Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

January 2019

General Instructions:

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

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

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

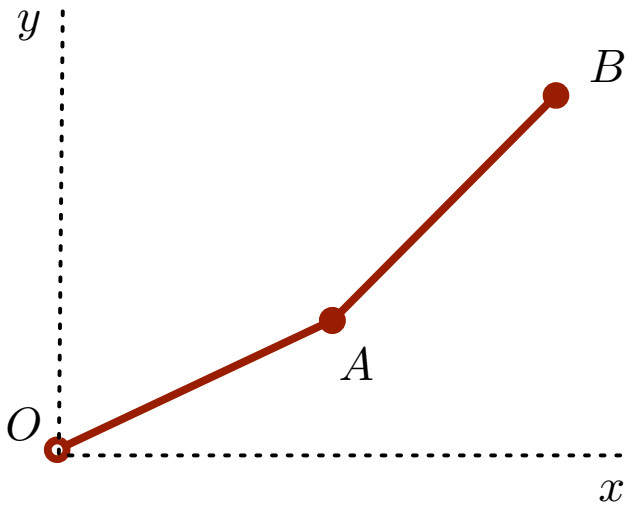
Write your ID number (not your name!) on each exam booklet.

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

Classical Mechanics 1

Linked rods in a plane

Two massless rods lie in the $x - y$ plane (neglect gravity). Each rod has length ℓ, and each rod has mass M at one end (points A and B below). The massless end of the first rod is hinged to a fixed pivot O, while its massive end is hinged at the point A to massless end of the second rod as shown below. The hinges at O and A are constructed so that the second rod can swing past past the first without obstruction.



(a) (7 points) Write down the Lagrangian of the system. Determine and interpret any integrals of motion.

(b) At time $t = 0$ both rods are aligned along the x axis. The mass at A moves with velocity v_0, while the mass at B moves with velocity $2v_0 + \Delta v$, with $\Delta v \ll v_0$.

i (3 points) Qualitatively describe the subsequent motion of the system.

ii (10 points) Determine the angles of the masses relative to the x axis as functions of time.

Solution:

(a) First we find the Lagrangian of the system. The generalized coordinates are ϕ_1 and ϕ_2. The coordinates of a point in A are

$$\boldsymbol{r}_A = (\ell\cos(\phi_1), \ell\sin(\phi_1))\,, \tag{1}$$

while the coordinates of B are

$$\boldsymbol{r}_B = \boldsymbol{x}_A + \ell(\cos(\phi_1+\phi_2), \sin(\phi_1+\phi_2))\,. \tag{2}$$

Here and below we will write $\phi_3 = \phi_1 + \phi_2$

Thus, the velocities are

$$\boldsymbol{v}_A = \ell(-\sin(\phi_1), \cos(\phi_1))\dot{\phi}_1\,, \tag{3}$$

and

$$\boldsymbol{v}_B = \boldsymbol{v}_A + \ell(-\sin(\phi_3), \cos(\phi_3))(\dot{\phi}_3)\,, \tag{4}$$

respectively. The kinetic energy is $\frac{1}{2}m\boldsymbol{v}_A^2 + \frac{1}{2}m\boldsymbol{v}_B^2$ yielding after some algebra

$$\begin{aligned} T =& \frac{1}{2}m\ell^2\dot{\phi}_1^2 + \left(\frac{1}{2}m\ell^2\dot{\phi}_1^2 + \frac{1}{2}m\ell^2\dot{\phi}_3^2, + m\ell^2\cos(\phi_3-\phi_1)\dot{\phi}_1\dot{\phi}_3\right)\,, & (5)\\ =& \frac{1}{2}m\ell^2\dot{\phi}_1^2 + \left(\frac{1}{2}m\ell^2\dot{\phi}_1^2 + \frac{1}{2}m\ell^2(\dot{\phi}_1+\dot{\phi}_2)^2 + m\ell^2\cos(\phi_2)\dot{\phi}_1(\dot{\phi}_1+\dot{\phi}_2)\right)\,, & (6)\\ =& \frac{1}{2}m\ell^2\dot{\phi}_1^2\,(3+2\cos(\phi_2)) + m\ell^2(1+\cos\phi_2)\dot{\phi}_1\dot{\phi}_2 + \frac{1}{2}m\ell^2\dot{\phi}_2^2\,. & (7)\end{aligned}$$

We have two integrals of motion. The first is the total energy of the system.

$$h = p_1\dot{\phi}_1 + p_2\dot{\phi}_2 - L\,. \tag{8}$$

We have

$$\begin{aligned} p_1 =& m\ell^2(3+2\cos(\phi_2))\dot{\phi}_1 + m\ell^2(1+\cos\phi_2)\dot{\phi}_2\,, & (9)\\ p_2 =& m\ell^2(1+\cos(\phi_2))\dot{\phi}_1 + m\ell^2\dot{\phi}_2\,, & (10)\end{aligned}$$

The Hamiltonian function reduces to simply to the kinetic energy

$$h = T = \frac{1}{2}m\ell^2\dot{\phi}_1^2\,(3+2\cos(\phi_2)) + m\ell^2(1+\cos\phi_2)\dot{\phi}_1\dot{\phi}_2 + \frac{1}{2}m\ell^2\dot{\phi}_2^2\,, \tag{11}$$

as one could expect.

The second is associated with the cyclic coordinate ϕ_1, which is the total angular momentum:

$$J = \frac{\partial\mathcal{L}}{\partial\dot{\phi}_1} = p_1\,. \tag{12}$$

(i) It is perhaps a good place to use some intuition. If the total angular momentum is large compared to the internal angular momentum. There will be a strong centrifugal force which will tend to align rod B with rod A. The resulting sytem will exhibit small oscillations around this configuration, while the center of mass will move at a constant rate around the circle.

(ii) We should expand near $\phi_2 = 0$. $\dot{\phi}_1$ is not small, but $\dot{\phi}_2$ and ϕ_2 are small. The Lagrangian in this case is

$$L = \frac{1}{2}m\ell^2\dot{\phi}_1^2(5 - \phi_2^2) + 2m\ell^2\dot{\phi}_1\dot{\phi}_2 + \frac{1}{2}m\ell^2\dot{\phi}_2^2 \,. \tag{13}$$

The angular momentum is

$$J = 5m\ell^2\dot{\phi}_1 + 2m\ell^2\dot{\phi}_2 \,. \tag{14}$$

The equation of motion for ϕ_2 is

$$\frac{d}{dt}(m\ell^2\dot{\phi}_2 + 2m\ell^2\dot{\phi}_1) = -m\ell^2\dot{\phi}_1^2\phi_2 \,. \tag{15}$$

On the RHS, which is already small, we can approximate

$$\dot{\phi}_1 = \frac{J}{5m\ell^2} \,, \tag{16}$$

so the RHS can be written

$$-m\ell^2\dot{\phi}_1^2\phi_2 = -\frac{J^2}{25m\ell^2}\phi_2 \,. \tag{17}$$

The LHS can also be approximated. Since

$$\frac{dJ}{dt} = 0 \,, \tag{18}$$

we have

$$5m\ell^2\ddot{\phi}_1 + 2m\ell^2\ddot{\phi}_2 = 0 \,. \tag{19}$$

So the LHS reads

$$m\ell^2\ddot{\phi}_2 + 2m\ell^2\ddot{\phi}_1 = m\ell^2\ddot{\phi}_2(1 - \frac{4}{5}) \,. \tag{20}$$

Then the equation of motion for ϕ_2 is

$$\frac{1}{5}m\ell^2\ddot{\phi}_2 = -\frac{J^2}{25m\ell^2}\phi_2 \,. \tag{21}$$

Thus the motion is periodic with frequency

$$\omega_0^2 = \frac{J^2}{5(m\ell^2)^2} \,. \tag{22}$$

Since

$$J \simeq 5m\ell v \,, \tag{23}$$

we have

$$\omega_0^2 = \frac{5v^2}{\ell^2}\,. \tag{24}$$

Putting together the results we have

$$\phi_2 = A\sin(\omega_0 t) + B\cos(\omega t) \tag{25}$$

$$\dot{\phi}_1 = \frac{J}{5m\ell^2} - \frac{2}{5}\dot{\phi}_2 \tag{26}$$

The second equation is integrated to yield

$$\phi_1 = \frac{Jt}{5m\ell^2} - \frac{2}{5}\phi_2 + \text{const} \tag{27}$$

At time $t = 0$, $\phi_1 = \phi_2 = 0$, so our solutions can be written

$$\phi_2(t) = \frac{C}{\omega_0}\sin(\omega_0 t) \tag{28}$$

$$\phi_1(t) = Dt - \frac{2}{5}\phi_2 \tag{29}$$

Then in order to match the initial condition we need

$$\dot{\phi}_1 = \frac{v_0}{\ell} \qquad \dot{\phi}_2 = \frac{\Delta v}{\ell} \tag{30}$$

So finally

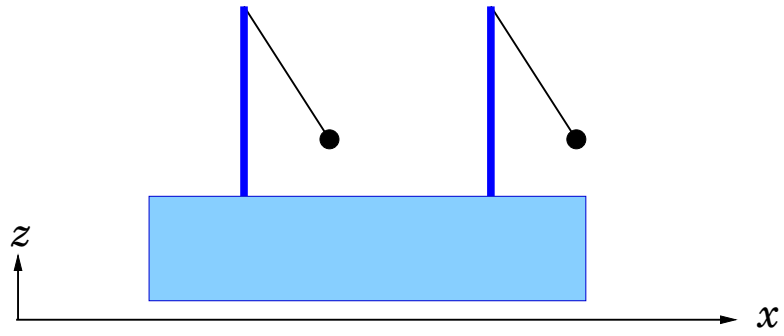
$$\phi_2(t) = \frac{\Delta v}{\ell\omega_0}\sin(\omega_0 t) \tag{31}$$

$$\phi_1(t) = \left(\frac{v_0}{\ell} + \frac{2\Delta v}{5\ell}\right)t - \frac{2}{5}\phi_2 \tag{32}$$

Classical Mechanics 2

Coupled pendulums

Two identical pendulums each have a point mass m suspended (in a uniform gravitational field) on a massless rigid rod of length ℓ hanging from a frictionless pivot. The pendulums are constrained to swing in the $x-z$ plane, and are mounted on a block of mass $M = 2m$ which is free to slide, without friction, in the x-direction.



(a) (10 points) Construct a Lagrangian of the system assuming small oscillations: (i) find the resulting normal modes and frequencies, (ii) interpret any zero modes, and (iii) qualitatively sketch the oscillation pattern for each mode.

(b) (6 points) Now the base (the block with mass $2m$) is pushed in the x-direction by an external force $F(t) = P_0\delta(t)$. Determine thee subsequent motion of the system, assuming that the impulse P_0 is so small that the subsequent oscillations may be treated in a harmonic approximation.

(c) (4 points) Now consider a time dependent force pushing the base in the x-direction:

$$F(t) \equiv F_0 e^{-|t|/\tau}\,, \tag{33}$$

where $\tau > 0$ is some characteristic time scale. Assuming that the system is at rest for $t \to -\infty$, determine the total work done on the system by the time dependent force as $t \to +\infty$.

Solution:

(a) First we coordinate the system. Choosing X to be the bottom of the center of mass of the base, and ϕ_1 and ϕ_2 to be the angles. The coordinates of the first mass is

$$x_1 = X + \ell \sin(\phi_1) \simeq X + \ell\phi_1 + O(\phi_1^3)\,, \tag{34}$$

$$y_1 = \ell(1 - \cos(\phi_1) \simeq \ell\frac{\phi^2}{2}\,, \tag{35}$$

with an analogous expression for the second mass. Here we have chose $y = 0$ to be the resting point of the two masses.

The kinetic energy

$$T = \frac{1}{2}M\dot{X}^2 + \frac{1}{2}m(\dot{X} + \ell\dot{\phi}_1)^2 + \frac{1}{2}m(\dot{X} + \ell\dot{\phi}_2)^2\,. \tag{36}$$

The potential energy is just

$$U = mgy_1 + mgy_2\,. \tag{37}$$

So the total Lagrangian is

$$L = m\dot{X}^2 + \frac{1}{2}m(\dot{X} + \ell\dot{\phi}_1)^2 + \frac{1}{2}m(\dot{X} + \ell\dot{\phi}_2)^2 + \frac{1}{2}mg\ell^2(\phi_1^2 + \phi_2^2)\,. \tag{38}$$

First we note that there is a zero mode associated with the x translation of the system

$$P_X = \frac{\partial L}{\partial \dot{X}} = 4m\dot{X} + m\ell\dot{\phi}_1 + m\ell\dot{\phi}_2\,. \tag{39}$$

This is clearly the momentum of the center of mass.

To find the equation of motion of the remaining coordinates it is useful to eliminate X (which is cyclic) and to focus on ϕ_1 and ϕ_2. This can be done using the Routh procedure. The Routhian, $-R \equiv L_{\text{eff}}$, is

$$L_{\text{eff}} = L - p_X\dot{X}\,, \tag{40}$$

and gives an effective Lagrangian for the remaining coordinates and a Hamilton equation of motion for X.

In addition, since only the sum $(\phi_1 + \phi_2)/2 = \phi_s$ couples to the center of mass, it is convenient to change coordinates to ϕ_s and $\phi_\Delta = (\phi_2 - \phi_1)/2$. This is also motivated by symmetry considerations. We note the following

$$\phi_1^2 + \phi_2^2 = 2\phi_s^2 + 2\phi_\Delta^2\,, \tag{41}$$

$$\dot{\phi}_1^2 + \dot{\phi}_2^2 = 2\dot{\phi}_s^2 + 2\dot{\phi}_\Delta^2\,. \tag{42}$$

We also note that the velocity of the center of mass is

$$P_X = 4m\dot{X} + 2m\ell\dot{\phi}_s\,. \tag{43}$$

$$\tag{44}$$

The effective Lagrangian evaluates to

$$L_{\text{eff}} = \frac{1}{2}m\ell^2\left(\dot{\phi}_1^2 + \dot{\phi}_2^2\right) - \frac{1}{2}mg\ell^2(\phi_1^2 + \phi_2^2) - \frac{1}{2}(4m)\dot{X}^2\,, \tag{45}$$

$$= m\ell^2\dot{\phi}_s^2 - mg\ell\phi_s^2 + m\ell^2\dot{\phi}_\Delta^2 - mg\ell\phi_\Delta^2 - \frac{(P_x - 2m\ell\dot{\phi}_s)^2}{2(4m)}\,. \tag{46}$$

Expanding the factor

$$-\frac{(P_X - 2m\ell\dot{\phi}_s)^2}{2(4m)} = -\frac{P_X^2}{2(4m)} + \frac{2P_x(2m\ell\dot{\phi}_s)}{8m} - \frac{(2m)^2\ell^2\dot{\phi}_s^2}{8m}\,, \tag{47}$$

$$= -\frac{P_X^2}{2(4m)} - \frac{1}{2}\frac{dP_X}{dt}\ell\dot{\phi} - \frac{1}{2}m\ell^2\dot{\phi}_s^2\,. \tag{48}$$

Recognizing that P_X is constant, the effective Lagrangian is

$$L_{\text{eff}} = \frac{1}{2}m\ell^2\dot{\phi}_s^2 - mg\ell\phi_s^2 + m\ell^2\dot{\phi}_\Delta^2 - mg\ell\phi_\Delta^2 + \text{const}\,. \tag{49}$$

From here the normal modes are simple. The first EOM

$$m\ell^2\ddot{\phi}_s + 2mg\ell\phi_s = 0\,, \tag{50}$$

yielding a resonance frequency (squared) of

$$\omega_1^2 = 2\frac{g}{\ell}\,. \tag{51}$$

The second normal mode associated with ϕ_Δ is a simple pendulum

$$\omega_2^2 = \frac{g}{\ell}\,. \tag{52}$$

(b) Now we add a force. After integrating the force on the block from $t = -\epsilon$ to $t = +\epsilon$, the momentum of the base is

$$(2m)\dot{X} = P_0\,. \tag{53}$$

The momentum of the balls is zero

$$m\dot{x}_1 = m\dot{X} + m\ell\dot{\phi}_1 = 0\,, \tag{54}$$

$$m\dot{x}_2 = m\dot{X} + m\ell\dot{\phi}_2 = 0\,. \tag{55}$$

This means that just after the impulse

$$P_X = P_0\,, \tag{56}$$

$$\dot{\phi}_s = -\frac{P_0}{2m\ell}\,, \tag{57}$$

$$\dot{\phi}_\Delta = 0\,. \tag{58}$$

The subsequent oscillator motion of ϕ_s is just given by a simple harmonic oscillator result

$$\phi_s(t) = -\frac{P_0}{2m\ell}\frac{\sin(\omega_1 t)}{\omega_1}\,, \tag{59}$$

with initial conditions described above. Similarly $P_X = P_0 = \text{const}$ and $\phi_\Delta = 0$.

We can find $X(t)$ from the Eq. (43) for the center of mass and our result for $\phi_s(t)$

$$P_0 = 4m\dot{X} - P_0\cos(\omega_1 t)\,, \tag{60}$$

Thus,

$$\dot{X} = \frac{P_0}{4m}(1+\cos(\omega_1 t))\,, \tag{61}$$

which is easily integrated to find

$$X(t) = \frac{P_0}{4m}t + \frac{P_0}{4m\omega_1}\sin(\omega_1 t)\,. \tag{62}$$

(c) Let us find the motion for an arbitrary force $F(t)$. In general

$$X(t) = \int_{-\infty}^{\infty} dt_0\, G_R(t-t_0)F(t_0)\,. \tag{63}$$

One should realize that the Green function is the response to an impulsive force $\delta(t-t_0)$, which was already found in part (b). We can use this to write

$$G_R(t-t_0) = \frac{1}{4m}(t-t_0) + \frac{1}{4m\omega_1}\sin(\omega_1(t-t_0))\,. \tag{64}$$

Its derivative is

$$\partial_t G_R(t-t_0) = \frac{1}{4m} + \frac{1}{4m}\cos(\omega_1(t-t_0))\,. \tag{65}$$

The work done is

$$W = \int dt F(t)\dot{X}(t)\,, \tag{66}$$

leading to

$$W = \int dt \int dt_0 F(t)\partial_t G_R(t-t_0)F(t_0)\,. \tag{67}$$

The Green function derivative consists of a constant, $1/4m$, and cos term

$$W = \frac{1}{4m}\left(\int dt F(t)\right)^2 + \frac{1}{4m}\int\int dt\, dt_0\, F(t)\cos(\omega_1(t-t_0))\,F(t_0)\,. \tag{68}$$

Writing the $\cos(\omega_1(t-t_0)) = (e^{i\omega_1(t-t_0)} + e^{-i\omega_1(t-t_0)})/2$ and performing the integrals, we find

$$\boxed{W = \frac{1}{4m}|\tilde{F}(0)|^2 + \frac{1}{4m}|\tilde{F}(\omega_1)|^2}\,, \tag{69}$$

where

$$\tilde{F}(\omega) = \int dt e^{i\omega t} F(t)\,, \tag{70}$$

is the Fourier transform of $F(t)$. Thus the work is only sensitive to the spectral density of the force at the resonant frequencies of the system, $\omega = 0$ and $\omega = \omega_1$.

For the current case the Fourier transform is

$$\tilde{F}(\omega) = \frac{2F_0\tau}{1 + (\omega\tau)^2} \tag{71}$$

Classical Mechanics 3

Scattering between two particles

An incoming particle (particle A) of mass m and velocity $\vec{v}$ and collides with a free particle (particle B) also of mass m, which is initially at rest in the laboratory frame. The two particles interact with a repulsive $1/r^2$ potential

$$U(r) = \frac{h}{r^2}\,, \quad h > 0\,,$$

where $\vec{r} = \vec{r}_A - \vec{r}_B$ is the relative coordinate of the two particles.

Find the angular distribution (the differential cross-section) of the deflected particles, $d\sigma(\theta)/d\theta$, where θ is the angle between $\vec{v}$ and particle A's velocity after the collision. Assume that the process is repeated many times with random impact parameter b, distributed so that the number of incident particles per transverse area is constant. In steps:

(a) (3 points) Write down the Lagrangian of the two particles. Introduce the center-of-mass and relative coordinates of the system, and show that the equation of motion of the relative coordinate $\vec{r}$ is that of a single (effective) particle in the potential $U(r)$. Express the energy E and angular momentum ℓ of the relative motion with respect to the origin of $\vec{r}$ in terms of the "laboratory" frame quantities m, v and b.

(b) (6 points) Find the trajectory $r(\phi)$, where the ϕ is the polar angle, of the effective particle with energy E and angular momentum ℓ moving in the potential $U(r)$. Follow the convention that $\phi = 0$ corresponds to the distance of closest approach as shown below.

(c) (6 points) Find the differential cross-section $d\sigma(\chi)/d\chi$ in the center-of-mass frame, where χ is the scattering angle in this frame.

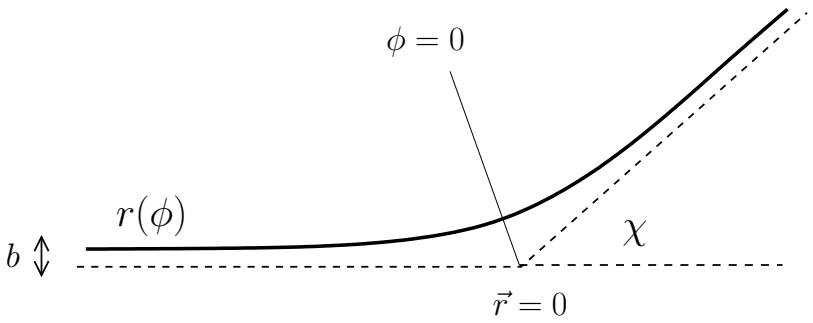


Figure 1: The scattering angle χ in the center-of-mass frame.

(d) (5 points) Convert $d\sigma(\chi)/d\chi$ into the initial "laboratory" frame to find $d\sigma(\theta)/d\theta$.

Solution

(a) Introducing the center-of-mass and relative coordinates: $\vec{r}_{c.m.} = (\vec{r}_1 + \vec{r}_2)/2$, and $\vec{r} = \vec{r}_1 - \vec{r}_2$, we see that the initial relative velocity is $\dot{\vec{r}} = \vec{v}$. The reduced mass of the relative motion is $m/2$. Therefore, the energy and the angular momentum of the relative motion are:

$$E = \frac{mv^2}{4}\,, \quad l = \frac{mv\rho}{2}\,.$$

(b) To find the trajectory, we evaluate the standard integral for the polar angle ϕ for motion in the central potential $U(r)$:

$$\phi = \frac{l}{\sqrt{m}} \int^r \frac{dr/r^2}{[E - (h + l^2/m)/r^2]^{1/2}} = -\int^{1/r} \frac{du}{[(mE/l^2) - (1 + mh/l^2)u^2]^{1/2}}$$

$$= \frac{1}{(1 + mh/l^2)^{1/2}} \arccos\Big(\frac{1/r}{\big[E/(h + l^2/m)\big]^{1/2}}\Big)\,.$$

The integration constant here was taken to be zero, the choice that makes $\phi = 0$ the pericenter. Finally, the trajectory is given by the following equation:

$$\frac{1}{r} = \Big(\frac{E}{h + l^2/m}\Big)^{1/2} \cos\big[(1 + mh/l^2)^{1/2}\phi\big]\,.$$

(c) This equation shows that the angle $2\phi_0$ between the incoming and outgoing directions of the particle scattered by the $1/r^2$ potential is:

$$2\phi_0 = \frac{\pi}{(1 + mh/l^2)^{1/2}}\,.$$

This means that the impact parameter $\rho = 2l/mv$ depends on the scattering angle $\chi = \pi - 2\phi_0$ as

$$\rho = \frac{(h/E)^{1/2}(\pi - \chi)}{\big[2\pi\chi - \chi^2\big]^{1/2}}\,.$$

Hence,

$$\frac{d\rho}{d\chi} = -\frac{(h/E)^{1/2}\pi^2}{\big[2\pi\chi - \chi^2\big]^{3/2}}\,,$$

and the differential cross section $d\sigma(\chi)/d\chi$ is:

$$\frac{d\sigma(\chi)}{d\chi} = \frac{\rho}{\sin\chi}\Big|\frac{d\rho}{d\chi}\Big| = \frac{h}{E\sin\chi}\,\frac{\pi^2(\pi - \chi)}{\chi^2(2\pi - \chi)^2} = \frac{4h}{mv^2\sin\chi}\,\frac{\pi^2(\pi - \chi)}{\chi^2(2\pi - \chi)^2}\,, \qquad \chi \in [0, \pi]\,.$$

(d) To convert this result into the laboratory frame, one needs to find the velocity of the scattered particle $\dot{\vec{r}}_1 = \dot{\vec{r}}_{c.m.} + \dot{\vec{r}}/2$. Since $\dot{\vec{r}}_{c.m.} = \vec{v}/2$, we see from this relation that the scattering angles in the center-of-mass and the laboratory frames are related simply as

$$\theta = \chi/2\,.$$

Equating the number of scattered particles in the two frames,

$$\frac{d\sigma}{d\chi}\sin\chi d\chi = \frac{d\sigma(\theta)}{d\theta}\sin\theta d\theta\,,$$

and using the relation between the scattering angles, we find finally:

$$\frac{d\sigma(\theta)}{d\theta} = 4\cos\theta\frac{d\sigma}{d\chi}\Big|_{\chi=2\theta} = \frac{h}{2mv^2\sin\theta}\,\frac{\pi^2(\pi-2\theta)}{\theta^2(\pi-\theta)^2}\,, \qquad \theta\in[0,\pi/2]\,.$$

Similarly, one can show that the angular distribution of the particles that initially were at rest is the same.

Electromagnetism 1

Radiation from an undulator

Consider an ultra-relativistic electron of charge q, mass m, and velocity v, propagating in the z direction with $\gamma \equiv 1/\sqrt{1 - v^2/c^2} \gg 1$. In the lab frame $\mathcal{F}_0$, the electron experiences a weak external sinusoidal magnetic field directed along the x axis:

$$\boldsymbol{B}(z) = B_0 \sin(kz)\, \hat{\boldsymbol{x}}\,. \tag{1}$$

The electron is only slightly deflected from its straight line motion as it propagates in the magnetic field.

In this problem we will compute the average energy radiated per unit time by the undulating electron in two ways. In parts $(a), (b), (c)$ we will work in a frame $\mathcal{F}$ moving (with the electron) at constant speed v in the z direction relative to the lab. In part (d) we will work directly in the lab frame $\mathcal{F}_0$.

(a) (4 points) Explicitly determine the external electromagnetic field in the moving frame $\mathcal{F}$ by making a Lorentz transformation. Compute the instantaneous Poynting vector in $\mathcal{F}$ (both magnitude and direction). Show that the transformed fields are equivalent to a plane wave. What is the wavelength and amplitude associated with these fields?

(b) (6 points) Determine the average energy radiated per unit time by the electron in frame $\mathcal{F}$.

(c) (4 points) Show that the energy radiated per unit time by an accelerating charged particle is invariant under Lorentz boosts in the z direction. What then is the average energy radiated per unit time in the lab frame $\mathcal{F}_0$ by the undulating electron?

Hint: Boost the radiated energy and momentum in a time interval Δt from the instaneous rest frame of the accelerating particle to a frame moving in the z direction.

(d) (6 points) The relativistic Larmor formula for the total energy W radiated per retarded time T is

$$\frac{dW}{dT} = \frac{2}{3}\left(\frac{q^2}{4\pi c^3}\right)\left(\gamma^6 \boldsymbol{a}_\parallel^2 + \gamma^4 \boldsymbol{a}_\perp^2\right)\,. \tag{2}$$

Here $\boldsymbol{a}_\parallel$ is the acceleration of the electron parallel to its velocity, and $\boldsymbol{a}_\perp$ is the acceleration perpendicular to its velocity.

Working in the lab frame, use Eq. (2) with the appropriate kinematic approximations to determine the average energy lost per time by the relativistic electron. Compare the result to that of part (c).

Solution

(a) We use the transformation rule

$$\underline{F}^{\mu\nu}(\underline{X}) = L^{\mu}_{\rho} L^{\nu}_{\sigma} F^{\rho\sigma}(X)\,, \tag{3}$$

to determine the field strength in the electron's frame. The only non-zero component of $F^{\rho\sigma}$ is $F^{yz} = -F^{zy} = B_x$, which follows from the relation, $F^{ij} = \epsilon^{ijk} B_k$. The matrix $(\mathcal{L})^{\mu}_{\nu} = L^{\mu}_{\nu}$ takes the form

$$\mathcal{L} = \begin{pmatrix} \gamma & 0 & 0 & -\gamma\beta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\gamma\beta & 0 & 0 & \gamma \end{pmatrix}, \tag{4}$$

and thus

$$\underline{F}^{\mu\nu} = L^{\mu}_{y} L^{\nu}_{\ z} F^{yz} - L^{\mu}_{z} L^{\nu}_{\ y} F^{yz}\,. \tag{5}$$

Looking at this formula, one of the indices in $\underline{F}^{\mu\nu}$ needs to be y. Thus, the non-zero components are $\underline{E}^{y} = \underline{F}^{0y}$ and $\underline{B}_x = F^{yz}$:

$$E^{y}(\underline{X}) = \underline{F}^{0y} = -\,L^{0}_{spz} L^{y}_{\ y} F^{yz} = \gamma\beta B_x(X)\,, \tag{6}$$

$$B^{x}(\underline{X}) = \underline{F}^{yz} = L^{y}_{y} L^{z}_{z} F^{yz} = \gamma B_x(X)\,. \tag{7}$$

We also need to express the coordinates of the lab frame in terms of the electrons coordinates, $X = (\mathcal{L}^{-1})\underline{X}$. This yields

$$ct = \gamma(c\underline{t}) + \gamma\beta\underline{z}\,, \tag{8}$$

$$z = \gamma\beta(c\underline{t}) + \gamma\underline{z}\,. \tag{9}$$

Thus, since $B_x(X) = B_0 \sin(kz)$ we find

$$B_x(X) = B_0 \sin\left(k\gamma v\underline{t} + k\gamma\underline{z}\right)\,, \tag{10}$$

and the fields in the ultra relativistic limit $\beta \simeq 1$ read

$$\underline{\boldsymbol{E}} = \gamma B_0 \sin\left(k\gamma\left(\underline{z} + c\underline{t}\right)\right)\,\hat{\boldsymbol{y}}\,, \tag{11}$$

$$\underline{\boldsymbol{B}} = \gamma B_0 \sin\left(k\gamma\left(\underline{z} + c\underline{t}\right)\right)\,\hat{\boldsymbol{x}}\,. \tag{12}$$

We note the similarity between these fields and a plane wave of light with wavenumber $k\gamma$ (wavelength $\lambda{=}2\pi/k\gamma$) moving in the negative z direction with amplitude γB_0. The Poynting vector $\boldsymbol{S} = c\boldsymbol{E} \times \boldsymbol{B}$ is

$$\boldsymbol{S} = -c\gamma^2 B_0^2 \sin^2(k\gamma\left(\underline{z} + c\underline{t}\right))\,\hat{\boldsymbol{z}}\,, \tag{13}$$

and is proportional to γ^2.

(b) In frame $\mathcal{F}$ the electric field of the incident plane wave is

$$\boldsymbol{E}(t,\boldsymbol{x}) = \mathcal{E}e^{-i\omega t+ikz}\hat{\boldsymbol{y}}\,, \tag{14}$$

where it is conventionally understood that we are to take the real part of this expression. From part (a), the amplitude of the electric field is $\mathcal{E} = \gamma B_0$.

For an electron at $z = 0$, the acceleration is given by Newton's law

$$\boldsymbol{a}(t) = \frac{q\mathcal{E}}{m}e^{-i\omega t}\hat{\boldsymbol{z}} \equiv \boldsymbol{a}_\omega e^{-i\omega t}\,. \tag{15}$$

The radiated power is

$$P = \frac{2}{3}\frac{q^2}{4\pi}\frac{a(t)^2}{c^3}\,, \tag{16}$$

and thus the time averaged radiated power reads

$$\overline{P} = \frac{1}{3}\frac{q^2}{4\pi}\frac{|a_\omega|^2}{c^3}\,. \tag{17}$$

Using the result from (a) that $\mathcal{E} = \gamma B_0$

$$\overline{P} = \left(\frac{1}{12\pi}\right)\frac{q^4}{m^2c^3}\gamma^2 B_0^2\,. \tag{18}$$

(c) In the rest frame, the energy radiated in a time Δt is $\Delta P^0 = \Delta E/c$. The momentum radiated in Δt is zero, $\Delta P^i = 0$. Over this time interval the change in the electron's four vector ΔX^μ is $(\Delta X^0, \Delta X^i) = (c\Delta t, \mathbf{0})$. We can now boost these four vectors in another frame.

Boosting the momentum in Z direction we find

$$\Delta\underline{P}^0 = \gamma\Delta P^0\,, \tag{19}$$

$$\Delta\underline{P}^z = -\gamma\beta\Delta P^0\,. \tag{20}$$

Boosting the coordinates yields

$$\Delta\underline{X}^0 = \gamma\Delta X^0\,, \tag{21}$$

$$\Delta\underline{X}^z = -\gamma\beta\Delta X^0\,. \tag{22}$$

Thus, in the new frame the energy radiated per time is

$$\frac{\Delta\underline{P}^0}{\Delta\underline{X}^0} = \frac{\gamma\Delta P^0}{\gamma\Delta X^0} = \frac{\Delta P^0}{\Delta X^0}\,, \tag{23}$$

establishing the invariance of this quantity.

Since the total power is Lorentz invariant it may be computed in the rest frame of the electron, and thus the frame $\mathcal{F}$ result of (b) holds in the lab frame $\mathcal{F}_0$

$$\overline{P} = \left(\frac{1}{12\pi}\right)\frac{q^4}{m^2c^3}\gamma^2 B_0^2\,. \tag{24}$$

(d) In the lab frame we can compute the acceleration of the electron using Newton's law

$$\frac{d\boldsymbol{p}}{dt} = q\,\frac{\boldsymbol{v}}{c} \times \boldsymbol{B}\,, \tag{25}$$

where

$$\boldsymbol{p} = \gamma m \boldsymbol{v}\,, \tag{26}$$

is the relativistic momentum. Here the particle is only scarcely deflected from its straight line motion. Thus, in a first approximation $\boldsymbol{v} \simeq c\,t\,\hat{\boldsymbol{z}}$, and the magnetic field then causes small deflections in the $\hat{\boldsymbol{z}} \times \hat{\boldsymbol{x}} = \hat{\boldsymbol{y}}$ direction. The acceleration in the y direction is approximately

$$a^y_\perp = \frac{dv^y}{dt} \simeq \frac{qv}{m\gamma c} B_0 \sin(kvt) \simeq \frac{q}{m\gamma} B_0 \sin(kct)\,. \tag{27}$$

The energy radiated is determined only by the transverse acceleration $\boldsymbol{a}_\perp$

$$\overline{\frac{dW}{dT}} = \frac{2}{3}\left(\frac{q^2}{4\pi c^3}\right)\gamma^4 \overline{\left(\frac{q^2}{\gamma^2}\,B_0^2\,\sin^2(kct)\right)} \tag{28}$$

$$= \frac{1}{12\pi}\frac{q^4}{m^2c^3}\gamma^2 B_0^2 \tag{29}$$

in agreement with part (d).

Electromagnetism 2

A current loop and a sphere

A circular loop of radius R, lying flat in the xy-plane with center at the origin, carries a uniform current I. A sphere of radius $a \ll R$ and permeability μ is placed at a height $h \gg a$ on the z axis above the xy-plane.

a. (6 points) Determine the magnetic field $\vec{\mathbf{B}}$ inside and outside the sphere.

b. (4 points) Determine the force between the sphere and the ring. Give a qualitative explanation for the direction of the force for both paramagnetic ($\mu > \mu_0$) and diamagnetic ($\mu < \mu_0$) materials.

c. (5 points) Determine the angular distribution of the force per area on the surface of the sphere to leading order in a/R.

d. (3 points) Integrate the force per area in (c) to find the total force and compare the result to (b). Do they agree? Why or why not? Explain.

e. (2 points) Now place the sphere in the center of the ring at zero height, $h = 0$. Is this configuration stable or unstable configuration? Explain. Consider both paramagnetic and diamagnetic materials.

Solution

a. The magnetic field created by the loop at a heigth h is

$$\vec{\mathbf{B}} = \oint_C \frac{I d\vec{l} \times \hat{R}_h}{R_h^2} = \frac{I 2\pi R^2}{R_h^3} \hat{z} = B_0(h)\hat{z} \tag{30}$$

with $R_h^2 = R^2 + h^2$. Throughout the coordinate system will be centered in the sphere. The corresponding applied magnetic potential $\vec{\mathbf{B}}_0 = -\vec{\nabla}\varphi_0$ is $\varphi_0 = -B_0(h)z/\mu_0$. When a sphere of radius $a \ll R$ is positioned at height h, we will assume that the outside potential around the sphere $\varphi_>$ asymptotes φ_0. Let $\varphi_<$ be the potential inside the sphere. Since both satisfy $\nabla^2\varphi_{<,>} = 0$, then for the lowest partial wave (dipole)

$$\varphi_> = \frac{A}{r^2}\cos\theta + \varphi_0 \qquad\qquad \varphi_< = Cr\cos\theta \tag{31}$$

subject to the continuity equations at $r = a$,

$$\phi_> = \phi_< \qquad\qquad \mu_0 \frac{\partial \varphi_>}{\partial r} = \mu \frac{\partial \varphi_<}{\partial r} \tag{32}$$

which gives

$$\varphi_< = \left(\frac{-3}{\mu + 2\mu_0}\right) B_0 z \qquad\qquad \mathbf{B}_< = -\mu\vec{\nabla}\varphi_< = \left(\frac{3\mu}{\mu + 2\mu_0}\right) \vec{\mathbf{B}}_0 \tag{33}$$

and similarly for $\vec{\mathbf{B}}_> = -\mu_0\vec{\nabla}\varphi_>$.

b. The magnetization follows as

$$\vec{\mathbf{B}}_< = \mu_0\left(\vec{\mathbf{H}} + \vec{\mathbf{M}}\right) = \mu\vec{\mathbf{H}} \tag{34}$$

and therefore

$$\vec{\mathbf{M}} = \frac{3(\mu - \mu_0)}{\mu_0(\mu + 2\mu_0)} \vec{\mathbf{B}}_0 \equiv \alpha\, \vec{\mathbf{B}}_0 \tag{35}$$

b. The energy of the sphere in the external field $\vec{\mathbf{B}}_0$ is

$$\mathcal{E} = -\left(\frac{4\pi a^3}{3}\vec{\mathbf{M}}\right) \cdot \vec{\mathbf{B}}_0 \tag{36}$$

The binary force between the loop and the sphere is along the z-axis by symmetry

$$F_z = -\frac{\partial \mathcal{E}}{\partial h} = \frac{18(\mu - \mu_0)}{\mu_0(\mu + 2\mu_0)} \frac{4\pi h a^3}{3R_h^2} B_0^2(h) \tag{37}$$

It is attractive for $\mu_0 < \mu$ and repulsive for $\mu_0 > \mu$.

d. To determine the angular distribution of the force around the sphere, we note that the surface current density is

$$\vec{\sigma}_M = \hat{r} \times (\vec{\mathbf{H}}_< - \vec{\mathbf{H}}_>) = \vec{\mathbf{M}} \times \hat{r} \tag{38}$$

since $\hat{r} \times (\vec{\mathbf{B}}_< - \vec{\mathbf{B}}_>)$. The pressure on the sphere or force per unit area is

$$\vec{f} \equiv \frac{d\vec{\mathbf{F}}}{dA} = \vec{\sigma}_M \times \vec{\mathbf{B}}_0 = \alpha((\vec{\mathbf{B}}_0 \times \hat{r}) \times \vec{\mathbf{B}}_0) = \alpha B_0^2(h)(\hat{r} - \hat{z}\,(\hat{r} \cdot \hat{z})) \tag{39}$$

which clearly shows that $f_z = 0$. The total force is

$$\vec{\mathbf{F}} = \alpha B_0^2(h) \int a^2 d\Omega\,(\hat{r} - \hat{z}\,(\hat{r} \cdot \hat{z})) \tag{40}$$

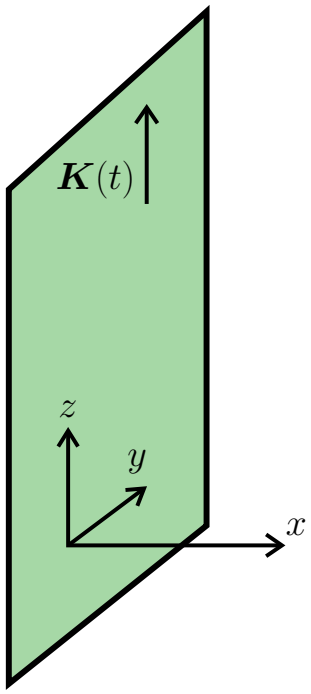
with manifest $\mathbf{F}_z = 0$. This is expected from the Lorentz character of the force on the surface currents on the sphere.

e. The expression of F_z in (37) shows that although $F_z = 0$ for $h = 0$, a small deviation up results in a repulsive force for $\mu_0 > \mu$ and an attractive force for $\mu_0 < \mu$. The former configuration is unstable, while the latter is stable.

Electromagnetism 3

A current sheet in an ohmic medium

Consider an infinite sheet lying in the zy plane carrying surface current[1], $\boldsymbol{K} = K_0\, e^{-i\omega t}\, \hat{\boldsymbol{z}}$. The current is driven by an external source which sustains the current's amplitude and frequency.



(a) (4 points) First consider the this current-carrying sheet in vacuum. Determine the magnetic and electric fields to lowest (non-trivial) order in the frequency. Sketch the amplitude of the electric field as a function of x for both positive and negative values of x. Do your results for the electromagnetic fields hold everywhere in space? Explain.

(b) (8 points) Now place the same current sheet into an ohmic medium of conductivity σ with[2] $\sigma \gg \omega$. Determine the (real) electric and magnetic fields everywhere in space. Sketch the amplitude of the electric field as a function of x for both positive and negative values of x.

Show how your results for the fields follow from the Maxwell equations and their boundary conditions. Assume that[3] $\epsilon = \mu = 1$.

(c) (8 points) Determine the total energy dissipated per time by the induced electric fields in the ohmic medium. Show that it equals the work done per time by the external source maintaining the surface current.

[1] The units of K_0 are amps/meter in SI units.
[2] In SI units this reads $\sigma/\epsilon_0 \gg \omega$.
[3] In SI units this reads $\epsilon = \epsilon_0$ and $\mu = \mu_0$.

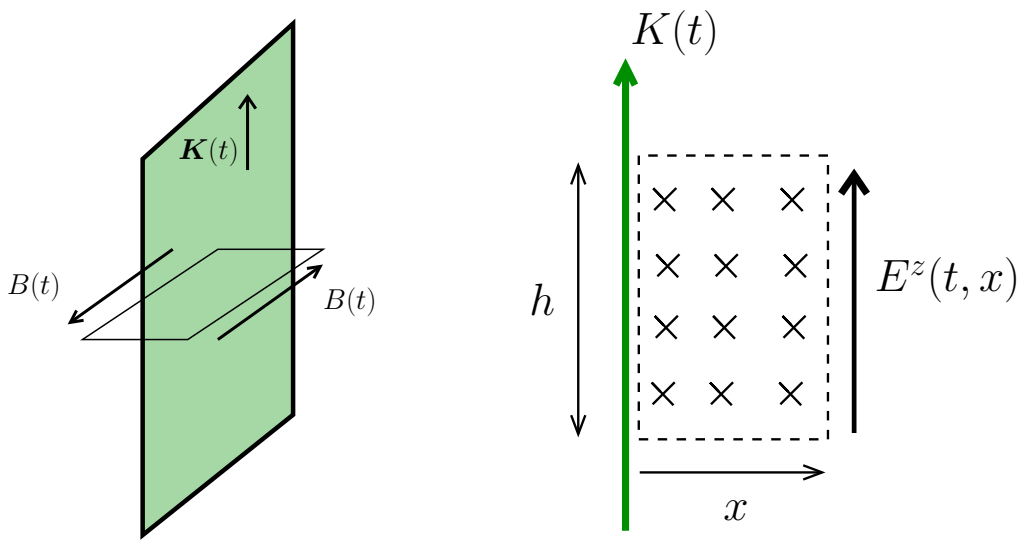


Figure 1: (a) Amperian loop used to determine the magnetic field. (b) Loop used to determine the electric field using Faraday's law.

Solution:

(a) Drawing an Amperian loop of length ℓ as shown in Fig. 1(a) we find

$$\oint \boldsymbol{B} \cdot d\boldsymbol{\ell} = \frac{I}{c}\,, \tag{41}$$

$$2B(t)\ell = \frac{K(t)}{c}\ell\,. \tag{42}$$

Reinserting the direction of the magnetic field we find

$$\boldsymbol{B}(t) = \begin{cases} \frac{K_0}{2c} e^{-i\omega t}\hat{\boldsymbol{y}} & x > 0 \\ -\frac{K_0}{2c} e^{-i\omega t}\hat{\boldsymbol{y}} & x < 0 \end{cases}\,. \tag{43}$$

One can also immediately check that the boundary conditions are satisfied:

$$\boldsymbol{n} \times (\boldsymbol{B}_2 - \boldsymbol{B}_1) = \frac{\boldsymbol{K}(t)}{c}\,, \qquad \text{or} \qquad B^y|_{x=0^+} - B^y|_{x=0^-} = \frac{K(t)}{c}\,. \tag{44}$$

To determine the induced electric field we use Faraday's Law in integral form

$$\oint \boldsymbol{E} \cdot d\boldsymbol{\ell} = -\frac{1}{c}\partial_t \int \boldsymbol{B} \cdot d\boldsymbol{a}\,. \tag{45}$$

Drawing a surface as shown in Fig. 1(b) for $x > 0$ we find

$$E^z(t)h = +\frac{1}{c}\partial_t B^y(t) h x\,, \tag{46}$$

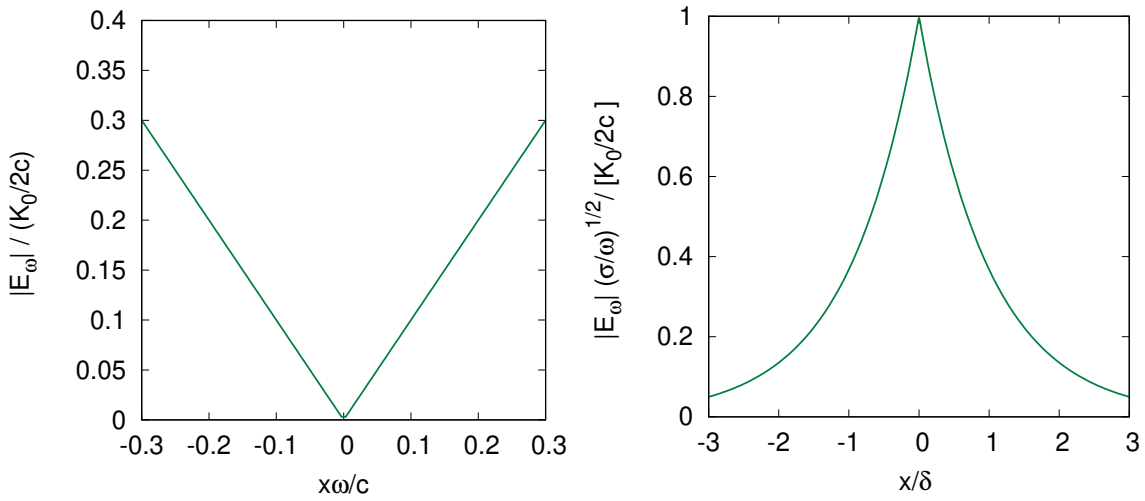


Figure 2: (a) The electric field in vacuum from part (a), Eq. (49). (b) The electric field in the ohmic medium, Eq. (64). In case (b) (in contrast to (a)) the work done by the external source is non-zero because the induced electric field does not vanish at $x = 0$.

where we have recognized that the normal to the surface is in the negative y direction for a loop as drawn in Fig. 1(b), and thus $\boldsymbol{B} \cdot d\boldsymbol{a} < 0$. For $x > 0$ the electric field reduces to

$$E^z(t) = \frac{-i\omega}{c} \frac{K_0}{2c} e^{-i\omega t} x \qquad x > 0\,. \tag{47}$$

A similar loop for $x < 0$ gives

$$E^z(t) = \frac{-i\omega}{c} \frac{K_0}{2c} e^{-i\omega t} (-x) \qquad x < 0\,, \tag{48}$$

leading to our final result

$$\boldsymbol{E}(t,x) = \mathrm{Re}\left[\frac{-i\omega K_0}{2c^2} e^{-i\omega t}|x|\right] \hat{\boldsymbol{z}}\,, \tag{49}$$

$$= -\frac{\omega|x|}{c} \sin(\omega t) \frac{K_0}{2c} \hat{\boldsymbol{z}}\,. \tag{50}$$

A graph of the electric field (amplitude) in the z direction is shown in Fig. 2(a). The amplitude of the electric field grows with x, and when

$$\frac{\omega x}{c} \sim 1\,, \tag{51}$$

the quasi-static approximation used here is no longer valid. At this point the electric field becomes comparable to the magnetic field.

(b) When the sheet is in an ohmic medium, we first derive the appropriate magnetic diffusion equation for magnetic field in conducting media. Writing $\boldsymbol{j} = \sigma \boldsymbol{E}$ we find

$$\nabla \times (\nabla \times \boldsymbol{B}) = \frac{\sigma}{c} \nabla \times \boldsymbol{E}\,. \tag{52}$$

Using

$$\nabla \times (\nabla \times \boldsymbol{B}) = \nabla(\nabla \cdot \boldsymbol{B}) - \nabla^2 \boldsymbol{B}\,, \tag{53}$$

and Faraday's Law

$$\nabla \times \boldsymbol{E} = -\frac{1}{c}\partial_t \boldsymbol{B}\,, \tag{54}$$

we find the magnetic diffusion equation

$$\nabla^2 \boldsymbol{B} = \frac{\sigma}{c^2}\partial_t \boldsymbol{B}\,. \tag{55}$$

In this problem we are motivated by the right hand rule to try a solution of the form

$$\boldsymbol{B}(t,x) = B_0 e^{ikx - i\omega t}\hat{\boldsymbol{y}}\,. \tag{56}$$

Substituting this ansatz into the diffusion equation, Eq. (55), and solving for k we find two possible values of k

$$k_\pm \equiv \pm\sqrt{i\frac{\sigma\omega}{c^2}} = \pm\frac{1}{\delta}(1+i)\ . \tag{57}$$

In the last step, we used the traditional definition of the skin depth

$$\delta \equiv \sqrt{\frac{2c^2}{\sigma\omega}}\,. \tag{58}$$

The solution must decay as $x \to \pm\infty$ and should have a symmetric character. Thus, the solution to the right and left of the current sheet takes the form

$$\boldsymbol{B} = \mathrm{Re}\begin{cases} B_0 e^{i(1+i)x/\delta} e^{-i\omega t}\hat{\boldsymbol{y}} & x > 0 \\ -B_0 e^{-i(1+i)x/\delta} e^{-i\omega t}\hat{\boldsymbol{y}} & x < 0 \end{cases}\,. \tag{59}$$

The coefficient B_0 can be found from the boundary conditions, Eq. (44),

$$B_0 = \frac{K_0}{2c}\,, \tag{60}$$

and the solution therefore takes the form

$$\boldsymbol{B} = \pm\frac{K_0}{2c} e^{-|x|/\delta}\cos(|x|/\delta - \omega t)\hat{\boldsymbol{y}}\,. \tag{61}$$

Here the positive sign is for $x > 0$ and the negative sign is for $x < 0$.

The electric field is found from Ampere's Law together with the constitutive relation $\boldsymbol{j} = \sigma\boldsymbol{E}$:

$$\nabla \times \boldsymbol{B} = \frac{\sigma \boldsymbol{E}}{c}\,. \tag{62}$$

Since B is the y direction

$$(\nabla \times \boldsymbol{B})_z = \partial_x B_y = ik_+ \frac{K_0}{2c} e^{ik_+ x - i\omega t}\,, \tag{63}$$

leading to our final result for $x > 0$

$$E^z(t,x) = -\,\mathrm{Re}\left[\frac{c(1-i)}{\sigma\delta}\frac{K_0}{2c}e^{ik_+x-i\omega t}\right], \tag{64}$$

$$= -\,\mathrm{Re}\left[\frac{\sqrt{2}c}{\sigma\delta}\,\frac{K_0}{2c}e^{-x/\delta}e^{ix/\delta-i\omega t-i\pi/4}\right], \tag{65}$$

$$= -\sqrt{\frac{\omega}{\sigma}}\left(\frac{K_0}{2c}\right)e^{-x/\delta}\cos(x/\delta-\omega t-\pi/4)\,. \tag{66}$$

In the last step we recognized that

$$\frac{\sqrt{2}c}{\sigma\delta} = \sqrt{\frac{\omega}{\sigma}}\,. \tag{67}$$

The solution for $x < 0$ is follows by the relacements $x \to |x|$. A graph of the amplitude, $|E_\omega| \propto e^{-|x|/\delta}$ is shown in Fig. 2(b).

(c) The work done per area per time can be found in at least three ways:

1. By calculating the work done by the battery, $-\boldsymbol{K}\cdot\boldsymbol{E}$. The work done by the battery on the currents is, $\boldsymbol{K}\cdot\boldsymbol{E}_{\rm batt}$. The battery must supply an additional field $\boldsymbol{E}_{\rm batt} = -\boldsymbol{E}$ to counter balance the induced field $\boldsymbol{E}$, and maintain the current $\boldsymbol{K}$.

2. By calculating the Poynting flux flowing out of the sheet.

3. By integrating the dissipation rate over the volume: $\int dV\,\boldsymbol{j}\cdot\boldsymbol{E} = \sigma\int dV E^2$

They should all agree. All of these calculations involve time averages of harmonic quantities, which are calculated as follows: if $A(t) = \mathrm{Re}[A_\omega e^{-i\omega t}]$ and $B(t) = \mathrm{Re}[B_\omega e^{-i\omega t}]$ then

$$\overline{A(t)B(t)} = \frac{1}{2}\mathrm{Re}[A_\omega B_\omega^*]\,. \tag{68}$$

The first method directly evaluates the work done by the battery

$$\frac{dW}{dt\,dA} = -\,\overline{\boldsymbol{K}\cdot\boldsymbol{E}}\big|_{x=0} \tag{69}$$

$$= -\,\frac{1}{2}\mathrm{Re}[K_\omega (E^z_\omega)^*] \tag{70}$$

$$= +\,\frac{1}{2}\mathrm{Re}[K_0\sqrt{\frac{\omega}{\sigma}}\frac{K_0^*}{2c}\frac{(1-i)}{\sqrt{2}}] \tag{71}$$

$$= \frac{|K_0|^2}{4c}\sqrt{\frac{\omega}{2\sigma}} \tag{72}$$

The Poynting flux methods is evaluated similarly. There are two sides to the sheet leading to a factor of two

$$\frac{dW}{dt\,dA} = 2c\,\overline{\boldsymbol{E}\times\boldsymbol{B}}\cdot\hat{\boldsymbol{x}}\,, \tag{73}$$

$$= -\,2c\,\frac{1}{2}\mathrm{Re}\left[\left(\frac{K_\omega}{2c}\right)(E^z_\omega)^*\right], \tag{74}$$

which clearly agrees with Eq. (70). (The minus in passing from the first to the second line follows from $\hat{\boldsymbol{z}} \times \hat{\boldsymbol{y}} = -\hat{\boldsymbol{x}}$.) We should expect agreement between these two methods since

$$-\nabla \cdot \boldsymbol{S} = \boldsymbol{j} \cdot \boldsymbol{E}\,, \tag{75}$$

Integrating $\nabla \cdot \boldsymbol{S}$ over a Gaussian "pillbox" shows directly that the Poynting flux out of the sheet equals the work done by the battery, $-\boldsymbol{K} \cdot \boldsymbol{E}$.

Finally, we integrate the ohmic dissipation over the volume. Here we evaluate the contribution from $x > 0$ and then multiply by a factor of two to account for $x < 0$:

$$\frac{dW}{dt\,dA} = 2\sigma \int_0^\infty dx \overline{E^2}\,, \tag{76}$$

$$= 2\sigma \int_0^\infty dx \frac{1}{2} \left(\frac{|K_0|^2}{4c^2} \frac{\omega}{\sigma} e^{-2x/\delta} \right)\,, \tag{77}$$

$$= \omega \frac{|K_0|^2}{8c^2}\,\delta\,, \tag{78}$$

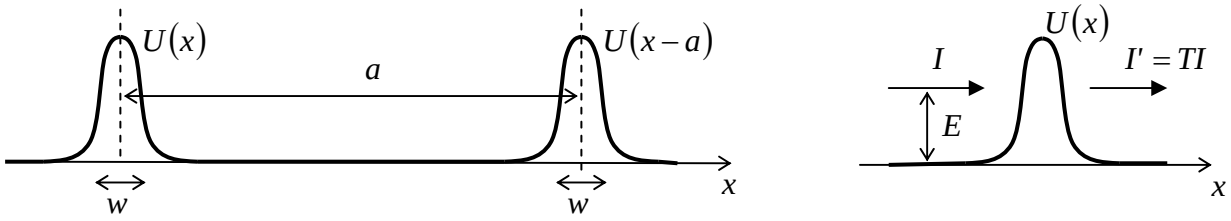
$$= \sqrt{\frac{\omega}{2\sigma}} \frac{|K_0|^2}{4c}\,. \tag{79}$$

All three methods thus give the same answer.

Quantum Mechanics 1

Resonant tunneling and state metastability

Your goal in this problem is to study and relate two basic quantum properties of a one-dimensional non-relativistic particle of mass m, moving in the system of two similar, symmetric potential barriers $U(x)$ of width scale w, separated by a much larger distance $a >> w$ – see the left panel in the figure below. Each barrier has a tunneling transparency $T \leq 1$ (which is some smooth function of the particle's energy E), defined as shown on the right panel of the figure, where I and I' are the probability currents of the incident and transferred monochromatic de Broglie waves.



A (4 points). Calculate the (similarly defined) transparency T' of the two-barrier system for a monochromatic de Broglie wave incident from afar, as a function of a, T, and the particle's energy E.

B (2 points). Sketch the calculated transparency as a function of a, and prove that its largest value, reached at certain resonance values a_{res}, equals 1, and hence may be larger than T. Give a physical interpretation of this fact.

C (4 points). For the case of a very low barrier transparency, $T << 1$, and the distance a close to one of its resonance values a_{res}, calculate the energy width δE of the transparency resonance. (For certainty, use the standard "FWHM" definition of the width as the energy interval within that the transparency is larger than ½.)

D (7 points). Now consider the situation when the particle is initially placed between the barriers (again with a very low transparency $T << 1$), in its lowest-energy state, which is metastable due to the tunneling through the barriers. Calculate the law of the time decay of the probability to find the particle between the barriers, in the lowest nonvanishing approximation in T.

E (3 points). Compare the characteristic time τ of the metastable state's decay to the energy width δE calculated in Task C, and comment. Explain why such "energy-time uncertainty relation" is less general than the canonical uncertainty relations - such as those between Cartesian components of the generalized coordinates and the corresponding momenta.

Hint: Working on Task D, it may be helpful to represent the standing de Broglie wave describing the metastable state as a sum of two waves traveling in opposite directions.

Solution:

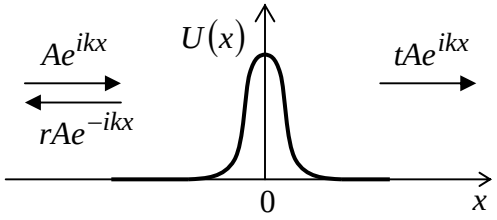
A (4 points): Outside of the barriers, i.e. in any region where $U(x) = 0$, the stationary 1D Schrödinger equation has the simple form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + E\psi = 0\,,$$

and hence is satisfied with any linear superposition of two de Broglie waves $\exp\{\pm ikx\}$, where the wave number k is determined by the particle's energy E:

$$\frac{\hbar^2 k^2}{2m} = E\,.$$

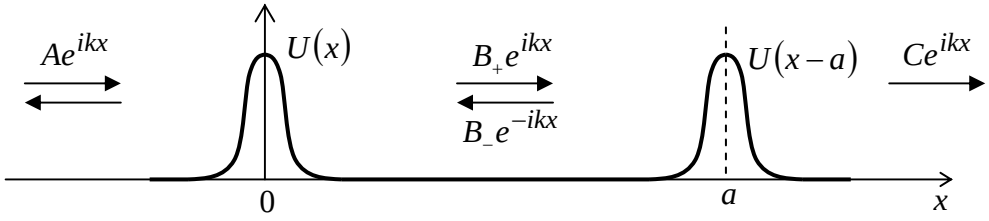
Due to the Schrödinger equation's linearity for any x, for a single barrier located at $x = 0$, with the wave incident from the left, the coefficients in such superpositions at $x < 0$ and $x > 0$ may be selected as shown in Fig. below.



Here t and r the (generally, complex) transmission and reflection coefficients, which may depend on the energy of the incident wave, but not its amplitude A. Since the corresponding probability currents I are proportional to the squares of the moduli of these coefficients, they are related by the probability conservation law as

$$|rA|^2 + |tA|^2 = |A|^2, \qquad \text{giving } |r|^2 = 1 - |t|^2 \equiv 1 - T\,. \tag{1}$$

For the system of two barriers, we may take the superpositions, in three regions outside the barriers, in the form shown in Fig. below.



Now requiring that the waves incident upon, transmitted through, and reflected from each barrier satisfy the same relations as for a single barrier, we get the following relations between the complex amplitudes of these waves:

$$B_+ = tA + rB_-\,, \qquad B_-e^{-ika} = rB_+e^{ika}\,, \qquad Ce^{ika} = tB_+e^{ika}\,.$$

This system of linear equations yields, in particular,

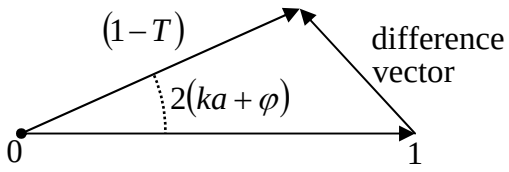
$$C = \frac{t^2 A}{1 - r^2 \exp\{2ika\}},$$

so that using Eq. (1), the transparency of the system may be represented as

$$T' \equiv \frac{I_C}{I_A} = \left|\frac{C}{A}\right|^2 = \left|\frac{t^2}{1 - r^2 \exp\{2ika\}}\right|^2 \equiv \frac{\left(|t|^2\right)^2}{\left|1 - |r|^2 \exp\{2i(ka + \varphi)\}\right|^2} = \frac{T^2}{\left|1 - (1 - T)\exp\{2i(ka + \varphi)\}\right|^2}, \quad (2)$$

where the real phase $\varphi \equiv \arg r$ may be also a (smooth) function of k, and hence of the energy E.

B (2 points). The easiest way to analyze T' as a function of a is to consider the denominator of the last form of Eq. (2) as the square of the length of the 2D vector that is the difference of two vectors: one of length 1, directed along some fixed axis, and the second vector of length $(1 - T)$, turned by the angle $2(ka + \varphi)$ – see Fig. below.

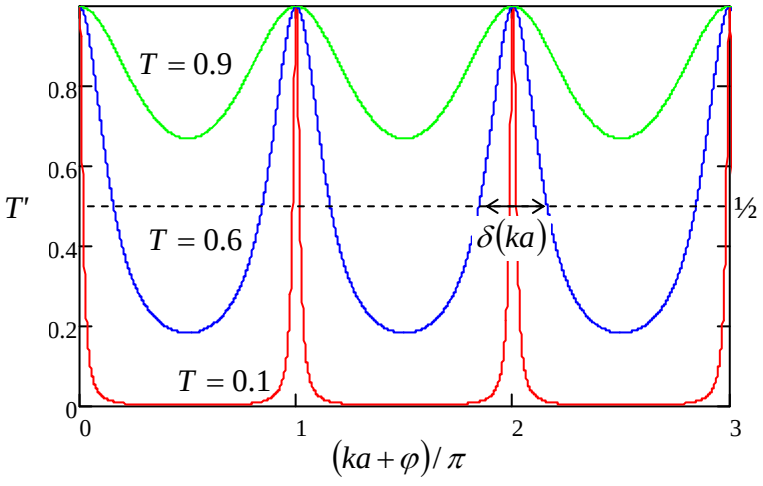


The change of a, which affects only this angle, leads to the mutual rotation of the two vectors with the period $\Delta(ka) = 2\pi$, and as a result, to oscillations of the denominator in Eq. (2), and hence of the transparency T', with the same period. This is the effect of resonant tunneling, physically arising from the interference of the de Broglie waves reflected from two potential barriers. The largest value of T' is reached when the two vector are exactly aligned, i.e. when

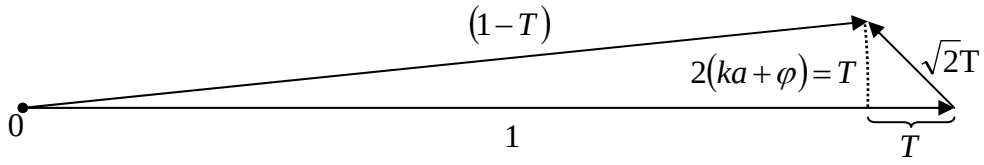
$$ka + \varphi = k_n a + \varphi \equiv \pi n, \quad (3)$$

where n is an integer, so that the vector of their difference has the length T, and Eq. (2) yields $T'_{max} = 1$. This value may be indeed larger than the transparency T of a single barrier, because due to the constructive interference of the reflected waves, the internal wave amplitudes $B_{\pm}$ are resonantly increased, resulting in the corresponding increase of the transmitted wave's amplitude C.

Figure below shows plots of Eq. (2) for several values of the parameter T. The smaller is T, the sharper is the resonance peak, i.e. the smaller is its FWHM (Full Width on Half-Maximum), $\delta(ka)$.



C (4 points). If the single barrier's transparency is very low, $T << 1$, the two vectors discussed above have very close lengths, so that the transparency decreases to ½ when the angle $2(ka + \varphi)$ between them is increased to a small amount equal to approximately $\pm T$ – see the vector diagram below.



The distance between these two values is

$$\delta\left[2(ka+\varphi)\right] \equiv 2(ka+\varphi)_{+} - 2(ka+\varphi)_{-} \approx 2T,$$

Since T (and hence r and t, including $\varphi \equiv \arg r$) are relatively slow functions of k, we may use this expression even if this change of the phase shift $2(ka + \varphi)$ is achieved using a small change δE of particle's energy, and hence of the wave vector, at constant $a \approx a_{res}$:

$$\delta k \approx \frac{T}{a}, \qquad \text{so that } \delta E \approx \frac{dE}{dk}\delta k = \frac{\hbar^2}{m} k \delta k \approx \frac{\hbar^2 k_n}{ma} T\,. \tag{4}$$

D (7 points). If $T = 0$, the particle placed between the barriers has genuine stationary states described by standing waves,

$$\psi_n(x) = B\sin(k_n x + \text{const}),$$

with the wave numbers given by Eq. (3). If T is nonvanishing but very small, this solution still may be used as a reasonable approximation, but due to the particle "leakage" (tunneling) through the barriers, the wavefunction has to be normalized not to unity, but to the probability W of finding the particle between the barriers at this particular instant, which may be less than 1:

$$\int_{\text{inside}} |\psi|^2 dx \equiv |B|^2 \int_{\text{inside}} \left|\sin(k_n x + \varphi)\right|^2 dx = W\,.$$

In the limit $w << a$, the exact interval of this integration are not important, and may be taken to be $[0, a]$. Since, according to Eq. (3), this interval contains an integer number of de Broglie half-waves, the integral equals $a/2$, and we get

$$|B|^2 \frac{a}{2} = W, \qquad \text{i.e. } |B|^2 = \frac{2W}{a}\,.$$

As suggested in the Hint, this solution may be represented in the same form as in Task A:

$$\psi_n(x) = B_{+}\exp\{+ik_n x\} + B_{-}\exp\{-ik_n x\}, \qquad \text{with } |B_{+}| = |B_{+}| = \frac{|B|}{2} = \left(\frac{W}{2a}\right)^{1/2}.$$

Each of these waves, hitting the corresponding barrier, induces beyond it an outgoing wave with the amplitude $C_{\pm} = tB_{\pm}$ and hence with the probability current

$$I_{\pm} = \pm\frac{\hbar k_n}{m}|C_{\pm}|^2 = I = \pm\frac{\hbar k_n}{m}|tB_{\pm}|^2 = \pm\frac{\hbar k_n}{m} T \frac{W}{2a}. \tag{5}$$

These leakage currents gradually reduce the probability W. The law of this reduction may be found from the general probability conservation law, in our case taking the form[1]

$$\frac{dW}{dt} + I_+ - I_- = 0 .$$

With the result (5), this law gives a simple differential equation

$$\frac{dW}{dt} = -\frac{W}{\tau}, \qquad \text{with } \frac{1}{\tau} = \frac{\hbar k_n}{ma} T , \tag{6}$$

with the elementary solution $W(t) = W(0)\exp\{-t/\tau\}$, so that the constant τ given by Eq. (6) is the metastable state's lifetime.

E (3 points). Comparing Eqs. (4) and (6), we see that their relation is remarkably simple:

$$\delta E = \frac{\hbar}{\tau}, \qquad \text{i.e. } \delta E\, \tau = \hbar . \tag{7}$$

This "energy-time uncertainty relation" is much more general than the analyzed situation, and is valid, in particular, for a broad class of metastable states. However, it is still *less* general than canonical uncertainty relation, in particular the Heisenberg's relation

$$\delta r_j\, \delta p_j \geq \frac{\hbar}{2}. \tag{8}$$

Indeed, in quantum mechanics, the Cartesian coordinates r_j of a particle, the Cartesian components p_j of its momentum, and the energy E are regular observables, represented by operators. In contract, the time is treated as a c-number argument, and is not represented by an operator, so that Eq. (7) cannot be derived using such general assumptions as Eq. (8). Thus the time-energy uncertainty relation should be applied with caution.

* * *

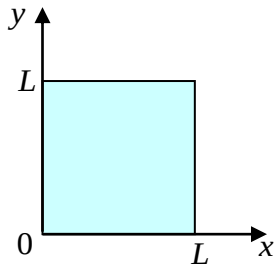
Finally, note that this the simple model discussed in this problem is a convenient platform for discussion of several conceptual issues of quantum mechanics, including the relation between closed (and hence energy-conserving) and open (and hence dissipative) systems, in particular their time reversibility and irreversibility, and also of the so-called "wave-packet reduction" at quantum measurements – see, e.g., Sec. 2.5 in https://commons.library.stonybrook.edu/egp/4/ .

[1] If the system is initially in one of its higher metastable states, with $k_n > (k_n)_{\min}$, the perturbation caused by the barrier transparency may also cause quantum transitions to lowest-energy states, thus affecting the probability conservation law. This is why this problem asks only the explore the lowest-energy state.

Quantum Mechanics 2

Orbital motion perturbations

A spinless point particle of mass *m* is confined to a square-shape two-dimensional region of size $L \times L$:



A (2 points). Write down the stationary wave functions and the corresponding eigenenergies of the particle.

B (5 points). Now consider there is a "point defect" inside the region, whose potential can be modeled as

$$U = \lambda L^2 \delta(\vec{r} - \vec{r}_0),$$

where $\vec{r}_0 = \{x_0, y_0\}$ is the location of the defect. Treating the potential as a perturbation, calculate the first-order corrections to the energies of the ground state and the first excited state. Find out the locations of the defect (inside the square), at which the 1st excited state remains degenerate.

C (7 points). Now consider a moving "defect", which oscillates along the *x*-direction at the center of the square:

$$\vec{r}_0 = \left\{ \frac{L}{2} + l \sin \omega t, \frac{L}{2} \right\},$$

where $l << L$. Find out the selection rule for the particle excitation from the ground state to an arbitrary excited state. Calculate the time-dependent probability for the charge to be in the first excited state, for $\omega << \omega_{fi}$, where $\hbar\omega_{fi}$ is the energy difference between the initial and final states, using the time-dependent perturbation theory.

D (6 points). At $\omega << \omega_{fi}$, the time evolution of the system obeys the adiabatic theorem. Use this fact to calculate the time-dependent transition probability from the ground state to the first excited state. Compare your result with what you got in Task C.

Solution:

a) The wave functions are standing waves which vanish at the edges of the region:

$$\Psi_{n_x,n_y} = |\mathrm{n}_x, n_y> = \frac{2}{L}\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_y\pi y}{L}\right)$$

where n_x, n_y = 1, 2, 3, ….. And the corresponding energies are:

$$\mathrm{E}_{n_x,n_y} = \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2 + n_y^2\right)$$

Ground state: $(n_x, n_y) = (1,1)$, not degenerate.

First excited state, $(n_x, n_y) = (1,2), (2,1)$, denegeracy=2.

b) Ground state is not degenerate, so the 1st order energy correction is:

$$\Delta\mathrm{E}_{11}^{(1)} = \langle 1,1|V'|1,1\rangle$$

$$= \frac{4}{L^2}\int dxdy \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right)\delta(x - x_0)\delta(y - y_0)\lambda L^2$$

$$= 4\lambda\sin^2\left(\frac{\pi x_0}{L}\right)\sin^2\left(\frac{\pi y_0}{L}\right)$$

For the first excited states: $|1,2>$ and $|2,1>$

$$\langle 1,2|V'|1,2\rangle = 4\lambda\sin^2\left(\frac{\pi x_0}{L}\right)\sin^2\left(\frac{2\pi y_0}{L}\right) \equiv a$$

$$\langle 1,2|V'|2,1\rangle = 4\lambda\sin\left(\frac{\pi x_0}{L}\right)\sin\left(\frac{2\pi x_0}{L}\right)\sin\left(\frac{2\pi y_0}{L}\right)\sin\left(\frac{\pi y_0}{L}\right) \equiv b$$

$$\langle 2,1|V'|1,2\rangle = 4\lambda\sin\left(\frac{2\pi x_0}{L}\right)\sin\left(\frac{\pi x_0}{L}\right)\sin\left(\frac{\pi y_0}{L}\right)\sin\left(\frac{2\pi y_0}{L}\right) = b$$

$$\langle 2,1|V'|2,1\rangle = 4\lambda\sin^2\left(\frac{2\pi x_0}{L}\right)\sin^2\left(\frac{\pi y_0}{L}\right) \equiv c$$

Solving:
$$\begin{pmatrix} a & b \\ b & c \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = E_2^{(1)}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

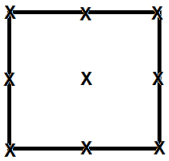
We get: $\Delta E_2^{(1)} = \frac{a+c\pm\sqrt{(a-c)^2+4b^2}}{2} = 0, a + c$

$$\frac{u_1}{u_2} = \frac{2b}{a + c \pm \sqrt{(a-c)^2 + 4b^2}}$$

Hence:
$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \frac{1}{\sqrt{1+\alpha^2}}\begin{pmatrix} \alpha \\ 1 \end{pmatrix}$$

For the 1st excited state to remain degenerate, $(a-c)^2 + 4b^2 = 0$, so $a = c$ and $b = 0$

Hence: $x_0 = 0, \frac{L}{2}, L$; and $y_0 = 0, \frac{L}{2}, L$

 (locations which do not break degeneracy for the 1st excited state)

b) First we can write down the time-dependent defect potential:

$$V' = \lambda L^2 \delta\left(x - \frac{L}{2} - l \cdot sin(\omega t)\right)\delta\left(y - \frac{L}{2}\right)$$

A transition from the ground state (1,1) to (n_x, n_y):

$$d(t) = \frac{-i}{\hbar}\int dxdy \int_0^t \frac{4}{L^2}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\lambda L^2 \delta\left(x - \frac{L}{2} - l\sin(\omega t')\right)\delta\left(y - \frac{L}{2}\right)e^{i\omega_{fi}t'}dt'$$

$$= \frac{-4\lambda i}{\hbar}\int_0^t \sin\left(\frac{\pi}{2} + \frac{\pi l \sin(\omega t')}{L}\right)\sin\left(\frac{\pi}{2}\right)\sin\left(\frac{n_x \pi}{2} + \frac{n_x \pi l \sin(\omega t')}{L}\right)\sin\left(\frac{n_y \pi}{2}\right)e^{i\omega_{fi}t'}dt'$$

Here $\omega_{fi} = \frac{E_f - E_i}{\hbar}$. And between the ground state and excited state (n_x, n_y), $\omega_{fi} = \frac{\pi^2\hbar^2}{2mL^2}\frac{n_x^2 + n_y^2 - 2}{\hbar}$.

For d(t) to be non-zero, n_y = 1,3,5…. For the 1st excited state, transition can only happen between (11,) and (2,1). So we only consider n_x=2, n_y=1.

Since $l \ll L$, assuming the time-dependent terms in sine are very small, the above can be approximated by:

$$d(t) = \frac{-4\lambda i}{\hbar}\int_0^t \frac{2\pi l \sin(\omega t')}{L}e^{i\omega_{fi}t'}dt'$$

$$= \frac{-4\lambda i}{\hbar}\frac{2\pi l}{L}\int_0^t \sin(\omega t')e^{i\omega_{fi}t'}dt'$$

$$= \frac{-4\lambda i}{\hbar}\frac{2\pi l}{L}\int_0^t \frac{1}{2i}\left(e^{i\omega t'} - e^{-i\omega t'}\right)e^{i\omega_{fi}t'}dt'$$

$$= \frac{-2\lambda}{\hbar}\frac{2\pi l}{L}\int_0^t \left[e^{i(\omega_{fi}+\omega)t'} - e^{i(\omega_{fi}-\omega)t'}\right]dt'$$

$$= \frac{2i\lambda}{\hbar}\frac{2\pi l}{L}\left[\frac{e^{i(\omega_{fi}+\omega)t} - 1}{\omega_{fi} + \omega} - \frac{e^{i(\omega_{fi}-\omega)t} - 1}{\omega_{fi} - \omega}\right]$$

For $\omega \ll \omega_{fi}$, this can be approximated by:

$$d(t) = \frac{2i\lambda}{\hbar}\frac{2\pi l}{L}\left[\frac{e^{i(\omega_{fi}+\omega)t}-1}{\omega_{fi}} - \frac{e^{i(\omega_{fi}-\omega)t}-1}{\omega_{fi}}\right]$$

$$= \frac{2i\lambda}{\hbar}\frac{2\pi l}{L}\left[\frac{e^{i(\omega_{fi}+\omega)t} - e^{i(\omega_{fi}-\omega)t}}{\omega_{fi}}\right]$$

Hence the transition probability is:

$$|d(t)|^2 = \left(\frac{4\pi l\lambda}{\hbar L}\right)^2 \frac{2-2\cos(2\omega t)}{\omega_{fi}^2}$$

$$= \frac{256m^2\lambda^2 l^2 L^2}{9\pi^2\hbar^4}\sin^2(\omega t)$$

d). Based on adiabatic theorem, the system starting from ground state would remain in ground state while been very slowly perturbed. Under the slow perturbation, at any given moment, the ground state is (from time-independent perturbation method):

$$|1{,}1\rangle = \left\{\left|1,1^{(0)}\right\rangle + \sum_{n_x,n_y}\left|n_x,n_y{}^{(0)}\right\rangle \frac{\left\langle n_x,n_y{}^{(0)}\middle|V'\middle|1,1^{(0)}\right\rangle}{E_{1,1}^{(0)}-E_{n_x,n_y}^{(0)}}\right\} e^{i\alpha(t)}$$

Here $\alpha(t)$ accounts for both dynamic and geometric phases. The transition to the 1st excited state is thus described by the projection of the 1st excited state on the perturbed ground state:

$$\left\langle 2,1^{(0)}\middle|1{,}1\right\rangle = \frac{\left\langle 2,1^{(0)}\middle|V'\middle|1,1^{(0)}\right\rangle}{E_{1,1}^{(0)}-E_{2,1}^{(0)}} e^{i\alpha(t)}$$

$$= \frac{\int \frac{4}{L^2}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\lambda L^2\delta\left(x-\frac{L}{2}-l\sin(\omega t')\right)\delta\left(y-\frac{L}{2}\right)dxdy}{E_{1,1}^{(0)}-E_{2,1}^{(0)}} e^{i\alpha(t)}$$

$$= 4\lambda\frac{\sin\left(\pi+\frac{2\pi l\sin(\omega t)}{L}\right)\sin\left(\frac{\pi}{2}+\frac{\pi l\sin(\omega t)}{L}\right)}{E_{1,1}^{(0)}-E_{2,1}^{(0)}} e^{i\alpha(t)}$$

$$\approx 4\lambda\frac{2mL^2}{\pi^2\hbar^2}\frac{\frac{2\pi l}{L}\sin(\omega t)}{3} e^{i\alpha(t)} = \frac{16m\lambda L l}{3\pi\hbar^2}\sin(\omega t)e^{i\alpha(t)}$$

And $\left\langle 1,2^{(0)}\middle|1{,}1\right\rangle = 0$ obviously, because $\left\langle 1,2^{(0)}\middle|V'\middle|1,1^{(0)}\right\rangle = 0$ from the selection rule in c).

So the probably for the system to transit from ground state to the 1st excited state is:

$$\left|\langle 2,1^{(0)}|1,1\rangle\right|^2 = \frac{256m^2\lambda^2l^2L^2}{9\pi^2\hbar^4}\sin^2(\omega t)$$

This is the same result as derived from the time-dependent perturbation method.

Quantum Mechanics 3

Two fermions on a ring

Consider two spin-1/2 fermions of mass m, with coordinates x_1 and x_2, confined to move on a circle of circumference L and interacting through a spin-dependent potential

$$V = -u\delta(x_1 - x_2)\vec{s}_1 \cdot \vec{s}_2\,, \quad u > 0,$$

where $\vec{s} = \{s_x, s_y, s_z\}$ is the operator of the spin 1/2 (in units of $\hbar$), so that the Hamiltonian H of the two-electron system (in the standard notations) is:

$$H = \frac{1}{2m}(p_1^2 + p_2^2) + V\,.$$

The circle is threaded by an infinitely-long solenoid which carriers a magnetic flux Φ, so that the electron momenta are

$$p_j = \frac{\hbar}{i}\frac{\partial}{\partial x_j} - eA\,,$$

where A is the vector potential produced by the magnetic flux, which can be taken to be constant along the circle, and e is the electron's charge.

(a) (4 points) What is the relation between A and Φ? Use this relation to write down the single-particle eigenstates $\psi_n(x)$ and eigenenergies E_n of one electron on the circle in terms of ϕ and other parameters in the problem.

(b) (3 points) Derive the boundary conditions for the orbital part $\psi(x_1, x_2)$ of the two-electron wavefunction at $x_1 = x_2$, if electron spins are in the triplet state.

(c) (4 points) Assuming that $|\Phi/(h/e)| < \frac{1}{2}$, find the ground-state energy $E_0^{(t)}$ and the orbital part $\psi_0^{(t)}(x_1, x_2)$ of the corresponding two-electron state.

(d) (4 points) Derive the same boundary conditions as in part (b) for electron spins in the singlet state.

(e) (5 points) For $\Phi = 0$, determine the ground-state energy $E_0^{(s)}$ and the orbital part $\psi_0^{(s)}(x_1, x_2)$ of the ground-state two-electron wavefunction in the singlet spin state in the limit of strong potential $u \to \infty$.

Solution

(a) By Stokes' theorem

$$\Phi = \int d\vec{s}\vec{B} = \int d\vec{s}\nabla \times \vec{A} = \int d\vec{l}\vec{A} = LA.$$

Since the wavefunctions on a circle should be periodic with the period L, the single-particle eigenstates are

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}, k_n = \frac{2\pi}{L} n\,, \quad n = 0, \pm 1, \pm 2, \ldots\,.$$

Acting on these wavefunctions with the kinetic energy operator $p^2/2m$, and using the relation between A and Φ, we get the eigenenergies that correspond to these eigenstates

$$E_n = \frac{(\hbar k_n - eA)^2}{2m} = \frac{(hn - eLA)^2}{2mL^2} = \frac{h^2(n-\phi)^2}{2mL^2}\,.$$

Here and below $\phi \equiv \Phi/(h/e)$.

(b) Any one of the triplet spin states is symmetric with respect to interchange of the two spins:

$$|S=1\rangle = \{|\uparrow\uparrow\rangle\,; |\downarrow\downarrow\rangle\,; \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle]\,\}\,.$$

Since the total wavefunction of the two electrons should be antisymmetric with respect to interchange of the electrons, the symmetric nature of the spin part of the wavefunction makes the orbital part $\psi(x_1, x_2)$ antisymmetric in the triplet states. This means that in this case, $\psi(x_1, x_2)\Big|_{x_1=x_2} = 0$, and $\psi(x_1, x_2)\delta(x_1 - x_2) \equiv 0$. Therefore, the interaction V does not have any effect on the wavefunction, and electrons in the triplet state behave as non-interacting, i.e. $\psi(x_1, x_2)$ is continuous together with its first derivatives at $x_1 = x_2$ as at all other points.

(c) Electrons in the triplet state behave as non-interacting. Since in the triplet state, the two electrons effectively have the same direction of spin, they can not occupy the same orbital state. The lowest energy of the two-electron state is reached then, when the two electrons occupy the two lowest-energy single-particle states. This means that for $\phi \in [0, 1/2]$,

$$E_0^{(t)} = E_0 + E_1 = \frac{h^2(1 - 2\phi + 2\phi^2)}{2mL^2}\,, \quad \psi_0^{(t)}(x_1, x_2) = \frac{1}{\sqrt{2}L}(e^{i2pix_1/L} - e^{i2pix_2/L}).$$

For $\phi \in [-1/2, 0]$,

$$E_0^{(t)} = E_0 + E_{-1} = \frac{h^2(1 + 2\phi + 2\phi^2)}{2mL^2}\,, \quad \psi_0^{(t)}(x_1, x_2) = \frac{1}{\sqrt{2}L}(e^{-i2pix_1/L} - e^{-i2pix_2/L}).$$

(d) For electrons in the singlet spin state,

$$|S=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\,,$$

the spin part of the wavefunction is antisymmetric, and the orbital part should be symmetric. in this case, the δ-functional potential affects the wavefunction. To find the magnitude of the potential, one needs to evaluate the magnitude of the spin part $\vec{s}_1 \cdot \vec{s}_2$ of the interaction V. As usual, making use of the operator $\vec{S} = \vec{s}_1 + \vec{s}_2$ of the total spin, we have

$$\vec{s}_1 \cdot \vec{s}_2 = [\vec{S}^2 - \vec{s}_1^2 - \vec{s}_2^2]/2 = \frac{1}{2}\vec{S}^2 - \frac{3}{4}\,,$$

In the singlet state $|S = 0\rangle$, this gives:

$$\vec{s}_1 \cdot \vec{s}_2 |S = 0\rangle = -\frac{3}{4}|S = 0\rangle\,,$$

i.e., the interaction V reduces to $V = (3u/4)\delta(x_1 - x_2)$, and its effect on $\psi(x_1, x_2)$ can be described in the same way as for the standard single-particle δ-function potential. Integrating the spatial Schrödinger equation over infinitesimal interval of x_1 around the point $x_1 = x_2$, one obtains that the wavefunction is continuous at $x_1 = x_2$ with discontinuous first derivative:

$$\frac{\partial\psi}{\partial x_1}\Big|_{x_1=x_2+0} - \frac{\partial\psi}{\partial x_1}\Big|_{x_1=x_2-0} = (3mu/2\hbar^2)\psi(x_1 = x_2)\,.$$

Similarly for x_2:

$$\frac{\partial\psi}{\partial x_2}\Big|_{x_2=x_1+0} - \frac{\partial\psi}{\partial x_2}\Big|_{x_2=x_1-0} = (3mu/2\hbar^2)\psi(x_1 = x_2)\,.$$

The fact that the wavefunction $\psi(x_1, x_2)$ is symmetric in the singlet state, implies that

$$\frac{\partial\psi}{\partial x_1}\Big|_{x_1=x_2-0} = \frac{\partial\psi}{\partial x_2}\Big|_{x_2=x_1-0}\,.$$

This equality transforms the first relation above into the sought boundary condition:

$$\Big(\frac{\partial\psi}{\partial x_1} - \frac{\partial\psi}{\partial x_2}\Big)\Big|_{x_1=x_2+0} = (3mu/2\hbar^2)\psi(x_1 = x_2)\,. \tag{80}$$

(e) The boundary condition (80) together with the fact that momenta are finite, means that $\psi(x_1 = x_2) = 0$ in the limit $u \to \infty$. One can immediately see that such symmetric wavefunction $\psi^{(s)}(x_1, x_2)$ vanishing at coincident coordinates can be constructed out of the antisymmetric wavefunction of noninteracting electrons $\psi^{(t)}(x_1, x_2)$,

$$\psi^{(t)}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_{n_1}(x_1)\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\psi_{n_2}(x_1)]$$

by the sign change:

$$\psi^{(s)}(x_1, x_2) = \psi^{(t)}(x_1, x_2)\,\mathrm{sgn}\,(x_1 - x_2)\,. \tag{81}$$

Such a sign change implies however, that as the function of one coordinate, e.g. x_1, $\psi^{(s)}$ aquires an extra phase π when increasing past x_2. As a result, the single-particle wavefunctions on a circle that could be used to build up $\psi^{(t)}$ and then $\psi^{(s)}$ should be antiperiodic, changing the quantization of momenta:

$$e^{ikL} = -1\,, \quad k = \pi\hbar(2n + 1)/L.$$

In this case, the lowest-energy state corresponds to $n_{1,2} = 0, -1$, giving the ground state energy

$$E_0^{(s)} = \frac{h^2}{4mL^2} \, .$$

The wavefunction that corresponds to this state is

$$\psi_0^{(s)}(x_1, x_2) = \frac{\sqrt{2}}{L} \sin\left(\frac{\pi}{L}|x_1 - x_2|\right) .$$

Statistical Mechanics 1

Ideal gas in gravitational potential

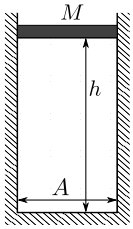
Consider an ideal gas of N indistinguishable molecules of mass m in a cylindrical volume $V = Ah$ with base area A and height h.

(a) (5 points) Calculate the canonical partition function of the ideal gas $Z^g(T, V)$, including the effect of gravity. You may find useful the integral $\int_0^\infty dt\, t^2\, e^{-t^2} = \sqrt{\pi}/4$.

(b) (4 points) Using the partition function, calculate the internal energy of the system. Then, determine the heat capacity in two limits, $T \gg mgh$ and $T \ll mgh$. You may find the Stirling approximation $N! \approx (N/e)^N$ helpful.

(c) (2 points) Write down the condition for when the effect of gravity is negligible compared to the thermal energy. What is the internal energy in that case? Neglecting internal degrees of freedom, estimate at what temperature the thermal energy for oxygen molecules O_2 (^{16}O) at 1m height is of the order of the potential energy.

Now assume that the top of the cylinder is a piston of mass M that can move vertically (change the height h), and that the gravity effects on the gas itself are *negligible*, so that the gas volume can change but the pressure is constant.



(d) (2 points) Write down the Hamiltonian of the combined piston + gas system H^{g+p}, and express the potential energy of the piston in terms of the pressure and the volume of the gas.

(e) (4 points) Find the canonical partition function Z^{g+p} of the system with the piston. One way to do this is to use the result for the partition function $Z^g(T, V)$ from part (a) (now neglecting the potential energy of the gas). First, show that Z^{g+p} is proportional to its Laplace transform

$$Z^{g+p}(T, P) = B \int_0^\infty dV e^{-\alpha V} Z^g(T, V) \tag{82}$$

for some B and α that you have to determine. Then compute Z^{g+p} as above (you may use the integral $\int_0^\infty dx\, x^N\, e^{-bx} = \frac{N!}{b^{N+1}}$).

(f) (3 points) Compute the variance of the piston height h and express it in terms of particle number N, piston mass M, and temperature T.
Hint: one way to do this is to use the pressure-dependent partition function $Z^{g+p}(T, P)$.

Solution:

(a) The partition function of the system is given by

$$Z^g = \frac{1}{N!}\left(z^{(1)}\right)^N \simeq \left(\frac{N}{e}z^{(1)}\right)^N , \tag{83}$$

with

$$z^{(1)} = \frac{1}{(2\pi\hbar)^3}\int d^3p\, d^3x\, e^{-\beta H^{(1)}} , \tag{84}$$

where

$$H^{(1)} = \frac{p^2}{2m} + mgy , \tag{85}$$

is the Hamiltonian for one particle with momentum p at height y, and $\beta = 1/T$.

Evaluating the integral in $z^{(1)}$,

$$\begin{aligned}
z^{(1)} &= \frac{4\pi}{(2\pi\hbar)^3}\int_0^\infty dp\, p^2\, e^{-\beta\frac{p^2}{2m}}\int_0^h Ae^{-\beta mgy}dy \\
&= \frac{4\pi}{(2\pi\hbar)^3}\left(\frac{2m}{\beta}\right)^{3/2}\int_0^\infty dt\, t^2\, e^{-t^2}\int_0^h Ae^{-\beta mgy}dy \\
&= \frac{4\pi}{(2\pi\hbar)^3}\left(\frac{2m}{\beta}\right)^{3/2}\frac{\sqrt{\pi}}{4}\int_0^h Ae^{-\beta mgy}dy \\
&= \frac{1}{(2\pi\hbar)^3}\left(\frac{2\pi m}{\beta}\right)^{3/2}\left[-\frac{A}{\beta mg}e^{-\beta mgy}\right]_0^h \\
&= \frac{1}{(2\pi\hbar)^3}\left(\frac{2\pi m}{\beta}\right)^{3/2}\frac{A}{\beta mg}\left(1-e^{-\beta mgh}\right) ,
\end{aligned}$$

one gets the partition function of the system

$$Z = \left[\frac{N}{e}\frac{1}{(2\pi\hbar)^3}\left(\frac{2\pi m}{\beta}\right)^{3/2}\frac{A}{\beta mg}\left(1-e^{-\beta mgh}\right)\right]^N = \left[\frac{N}{e}\frac{A}{\lambda_T^3\beta mg}\left(1-e^{-\beta mgh}\right)\right]^N , \tag{86}$$

where $\lambda_T = \sqrt{\frac{2\pi\hbar^2\beta}{m}}$ is the thermal wavelength.

(b) The internal energy of the system is given by

$$\begin{aligned}
U =& -\frac{\partial}{\partial\beta}\ln Z = -\frac{\partial}{\partial\beta}\left\{N\ln\left[\frac{N}{e}\left(\frac{2\pi m}{\beta(2\pi\hbar)^2}\right)^{3/2}\frac{A}{\beta mg}\left(1-e^{-\beta mgh}\right)\right]\right\} \\
=& -\frac{\partial}{\partial\beta}\left[N\left(\ln N - 1 - \frac{3}{2}\ln\beta - \ln\beta + \ln(1-e^{-\beta mgh}) + \ln\frac{A}{mg} - \frac{3}{2}\ln\frac{2\pi\hbar^2}{m}\right)\right] \\
=& \frac{5}{2}\frac{N}{\beta} + N\frac{mgh}{1-e^{\beta mgh}}
\end{aligned}$$

(c) Gravity becomes relevant when $\varepsilon = \frac{mgh}{kT} \sim 1$, i.e., the potential energy is on the order of the thermal energy at temperature T. For $\varepsilon \ll 1$, we can neglect gravity. To get the internal energy in this case, we expand the exponential:

$$\begin{aligned} U &= \frac{5}{2}\frac{N}{\beta} + N\frac{mgh}{1-e^{\beta mgh}} \simeq \frac{5}{2}\frac{N}{\beta} + N\frac{mgh}{1-1-\beta mgh-\frac{1}{2}(\beta mgh)^2+\mathcal{O}(\varepsilon^3)} \\ \Leftrightarrow U &= \frac{5}{2}\frac{N}{\beta} - N\frac{mgh}{\beta mgh(1+\frac{1}{2}\beta mgh)} \\ \Leftrightarrow U &= \frac{3}{2}NkT\left(1+\mathcal{O}\left(\frac{mgh}{kT}\right)\right), \end{aligned}$$

which in this limit is the well known internal energy of an ideal gas of non-interacting particles.

The temperature at which ε becomes one for $h = 1\,\mathrm{m}$, $m = 32u = 5.312 \cdot 10^{-26}\,\mathrm{kg}$, is

$$T \approx \frac{mgh}{k} = \frac{5.312 \cdot 10^{-26}\, 9.8\,\mathrm{m^2\,kg\,s^{-2}}}{1.38 \cdot 10^{-23}\,\mathrm{m^2\,kg\,s^{-2}\,K^{-1}}} = 0.038\,\mathrm{K} \tag{87}$$

Normal room temperature is 273.15 K, so the effect of gravity is negligible for oxygen at room temperature, according to this simplified estimate.

(d) The pressure on the system, exerted on the gas by the piston is $P = Mg/A$. The potential energy of the piston is $Mgh = AhP = VP$. With that, the Hamiltonian of the combined sytem is

$$H^{g+p} = H^g + k^2/2M + PV\,, \tag{88}$$

where $H^g = \sum_i^N H^{(i)}$ is the Hamiltonian of the entire gas, and k is the momentum of the piston in the z direction.

(e) With the Hamiltonian H^{g+p} above, the canonical partition function becomes

$$Z^{g+p}(T,P) = \frac{1}{N!}\int d\omega^g \int \frac{dhdk}{2\pi\hbar}\exp[-\beta(H^g + k^2/2M + PV)]\,, \tag{89}$$

where $\int d\omega^g$ is the phase space integral for the whole gas, assuming a constant volume $V = Ah$. One can first formally integrate the gas degrees of freedom,

$$Z^{g+p}(T,P) = \int \frac{dhdk}{2\pi\hbar}\, e^{-\beta(k^2/2M+PV)}\left[\frac{1}{N!}\int d\omega^g e^{-\beta H^g}\right] = \int \frac{dVdk}{2\pi\hbar A}\, e^{-\beta(k^2/2M+PV)} Z^g(T,V)\,, \tag{90}$$

where $Z^g(T,V)$ is the gas partition function and $dV = A\,dh$. Integrating out the piston momentum k, one gets

$$Z^{g+p}(T,P) = \frac{1}{A}\sqrt{\frac{M}{2\pi\hbar^2\beta}}\int dV\, e^{-\beta PV}\, Z^g(V,T)\,. \tag{91}$$

Thus, the partition function for constant pressure is the Laplace transform of that at constant volume, as given in part (e) with $\alpha = \beta P$ and $B = \frac{1}{A}\sqrt{\frac{M}{2\pi\hbar^2\beta}}$.

In the high-temperature limit $\beta \to 0$, the partition function of the gas Z^g simplifies to

$$Z^g(T,V) \approx \frac{1}{N!}\left[\left(\frac{M}{2\pi\hbar^2\beta}\right)^{3/2}\frac{A}{\beta mg}(1-1+\beta mgh)\right]^N = \frac{1}{N!}\lambda^{-3N}V^N \tag{92}$$

and its Laplace transform is given by

$$Z^{g+p}(T,P) = B\int dV e^{-\alpha V}\frac{1}{N!}\lambda_T^{-3N}V^N = B\lambda_T^{-3N}\cdot\frac{1}{N!}\frac{N!}{\alpha^{N+1}} = \frac{1}{A\Lambda_T\lambda_T^{3N}}\left(\frac{T}{P}\right)^{N+1} \tag{93}$$

where $\Lambda_T = \sqrt{\frac{2\pi\hbar^2\beta}{M}}$ is the thermal wavelength of the piston.

(f) The variance of the piston height is essentially the variance of the volume of the gas at constant pressure, $\langle(\delta h)^2\rangle = \frac{1}{A^2}\langle(\delta V)^2\rangle$, and can be found from the equipartition theorem for the oscillating piston supported by the ideal gas with the isothermal compressibility $\kappa_T = \frac{1}{V}\left(-\left(\frac{\partial V}{\partial P}\right)_T\right) = N\frac{T^2}{P^2}$. It is more fun, however, to use the machinery of the pressure-dependent partition function developed in parts (e,d). The volume and its fluctuation can be found as partial derivatives of $\big[-\ln Z^{g+p}(T,P)\big]$ with respect to the pressure,

$$\langle V\rangle = -\frac{1}{\beta}\frac{1}{Z^{g+p}}\left(\frac{\partial Z^{g+p}}{\partial P}\right)_T = -\frac{1}{\beta}\left(\frac{\partial \ln Z^{g+p}}{\partial P}\right)_T = \left(\frac{\partial\big(-T\ln Z^{g+p}(T,P)\big)}{\partial P}\right)_T, \tag{94}$$

$$\begin{aligned}\langle(\delta V)^2\rangle &= \langle V^2\rangle - \langle V\rangle^2 = \frac{1}{\beta^2}\frac{1}{Z^{g+p}}\left(\frac{\partial^2 Z^{g+p}}{\partial P^2}\right)_T - \left(-\frac{1}{\beta}\frac{1}{Z^{g+p}}\left(\frac{\partial Z^{g+p}}{\partial P}\right)_T\right)^2 \\ &= \frac{1}{\beta^2}\left(\frac{\partial^2 \ln Z^{g+p}}{\partial P^2}\right)_T = -T\left(\frac{\partial^2\big(-T\ln Z^{g+p}(T,P)\big)}{\partial P^2}\right)_T,\end{aligned} \tag{95}$$

and thus one can identify $\big(-T\ln Z^{g+p}(T,P)\big)$ with the Gibbs potential. Using the expression for Z^{g+p} from above, one gets

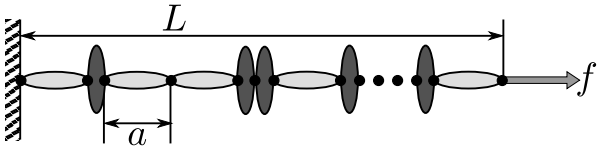
$$\langle(\delta V)^2\rangle = T^2\left(\frac{\partial^2 \ln Z^{g+p}}{\partial P^2}\right)_T = T^2\left(\frac{\partial^2\big[(N+1)\big(-\ln P\big)+f(T)\big]}{\partial P^2}\right)_T = (N+1)\frac{T^2}{P^2} \approx \frac{1}{N}V^2, \tag{96}$$

and the piston height fluctuation is

$$\delta h = \frac{\delta V}{A} \approx \frac{1}{\sqrt{N}}\frac{V}{A} = \frac{h}{\sqrt{N}} = \frac{1}{\sqrt{N}}\frac{T}{Mg}. \tag{97}$$

Statistical Mechanics 2

Thermodynamics of a polymer molecule



Consider a single polymer molecule that consists of $N \gg 1$ connected elementary identical links. These links may be either "folded" (zero length) or extended (to length a) in the same direction, and have the same intrinsic energy in both states. One end of the molecule is fixed, and tension f may be applied to the other end.

(a) (3 points) Find the average length L_0 of the molecule when no tension is applied to the molecule ($f = 0$). How does L_0 depend on temperature? What is the variance of the length $\langle(\delta L)^2\rangle$ (assuming constant temperature)?

Hint: Throughout the problem, assume that the change in the length of the molecule is small, $\Delta L \ll L_0$.

(b) (4 points) The molecule is "stretched" to fixed length $L = L_0 + \Delta L$. How many microscopic states of the molecule correspond to this state, and what is the corresponding entropy? You may use the Stirling approximation $\ln n! = (n \ln n - n)$.

(c) (3 points) Calculate the tension f required to stretch the molecule in part(b) to length $L = L_0 + \Delta L$, and its elasticity k_T at constant temperature T.

(d) (3 points) Now assume that the heat capacity of the unstretched molecule $C(L_0) \equiv C_0$ is independent of temperature. Calculate the heat capacity C_f for a molecule stretched by a constant force f.

(e) (3 points) What is the adiabatic elasticity k_S if the molecule?

(f) (4 points) Suggest a design for a heat engine based on the temperature dependence of the elasticity $k_T(T)$ and calculate its efficiency. Draw the engine's operating cycle in the (L, T) plane and show the direction of the cycle.

Solution

This problem can be solved using either microcanonical or canonical (Gibbs) distribution. The solution here takes the microcanonical approach, which somewhat more complicated bit is equally valid, but has the advantage of emphasizing how the tension in the rubber band appears from the entropy if its disordered links.

(a) Since both states of each link have the same energy, their probabilities are the same and equal to $\frac{1}{2}$ and independent of the temperature. The average length then is

$$L_0 = \langle L \rangle_{f=0} = N \cdot \big(\frac{1}{2} \cdot 0 + \frac{1}{2} \cdot a\big) = a\frac{N}{2}$$

and also does not depend on the temperature. The number of extended links is given by the binomial distribution, so its variance $(\delta N_+)^2 = N \cdot 1 \cdot (1 - \frac{1}{2}) = \frac{1}{4}N$ gives the fluctuation of the length $\delta L = a\,\delta N_+ = \frac{1}{2}a\sqrt{N}$. Alternatively, one can consider the fluctuation of the length of one (i-th) link,

$$(\delta l_i)^2 = \langle (\Delta l_i)^2 \rangle = \langle l_i^2 \rangle - \langle l_i \rangle^2 = \frac{1}{2}a^2 - (\frac{a}{2})^2 = \frac{1}{4}a^2\,, \tag{98}$$

which gives the same answer for N independent links $(\delta L)^2 = N(\delta l_i)^2 = \frac{1}{4}a^2 N$.

(b) If the length of the molecule is known, then the precise number of extended N_+ and folded N_- links can be determined:

$$L = L_0 + \Delta L = aN_+ \quad \Leftrightarrow \quad N_+ = \frac{N}{2}\big(1 + \frac{\Delta L}{L_0}\big)\,, \quad N_- = N - N_+ = \frac{N}{2}\big(1 - \frac{\Delta L}{L_0}\big)$$

The number of microscopic states, or the statistical weight Γ, corresponding to the molecule having length L, is given by the number of all combinations of stretched N_+ and folded N_- links out of the total $N = N_+ + N_-$ links,

$$\Gamma(L) = \frac{N!}{N_+!N_-!}\,,$$

from which it is easy to compute the entropy using the Stirling formula $\ln n! \approx (n \ln n - n)$:

$$\begin{aligned} S_d(L) = \ln \Gamma(L) &\approx N \ln N - N - (N_+ \ln N_+ - N_+) - (N_- \ln N_- - N_-) \\ &= -N_+ \ln \frac{N_+}{N} - N_- \ln \frac{N_-}{N} \\ &= -\frac{N}{2}\Big\{\Big(1 + \frac{\Delta L}{L_0}\Big) \ln \Big[\frac{1}{2}\Big(1 + \frac{\Delta L}{L_0}\Big)\Big] + \Big(1 - \frac{\Delta L}{L_0}\Big) \ln \Big[\frac{1}{2}\Big(1 - \frac{\Delta L}{L_0}\Big)\Big]\Big\} \\ &\approx N\Big[\ln 2 - \frac{1}{2}\Big(\frac{\Delta L}{L_0}\Big)^2\Big] \end{aligned}$$

In the last line, the expansion $\ln(1 + x) = x - \frac{1}{2}x^2 + O(x^3)$ was used. The first term is the entropy of a molecule without load (at $f = 0$), in which any link can be in two equally

probable states, whereas the second reflects the decrease in the entropy as the molecule is stretched (or compressed) and more links become extended (or folded) than $N/2$.

The fluctuation of the length can also be easily found from the Gaussian probability distribution $p(L) \propto \Gamma(L) = e^{S_d(L)}$:

$$p(L) \propto \exp\Big[-\frac{N}{2}\Big(\frac{\Delta L}{L_0}\Big)^2 \Big] \quad \Longrightarrow \quad \langle (\Delta L)^2 \rangle = \frac{L_0^2}{N}\,, \quad \text{or } \delta L = \sqrt{\langle (\Delta L)^2 \rangle} = \frac{L_0}{\sqrt{N}} = \frac{1}{2} a \sqrt{N}\,.$$

(c) If the molecule is stretched at constant temperature, the change in the free energy is

$$dF = -S\,dT + f\,dL \overset{T=const}{=} f\,dL \tag{99}$$

(note that when the molecule is stretched the external force performs work $\delta W_{\rm ext} = f\,dL$). Alternatively, the free energy for the constant temperature also can be found from the number of microscopic states above,

$$F(T,L) - F(T, L = L_0) = -T \ln \frac{Z(T,L)}{Z(T,L_0)} = -T \ln \frac{\Gamma(T,L)}{\Gamma(T,L_0)} \approx \frac{1}{2} T N \Big(\frac{\Delta L}{L_0}\Big)^2$$

where the difference in the Gibbs partition functions is given only by the disorder of the links because the energies of links in both states are the same. Finally, the tension in the molecule is

$$f = \left(\frac{\partial F}{\partial L}\right)_T = TN \frac{\Delta L}{L_0^2} = \frac{2T}{a} \frac{\Delta L}{L_0}\,,$$

and the isothermal elasticity is

$$k_T = \left(\frac{\partial f}{\partial L}\right)_T = \frac{2T}{a L_0}\,.$$

Note that this elasticity is different from the elasticity of a thermally insulated molecule k_S because the work done by the external force f may produce heat and change the temperature of the molecule, leading to an additional change in the tension f.

(d) First, note that the internal energy of the molecule is independent of its length $L = L_0 + \Delta L$ because there is no energy difference between the different states of the links. Therefore, all the internal energy is given by its "thermal" energy and does not depend on the elongation ΔL,

$$E(T,L) = C_0 T$$

neither does its heat capacity at constant length $C_L(T,L) = C_0 = \text{const}$. However, the heat capacity at constant tension f is larger than $C_L = C_0$ because of the work *performed by the molecule as it shrinks* with increasing temperature:

$$C_f(T,f) = \left(\frac{\partial E}{\partial T}\right)_f - f \left(\frac{\partial L}{\partial T}\right)_f\,,$$

(the minus sign is due to the relation $T\,dS = dE - f\,dL$ where $f\,dL$ is the work performed by the external force). Since the internal energy is independent of L, it is also independent

of f, therefore $\left(\frac{\partial E}{\partial T}\right)_f = C_0$. The length of the molecule can be found from the equation in (c): $\Delta L = \frac{aL_0}{2T} f$, and

$$C_f(T,f) = C_0 + \frac{aL_0}{2T^2} f^2 = C_0 + 2\frac{L_0}{a}\Big(\frac{\Delta L}{L_0}\Big)^2 = C_0 + N\Big(\frac{\Delta L}{L_0}\Big)^2 > C_L = C_0$$

(e) One elegant solution is to compute the ratio of the adiabatic to the isothermic elasticities using the chain rule for determinants,

$$\frac{k_S}{k_T} = \frac{\partial(f,S)}{\partial(L,S)} \cdot \frac{\partial(L,T)}{\partial(f,T)} = \frac{\partial(f,S)}{\partial(f,T)} \cdot \frac{\partial(L,T)}{\partial(L,S)} = \frac{C_f}{C_L} = 1 + \frac{N}{C_0}\Big(\frac{\Delta L}{L_0}\Big)^2$$

and use the expression for k_T from above. Alternatively, one can evaluate the partial derivative $\left(\frac{\partial f}{\partial L}\right)_S$ by changing the variables $(L,S) \to (L,T)$ and using the molecule's "equation of state" $f = \frac{2T}{a}\frac{\Delta L}{L_0}$:

$$k_S = \left(\frac{\partial f}{\partial L}\right)_S = \left(\frac{\partial f}{\partial L}\right)_T + \left(\frac{\partial f}{\partial T}\right)_L \cdot \left(\frac{\partial T}{\partial L}\right)_S = k_T + \frac{2}{a}\frac{\Delta L}{L_0}\left(\frac{\partial T}{\partial L}\right)_S$$

The derivative $\left(\frac{\partial T}{\partial L}\right)_S$ may be evaluated using the 1st law of thermodynamics and $dE = C_0 dT$:

$$dE - f\,dL = C_0 dT - \frac{2T}{a}\frac{\Delta L}{L_0} dL = T\,dS = 0 \quad \Rightarrow \quad \left(\frac{\partial T}{\partial L}\right)_S = \frac{2T}{aC_0}\frac{\Delta L}{L_0}$$

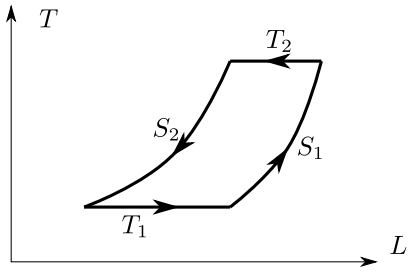
and, finally,

$$k_S = k_T + \frac{4T}{a^2 C_0}\Big(\frac{\Delta L}{L_0}\Big)^2 = k_T\Big[1 + \frac{2L_0}{aC_0}\Big(\frac{\Delta L}{L_0}\Big)^2\Big] = k_T\Big[1 + \frac{N}{C_0}\Big(\frac{\Delta L}{L_0}\Big)^2\Big],$$

consistent with the previuos answer.

(f)

The simplest solution is to implement the Carnot cycle which has efficiency $\eta = 1 - T_1/T_2$ shown on the right. Note that the entropy $S_2 > S_1$ because the shorter (less stretched) molecule has larger entropy. Thus, the molecule has to be cooled ($S_1 - S_2 < 0$) as it is stretched at T_1 and heated ($S_2 - S_1 > 0$) as it is released at temperature T_2.



To draw the diagram in (L,T) axes, we need to find how the temperature changes when the molecule is stretched adiabatically. For $S = \text{const} \Leftrightarrow dS = 0$, we have

$$0 = TdS = dE - f\,dL \quad \Leftrightarrow \quad C_0\,dT = \frac{2T}{a}\frac{\Delta L}{L_0}\,dL \quad \Leftrightarrow \quad T = T_0 \exp\big[\frac{(\Delta L)^2}{aC_0 L_0}\big]$$

and the dependency of the temperature on the elongation is exponential (for $\Delta L \ll L_0$).

Statistical Mechanics 3

The thermoelectric effect

A (3 points). For a gas of similar non-relativistic particles, write:

- the Liouville theorem,
- the Boltzmann transport equation in its general form, and
- the Boltzmann equation in the relaxation-time approximation.[1]

B (2 points). Spell out the last equation for a free, isotropic Fermi gas of particles with electric charge q, in the presence of a uniform, time-independent external electric field $\mathbf{E}$.

C (4 points). Solve the obtained equation in the linear approximation in the weak applied field $\mathbf{E}$, and use the result to express the densities of the electric current ($\mathbf{j}_e$) and of the heat flow ($\mathbf{j}_h$) as integrals over the single-particle energy ε.

Hint 1: The heat flow density in a gas with the single-particle probability distribution $w(\mathbf{r}, \mathbf{p})$ may be calculated as

$$\mathbf{j}_h = \int (\varepsilon - \mu)\mathbf{v}\, w d^3 p\,,$$

where μ its chemical potential, and $\mathbf{v}$ is the particle's velocity.

D (2 points). Give a physical interpretation of the formula given in *Hint 1*.

E (2 points). Use the first result of Task C to obtain an explicit expression for the Ohmic conductivity σ (defined as the coefficient in the differential form $\mathbf{j}_e = \sigma\mathbf{E}$ of the Ohm law) via the gas density n, particle's charge q and mass m, and the relaxation time τ, for arbitrary temperature.

F (3 points). For a degenerate Fermi gas, use the second result of Task C and the Sommerfeld expansion formula to calculate the so-called *Peltier coefficient* in the linear relation $\mathbf{j}_h = \Pi\mathbf{j}_e$.

Hint 2: The Sommerfeld expansion may be represented in several forms; for this problem, the most useful of them is

$$\int_0^\infty \varphi(\varepsilon)\left(-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right) d\varepsilon \approx \varphi(\mu) + \frac{\pi^2}{6} T^2 \frac{d^2\varphi(\varepsilon)}{d\varepsilon^2}\Big|_{\varepsilon=\mu}, \qquad \text{at } T << \mu\,,$$

where $\varphi(\varepsilon)$ is a smooth function equal to zero at $\varepsilon = 0$, and $f(\varepsilon)$ is the Fermi-Dirac distribution.

G (4 points). Suggest a simple method to measure the coefficient Π experimentally.

Hint 3: Think about a loop made of two different conducting materials, one of them with a known Π.

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[1] The approximation is sometimes called the BGK model.

Solution

A (3 points). The general form of the Liouville theorem is

$$\frac{dw}{dt} \equiv \frac{\partial w}{\partial t} + \sum_{j=1}^{d} \left(\frac{\partial w}{\partial q_j} \dot{q}_j + \frac{\partial w}{\partial p_j} \dot{p}_j \right) = 0 ,$$

where $w(\{q_j\}, \{p_j\}, t)$ is the probability density to find the particle in the $(2d + 1)$-dimensional space of its d generalized coordinates q_j, d generalized momenta p_j, and time t. For a non-relativistic gas of 3D particles ($d = 3$, $\{q_1, q_2, q_3\} = r$), each under the effect of an external force $\mathbf{F}(\mathbf{r}, t)$ but otherwise free to move, the equation takes the form

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla_r w + \mathbf{F} \cdot \nabla_p w = 0 ,$$

where $\mathbf{v}$ is the particle's velocity, and ∇_r and ∇_p are the del operators in the coordinate and momentum spaces.

The Boltzmann transport equation differs from the Liouville theorem by addition of the so-called scattering integral, giving an approximate account of relatively rare particle scattering events, for example in the form

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla_r w + \mathbf{F} \cdot \nabla_p w = \int d^3 p' \left[\Gamma_{\mathbf{p}' \to \mathbf{p}} w(\mathbf{r}, \mathbf{p}', t) - \Gamma_{\mathbf{p} \to \mathbf{p}'} w(\mathbf{r}, \mathbf{p}, t) \right],$$

where Γ are the rates of the corresponding scattering events.

This equation is most frequently used in a simpler form further by assuming that the scattering integral is proportional to the local deviation,

$$\tilde{w} \equiv w - w_0 ,$$

of the probability density from its value w_0 in equilibrium, so that equation takes the form

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla_r w + \mathbf{F} \cdot \nabla_p w = -\frac{\tilde{w}}{\tau} ,$$

where τ is a phenomenological constant, called the relaxation time. (Physically, this is the average time a particle moves between two consequent scattering events.)

B (2 points). For a free, isotropic Fermi gas

$$w_0 = \frac{g}{(2\pi\hbar)^3} f(\varepsilon), \qquad (1)$$

where $g = 2s + 1$ is the spin degeneracy, and $f(\varepsilon)$ is the Fermi-Dirac distribution

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon - \mu)/T} \pm 1} ,$$

$\varepsilon = p^2/2m$ is the single-particle energy, μ is the chemical potential, and T is temperature in energy units. For particles with electric charge q in an electric field **E**, in the absence of other forces, we may write **F** = q**E**. If **E** is time- and space-independent, so should be w, so that the Boltzmann equation, in the relaxation-time approximation, reduces to

$$q\mathbf{E}\cdot\nabla_p\left(w_0+\tilde{w}\right)=-\frac{\tilde{w}}{\tau}. \qquad (2)$$

C (4 points). If the applied electric field is relatively weak ($qEv\tau << T, \mu$), it may cause only a weak deviation of the probability density from its equilibrium value (1), so that in the linear approximation in **E** we may neglect $\tilde{w}$ in comparison with w_0 on the left-hand side of Eq. (2), and it may be readily solved:

$$\tilde{w}=-q\tau\,\mathbf{E}\cdot\nabla_p w_0 .$$

Since, according to Eq. (1), w_0 depends on **p** only via the energy $\varepsilon = p^2/2m$, we may write $\nabla_p w_0 = (\partial w_0/\partial\varepsilon)\nabla_p\varepsilon$. But the j^{th} Cartesian component of this vector,

$$\left(\nabla_p\varepsilon\right)_j\equiv\frac{\partial}{\partial p_j}\varepsilon=\frac{\partial}{\partial p_j}\frac{p_1^2+p_1^2+p_1^2}{2m}=\frac{p_j}{m}=v_j,$$

so that the gradient $\nabla_p\varepsilon$ is just the particle's velocity **v**, and we may write

$$\tilde{w}=\tau\,q\,\mathbf{E}\cdot\mathbf{v}\left(-\frac{\partial w_0}{\partial\varepsilon}\right).$$

Let us first use this expression for the calculation of the electric current density

$$\mathbf{j}_{\text{e}}=\int q\mathbf{v}w\,d^3p\equiv q\int\mathbf{v}\left(w_0+\tilde{w}\right)d^3p .$$

Since in the equilibrium state (with $w = w_0$), the net current density has to equal zero, the integral of the first term in the parentheses has to vanish. For the integral of the second term, we get

$$\mathbf{j}_{\text{e}}=q^2\tau\int\mathbf{v}\left(\mathbf{E}\cdot\mathbf{v}\right)\left(-\frac{\partial w_0}{\partial\varepsilon}\right)d^3p=\frac{gq^2\tau}{\left(2\pi\hbar\right)^3}\int\mathbf{v}\left(\mathbf{E}\cdot\mathbf{v}\right)\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]d^3p .$$

Due to axial symmetry of this expression, the vector **j** is directed along the applied field,

$$\mathbf{j}_{\text{e}}=\frac{gq^2\tau\,\mathbf{E}}{\left(2\pi\hbar\right)^3}\int v^2\cos^2\theta\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]d^3p ,$$

where Here θ is the angle between the field **E** and the vector **p** = m**v**. Transferring to the polar coordinates, and performing an easy angular integration, we get

$$\mathbf{j}_{\text{e}}=\frac{gq^2\tau\,\mathbf{E}}{\left(2\pi\hbar\right)^3}\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta d\theta\cos^2\theta\int_0^{\infty}p^2dp\,v^2\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]=\frac{gq^2\tau\mathbf{E}}{\left(2\pi\hbar\right)^3}\frac{4\pi}{3}\int_0^{\infty}p^2dp\,v^2\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right].$$

As requested in the assignment, the remaining, one-dimensional integral may be readily recast to that over particle energies $\varepsilon = p^2/2m$: $p^2 = 2m\varepsilon$, so that $p = (2m\varepsilon)^{1/2}$, $dp = (m/2\varepsilon)^{1/2}$, and $v^2 = 2\varepsilon/m$:

$$\mathbf{j}_e = \frac{gq^2\tau\mathbf{E}}{(2\pi\hbar)^3}\frac{4\pi}{3}\int_0^\infty (8m\varepsilon^3)^{1/2}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]d\varepsilon \ . \qquad (3)$$

Now according to the expression for the heat flow density $\mathbf{j}_h$ given in *Hint 1*, it may be obtained from Eq. (3) for $\mathbf{j}_e$ by the replacement $q \to (\varepsilon - \mu)$, immediately giving

$$\mathbf{j}_h = \frac{gq\tau\mathbf{E}}{(2\pi\hbar)^3}\frac{4\pi}{3}\int_0^\infty (8m\varepsilon^3)^{1/2}(\varepsilon-\mu)\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]d\varepsilon \ . \qquad (4)$$

D (2 points). By definition, the chemical potential μ of a system of independent particles is just an average energy of a particle, and a deviation $(\varepsilon - \mu)$ of the particle's energy ε from this average may be interpreted as its thermal energy.

Another possible explanation is that for a uniform gas of N particles, the factor $(\varepsilon - \mu)$ in the expression for $\mathbf{j}_h$ may be represented as $(E - G)/N$, where E is the total energy, and G the Gibbs energy of the system. But according to the basic thermodynamics,

$$E - G = TS - PV \ ,$$

where S is entropy, P the pressure, and V the volume of the gas. The full differential of this difference,

$$d(E-G) = TdS + SdT - PdV - VdP \ .$$

so that in the absence of mechanical work $d\mathcal{W} = -PdV$ and of changes of pressure and temperature (as in our current problem), the differential is reduced to just TdS, i.e. to the elementary heat dQ.

E (2 points). We may take the integral in Eq. (3) by parts. Since the function under it vanishes at both ends of the integration interval (at $\varepsilon = 0$, due to the factor $\varepsilon^{3/2}$, and at $\varepsilon \to +\infty$, due to the exponentially decreasing Fermi distribution function f), the result is

$$\sigma = \frac{gq^2\tau}{(2\pi\hbar)^3}\frac{4\pi}{3}\int_0^\infty f(\varepsilon)d\left[(8m\varepsilon^3)^{1/2}\right] \equiv \frac{gq^2\tau}{(2\pi\hbar)^3}\frac{4\pi}{3}(8m)^{1/2}\int_0^\infty f(\varepsilon)\frac{3}{2}\varepsilon^{1/2}d\varepsilon$$
$$\equiv \frac{q^2\tau}{m}\times\frac{gm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^\infty f(\varepsilon)\varepsilon^{1/2}d\varepsilon.$$

But the factor following the multiplication sign is just the well-known expression for the density $n \equiv N/V$ of the gas in thermal equilibrium. Indeed, using Eq. (1), and the substitutions listed just before Eq. (3), we get

$$n = \int w_0 d^3p = \frac{g}{(2\pi\hbar)^3}\int f(\varepsilon)d^3p = \frac{g}{(2\pi\hbar)^3}4\pi\int_0^\infty p^2dpf(\varepsilon) = \frac{gm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^\infty \varepsilon^{1/2}d\varepsilon\, f(\varepsilon). \qquad (5)$$

Hence in the relaxation-time approximation, the Ohmic conductivity may be expressed by the Drude formula,

$$\sigma = \frac{q^2\tau}{m}n \ , \qquad (6)$$

at arbitrary temperature.

F (3 points). Applying the Sommerfeld expansion formula, given in *Hint 2*, with $\varphi(\varepsilon) = \varepsilon^{3/2}(\varepsilon - \mu) \equiv \varepsilon^{5/2} - \mu\varepsilon^{3/2}$, i.e. with $\varphi(\mu) = 0$ and $d^2\varphi(\varepsilon)/d\varepsilon^2|_{\varepsilon=\mu} = 3\mu^{1/2}$, to Eq. (4), for the ratio $\mathbf{j}_h/\mathbf{E} \equiv \sigma\Pi$ we get

$$\sigma\Pi \approx \frac{gq\tau}{(2\pi\hbar)^3}\frac{4\pi}{3}\frac{\pi^2T^2}{6}3(8m\mu)^{1/2}, \qquad \text{for } T << \mu. \tag{7}$$

This expression may be further simplified taking into account that for the degenerate Fermi gas, at $T << \mu(T) \approx \mu(0) \equiv \varepsilon_F$, the Fermi distribution becomes very simple,

$$f(\varepsilon) \approx \begin{cases} 1, & \text{for } \varepsilon < \varepsilon_F, \\ 0, & \text{for } \varepsilon_F < \varepsilon, \end{cases}$$

enabling a simple integration in Eq. (5):

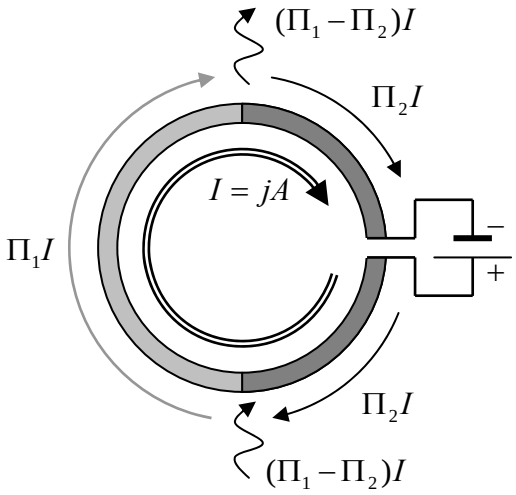
$$n \approx \frac{gm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^{\varepsilon_F}\varepsilon^{1/2}d\varepsilon = \frac{gm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\frac{2}{3}\varepsilon_F^{3/2}.$$

Plugging this expression into Eq. (6) for σ, and the result into Eq. (7), we get simply

$$\Pi = \frac{\pi^2}{2q}\frac{T^2}{\varepsilon_F}, \qquad \text{for } T << \varepsilon_F.$$

We see that the phenomenological relaxation time τ has canceled, implying that the last result is more robust to violations of the relaxation-time approximation.

G (4 points). Figure below shows the traditional (and apparently the easiest) way to measure the Peltier coefficient.



An external voltage source drives a certain dc current $I = j_e A$ (where A is the conductors' cross-section area), the same in the whole loop. However, if the materials 1 and 2 are different, the power $\mathscr{P} \equiv$

$j_h A$ of the voltage-induced heat flow[2] may be different in two parts of the loop. Indeed, if the whole system is kept at the same temperature, the integration of the relation $\mathbf{j}_h = \Pi \mathbf{j}_e$ over the cross-sections of each part yields

$$\mathcal{P}_{1,2} = \Pi_{1,2} A_{1,2} j_{1,2} = \Pi_{1,2} I_{1,2} = \Pi_{1,2} I .$$

This equality means that in order to sustain a constant temperature, the following power difference,

$$\Delta\mathcal{P} = (\Pi_1 - \Pi_2) I ,$$

has to be extracted from one junction of the two materials (in the Fig. above, shown on the top), and inserted into the counterpart junction.

This is the *thermoelectric* (or *Peltier*) *effect*, may be used, in particular, for the measurement of the coefficient Π of one of the materials, provided that its value in the counterpart material is known. Another, much more common, application of this effect is for *thermoelectric cooling*. Indeed, if a constant temperature is *not* maintained, one of the junctions is heated (in excess of the bulk, Joule heating), while the latter one is cooled. Such *Peltier refrigerators*, which require neither moving parts nor fluids, are very convenient for modest (by a few tens °C) cooling of relatively small components of various systems - from sensitive radiation detectors on mobile platforms (including spacecraft), all the way to cold drinks in vending machines.

[2] Note that we are discussing the heat *transferred* through the conductors, not the additional Joule heat *generated* in them by the current. (The latter heat, with the power density $j_e E = \sigma E^2$, is proportional to the square of the applied voltage V, rather than proportional to it as the Peltier heat.)