omega_{i}}-1} = \left(\frac{\beta\hbar}{2} - \frac{\beta\hbar e^{\beta\hbar\omega_{l}}}{e^{\beta\hbar\omega_{l}}-1}\right) Z \\ \frac{\partial^{2}Z}{\partial \omega_{l}^{2}} &= \left[-\frac{(\beta\hbar)^{2}e^{\beta\hbar\omega_{l}}}{e^{\beta\hbar\omega_{l}}-1} + \frac{(\beta\hbar)^{2}e^{2\beta\hbar\omega_{l}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}}\right] Z + \left(\frac{\beta\hbar}{2} - \frac{\beta\hbar e^{\beta\hbar\omega_{l}}}{e^{\beta\hbar\omega_{l}}-1}\right)^{2} Z \\ &= \left[\frac{(\beta\hbar)^{2}e^{\beta\hbar\omega_{l}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}} + \left(\frac{\beta\hbar}{2}\right)^{2} - \frac{(\beta\hbar)^{2}e^{\beta\hbar\omega_{l}}}{e^{\beta\hbar\omega_{l}}-1} + \frac{(\beta\hbar)^{2}e^{2\beta\hbar\omega_{l}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}}\right] Z = (\beta\hbar)^{2} \left[\frac{1}{4} + \frac{2e^{\beta\hbar\omega_{l}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}}\right] Z \\ &\left\langle n_{l}^{2} \right\rangle = \frac{1}{4} + \frac{2e^{\beta\hbar\omega_{l}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}} - \overline{n_{l}} - \frac{1}{4} = \frac{2e^{\beta\hbar\omega_{l}}}{(e^{\beta\hbar\omega_{l}}-1)^{*}} - \frac{1}{e^{\beta\hbar\omega_{l}}-1} = \frac{e^{\beta\hbar\omega_{l}}+1}{(e^{\beta\hbar\omega_{l}}-1)^{*}} \end{split}$$

$$\left\langle n_{l}^{2}\right\rangle - \left\langle n_{l}\right\rangle^{2} = \frac{e^{\beta\hbar\omega_{l}} + 1}{\left(e^{\beta\hbar\omega_{l}} - 1\right)^{2}} - \frac{1}{\left(e^{\beta\hbar\omega_{l}} - 1\right)^{2}} = \frac{e^{\beta\hbar\omega_{l}}}{\left(e^{\beta\hbar\omega_{l}} - 1\right)^{2}}$$

The statistical dispersion of the phonon number for mode *l* is $\frac{e^{\frac{\beta\hbar\omega_l}{2}}}{e^{\beta\hbar\omega_l}-1}$

F) Total phonon number:

$$\sum g(\omega_l) n_l \approx \int_0^{\omega_D} \frac{\omega A}{2\pi c^2} \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} d\omega$$

High temperature limit: $\beta \hbar \omega_D \rightarrow 0$

$$e^{-\beta\hbar\omega} \approx 1 - \beta\hbar\omega$$

$$\int_{0}^{\omega_{D}} \frac{\omega A}{2\pi c^{2}} \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} d\omega \approx \int_{0}^{\omega_{D}} \frac{\omega A}{2\pi c^{2}} \frac{1}{\beta\hbar\omega} d\omega = \frac{A\omega_{D}}{2\pi c^{2}\hbar\beta} = \frac{A\omega_{D}k_{B}T}{2\pi c^{2}\hbar} = \sqrt{\frac{2NA}{\pi}} \frac{k_{B}T}{\hbar c}$$

Low temperature limit: $\beta \hbar \omega_D \rightarrow \infty$

$$\int_{0}^{\omega_{D}} \frac{\omega A}{2\pi c^{2}} \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} d\omega = \frac{A}{2\pi c^{2}\beta^{2}\hbar^{2}} \int_{0}^{\beta\hbar\omega_{D}} \frac{x}{e^{x} - 1} dx \approx \frac{A}{2\pi c^{2}\beta^{2}\hbar^{2}} \int_{0}^{\infty} \frac{x}{e^{x} - 1} dx = \frac{A\pi k_{B}^{2}T^{2}}{12c^{2}\hbar^{2}}$$

Statistical Mechanics 3

Boltzmann equation

The relaxation-time approximation $(RTA)^1$ is the following simple model for the scattering term in the Boltzmann kinetic equation:

$$\frac{dw}{dt} = -\frac{w - w_0}{\tau}$$

where $w(\mathbf{r}, \mathbf{p}, t)d^3rd^3p$ is the mean number of particles in the phase space element d^3rd^3p , dw/dt is the full derivative of this function, w_0 is its equilibrium value at the given energy and temperature, and τ is some effective time constant.

A (2 points). Specify w_0 for the case of non-interacting Fermi-particles.

B (4 points). Write the RTA Boltzmann equation for a diluted gas of charged particles, placed into a uniform, time-independent electric field \mathbf{E} , but otherwise free to move.

C (6 points). Find the stationary solution of the equation in the 1st approximation in low electric field, and use it to derive the general expression for the dc Ohmic conductivity σ of the gas.

D (4 points). Spell out the expression for σ in the limits of degenerate and non-degenerate (classical) Fermi gases. Assuming that τ is temperature-independent, how does σ depend on temperature in each of these limits?

E (4 points). Compare your results with the classical Drude formula for σ , and discuss the physical sense of the constant τ . Discuss the most evident shortcomings of the RTA model.

Hint: You may like to use the following integral: $\int_{0}^{\infty} \xi^{3/2} e^{-\xi} d\xi = \Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\pi^{1/2}.$

¹ Alternatively, this approximation is called the BGK model, after P. Bhatnager, E. Gross, and M. Krook, who suggested it in 1954. (The same year, a similar model was discussed by P. Welander.)

Solution

A (3 points). At equilibrium, $w(\mathbf{r}, \mathbf{p}, t)$ of a gas of non-interacting particles is a product of the density *n* of the orbital states, by the spin degeneracy factor g = 2s + 1 of each orbital state (for electrons, which are spin- $\frac{1}{2}$ particles, g = 2), by the average occupancy $\langle N \rangle$ of each state, given by the Fermi-Dirac distribution:

$$w = w_0 = gn \langle N \rangle = 2 \frac{1}{(2\pi\hbar)^3} \frac{1}{e^{(\varepsilon - \mu)/T} + 1},$$
(1)

where μ is the chemical potential, $T = k_B T_K$ is temperature in energy units, and ε is the single-particle energy. For a free gas, the energy includes only the kinetic component:

$$\varepsilon = \frac{p^2}{2m},\tag{2}$$

and hence does not depend on \mathbf{r} (and t).

B (3 points). In the absence of scattering, the Boltzmann equation is reduced to the fundamental Liouville equation

$$\frac{dw}{dt} = 0,$$

which expresses the conservation of the number of particles in an elementary volume d^3pd^3r moving with the particle flow. Spelling out, in the usual way, the full derivative d/dt for this function of **r**, **p** (with 3 spatial equations each) and *t*, we get

$$\frac{\partial w}{\partial t} + \sum_{j=1}^{3} \left(\frac{\partial w}{\partial r_j} \frac{\partial r_j}{\partial t} + \frac{\partial w}{\partial p_j} \frac{\partial p_j}{\partial t} \right) = 0.$$

Since this equality is valid in the reference frame moving, at the considered instant, with the particles, the partial derivatives $\partial r_j/\partial t$ are the Cartesian components v_j of their velocity v. If, in addition, the frame is inertial, the derivatives $\partial p_j/\partial t$ are the Cartesian components F_j of the force $\mathbf{F} = q\mathbf{E}$ applied to each particle. As a result, the Liouville equation may be written as

$$\frac{\partial w}{\partial t} + \sum_{j=1}^{3} \left(v_j \frac{\partial w}{\partial r_j} + qE_j \frac{\partial w}{\partial p_j} \right) \equiv \frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla_r w + q\mathbf{E} \cdot \nabla_p w = 0.$$

Now adding the scattering term in its RTA form, we get the corresponding Boltzmann equation:

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla_r w + q \mathbf{E} \cdot \nabla_p w = -\frac{w - w_0}{\tau}$$

C (3 points). If the electric field is constant, the first term in the Boltzmann equation vanishes, and if the gas is space-uniform, the second term vanishes as well, so that the equation is reduced to

$$q\mathbf{E}\cdot\nabla_p(w_0+\widetilde{w})=-\frac{\widetilde{w}}{\tau}, \quad \text{where } \widetilde{w}\equiv w-w_0.$$

Since $\tilde{w} \to 0$ at $\mathbf{E} \to 0$, in the linear approximation in \mathbf{E} we may neglect \tilde{w} in the left-hand part of this equation, so that it immediately yields

$$\widetilde{w} = -q \,\tau \,\mathbf{E} \cdot \boldsymbol{\nabla}_{p} w_{0}$$

Since w_0 depends on **p** only via its dependence on ε , we may continue as

$$\widetilde{w} = -q \tau \mathbf{E} \cdot \left(\nabla_{p} \varepsilon \right) \frac{\partial w_{0}}{\partial \varepsilon} \equiv -q \tau \mathbf{E} \cdot \mathbf{v} \frac{\partial w_{0}}{\partial \varepsilon}, \qquad (2)$$

where the partial derivative denotes the constancy of μ and T, and $\mathbf{v} \equiv \nabla_p \varepsilon$ is just the particle's group velocity. (In our isotropic, parabolic model given by Eq. (2), $\mathbf{v} = \mathbf{p}/m$.)

D (3 points). The electric current's density may be calculated as

$$\mathbf{j} = \int q \mathbf{v} w d^3 p \equiv q \int \mathbf{v} (w_0 + \widetilde{w}) d^3 p \, .$$

Since in the equilibrium state, with $w = w_0$, the current has to be zero, the integral of the first term in the parentheses has to vanish. For the integral of the second term, plugging in Eq. (2), and taking into account Eq. (1), we get

$$\mathbf{j} = q^2 \tau \int \mathbf{v} \left(\mathbf{E} \cdot \mathbf{v} \right) \left(-\frac{\partial w_0}{\partial \varepsilon} \right) d^3 p \equiv \frac{2q^2 \tau}{\left(2\pi\hbar\right)^3} \int \mathbf{v} \left(\mathbf{E} \cdot \mathbf{v} \right) \left(-\frac{\partial \langle N \rangle}{\partial \varepsilon} \right) d^3 p$$

This is the famous *Sommerfeld formula*, valid even for materials with non-spherical Fermi surfaces. For our isotropic case (2), it is reduced to the Ohm law $\mathbf{j} = \sigma \mathbf{E}$, with

$$\sigma = \frac{2q^2\tau}{(2\pi\hbar)^3} \int v^2 \cos^2\theta \left(-\frac{\partial \langle N \rangle}{\partial \varepsilon}\right) d^3p \equiv \frac{2q^2\tau}{(2\pi\hbar)^3} 2\pi \int_0^\infty v^2 \left(-\frac{\partial \langle N \rangle}{\partial \varepsilon}\right) p^2 dp \int_0^\pi \cos^2\theta \sin\theta d\theta,$$

where θ is the angle between the vectors **p** and **E**. The integral over the angle is elementary and equal to 2/3, so that using Eq. (2) to transfer the first integral from the momentum's magnitude *p* to the energy $\varepsilon = p^2/2m$ (so that $d\varepsilon = pdp/m$, and $dp = (m/p)d\varepsilon = (m/2\varepsilon)^{1/2}d\varepsilon$), we get

$$\sigma = \frac{2q^2\tau}{(2\pi\hbar)^3} \frac{4\pi}{3} \int_0^\infty v^2 \left(-\frac{\partial \langle N \rangle}{\partial \varepsilon}\right) p^2 dp = \frac{2q^2\tau}{(2\pi\hbar)^3} \frac{4\pi}{3} \int_0^\infty (8m\varepsilon^3)^{1/2} \left(-\frac{\partial \langle N \rangle}{\partial \varepsilon}\right) d\varepsilon .$$
(3)

E (4 points). In the limit of a degenerate Fermi gas, with the Fermi energy $\varepsilon_{\rm F} \approx \mu$ much larger than *T*, the Fermi distribution $\langle N \rangle$ switches from 1 to 0 very fast at the energy $\varepsilon \approx \varepsilon_{\rm F}$, so that $(-\partial \langle N \rangle / \partial \varepsilon)$ may be replaced with the delta-function $\delta(\varepsilon - \varepsilon_{\rm F})$, and Eq. (3) yields

$$\sigma = \frac{2q^2\tau}{(2\pi\hbar)^3} \frac{4\pi}{3} \left(8m\varepsilon_{\rm F}^3\right)^{1/2}.$$
 (4)

In this limit, the Ohmic conductivity σ is temperature-independent, besides the possible change of the relaxation time τ . (For electron scattering dominated by impurities, τ is also virtually a constant at low temperatures.)

In the opposite limit of high temperatures, $T >> \varepsilon_{\rm F}$, i.e. for an essentially classical gas, the Fermi-Dirac distribution is reduced to the exponential one,

$$\langle N(\varepsilon)\rangle = \exp\left\{\frac{\mu-\varepsilon}{T}\right\},\,$$

giving in particular

$$-\frac{\partial \langle N(\varepsilon) \rangle}{\partial \varepsilon} = \frac{1}{T} \exp\left\{\frac{\mu - \varepsilon}{T}\right\}.$$

With this substitution, Eq. (3) yields

$$\sigma = \frac{2q^2\tau}{(2\pi\hbar)^3} \frac{4\pi}{3} \frac{1}{T} e^{\mu/T} \int_0^\infty (8m\varepsilon^3)^{1/2} e^{-\varepsilon/T} d\varepsilon = \frac{2q^2\tau}{(2\pi\hbar)^3} \frac{4\pi}{3} e^{\mu/T} (8mT^3)^{1/2} \int_0^\infty \xi^{3/2} e^{-\xi} d\xi$$

Using the last integral, provided in the Hint, we finally get

$$\sigma = \frac{2q^2\tau}{(2\pi\hbar)^3} \frac{4\pi}{3} e^{\mu/T} \left(8mT^3\right)^{1/2} \frac{3}{4} \pi^{1/2} \equiv \frac{q^2\tau}{m} \frac{2e^{\mu/T}}{\left(2\pi\hbar^2/mT\right)^{3/2}}.$$
(5)

But the last fraction is just the well-known expression for the density N/V of a classical gas, so that is does not depend on temperature either. (Note that at higher temperatures, τ in actual conductors typically drops with *T* in particular, due to the growing phonon scattering.)

F (2 points). Eq. (5) may be immediately rewritten as

$$\sigma = \frac{q^2 \tau}{m} \frac{N}{V}.$$
 (6)

But this is just the standard form of the (dc) Drude formula. Now coming back to Eq. (4), the density of particles in the degenerate Fermi gas may be calculated as

$$\frac{N}{V} = \frac{2}{(2\pi\hbar)^3} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} 4\pi \int_0^{p_{\rm F}} p^2 dp \equiv \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^3}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} \equiv \varepsilon_{\rm F} + \frac{1}{2} \int \langle N \rangle d^3 p = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \text{where } \frac{p_{\rm F}^2}{2m} = \frac{2}{(2\pi\hbar)^3} \frac{4\pi p_{\rm F}^2}{3}, \qquad \frac{p_{\rm F}^2}{2m} = \frac{2}{(2\pi\hbar)^3} \frac{2\pi p_{\rm F}^2}{3}, \qquad \frac{p_{\rm F}^2}{2m} = \frac{2}{(2$$

Comparing this expression with Eq. (4), we see that the latter relation is also reduced to the Drude formula (6).

As the well-known classical derivation of Eq. (6) shows, τ has the sense of the average time interval between scatterings of a particle, leading to the loss of the additional momentum picked up by it from the external electric field.

G (2 points). The most important shortcoming of the RTA model is the independence of τ of the direction of the momentum change $\Delta \mathbf{p}$ at scattering. As a result, in this model, the energy relaxation at inelastic scattering (with $\Delta \mathbf{p}$ nearly parallel to \mathbf{p}) takes the same time as the momentum relaxation at elastic scattering (with $\Delta \mathbf{p}$ nearly normal to \mathbf{p}), while in real materials these processes may have completely different time scales.