Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

Fall 2020

General Instructions:

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

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

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

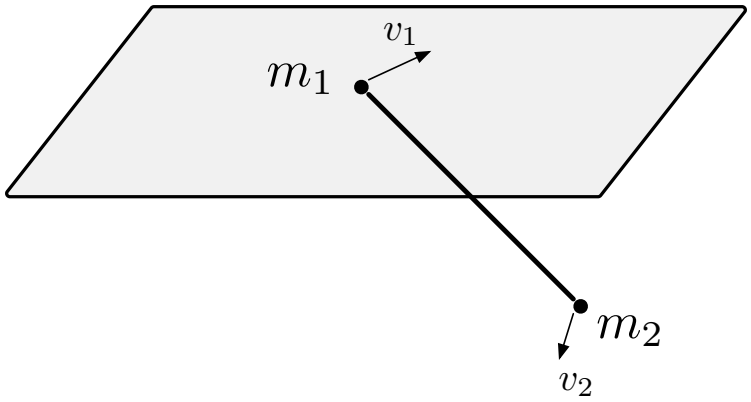
Write your ID number (not your name!) on each exam booklet.

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

Classical Mechanics 1

A sliding conical pendulum

Consider two beads connected by a rod of length ℓ. The first bead has mass m_1 and is constrained to lie in the x, y plane, but may move freely in this plane. The second bead has mass m_2 and can move freely in all three dimensions, and can pass freely through the x, y plane. The system sits in the earths gravitational field $\boldsymbol{g} = -g\,\hat{\boldsymbol{z}}$.

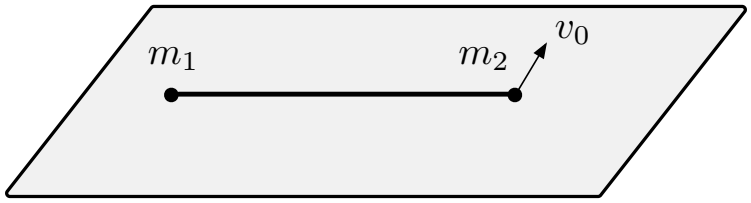


(a) (0 points) Determine the distance from m_1 to the center of mass.

(b) (6 points) Clearly define some appropriate generalized coordinates for the system, and write down the Lagrangian of the system in terms of these coordinates.

(c) (5 points) Identify all integrals of the motion.

Now consider the case where the first bead is initially at rest and the second bead initially has velocity v_0 in the x, y plane, and perpendicular to the rod, before beginning to fall (see below).



(d) (1 points) Describe qualitatively the subsequent motion of the system. In what Galilean frame is the motion periodic? Explain.

(e) (8 points)

(i) The pendulum swings down from an initial angle of $\pi/2$ relative to the vertical to a minimum angle. Determine this minimum angle.

(ii) Determine the associated period of the motion. You may leave any dimensionless integrals unevaluated. Define what is meant by large and small v_0 and describe the motion qualitatively in these two limits.

Solution

(a) From the picture, the center of mass is a distance $m_2\ell/M \equiv \alpha\ell$ from the first particle m_1 which is attached to the plane.

(b) It makes sense to use center of mass coordinates. Let us denote $M = m_1 + m_2$ as the total mass. The center of mass is mass coordinate $\boldsymbol{R} = (X, Y, Z)$

$$\boldsymbol{R} = \frac{m_1}{M}\boldsymbol{r}_1 + \frac{m_2}{M}\boldsymbol{r}_2\,. \tag{1}$$

The relative coordinate is $\boldsymbol{r} = (x, y, z)$ is

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2\,, \tag{2}$$

and the reduced mass is $\mu = m_1 m_2/(m_1 + m_2)$. The kinetic energy is

$$T = \frac{1}{2}M\dot{\boldsymbol{R}}^2 + \frac{1}{2}\mu\dot{\boldsymbol{r}}^2\,. \tag{3}$$

The vector $\boldsymbol{r}$ has a fixed length and is conveniently parameterized by two angles

$$x = \ell\sin(\theta)\cos\phi\,, \tag{4}$$
$$y = \ell\sin(\theta)\sin\phi\,, \tag{5}$$
$$z = \ell\cos(\theta)\,. \tag{6}$$

Now the angle θ is related to the height of the center of mass. From the picture, the center of mass is a distance $m_2\ell/M \equiv \alpha\ell$ from the first particle m_1 which is attached to the plane. We have from geometry

$$Z = -\alpha\ell\cos\theta\,. \tag{7}$$

Thus

$$\dot{Z} = \alpha\ell\sin\theta\,\dot{\theta}\,, \tag{8}$$

and then the kinetic energy is

$$T = \frac{1}{2}M(\dot{X}^2 + \dot{Y}^2 + \alpha^2\ell^2\sin^2(\theta)\dot{\theta}^2) + \frac{1}{2}\mu\ell^2(\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2)\,. \tag{9}$$

The potential energy is $U = MgZ$. Thus the full Lagrangian is

$$L = \frac{1}{2}M(\dot{X}^2 + \dot{Y}^2 + \alpha^2\ell^2\sin^2\theta\dot{\theta}^2) + \frac{1}{2}\mu\ell^2(\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2) + Mg\alpha\ell\cos\theta\,. \tag{10}$$

Since two of the terms are very similar, we define

$$m_0(\theta) = M\alpha^2\sin^2\theta + \mu\,, \tag{11}$$

leading to our final result

$$L = \frac{1}{2}M(\dot{X}^2 + \dot{Y}^2) + \frac{1}{2}m_0(\theta)\ell^2\dot{\theta}^2 + \frac{1}{2}\mu\ell^2\sin^2\theta\dot{\phi}^2 + Mg\alpha\ell\cos\theta\,. \tag{12}$$

(c) The are several cyclic coordinates owing to the symmetries of the problem.First there is the total momentum of the system

$$p_X = \frac{\partial L}{\partial \dot{X}} = M\dot{X}\,, \tag{13}$$

$$p_Y = \frac{\partial L}{\partial \dot{Y}} = M\dot{Y}\,. \tag{14}$$

Then there is the angular momentum around the Z axis.

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = \mu\ell^2 \sin^2\theta\dot{\phi}\,. \tag{15}$$

Finally there is the total energy of the system

$$E = \frac{p_X^2}{2M} + \frac{p_Y^2}{2m} + \frac{1}{2}m_0(\theta)\ell^2\dot{\theta}^2 + \frac{p_\phi^2}{2\mu\ell^2\sin^2(\theta)} - Mg\alpha\ell\cos\theta\,. \tag{16}$$

(d) In a frame which moves with the center of mass the motion will be periodic. The initial momenta are $p_1^y = 0$ and $p_2^y = m_2 v_0$ and

$$p_X = 0\,, \tag{17}$$

$$p_Y = m_2 v_0\,, \tag{18}$$

and thus if we look at the motion in a frame which moves in the y-direction with velocity $v_Y = m_2 v_0/M$ the motion will be periodic.

(e) (i) The initial conditions also excites internal oscillations and orbital motion. Similarly using a bit of geometry of we have that in the center of mass frame $\dot{\phi} = v_0/\ell$ and thus ϕ angular motion is determined by the angular momentum variable

$$p_\phi = \mu\ell v_0\,. \tag{19}$$

Finally the energy is constant and is determined by the initial conditions

$$E_0 = \frac{1}{2}m_2 v_0^2 = \underbrace{\frac{1}{2}\frac{m_2^2}{M}v_0^2}_{\text{init translational KE}} + \underbrace{\frac{1}{2}\mu v_0^2}_{\text{init rotational KE}}\,. \tag{20}$$

So setting $E = E_0$, we have after minor manipulations

$$\frac{1}{2}m_0(\theta)\ell^2\dot{\theta}^2 + \frac{\mu v_0^2}{2\sin^2\theta} - Mg\alpha\ell\cos\theta = \frac{1}{2}\mu v_0^2\,. \tag{21}$$

Then we have

$$\frac{1}{2}m_0(\theta)\ell^2\dot{\theta}^2 = -\frac{1}{2}\mu v_0^2\cot^2\theta + Mg\alpha\ell\cos\theta\,. \tag{22}$$

Solving for $\dot{\theta}$

$$\frac{d\theta}{dt} = \pm\frac{v_0}{\ell}\sqrt{\frac{\mu}{m_0(\theta)}}\sqrt{-\frac{\cos^2\theta}{\sin^2\theta} + u\cos\theta}\,, \tag{23}$$

where we have defined:

$$u \equiv \frac{Mg\alpha\ell}{\frac{1}{2}\mu v_0^2}\,. \tag{24}$$

u is a dimensionless number, which is the ratio of the initial potential to initial rotational kinetic energy. τ is a timescale set by the internal energy. Since the angle is decreasing (initially) we take the negative root for the first half period.

The turning points are when $\dot{\theta}$ is zero. Solving the equation for the turning points we have

$$\cos\theta_0 = 0 \qquad\qquad \theta_+ = \pi/2\,, \tag{25}$$

$$\cos\theta_- = \frac{-1+\sqrt{1+4u^2}}{2u} \qquad\qquad \theta_- < \pi/2\,. \tag{26}$$

Finally there is an unphysical turning point when the pendulum has angle greater than $\pi/2$.

(ii) Integrating the equation of motion Eq. (23) we find

$$\int_0^t dt = -\frac{\ell}{v_0}\int_{\pi/2}^{\theta(t)} d\theta \sqrt{\frac{1+r\sin^2\theta}{-\cot^2(\theta)+u\cos(\theta)}}\,, \tag{27}$$

with $r = m_2/m_1$. Here we have recognized that

$$\frac{m_0(\theta)}{\mu} = \frac{1}{\mu}\left(M\alpha^2\sin^2(\theta)+\mu\right) = 1 + r\sin^2\theta\,. \tag{28}$$

The pendulum swings down from $\theta{=}\pi/2$ to $\theta{=}\theta_-$) and back. One half of the pendulum's period is spent swinging down. Thus the full period is

$$T = \frac{2\ell}{v_0}\int_{\theta_-}^{\pi/2} d\theta \sqrt{\frac{1+r\sin^2\theta}{-\cot^2(\theta)+u\cos(\theta)}}\,. \tag{29}$$

$$= \frac{2\pi\ell}{v_0} f(u,r) \tag{30}$$

where $f(u,r)$ is a dimensionless function of u and r

Discussion: For simplicity let us set $r = m_2/m_1 = 1$. At small u, gravity's potential energy is very small compared the very large kinetic energy. Then the system makes very small oscillations between $\theta = \pi/2$ and $\theta = \pi/2-$tinybit. The period of oscillations can be worked out analytically in this case leading to

$$T = \frac{2\pi\ell}{v_0}\sqrt{2} \qquad u \ll 1 \tag{31}$$

This is suggested as an exercise.

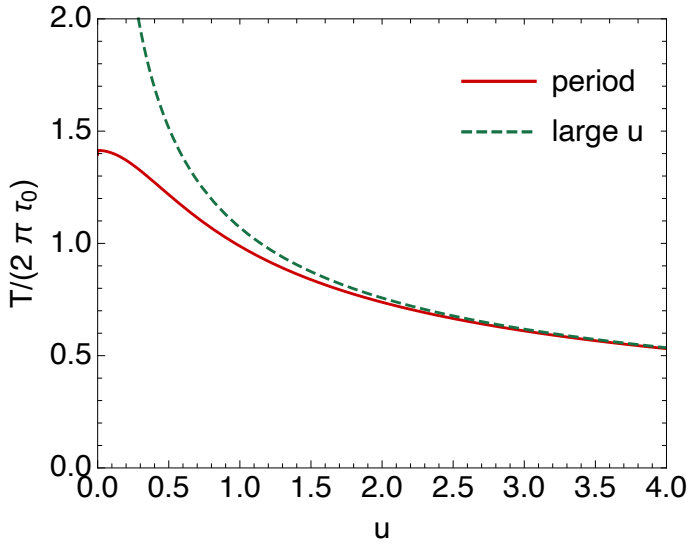


Figure 1: The period of the motion (normalized by $2\pi\ell/v_0$) as a function of u (see text).

At large u the system just falls, and the angular momentum can be neglected. Dimensional analysis in this limit says that the period is proportional to $\sqrt{\ell/g}$:

$$T = 2\pi\sqrt{\frac{\ell}{g}} \times \text{const} \tag{32}$$

This implies that $f(u,1) \to \text{const}/\sqrt{u}$ for $u \to \infty$. The integral can be done analytically in the limit that u is large, yielding

$$T = \frac{2\pi\ell}{v_0}\left(\frac{1.07}{\sqrt{u}}\right) \qquad u \gg 1 \tag{33}$$

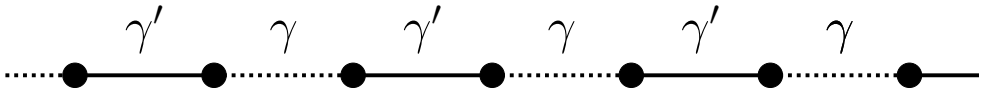
at large u.

Fig. 1 shows the period as a function of u, and the limits we have outlined.

Classical Mechanics 2

Waves from coupled springs

Consider a one dimensional system of springs, consisting of alternating spring constants γ and γ', and particles of mass m as shown below[1]. At rest the springs are unstretched and are separated by a distance a. Let x_i and u_i respectively denote the equilibrium position and small longitudinal displacement of the i-th oscillator.



(a) (7 points) Write down the Lagrangian for the system of springs and determine the equations of motion. Show that the normal modes of the system take the form

$$u_i = A\,\xi_1\, e^{-i\omega t + k x_i}\,, \tag{1a}$$

$$u_{i+1} = A\,\xi_2\, e^{-i\omega t + k x_{i+1}}\,, \tag{1b}$$

where i runs over the even sites. Explicitly write down the system of equations (in matrix form) that must be solved to determine the eigen-frequencies and associated vectors $\vec{\xi} = (\xi_1, \xi_2)$, but *do not* try to solve this system explicitly yet.

(b) (6 points) Determine the eigen-frequencies $\omega_\pm^2(k)$. Expand your eigen-frequencies at small k to quadratic order, and sketch the behavior of $\omega_+(k)$ and $\omega_-(k)$ at small k.

(c) For long wavelengths $ka \ll 1$ the fluctuations of the oscillators can be treated as a continuous system with a field $u(t,x)$ proportional to the displacements. Consider a continuous action of the form

$$S[u(t,x)] = \int dt\, dx\ \left(\partial_t u(t,x)\right)^2 - c_1 (\partial_x u(t,x))^2 - c_2\, (u(t,x))^2\,, \tag{2}$$

where c_1 and c_2 are constants.

(i) (4 points) Determine the equation of motion for $u(t,x)$ from this action, and compute the dispersion relation $\omega^2(k)$ from the resulting equation.

(ii) (3 points) How should the "low-energy" constants c_1 and c_2 be chosen to correctly model the fluctuations of part (c) for the positive mode $\omega_+(k)$, and how should they be chosen to correctly model the negative mode $\omega_-(k)$.

[1] To avoid confusion with the wavenumber k in Eq. (1), we are using γ and γ' for the spring constants instead of k and k'.

Solution

(a) We write

$$L = \sum_{i=\text{even}} \frac{1}{2}m\dot{u}_i^2 + \frac{1}{2}m\dot{u}_{i+1}^2 - \frac{1}{2}\gamma\left(u_{i+2} - u_{i+1}\right)^2 - \frac{1}{2}\gamma'(u_{i+1} - u_i)^2 \,. \tag{3}$$

Then the equation of motion read

$$m\ddot{u}_i = \gamma(u_{i+1} - u_i) - \gamma'(u_i - u_{i-1}) \,, \tag{4}$$

$$m\ddot{u}_{i+1} = \gamma'(u_{i+2} - u_{i+1}) - \gamma(u_{i+1} - u_i) \,, \tag{5}$$

Substituting the suggested ansatz

$$u_i = A\xi_1 e^{-i\omega t} e^{ikx_i} \,, \tag{6}$$

$$u_{i+1} = A\xi_2 e^{-i\omega t} e^{ikx_{i+1}} \,, \tag{7}$$

we find after minor algebra

$$-m\omega^2 \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \begin{pmatrix} -(\gamma+\gamma') & (\gamma e^{ika} + e^{-ika}\gamma') \\ (\gamma e^{-ika} + e^{ika}\gamma') & -(\gamma+\gamma') \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} . \tag{8}$$

(b) Separating the real and imaginary parts we have the matrix

$$\begin{pmatrix} -2\overline{\gamma} & 2\overline{\gamma}\cos(ka) - i(\gamma'-\gamma)\sin(ka) \\ 2\overline{\gamma}\cos(ka) + i(\gamma'-\gamma)\sin(ka) & -2\overline{\gamma} \end{pmatrix}$$
$$= -2\overline{\gamma}\mathbb{I} + 2\overline{\gamma}\cos(ka)\sigma_x + (\gamma'-\gamma)\sin(ka)\sigma_y \,, \tag{9}$$

where σ_x and σ_y are the Pauli matrices, and we have defined $\overline{\gamma} = (\gamma+\gamma')/2$.

The eigenvalues are therefore

$$m\omega_\mp^2 = 2\overline{\gamma} \mp \sqrt{4\overline{\gamma}^2\cos^2(ka) + (\gamma'-\gamma)^2\sin^2(ka)} \,, \tag{10}$$

If $\gamma' = \gamma$ then $m\omega_-^2 = 4\overline{\gamma}\sin^2(ka/2)$, which is the familiar Debye dispersion curve.

At small k, $\cos^2(ka) \simeq 1 - (ka)^2$, and thus

$$m\omega_\mp^2 \simeq 2\overline{\gamma} \mp 2\overline{\gamma}\left(1 - \tfrac{1}{2}u(ka)^2\right) \tag{11}$$

where

$$u = 1 - \frac{(\gamma'-\gamma)^2}{4\overline{\gamma}^2} > 0 \,. \tag{12}$$

So we find

$$\omega_-^2 \simeq \frac{\overline{\gamma}}{m}u(ka)^2 \,. \tag{13}$$

Taking the square root we find

$$\omega_-(k) = \pm v_0 k \,, \qquad v_0 \equiv a\sqrt{(\overline{\gamma}/m)u} \,. \tag{14}$$

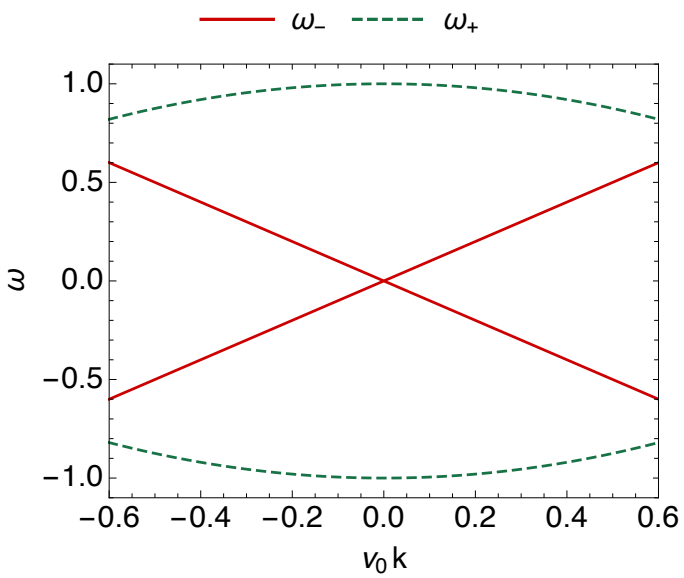


Figure 1: The allowed frequencies as a function of k

The plus mode has

$$\omega_+^2 \simeq \frac{4\overline{\gamma}}{m} - \frac{\overline{\gamma}}{m} u(ka)^2 \,, \tag{15}$$

and taking the square root yields

$$\omega_+(k) = \pm\omega_0 \left(1 - \frac{1}{2\omega_0^2}(v_0 k)^2\right) \,, \qquad \omega_0 = \sqrt{\frac{4\overline{\gamma}}{m}} \,. \tag{16}$$

The allowed values ω_- and ω_+ are shown in the figure in Fig. 1. See below for a discussion of the physics of these modes.

(c) Varying the action gives the equation of motion

$$-\partial_t^2 u + c_1 \partial_x^2 u - c_2 u = 0 \,. \tag{17}$$

Substituting $e^{-i\omega t + ikx}$ gives

$$\omega^2 - c_1 k^2 - c_2 = 0 \,, \tag{18}$$

or

$$\omega^2 = c_1 k^2 + c_2 \,. \tag{19}$$

(d) For the continuous action to reproduce the minus dispersion curve we must have

$$c_1 = v_0^2 \,, \qquad c_2 = 0 \,. \tag{20}$$

For the continuous action to reproduce the plus dispersion curve we must have

$$c_2 = \omega_0^2 \qquad c_1 = -v_0^2 \,. \tag{21}$$

Discussion: The minus mode is not gapped, which means that the waves have a frequency that approaches zero as $k \to 0$. The plus mode is gapped, but the frequency decreases as k increases. This is why $c_1 = -v_0^2$ is negative in this case. The term in the action $\propto (\partial_x u)^2$ has the opposite sign from a typical relativistic scalar field theory where c_1 must be postive. Some people like to think of this as a "negative effective mass":

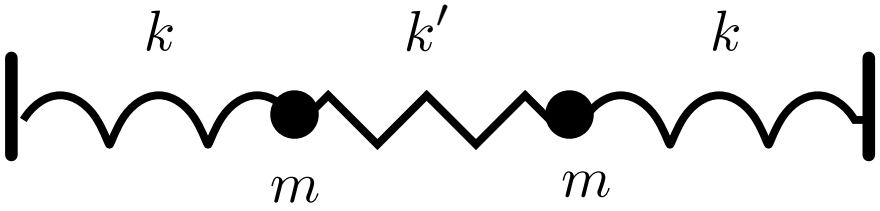
$$\omega_+(k) - \omega_0 = \frac{k^2}{2m_{\text{eff}}} = -\frac{k^2}{2|m_{\text{eff}}|}\,, \tag{22}$$

where $m_{\text{eff}} = -\omega_0/v_0^2$

Classical Mechanics 3

Oscillations with similar frequencies

Consider two particles of mass m coupled to the walls via springs with spring constant $k = m\omega_0^2$. The two particles are weakly coupled by a third spring with spring constant $k' = m\omega'^2$ as shown below. The particles can move only in the x-direction, and the springs are unstretched when the system is at rest. Assume that $\omega' \ll \omega_0$.



(a) (3 points) If at time $t = 0$ the left particle is displaced by an initial position x_0 and the right particle is at rest, determine the subsequent oscillations of the system.

(b) (4 points) Plot qualitatively $x_1(t)$ and $x_2(t)$. Show all relevant features, minding the strong inequality $k' \ll k$.

Now consider the case when the particles also experience dissipation. The drag force on the particles is

$$F_{\text{drag}} = -m\eta\frac{dx}{dt}\,, \tag{1}$$

and the drag coefficient is small $\eta \ll \omega' \ll \omega_0$. Starting at t=0, external forces are applied to the particles. The forces on the first and second particles are $F(t)$ and $-F(t)$ respectively. The particles are at rest for $t < 0$.

(c) (6 points) Determine the positions of the particles for $t > 0$ as an explicit integral over $F(t)$.

(d) (3 points) Determine the energy of the system for $t > 0$ as a double integral over $F(t)$.

(e) (4 points) If $F(t)$ is a time-dependent random force satisfying[2]

$$\begin{aligned}\langle F(t)\rangle &= 0\,,\\ \langle F(t)F(t')\rangle &= 2Tm\eta\delta(t-t')\,.\end{aligned}$$

Determine how the energy of the system evolves in time.

Here T is a constant parameter that can be interpreted as the temperature of an external bath provided the force $F(t)$.

[2]Imagine discrizing the system into steps of size Δt, the force in each Δt is $F(t) = \pm 2Tm\eta/\sqrt{\Delta t}$ where each sign occurs with 50% probability.

Solution

The equations of motion are given by Newtons Laws.

(a) The equations of motion are

$$m\ddot{x}_1 = -kx_1 + k'(x_2 - x_1)\,, \tag{2}$$
$$m\ddot{x}_2 = -k'(x_2 - x_1) - kx_2\,. \tag{3}$$

The matrix reads

$$-m\omega^2 \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = -\begin{pmatrix} (k+k') & k' \\ k' & (k+k') \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}\,. \tag{4}$$

The matrix has the form $(k+k')\mathbb{I} + k'\sigma_x$ where σ_x is the pauli matrix. In the eigen-basis of σ_x we have

$$m\omega_\pm^2 = (k+k') \pm k'\,. \tag{5}$$

The eigenvectors of σ_x are

$$E_\pm = \begin{pmatrix} 1 \\ \mp 1 \end{pmatrix} \tag{6}$$

To a good approximation since $k \gg k'$ we have

$$\omega_\pm = \overline{\omega} \pm \Delta\omega\,, \tag{7}$$

where

$$\overline{\omega} = \frac{k+k'}{m}\,, \tag{8}$$
$$\Delta\omega = \frac{(\omega')^2}{2\overline{\omega}}\,. \tag{9}$$

The initial conditions a simple 50-50 superposition of E_+ and E_- leading to the solution

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{x_0}{2} e^{-i\omega_+ t} E_+ + \frac{x_0}{2} e^{-i\omega_- t} E_-\,. \tag{10}$$

(b) We have a superposition of sinusoids with nearly equal frequency and equal amplitude. This is a setup for very strong beats. Indeed we have taking the real part of

$$x_1 = x_0 \cos(\overline{\omega}t)\cos(\Delta\omega t)\,, \tag{11}$$
$$x_2 = -x_0 \sin(\overline{\omega}t)\sin(\Delta\omega t)\,. \tag{12}$$

Fig. 1 shows the solution for $\overline{\omega} = 30\Delta\omega$

(c) Now the equations of motion are modified

$$m\ddot{x}_1 = -kx_1 - m\eta\dot{x}_1 + k'(x_2 - x_1) + F(t)\,, \tag{13}$$
$$m\ddot{x}_2 = -k'(x_2 - x_1) - m\eta\dot{x}_2 - kx_2 - F(t)\,. \tag{14}$$

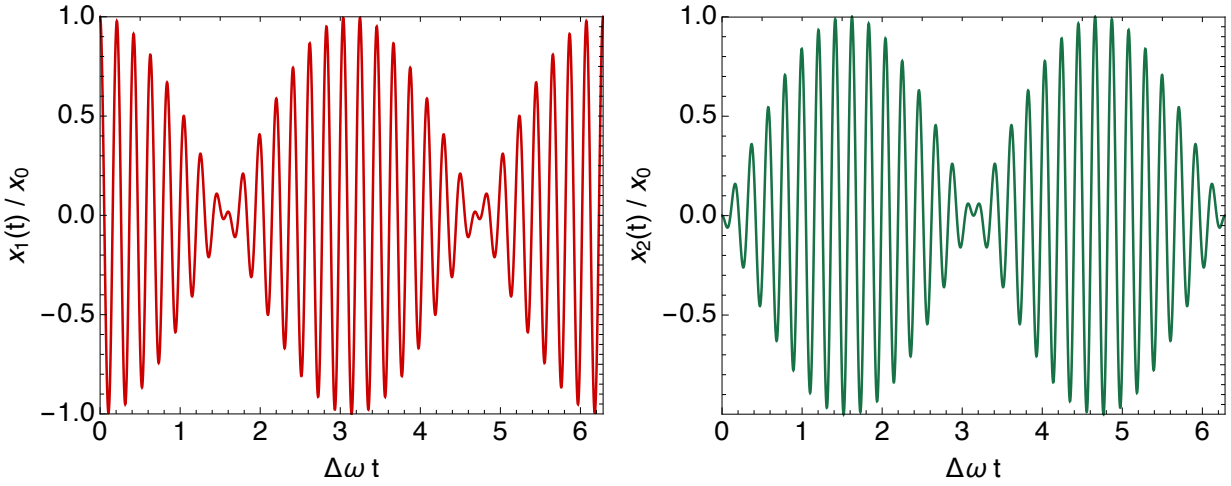


Figure 1: The solution for $\overline{\omega} = 30\Delta\omega$

Since the dissipation matrix is proportional to the identity, the eigen-vectors are still a good basis. Writing

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = q_+(t)E_+ + q_-(t)E_- \,, \tag{15}$$

we find the equations of motion

$$m\ddot{q}_+ = -\omega_+^2 q_+ - m\eta\dot{q}_+ + F(t)\,, \tag{16}$$

$$m\ddot{q}_- = -\omega_-^2 q_+ - m\eta\dot{q}_-\,. \tag{17}$$

Clearly only the amplitude of the plus mode is affected by the force. The Green function of the simple harmonic oscillator is

$$G(t,t') = \theta(t,t')e^{-\eta(t-t')/2}\sin(\omega_+(t-t'))\,. \tag{18}$$

Then

$$q_+(t) = \int_0^t \frac{F(t')}{m\omega_+} e^{-\eta(t-t')/2}\sin(\omega_+(t-t'))dt'\,, \tag{19}$$

$$q_-(t) = 0\,. \tag{20}$$

(d) The energy is

$$E = \frac{1}{2}m\dot{q}_+^2 + \frac{1}{2}m\omega_+^2 q^2(t)\,, \tag{21}$$

$$\simeq \int_0^t dt_1 \int_0^t dt_2 \, \frac{F(t_1)F(t_2)}{m^2\omega_+^2}\, e^{-\frac{1}{2}\eta(t-t_1)}e^{-\frac{1}{2}\eta(t-t_2)}m\omega_+^2 \times \left[\cos(\omega_+(t-t_1))\cos(\omega_+(t-t_2)) + \sin(\omega_+(t-t_1)\sin(\omega_+(t-t_2))\right]\,. \tag{22}$$

(e) Then using the statistics we find

$$E = \int_0^t dt_1 T\eta e^{-\eta(t-t_1)}\,, \tag{23}$$

$$= T\left(1 - e^{-\eta t}\right)\,. \tag{24}$$

Discussion. At late times the energy is given by $E = T$ as required by the equipartition theorem. The equations we have described with dissipation and a stochastic random force (with a variance that is precisely related to the dissipation) is known in statistical mechanics as the Langevin equations. The noise must be precisely related to the dissipation or the system will not reach thermal equilibrium at late times. What is happening is that the dissipation is taking energy away, while the noise is putting it back. If these processes are related, the system will equilibrate. The final energy of the oscillator is given by the equipartition theorem, which states that in classical statistical mechanics the energy of a system is given by $\frac{1}{2}T$ per quadratic form in the Hamiltonian. Here the Hamiltonian is

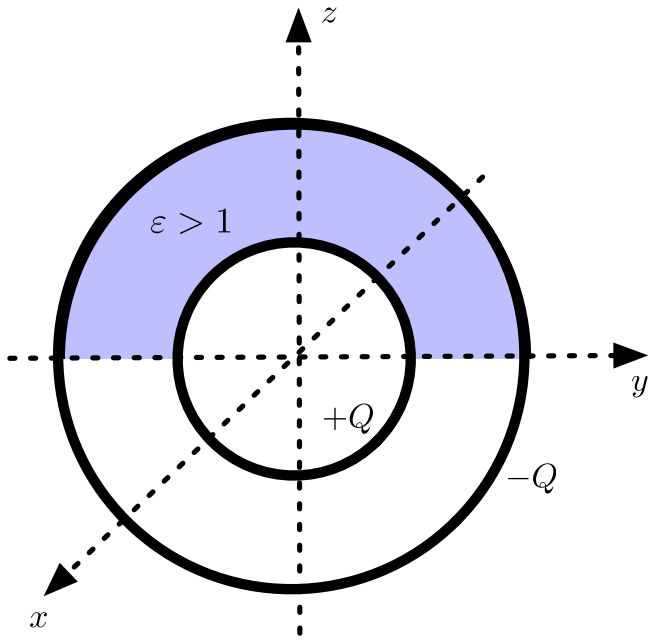
$$H = \frac{p_+^2}{2m} + \frac{1}{2}m\omega_+^2 x^2 \tag{25}$$

where $p_+ = m\dot{q}_+$. Since there are two quadratic forms – the kinetic energy, and the potential energy – the final equilibrium energy of the system is $\frac{1}{2}T + \frac{1}{2}T = T$.

Electromagnetism 1

Half-spherical capacitor

Two concentric conducting spheres of inner and outer radius a and b respectively, carry charges $\pm Q$. The empty space between the spheres is half-filled by a shell of dielectric with dielectric constant ϵ as illustrated in the figure.



(a) (8 points) Find the electric field everywhere between the spheres.

Hint: Assume that the electric field is directed radially and show that the equations of motion and all electrostatic boundary conditions are satisfied with this ansatz.

(b) (6 points) Calculate the charge per area on the inner sphere, and the polarization charge per area induced on the surface of the dielectric at $r = a$.

(c) (6 points) Calculate the magnitude and direction of the net electrostatic force on the inner sphere.

Solution

a. Azimuthal symmetry implies that the potential is $\Phi(r,\theta)$ or φ-independent. The solution to Gauss law splits for the upper and lower hemispheres

$$\begin{aligned}\Phi_U(r,\theta) &= \sum_l (A_l r^l + B_l r^{-(l+1)}) P_l(\cos\theta) \\ \Phi_L(r,\theta) &= \sum_l (C_l r^l + D_l r^{-(l+1)}) P_l(\cos\theta)\end{aligned} \tag{1}$$

The potential on the edges of the lower conducting shell is constant whatever θ

$$\begin{aligned}\Phi_L(a,\theta) &= \sum_l (C_l a^l + D_l a^{-(l+1)}) P_l(\cos\theta) = \mathbb{C} \\ \Phi_L(b,\theta) &= \sum_l (C_l b^l + D_l b^{-(l+1)}) P_l(\cos\theta) = \mathbb{D}\end{aligned} \tag{2}$$

which implies that only the $l = 0$ contributes. The same reasoning applies to the upper shell, thus

$$\begin{aligned}\Phi_U(r) = A_0 + B_0 r^{-1} &\to \vec{E}_U = \frac{B_0\,\hat{r}}{r^2} \to \vec{D}_U = \epsilon \frac{B_0\,\hat{r}}{r^2} \\ \Phi_L(r) = C_0 + D_0 r^{-1} &\to \vec{E}_L = \frac{D_0\,\hat{r}}{r^2} \to \vec{D}_L = \vec{E}_L\end{aligned} \tag{3}$$

with $B_0 = D_0$ since at the interface of the dielectric

$$(\vec{E}_U - \vec{E}_L)\cdot\hat{r} = 0 \qquad \text{and} \qquad (\vec{D}_U - \vec{D}_L)\times\hat{\theta} = 4\pi\sigma_F \tag{4}$$

B_0 is fixed by Gauss law on the inner shell,

$$2\pi\,\epsilon B_0\,[-\cos\theta]_0^{\frac{\pi}{2}} + 2\pi\,B_0\,[-\cos\theta]_{\frac{\pi}{2}}^{\pi} = 4\pi\,Q \to B_0 = \frac{2Q}{1+\epsilon} \tag{5}$$

b. The charge on the inner sphere follows from

$$\begin{aligned}\left(\vec{D}_L\cdot\hat{r}\right)_{r=a} &= 4\pi\sigma_L \to \sigma_L = \frac{1}{4\pi a^2}\frac{Q}{1+\epsilon} \\ \left(\vec{D}_U\cdot\hat{r}\right)_{r=a} &= 4\pi\sigma_U \to \sigma_U = \frac{1}{4\pi a^2}\frac{\epsilon Q}{1+\epsilon}\end{aligned} \tag{6}$$

since the inner sphere is a conductor with zero fields. The polarization charge induced on the surface of the dielectric material (upper part) at $r = a$ is

$$\sigma_P = \left(- \vec{P}_U \cdot \hat{r} \right)_{r=a} = \left(- (\epsilon - 1) \vec{E}_U \cdot \hat{r} \right)_{r=a} = \frac{1 - \epsilon}{1 + \epsilon} \frac{2Q}{a^2} \tag{7}$$

No dielectric is present in the lower part and thus no polarization charge.

c. In the absence of the dielectric, the net force on the inner sphere is zero. In the presence of the dielectric, the charges migrate and reorganize, with a deficiency in the upper-outer shell characterized by σ_P at $r = b$ (negative), and a surplus in the lower-inner shell characterized by σ_L at $r = a$ (positive). (The net total charge is still unchanged).

The net force is attractive and upward. To estimate it, consider the change in the electric energy stored in the shell due to the dielectric

$$\Delta W_E = \int_U d^3r \, \frac{1}{8\pi} \vec{E}_U \cdot \vec{D}_U - \int_U d^3r \, \frac{1}{8\pi} \vec{E}_L^2 = \frac{(\epsilon - 1)}{(\epsilon + 1)^2} \, Q^2 \left(\frac{1}{a} - \frac{1}{b} \right) \tag{8}$$

The force on the inner shell is

$$F_E = - \frac{\partial}{\partial a} \, \Delta W_E = \frac{(\epsilon - 1)}{(\epsilon + 1)^2} \frac{Q^2}{a^2} \tag{9}$$

Electromagnetism 2

Radiation from non-relativistic motion

(a) (8 points) Consider a relativistic charged particle of charge q and trajectory $\boldsymbol{r}_0(t)$. Recall that the Lienard-Wiechert potentials are[3]

$$\varphi(t,\boldsymbol{r}) = \frac{q}{4\pi\epsilon_0}\left[\frac{1}{R(1-\boldsymbol{n}\cdot\boldsymbol{v}_0/c)}\right]_{\text{ret}}, \tag{1a}$$

$$\boldsymbol{A}(t,\boldsymbol{r}) = \frac{q}{4\pi\epsilon_0 c}\left[\frac{\boldsymbol{v}_0/c}{R(1-\boldsymbol{n}\cdot\boldsymbol{v}_0/c)}\right]_{\text{ret}}, \tag{1b}$$

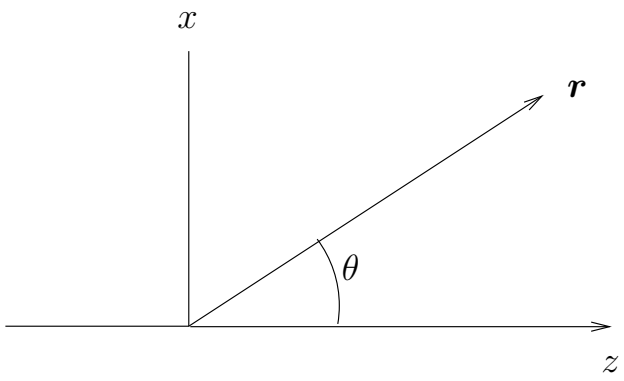
where $\boldsymbol{v}_0 = \dot{\boldsymbol{r}}_0$, $\boldsymbol{R} \equiv \boldsymbol{r} - \boldsymbol{r}_0$, and $\boldsymbol{n} = \boldsymbol{R}/R$. $[]_{\text{ret}}$ indicates that $\boldsymbol{r}_0$ and $\boldsymbol{v}_0$ are to be evaluated at the *retarded* time $T \equiv t - |\boldsymbol{r} - \boldsymbol{r}_0(T)|/c$.

(i) Find approximate expressions for these potentials in the far field limit (large $\boldsymbol{r}$), and for non-relativistic particles to first order in $\boldsymbol{v}_0/c$.

(ii) Derive an expression for the corresponding electric field $\boldsymbol{E}(t,\boldsymbol{r})$ (in the far field and non-relativistic limits) directly from the definition of field strength tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and the potentials of (i).

(b) (8 points) Consider a plane wave of light propagating in the z direction which is polarized in the x direction, $\boldsymbol{E}(t,\boldsymbol{r}) = E_0\cos(\omega t - kz)\hat{\boldsymbol{x}}$ (see below). The incoming light is incident upon an electron of charge q and mass m situated at the origin. The motion of the electron is non-relativistic.

Determine the radiated electric field in the far field at an angle θ relative to the z axis, and in the xz plane (see below). For these conditions, give explicit expressions for the Cartesian components of the (real) electric field as a function of r, θ, and time t.



[3]We have given the potentials in the SI system of units. In Gaussian units we substitute $q/(4\pi\epsilon_0) \to q$ and $q/(4\pi\epsilon_0 c) \to q$ in the equations φ and $\boldsymbol{A}$ respectively. In the Heavyside Lorentz units we substitute $q/(4\pi\epsilon_0) \to q/4\pi$ and $q/(4\pi\epsilon_0 c) \to q/4\pi$.

(c) (4 points) Determine the power per unit solid angle scattered at the angle θ of part (b) for light polarized in the xz plane, $dP_{xz}(\theta)/d\Omega$, and out of the xz plane, $dP_y(\theta)/d\Omega$. Give a qualitative explanation for the differences in the scatted intensities for the two cases.

Solution

(a) (i) In the far field limit, the retarded time is approximated

$$T \simeq t - r/c + \boldsymbol{n} \cdot \boldsymbol{r}_0/c\,, \tag{2}$$

where $\boldsymbol{n} = \boldsymbol{r}/r$ is the unit vector in the direction of $\boldsymbol{r}$. In a non-relativistic approximation $\boldsymbol{n} \cdot \boldsymbol{r}_0/c \ll t - r/c$. With both of these approximations

$$T \simeq t - r/c \equiv t_r\,. \tag{3}$$

Thus to first order in $\boldsymbol{v}_0/c$ we have

$$\varphi = \frac{q}{4\pi r}\left(1 + \boldsymbol{n} \cdot \boldsymbol{v}_0(t_r)/c\right)\,, \tag{4}$$

$$\boldsymbol{A} = \frac{q\boldsymbol{v}_0(t_r)/c}{4\pi r}\,. \tag{5}$$

(ii) First note that

$$\partial_i t_r = -n_i/c\,, \qquad \partial_t t_r = 1\,. \tag{6}$$

The electric field is then

$$E_i = -\frac{1}{c}\partial_t A_i - \partial_i \varphi\,, \tag{7}$$

$$= \frac{q}{4\pi r c^2}(-(a_0)_i + n_i(\boldsymbol{n} \cdot \boldsymbol{a}_0))\,. \tag{8}$$

It is notable how the longitudinal components of these derivatives (i.e. the term proportional to $(\boldsymbol{n} \cdot \boldsymbol{a}_0)n_i$ in $\partial_t A_i$ and $\partial_i \varphi$) cancel when computing the field strength. This cancelation is ultimately a consequence of the gauge invariance of the theory, and causes the outgoing wave to be transverse to the direction of propagation.

(b) We use the Larmour result of part (a). Here the external electric field induces an acceleration

$$\boldsymbol{a}_0(t) = \frac{\vec{F}}{m} = \frac{qE_0}{m}\cos(\omega t)\hat{\boldsymbol{x}}\,. \tag{9}$$

Then writing

$$\boldsymbol{n} = \cos(\theta)\hat{\boldsymbol{z}} + \sin(\theta)\hat{\boldsymbol{x}}\,. \tag{10}$$

we find

$$-\boldsymbol{a}_0(t_r) + \boldsymbol{n}(\boldsymbol{n} \cdot \boldsymbol{a}_0(t_r)) = -a_0(t_r)\cos(\theta)\vec{\epsilon}_1\,, \tag{11}$$

where $\vec{\epsilon}_1 = -\sin(\theta)\hat{\boldsymbol{z}} + \cos(\theta)\hat{\boldsymbol{x}}$, and the acceleration is to be evaluated at $t_r = t - r/c$. The vector $\vec{\epsilon}_1$ is shown in the figure below. Thus the scattered electric field is

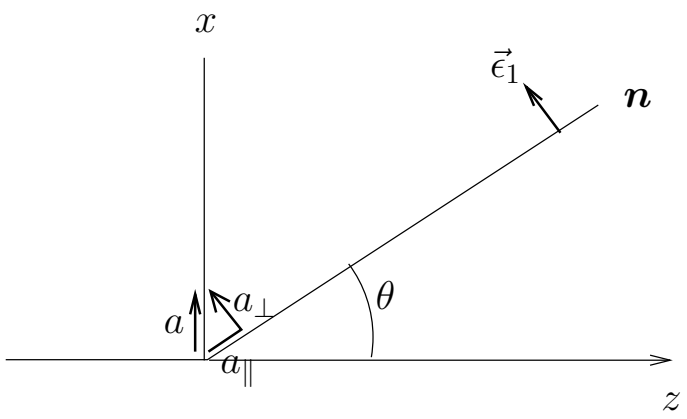
$$\boldsymbol{E}_{\text{scat}} = -\frac{q}{4\pi r c^2}\frac{qE_0}{m}\cos(\omega(t - r/c))\cos(\theta)\vec{\epsilon}_1\,, \tag{12}$$

and the x, y, z components are explicitly

$$E_{\text{scat,x}} = -\frac{q}{4\pi r c^2}\frac{qE_0}{m}\cos(\omega(t - r/c))\cos^2\theta\,, \tag{13}$$

$$E_{\text{scat,y}} = 0\,, \tag{14}$$

$$E_{\text{scat,z}} = \frac{q}{4\pi r c^2}\frac{qE_0}{m}\cos(\omega(t - r/c))\cos\theta\sin\theta\,. \tag{15}$$



(c) The electric field is clearly polarized in the plane along $\vec{\epsilon}_1$. Thus the power scattered with polarization out of plane is zero.

$$\frac{dP_y}{d\Omega} = 0\,. \tag{16}$$

The time averaged power scattered in the plane is

$$\frac{dP_{xz}}{d\Omega} = c\overline{|rE_{\rm scat}|^2} = \frac{q^4}{16\pi^2(mc^2)^2} cE_0^2 \cos^2\theta \overline{\cos^2(\omega t)}\,, \tag{17}$$

$$= \frac{q^4}{32\pi^2(mc^2)^2}\; cE_0^2 \cos^2(\theta)\,, \tag{18}$$

$$= \frac{3}{16\pi}\sigma_T\; cE_0^2 \cos^2(\theta)\,. \tag{19}$$

The result is proportional to the Thompson cross section (the total cross section for light electron scattering)

$$\sigma_T = \frac{q^2}{6\pi(mc^2)^2} \simeq 0.66\,\text{barns} \tag{20}$$

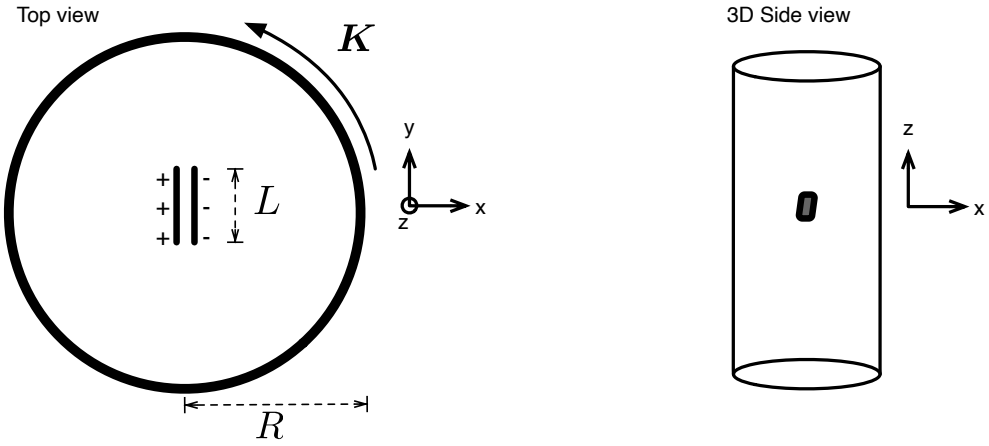
times the incoming intensity $\propto cE_0^2$.

Discussion: The result is clear physically (see figure). The charge accelerates in the $\hat{\boldsymbol{x}}$ direction and provides the source for electromagnetic waves. The polarization of the outgoing light reflects the oscillation direction of this source. Thus, the polarization of the outgoing electromagnetic waves thus lies in the xz plane, and the scattered light has no electric field component in the $\hat{\boldsymbol{y}}$ direction (out of plane). Only the compononent of the acceleration parallel to $\vec{\epsilon}_1$ ($a_\perp$ in the figure) contributes to the radiation. At an angle of $\theta = \pi/2$, the acceleration is parallel to the direction of the scattered light $\boldsymbol{n}$ and the scattered intensity is zero. This reflects the fact that the electric field of the outgoing wave must be transverse to the direction of propagation $\boldsymbol{n}$, and would therefore point in the $-\hat{\boldsymbol{z}}$ direction at $\theta = \pi/2$. There is no component of the acceleration which oscillates in the $-\hat{\boldsymbol{z}}$ direction.

Electromagnetism 3

A capacitor in a magnetic field

Consider two square non-conducting uniformly charged parallel plates of mass M, charge $\pm Q$, area $A = L^2$, and fixed separation d, with $d \ll L$. The center of plate assembly is placed precisely at the center of a long conducting tube of radius R, with $R \gg L$. The normal vector to the plates points along the x-axis, with the positively charged plate on the left at $x = -d/2$ when viewed from above (see below). Initially, the tube carries surface current $\boldsymbol{K} = K_0\,\hat{\boldsymbol{\phi}}$ as shown below.



(a) (2 points) Compute the magnitude and direction of the momentum $\boldsymbol{P}_{\text{field}}$ stored in the initial configuration of electromagnetic fields, *neglecting* the fringing electric fields of the plates.

In part (d), you will show that the total momentum in the fields, *including* the fringing fields, is exactly half of this partial result.

(b) (6 points) At $t = 0$ the current is slowly switched off over a time T, $K(t) = K_0\,(1 - t/T)$. Starting with the Lorenz force law,

$$F = q(\boldsymbol{E} + \frac{v}{c} \times \boldsymbol{B})\,, \tag{21}$$

determine the magnitude and direction of the force on each plate. Compute the total impulse $\Delta\boldsymbol{P}$ (both magnitude and direction) delivered to the plates over time T. Is this the same as part (a)? Explain.

(c) (6 points) If the parallel plates are replaced by an assembly consisting of two irregularly shaped non-conducting objects of charges $\pm Q$ and characteristic size $L \ll R$ and arbitrary orientation, show that the net force on the assembly is determined by its electric dipole moment and the changing magnetic field, $\dot{\boldsymbol{B}}$. Check that your general result is consistent with (b).

(d) (6 points) Recompute the total momentum stored in the initial fields of part (a), this time *including* the fringing electric fields. Show that the result is exactly half of (a) and related to the electric dipole moment of the the plates.

Hint: Prove the vector identity $\int_V d^3\boldsymbol{r}\, E_i = -\oint_{\mathcal{S}} da_i\, \phi$ where ϕ is the scalar potential, and use the result to rewrite the total momentum stored in the field as a surface integral over the cylinder (where the dipole approximation for the electric field is valid). Some elementary integrals are given below.

Elementary integrals:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}x}{(1+x^2)^{n/2}} = \begin{cases} \pi & n=2 \\ 2 & n=3 \\ \frac{\pi}{2} & n=4 \\ \frac{4}{3} & n=5 \end{cases} \tag{22}$$

Solution:

(a) The electric field is $E = \sigma\,\hat{\boldsymbol{x}}$, where $\sigma_0 = Q/A$ by Gauss Law. The magnetic field is $\boldsymbol{B} = (K_0/c)\,\hat{\boldsymbol{z}}$ by Ampere Law. We have

$$\boldsymbol{P}_{\rm field} = \frac{1}{c}\int_V d^3\boldsymbol{r}\,(\boldsymbol{E}\times\boldsymbol{B}) = \frac{1}{c^2}Ad\,\sigma_0 K_0(\hat{\boldsymbol{x}}\times\hat{\boldsymbol{z}}) = \frac{1}{c^2}Ad\,\sigma_0 K_0(-\hat{\boldsymbol{y}})\,. \tag{23}$$

(b) First we determine the induced field using Faraday's Law:

$$\oint \boldsymbol{E}_{\rm ind}\cdot {\rm d}\boldsymbol{\ell} = -\frac{1}{c}\partial_t \int \boldsymbol{B}\cdot {\rm d}\boldsymbol{a} \tag{24}$$

An elementary computation gives

$$2\pi\rho E^\phi = \frac{K_0}{Tc^2}\pi\rho^2\,, \tag{25}$$

and thus in Cartesian coordinates

$$\boldsymbol{E}_{\rm ind} = (E^x, E^y, E^z) = \frac{K_0}{2Tc^2}(-y, x, 0)\,. \tag{26}$$

We then find that the left plate experiences a force

$$F^y_L = \sigma_0\int_{x=-d/2,{\rm area}} E^y_{\rm ind,L} = -\frac{Ad}{4}\frac{\sigma_0 K_0}{Tc^2}\,. \tag{27}$$

The right plate as

$$F^y_R = -\sigma_0\int_{x=d/2,{\rm area}} E^y_{\rm ind,R} = -\frac{Ad}{4}\frac{\sigma_0 K_0}{Tc^2}\,, \tag{28}$$

and the net impulse is

$$\Delta P^y = (F^y_L + F^y_R)T = -Ad\,\frac{\sigma_0 K_0}{2c^2}\,. \tag{29}$$

This is half the momentum in the non-fringing electric fields. For the resolution of this inconsistently see (d), where the momentum in the fields is computed correctly.

(c) The net force on the "plates" is

$$F_i = \int dV\,\rho(\boldsymbol{x})E_i(\boldsymbol{x})\,. \tag{30}$$

Since the object is small in comparison to the lengths associated with $\boldsymbol{E}$, we can expand the electric field near the center of the object $\boldsymbol{x}_0$

$$E_i(\boldsymbol{x}_0+\delta\boldsymbol{x}) = E_i(\boldsymbol{x}_0) + \delta x^j\,\partial_j E_i(\boldsymbol{x}_0) \tag{31}$$

with $\delta\boldsymbol{x} = \boldsymbol{x} - \boldsymbol{x}_0$. So we have

$$F_i = \left[\int dV\,\rho(\boldsymbol{x})\right]E_i(\boldsymbol{x}_0) + \left[\int dV\,\rho(\boldsymbol{x})\,\delta x^j\right]\partial_j E_i(\boldsymbol{x}_0)\,. \tag{32}$$

The first term vanishes since the plates have no charge, and the dipole moment appears naturally in the second term

$$\boldsymbol{p} = \int dV \rho(\boldsymbol{x}) \delta \boldsymbol{x} \tag{33}$$

Then we write

$$\partial_j E_i = \frac{1}{2}(\partial_j E_i + \partial_i E_j) + \frac{1}{2}(\partial_j E_i - \partial_i E_j)\,, \tag{34}$$

and note that the symmetric (first) term vanishes for the field in Eq. (26), while the anti-symmetric (second) term is the curl:

$$\partial_j E_i - \partial_i E_j = (\nabla \times \boldsymbol{E})^k \epsilon_{jik}\,. \tag{35}$$

Using $\nabla \times \boldsymbol{E} = -\dot{\boldsymbol{B}}/c$ we find

$$F_i = -\frac{1}{2} p^j \epsilon_{jik} \frac{\dot{B}^k}{c}\,. \tag{36}$$

or

$$\boldsymbol{F} = \frac{1}{2c} \boldsymbol{p} \times \dot{\boldsymbol{B}}\,. \tag{37}$$

For the case of the plates

$$\boldsymbol{p} = \sigma_0 A d(-\hat{\boldsymbol{x}})\,, \qquad \dot{\boldsymbol{B}} = -\frac{K_0}{Tc}\,\hat{\boldsymbol{z}}\,, \tag{38}$$

and we have

$$\Delta \boldsymbol{P} = \boldsymbol{F} T = -Ad\,\frac{\sigma_0 K_0}{2c^2}\,\hat{\boldsymbol{y}}\,. \tag{39}$$

This agrees with part (b).

(d) Now let us re-compute the initial momentum stored in the fields including the fringing fields.

$$\boldsymbol{P}_{\text{field}} = \frac{1}{c}\int_V (\boldsymbol{E} \times \boldsymbol{B}) \tag{40}$$

Then $\boldsymbol{B}$ is constant and comes out of the integral

$$\boldsymbol{P}_{\text{field}} = -\frac{K_0}{c^2}\,\hat{\boldsymbol{z}} \times \int_V \boldsymbol{E} \tag{41}$$

We can use the identity

$$\int_V E_i = -\int da_i\,\phi \tag{42}$$

to rewrite the potential as a surface integral over the cylinder.

$$\int_V E_i = -\int da_i\,\frac{\boldsymbol{p}\cdot\boldsymbol{n}}{4\pi r^2} \tag{43}$$

Now $\boldsymbol{p} = p_0(-\hat{\boldsymbol{x}})$ where $p_0 = Ad\sigma_0$. Then a bit of geometry shows

$$\mathrm{d}a_x = R\mathrm{d}\phi\mathrm{d}z\cos\phi\,, \tag{44}$$

$$\mathrm{d}a_y = R\mathrm{d}\phi\mathrm{d}z\sin\phi\,, \tag{45}$$

$$\boldsymbol{p}\cdot\boldsymbol{n} = -\,p_0\cos\theta\cos\phi = -\frac{p_0 R\cos\phi}{(R^2+z^2)^{1/2}}\,, \tag{46}$$

$$r^2 = R^2 + z^2\,. \tag{47}$$

We find

$$\int_V E_x = \frac{1}{4\pi}\int_0^{2\pi}\mathrm{d}\phi\int_{-\infty}^{\infty}\mathrm{d}z\,\frac{p_0 R^2\cos^2\phi}{(R^2+z^2)^{3/2}}\,, \tag{48}$$

$$= \frac{p_0}{4}\int_{-\infty}^{\infty}\mathrm{d}z\,\frac{R^2}{(R^2+z^2)^{3/2}}\,, \tag{49}$$

$$= \frac{p_0}{2}\,. \tag{50}$$

The other components, $\int_V E_y$ and $\int_V E_z$ are zero. Thus we have shown that the total momentum stored in the initial field configuration is precisely half of what was computed in (a) :

$$\boldsymbol{P}_{\text{field}} = \frac{K_0 p_0}{2c^2}(-\hat{\boldsymbol{z}}\times\hat{\boldsymbol{x}})\,, \tag{51}$$

$$= \frac{K_0\sigma_0 Ad}{2c^2}(-\hat{\boldsymbol{y}})\,. \tag{52}$$

The increase in momentum of the plates $\Delta\boldsymbol{P}$ is a result of the momentum transfer of $\boldsymbol{P}_{\text{field}}$ from the field to the plates.

Quantum Mechanics 1

1D hydrogen atom

An image force attracts an electron to a flat surface. The dynamics of the electron at a distance x from the surface is governed then by the Hamiltonian

$$H = \frac{p^2}{2m} + V(x)\,, \quad V(x) = \begin{cases} +\infty\,, & x < 0\,, \\ -k/x\,, & x > 0\,, \end{cases}$$

where $k > 0$ is a constant.

(a) *(2 pts)* Write down the WKB quantization condition appropriate for the potential $V(x)$.

(b) *(4 pts)* Find explicitly the energies E_n of the stationary states of the electron bound to the surface in the WKB approximation.

In the rest of the problem you need to find the energies E_n exactly by solving the Schrödinger equation using the method of the series expansion of the solution.

(c) *(4 pts)* Write down the Schrödinger equation and find the main part, $a(x)$, of the asymptotic behavior of the wavefunctions $\psi(x)$ of the bound states at $x \to \infty$: $\psi(x) \simeq a(x)$. Derive the form of the Schrödinger equation this equation takes in terms of $f(x)$ that is defined as the remaining part of $\psi(x)$: $\psi(x) = f(x)a(x)$.

(d) *(4 pts)* Representing $f(x)$ as a power series, obtain the recurrence relation the coefficients of this series from the Scrödinger equation.

(e) *(4 pts)* Use the recurrence relation derived in (d) to find the energies E_n of the stationary states. Very briefly compare the exact energies E_n to their values in the WKB approximation.

(f) *(2 pts)* Find the wavefunction of the ground state of this "1D hydrogen atom".

Solution

(a) Classically, the motion of the electron bound to the surface has two turning points, $x = 0$ and $x = x_0 = k/|E|$, where $E < 0$ is the electron energy. The phase shift of the wavfunction upon reflection from the infinite potential wall at $x = 0$ is π, and the phase shift at x_0 is $\pi/2$. With these phase shifts, the WKB quantization condition is

$$\int_0^{x_0} dx[2m(E + k/x)]^{1/2} = \pi\hbar(n + 3/4)\,, \quad n = 0, 1, 2, \ldots\,.$$

(b) To find the energies E_n of the stationary bound states, one need to evaluate the integral in teh quatization condition. This can be done by two substitutions, first $x = u^2$, and then $u = \sqrt{x_0}\sin\phi$:

$$\int_0^{x_0} dx[2m(E + k/x)]^{1/2} = (2m|E|)^{1/2}\int_0^{x_0} dx[(x_0 - x)/x]^{1/2}$$

$$= (8m|E|)^{1/2}\int_0^{\sqrt{x_0}} du[x_0 - u^2]^{1/2} = x_0(8m|E|)^{1/2}\int_0^1 dz[1 - z^2]^{1/2}$$

$$= (8mk^2/|E|)^{1/2}\int_0^{\pi/2} d\phi(\cos\phi)^2 = \pi(mk^2/2|E|)^{1/2}\,.$$

From this integral, the energies E_n in the quasiclassical approximation are:

$$E_n = -\frac{mk^2}{2\hbar^2}\frac{1}{(n + 3/4)^2}\,, \quad n = 0, 1, 2, \ldots\,.$$

(c) The stationary Schrödinger equation can be written as:

$$\psi''(x) + \Big(\frac{2mk}{\hbar^2}\frac{1}{x} - \kappa^2\Big)\psi(x) = 0\,, \quad \kappa^2 \equiv -\frac{2mE_n}{\hbar^2}\,.$$

At $x \to \infty$ the potential energy term in this equation vanishes, and the solution has the form

$$\psi(x) \propto e^{-\kappa x}.$$

Introducing $f(x)$ by the relation $\psi(x) = f(x)e^{-\kappa x}$, i.e.,

$$\psi'(x) = [f'(x) - \kappa f(x)]e^{-\kappa x}, \quad \psi''(x) = [f''(x) - 2\kappa f'(x) + \kappa^2 f(x)]e^{-\kappa x},$$

one can directly express the Schrödinger equation as follows

$$xf''(x) - 2\kappa x f'(x) + \frac{2mk}{\hbar^2}f(x) = 0$$

(d) Since the wavefunction, and therefore the function f(x), should vanish at $x = 0$, where the potential is infinite: $f(x = 0) = 0$, expansion of $f4(x)$ in the power series should contain only the positive powers of x. It is conveniently to write the coefficients of this series as

$$f(x) = \sum_{n=1}^{\infty}\frac{a_n}{n!}x^n\,.$$

Inserting this series into the Schrödinger equation expressed through $f(x)$, and equating the coefficients with the same powers of x, we get the following recurrence relation for a's:

$$a_{n+1} = (2\kappa - \frac{2mk}{\hbar^2 n})a_n \, .$$

(e) If the recurrence relation obtained in part (d) is iterated to infinity, one sees that at large n,

$$a_n|_{n\to\infty} \sim (2\kappa)^n,$$

the coefficients that would imply that $f(x) \sim e^{2\kappa x}$ and result in the wavefunction diverging at large x. This means that the converging wavefunction of a bound states can be obtained only if the recurrence relation stops at some n, i.e., if

$$2\kappa - \frac{2mk}{\hbar^2 n} = 0 \quad \Rightarrow \quad \kappa = \frac{mk}{\hbar^2 n} \, .$$

This condition determines the possible energies E_n of the bound states:

$$E_n = -\frac{\hbar^2\kappa^2}{2m} = -\frac{mk^2}{2\hbar^2 n^2} \, , \quad n = 1, 2, \ldots \, .$$

We see that this equation is very close to the WKB result. The WKB energies are different from the exact ones only by $1/4$ subtracted from each quantum number n.

(f) For $n = 1$ and $E = E_1$, the only nonvanishing coefficient in the power series is a_1, which is determined only by the normalization condition of the wavefunction. Thus, the wavefunction of the ground state is

$$\psi_1(x) \propto x \exp\{-\frac{mk}{\hbar^2}x\} \, ,$$

and calculating the normalization factor, we get finally:

$$\psi_1(x) = \frac{2x(mk)^{3/2}}{\hbar^3} \exp\{-\frac{mk}{\hbar^2}x\} \, .$$

Quantum Mechanics 2

Spin angular momentum and an antiferromagnetic spin chain

Consider the spin operators in units of $\hbar$, $\hat{S}^\alpha$ with α=x, y, z, which satisfy the usual commutation relations $[\hat{S}^\alpha, \hat{S}^\beta] = i\sum_\gamma \varepsilon_{\alpha\beta\gamma}\hat{S}^\gamma$. The spin raising and lowering operators are $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$. The spin magnitude S can take any half-integer or integer value, and is given by the standard relation $S(S+1) = \sum_\alpha (\hat{S}^\alpha)^2$.

(a) (4 pts) Use the commutation relations between the $\hat{S}^\pm$ and $\hat{S}^z$ operators to show that under the rotation $U_z(\theta) = e^{-i\theta\hat{S}^z}$ the operator $\hat{S}^\pm$ transforms as $U_z(\theta)\hat{S}^\pm U_z(\theta)^\dagger = e^{\mp i\theta}\hat{S}^\pm$. Use this result and the permutation $x \to z \to y$ to show that $e^{-i\pi\hat{S}^y}\hat{S}^z e^{i\pi\hat{S}^y} = -\hat{S}^z$.

Now consider a chain of such spins on N sites (with N even) interacting with a nearest-neighbor antiferromagnetic Heisenberg interaction. The sites are labeled from $j = -N/2$ to $j = N/2-1$ and arranged in a circle, so that the $(N/2)$-th site is the same as $(-N/2)$-th site. The Hamiltonian of the chain is then:

$$H = \sum_{j=-N/2}^{N/2-1} (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \hat{S}_j^z \hat{S}_{j+1}^z) = \sum_{j=-N/2}^{N/2-1} \Big[\frac{1}{2}(\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+) + \hat{S}_j^z \hat{S}_{j+1}^z\Big]. \quad (1)$$

The chain is invariant under: (i) spatial translations, (ii) spatial reflections, and (iii) rotations of the spin operators, as illustrated below. The reflection can be about any site, but we will only consider the reflection about the origin, $j = 0$.

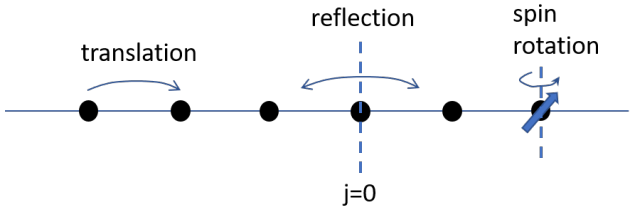


Figure 1: A linear chain of spins with $N = 6$ sites.

(b) (2 points) Prove that the Hamiltonian is invariant under a global rotation of spins via the rotation operator, $U_z(\theta) = e^{-i\theta\sum_j \hat{S}_j^z}$, i.e. show that $U_z(\theta)HU_z(\theta)^\dagger = H$.

The Hamiltonian is also obviously invariant under the translations and reflections.

(c) (4 points) The ground state of the chain $|\psi_0\rangle$ has energy e_0 per site, i.e.

$$H|\psi_0\rangle = Ne_0|\psi_0\rangle.$$

Assume that this ground state respects the symmetries of the Hamiltonian, including the rotation symmetry, which makes the x, y, z axes of the coordinate system equivalent. Use this assumption to determine the expectation values $\langle\psi_0|\hat{S}^+_j\hat{S}^-_{j+1}|\psi_0\rangle$ and $\langle\psi_0|\hat{S}^-_j\hat{S}^+_{j+1}|\psi_0\rangle$ in terms of e_0.

(d) (5 points) Now consider a non-uniform rotation $U_{\rm NU}$ which acts on the middle $(2n+1)$ sites of the chain $j \in [-n, n]$ with $n < N/2$, and rotates each spin in this range by a site-dependent angle θ_j that increases linearly with j from zero to 2π:

$$U^\dagger_{\rm NU} \equiv \exp\left(i\sum_{j=-n}^{n}\theta_j\hat{S}^z_j\right), \quad \text{where} \quad \theta_j \equiv \pi(j+n)/n\,. \tag{2}$$

The operator $U_{\rm NU}$ changes the ground state into another state $|\psi_1\rangle \equiv U^\dagger_{\rm NU}|\psi_0\rangle$, creating an excitation of length $2n+1$.

(i) Determine how $U^\dagger_{\rm NU}$ transforms under the combination of the reflection with respect to the origin, and a uniform spin rotation by π around y axis.
Hint: The combined action of these transformations on a single site operator $\hat{S}^z_j$ is such that $\hat{S}^z_j \to -\hat{S}^z_{-j}$.

(ii) Use the result of (i) to show that $\langle\psi_1|\psi_0\rangle = 0$, when the spin magnitude S on each site is a half-integer.

(e) (5 points) Calculate the energy difference between the states $|\psi_1\rangle$ and $|\psi_0\rangle$:

$$\delta E \equiv \langle\psi_1|H|\psi_1\rangle - \langle\psi_0|H|\psi_0\rangle. \tag{3}$$

Show that the energy difference is of order $\mathcal{O}(1/n)$ and approaches zero for large n.

Hint: Use the results of parts (a) and (c) applied to the chain.

This problem shows that $|\psi_1\rangle$ is orthogonal to $|\psi_0\rangle$ and has the approximately the same energy for large wavelengths, $n \to \infty$. The problem provides one particular example of the so-called Lieb-Schultz-Mattis (LSM) theorem which states that a 1D spin system with translation and spin rotation symmetry, and half-integer spin per unit cell, does not admit a gapped symmetric non-degenerate ground state.

Solution

(a) The simplest way to prove the first identity is to notice that the standard commutation relation:

$$[\hat{S}^{\pm}, \hat{S}^z] = \mp \hat{S}^{\pm}$$

can be rewritten as $\hat{S}^{\pm}\hat{S}^z = (\hat{S}^z \mp 1)\hat{S}^{\pm}$ and, in this form, generalizes immediately to an arbitrary function $f(\hat{S}^z)$ of $\hat{S}^z$:

$$\hat{S}^{\pm} f(\hat{S}^z) = f(\hat{S}^z \mp 1)\hat{S}^{\pm}.$$

This relation produces the required identity, if one takes $f(\hat{S}^z) = e^{i\theta\hat{S}^z}$.

The second identity can be proven using the previous result. Since $\hat{S}^x = (\hat{S}^+ + \hat{S}^-)/2$ and $\hat{S}^y = (\hat{S}^+ - \hat{S}^-)/2i$, the transformation properties of $\hat{S}^{\pm}$ show directly that

$$U_z(\theta)\hat{S}^x U_z(\theta)^{\dagger} = \cos\theta \hat{S}^x + \sin\theta \hat{S}^y.$$

Then, applying the permutation $x \to z \to y$ and setting $\theta = \pi$, we have

$$e^{-i\pi\hat{S}^y}\hat{S}^z e^{i\pi\hat{S}^y} = -\hat{S}^z.$$

The last identiy can also be proven by using the Baker-Hausdorff formula:

$$e^{-i\beta\hat{S}^y}\hat{S}^z e^{i\beta\hat{S}^y} = \hat{S}^z - i\beta[\hat{S}^y, \hat{S}^z] + \frac{(-i\beta)^2}{2}[\hat{S}^y, [\hat{S}^y, \hat{S}^z]] + ... + \frac{(-i\beta)^k}{k!}[\hat{S}^y, [\hat{S}^y, ...[\hat{S}^y, \hat{S}^z]...]] + ... \,,$$

where the last (general) terms contains k commutators.

$$[\hat{S}^y, \hat{S}^z] = i\hat{S}^x \,, \quad [\hat{S}^y, \hat{S}^x] = -i\hat{S}^z \,,$$

we see that the operator part of all odd terms in the series is equal to $\hat{S}^x$, while of all even terms – $\hat{S}^z$, while the numerical factors sum up to sine and cosine, respectively:

$$e^{-i\beta\hat{S}^y}\hat{S}^z e^{i\beta\hat{S}^y} = \hat{S}^z \cos\beta + \hat{S}^x \sin\beta \,.$$

For $\beta = \pi$, we get the required identity.

(b) Invariance of the Hamiltonian with respect to global rotations in the spin space follows immediately from the first relation proven in part (a) by noticing that the operators $\hat{S}^z$ are unchanged by the rotation, while the $\hat{S}^{\pm}$ operators acquire the phase factors with the opposite phases which cancel out in the products.

(c) The spin rotation symmetry means that the designation of the x, y, and z axis is arbitrary, and the contribution of each spin component to energy should be the same:

$$\langle\psi_0|\hat{S}^x_j\hat{S}^x_{j+1}|\psi_0\rangle = \langle\psi_0|\hat{S}^y_j\hat{S}^y_{j+1}|\psi_0\rangle = \langle\psi_0|\hat{S}^z_j\hat{S}^z_{j+1}|\psi_0\rangle = e_0/3 \,.$$

This, together with the reflection symmetry, immediately gives that

$$\langle\psi_0|\hat{S}^+_j\hat{S}^-_{j+1}|\psi_0\rangle = \langle\psi_0|\hat{S}^-_j\hat{S}^+_{j+1}|\psi_0\rangle = 2e_0/3 \,.$$

(d) Reflection with respect to the origin, changes the sign of the site index: $j \to -j$, while, as shown in part (a), the uniform rotation by π around y axis changes the sign of the $\hat{S}^z$. In total, this indeed gives: $\hat{S}^z_j \to -\hat{S}^z_{-j}$. This transformation has the following effect on the operator $U_{\rm NU}$:

$$\sum_{j=-l}^{l}(j+l)/l\cdot\hat{S}^z_j \to \sum_{j=-l}^{l}(-j-l)/l\cdot\hat{S}^z_{-j} = \sum_{j=-l}^{l}(j-l)/l\cdot\hat{S}^z_j = \sum_{j=-l}^{l}(j+l)/l\cdot\hat{S}^z_j - 2\sum_{j=-l}^{l}\hat{S}^z_j,$$

i.e.

$$U^\dagger_{\rm NU} \to U^\dagger_{\rm NU} e^{-i2\pi\sum_{j=-l}^{l}\hat{S}^z_j}.$$

This means that the difference between the original and transformed operator $U^\dagger_{\rm NU}$ is the rotation of the (2l+1) spins by 2π around the z axis. Since the state of each half-odd integer spin S is multiplied by (-1) as a result of 2π rotation, the two operators differ by the factor (-1). The fact that the ground state $|\psi_0\rangle$ is invariant with respect to the inversion and global rotations means that

$$\langle\psi_0|\psi_1\rangle = \langle\psi_0|U^\dagger_{\rm NU}|\psi_0\rangle = -\langle\psi_0|U^\dagger_{\rm NU}|\psi_0\rangle = -\langle\psi_0|\psi_1\rangle\,.$$

Thus,

$$\langle\psi_0|\psi_1\rangle = 0\,.$$

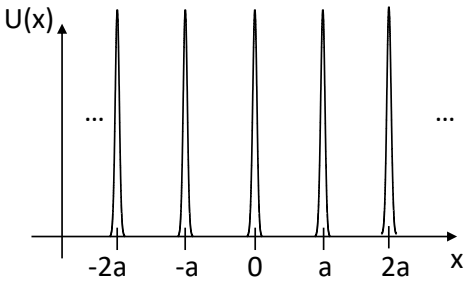
(e) From the results of (a) and (c) we know that the nonuniform rotation $U_{\rm NU}$ leaves the $\hat{S}^z$ part of the Hamiltonian unchanged, while multiplying the contribution from each edge between the rotated sites to the $\hat{S}^\pm$ part of the energy by the factor $\cos(\pi/l)$. This means that the total energy difference is:

$$\delta E = \frac{4le_0}{3}\cdot[\cos(\pi/l)-1]|_{l\to\infty} \approx \mathcal{O}(1/l)\,.$$

Quantum Mechanics 3

Particle in a periodic potential

Consider a particle of mass m in a periodic potential made of delta functions $U(x) = \alpha \sum_{n=-\infty}^{\infty} \delta(x - na)$ representing an idealized one-dimensional crystal. This problem will consider the energy spectrum of the particle in the potential, both for the case of discrete translational invariance, and for the case of an additional localized defect.



In the "potential-free" regions $na < x < (n+1)a$, the wavefunction ψ of the particle can be written as a superposition of plane waves, $A_n e^{ik(x-na)} + B_n e^{-ik(x-na)}$, where $k = k(E) = \sqrt{2mE/\hbar^2}$ is the wavenumber and E is the particle's energy.

(a) (3 points) Provide arguments to show that $\psi(x)$ must fulfill the condition $\psi(x+a) = \mu\psi(x)$. What are the possible values of μ? Relate μ to the so-called quasimomentum q, where $q \in [-\pi/a, \pi/a]$. (Note: this is known as Bloch's theorem.)

(b) (6 points) From the Schrödinger equation, find the matching conditions for ψ and its spatial derivative at the points $x = na$. Using these conditions, show that the relationship between E and μ can be written as

$$\mu^2 - 2\mu f(E) + 1 = 0$$

and find $f(E)$ in terms of the wavenumber $k = k(E)$.

(c) (3 points) From the constraint on μ, find the range of allowed values of $f(E)$.

(d) (5 points) The function $f(E)$ encodes the spectrum of the particle in the potential. Use Bloch's theorem and the result from the previous part to derive an equation that relates $f(E)$ to the quasimomentum q. Solve the obtained relation by iteration in the limit of a large potential, $\alpha \to \infty$ (introducing the dimensionless parameter $\lambda \equiv \alpha ma/\hbar^2$) to get the terms up to and including the order $1/\alpha$. Provide a very brief interpretation of the zero-order and the first order terms in $1/\alpha$.

(e) (3 points) Based on the above, sketch the function $E = E(q)$, indicating bands and band gaps, and briefly discuss the qualitative behavior of this function for arbitrary potential strength.

Solution

(a) Because of the discrete translational invariance, the shift of the wavefunction by the lattice period produces effectively the same state, with a wavefunction that can be different at most by a phase factor, i.e., we must have $|\mu| = 1$. In terms of the quasimomentum q, this factor is written as $\mu = e^{iqa}$.

(b) Integration of the Schrödinger equation $-\frac{\hbar^2}{2m}\psi'' + \alpha\delta(x - na)\psi = E\psi$ over an interval $[na - \epsilon, na + \epsilon]$ with $\epsilon \to 0$ yields

$$\psi(na + 0) = \psi(na - 0) \quad \text{and} \quad \psi'(na + 0) - \psi'(na - 0) = \frac{2m\alpha}{\hbar^2}\psi(na) \tag{1}$$

Applying the matching conditions for $x = na$ one then obtains

$$A_n + B_n = A_{n-1}e^{ika} + B_{n-1}e^{-ika}\,,$$

$$\left[1 + i\frac{2m\alpha}{\hbar^2 k}\right] A_n - \left[1 - i\frac{2m\alpha}{\hbar^2 k}\right] B_n = A_{n-1}e^{ika} - B_{n-1}e^{-ika}.$$

In addition, the condition $\psi(x + a) = \mu\psi(x)$ yields the relations

$$A_n = \mu A_{n-1} \quad \text{and} \quad B_n = \mu B_{n-1}\,,$$

which reduce the system of equations derived above to the equations for A_{n-1} and B_{n-1}. To simplify algebra, one can use explicitly the variables $u = A_{n-1} + B_{n-1}$ and $v = A_{n-1} - B_{n-1}$. In terms of these variables, the two linear equations for A_{n-1} and B_{n-1} take the following form:

$$\mu u = u\cos ka + iv\sin ka\,,$$

$$i\frac{2m\alpha}{\hbar^2 k}u + \mu v = v\cos ka + iu\sin ka\,.$$

This homogeneous system of equations can only be solved if the determinant is equal to zero:

$$\mu^2 - 2\mu f + 1 = 0, \quad \text{where} \quad f = \cos ka + \frac{m\alpha}{\hbar^2 k}\sin ka \tag{2}$$

(c) To find the physically relevant range for $f(E)$, we take into account that the solution of the quadratic equation for μ derived above is:

$$\mu = f \pm \sqrt{f^2 - 1}\,, \quad \text{if} \quad |f| > 1\,,$$

or

$$\mu = f \pm i\sqrt{1 - f^2}\,, \quad \text{if} \quad |f| \le 1\,.$$

One can see explicitly that only the last equation gives μ that satisfies the requirement $|\mu| = 1$. Thus, the range of physically relevant values of $f(E)$, which corresponds to allowed values of the eigenenergy E of the the particle in this periodic potential is

$$-1 \le f(E) \le 1\,.$$

(d) From the previous part, we see that the values of energy E for which $f(E) = \pm 1$, separate the regions of allowed values of energy with energy eigenstates of the particle in the potential (energy bands) from the regions where there are no energy eigenstates (energy gaps). To find them more quantitatively, we take the real part of the relation between μ and f to get

$$Re[\mu] = \cos qa = f = \cos \frac{\sqrt{2mE}}{\hbar} a + \frac{\alpha}{\hbar}\sqrt{\frac{m}{2E}} \sin \frac{\sqrt{2mE}}{\hbar} a \tag{3}$$

after substituting $k(E)$. The RHS is an oscillatory function of $\sqrt{E}$ with an amplitude that exceeds 1, while the LHS is between -1 and 1. This means that for energies for which the RHS exceeds unity, there is no solution (band gaps). On the other hand, because of the oscillatory behavior of the RHS, if there is a solution, it is not unique for a given q - there is a whole series $E = E_n$ $(n = 1, 2, 3, ...)$ for which the RHS matches the LHS. In other words, the solutions $E(q) = E_n(q)$ form bands, where the integer n is the band index.

One can see this directly in the limit of of strong potential $\alpha \to \infty$. Introducing a dimensionless parameter

$$\lambda \equiv \frac{\alpha m a}{\hbar^2}$$

characterizing potential strength, we can rewrite Eq. (3) in the form convenient for iteration

$$\frac{\sin ka}{ka} = \frac{1}{\lambda}(\cos qa - \cos ka)\,.$$

In the zeroth order of parameter $1/\lambda$ this equation is

$$\sin ka = 0\,,\ k \neq 0\,, \quad \text{i.e. } k = \frac{\pi n}{a} \equiv k_n\,,\ n = 1, 2, \ldots\,.$$

Thus, in this order, the eigenenergies E_n are independent of the quasimomentum q

$$E_n = \frac{\hbar^2 k_n^2}{2m} \equiv E_n^{(0)}\,.$$

A simple interpretation of this result is that in this approximation, the δ-functions of the potential are so strong that the tunneling is completely suppressed and the energy eigenstates are the states in the individual square wells of width a.

Using the fact that $\sin(\pi n + \xi)|_{\xi \ll 1} = (-1)^n \xi$, we see that in the next order, solution of the Eq. (3) is:

$$k = k_n[1 + \frac{1}{\lambda}((-1)^n \cos qa - 1)]\,,$$

and finally

$$E_n(q) = E_n^{(0)}[1 + \frac{2}{\lambda}((-1)^n \cos qa - 1)]\,.$$

The first-order correction describes finite tunneling through the δ-functions which broadens the states in each well into the energy bands of the width $4E_n^{(0)}/\lambda$.

(e) A sketch of $E(q)$ is given in Fig. 1. Qualitative features of the energy bands and gaps remain the same for arbitrary potential strength, with the width of the energy bands increasing, and energy gaps decreasing, with the decreasing strength of the periodic potential.

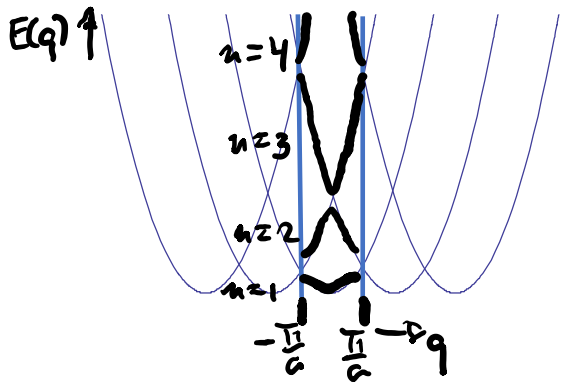


Figure 1: Qualitative sketch of $E(q)$.

Statistical Mechanics 1

Vibrations of a string

Consider a uniform violin string of length L with constant tension σ and total mass $M = \rho L$. Both ends of the string ($x = 0$ and $x = L$) are fixed. This string may have small vibrations in the perpendicular directions $|y|, |z| \ll L$

$$y_n(x,t) = A_n \sin(\frac{\pi n}{L} x) \cos(\omega_n t + \phi_n)\,, \quad n = 1, 2, \dots\,,$$

with kinetic and potential energies

$$U_n = \sigma \Delta L = \sigma \int_0^L dx \left(\sqrt{1 + (y')^2} - 1\right) \approx \frac{\pi^2 n^2 \sigma}{4L} A_n^2 \cos^2(\omega_n t + \phi_n)\,,$$
$$K_n \approx \int_0^L dx\, \frac{1}{2}\rho\, \dot{y}^2 = \frac{1}{4}\rho L\, A_n^2 \omega_n^2\, \sin^2(\omega_n t + \phi_n)$$

and similarly in the z direction (any longitudinal or twisting motion is neglected).

(A) (2 pts) Demonstrate that a vibrational mode with $(n-1)$ nodes has frequency $\omega_n = \omega_0 n$ and find ω_0.

Assume below that the temperature is always such that $T \gg \hbar\omega_0$.

(B) (4 pts) Find the partition function, free energy, and entropy for a single mode of vibration in plane (y, z) as function of temperature T.

(C) (6 pts) Now find the entropy, heat capacity, and energy of free vibrations of the string. at high temperature $T \gg \omega_0$.

(D) (4 pts) Calculate the mean squared *velocity* at the **midpoint** of the string $\langle \overline{\dot{y}^2 + \dot{z}^2} \rangle_{x=L/2}$.

(E) (4 pts) Calculate the transverse fluctuation of the **midpont** of the string $\langle \overline{y^2 + z^2} \rangle_{x=L/2}$.

Hint: In parts (D) and (E), remember to average over both time and the statistical ensemble.

You may find the following formulas useful:

$$\int_0^\infty dx\, \ln \frac{1}{1 - e^{-x}} = \int_0^\infty \frac{x\, dx}{e^x - 1} = \frac{\pi^2}{6}\,,$$
$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}\,, \quad \sum_{n\ \text{even}}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{24}\,, \quad \sum_{n\ \text{odd}}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{8}\,.$$

Vibrations of a string: solutions

(A) [2pt] The motion of the string in each mode is equivalent to an independent harmonic oscillator. The frequency ω_n can be found from equality of maximal kinetic and potential energies,

$$U_{\max} = K_{\max} \quad \Longrightarrow \quad \omega_n = \frac{\pi n}{L}\sqrt{\frac{\sigma}{\rho}} \tag{1}$$

so that $\omega_0 = \frac{\pi}{L}\sqrt{\frac{\sigma}{\rho}}$.

(B) [4pt] For a single node, the answers are the same as for the usual quantum harmonic oscillator (the ground-state energy is not included):

$$Z_n = \left(1 - e^{-\hbar\omega_n/T}\right)^{-1}, \tag{2}$$

$$F_n = -T \log Z_n = T \, \log\left(1 - e^{-\hbar\omega_n/T}\right), \tag{3}$$

$$E_n = T^2 \frac{\partial \log Z_n}{\partial T} = \frac{\hbar\omega_n}{e^{\hbar\omega_n/T} - 1} = \hbar\omega_n N_n \,, \tag{4}$$

$$S_n = \frac{E_n - F_n}{T} = \frac{\hbar\omega_n/T}{e^{\hbar\omega_n/T} - 1} - \log\left(1 - e^{-\hbar\omega_n/T}\right) = (N_n + 1)\log(N_n + 1) - N_n \log N_n \,, \tag{5}$$

where $N_n = \left(e^{\hbar\omega_n/T} - 1\right)^{-1}$ is the average excitation level of mode n.

(C) [6pt] In order to solve this problem, one has to sum the free energy over the modes,

$$F = 2\sum_{n=1}^{\infty} F_n = 2\sum_{n=1}^{\infty} T \log\left(1 - e^{-n\hbar\omega_0/T}\right), \tag{6}$$

where the factor of 2 accounts for independent vibrations in y and z transverse directions. Since the number of active modes $\propto \frac{T}{\omega_0}$ is large, the sum can be approximated by an the integral over the harmonic oscillator quantum $\varepsilon_n = \hbar\omega_n = \hbar\omega_0 n$ by replacing $\sum_n \longrightarrow \int \frac{d\varepsilon}{\hbar\omega_0}$:

$$F \approx 2\int_0^{\infty} \frac{d\varepsilon}{\hbar\omega_0} \, T \log\left(1 - e^{-\varepsilon/T}\right) = \frac{2T^2}{\hbar\omega_0}\int_0^{\infty} dx \log\left(1 - e^{-x}\right). \tag{7}$$

This expression is very similar to the black body radiation; the only difference is that here the number of dimensions is one. Integrating by parts,

$$F \approx -\frac{2T^2}{\hbar\omega_0}\int_0^{\infty} \frac{x\,dx}{e^x - 1} = -\frac{\pi^2 T^2}{3\hbar\omega_0}, \tag{8}$$

from which the entropy, energy, and heat capacity are easily computed:

$$S = -\left(\frac{\partial F}{\partial T}\right)_L = \frac{2\pi^2 T}{3\hbar\omega_0},$$

$$C = T\left(\frac{\partial S}{\partial T}\right)_L = \frac{2\pi^2 T}{3\hbar\omega_0},$$

$$E = F + TS = \frac{\pi^2 T^2}{3\hbar\omega_0}$$

The length of the string must be kept constant when computing partial derivatives because it determines the mode frequencies $\omega_n = \omega_0 n$ and thus plays the role of the "volume".

(D) [4pt] The fluctuations of the string's center add up from independent thermal fluctuations in each mode. In order to find the total fluctuation, one should

- average coordinates in each mode over time, and
- average the amplitude of each mode over the statistical ensemble, and
- sum over modes and directions ("polarizations") y, z.

Time averaging yields factor 1/2 in both kinetic/potential energies,

$$\overline{K_n} = \frac{1}{8}\rho L \omega_n^2 A_n^2\,, \qquad \overline{U_n} = \frac{1}{8}\sigma \frac{\pi^2 n^2}{L} A_n^2\,, \tag{9}$$

and the virial or equipartitioning theorem

$$\overline{\langle K_n \rangle} = \overline{\langle U_n \rangle} = \frac{1}{2}\frac{\varepsilon_n}{e^{\varepsilon_n/T}-1} \overset{\varepsilon_n \ll T}{\approx} \frac{T}{2}\,, \tag{10}$$

from which we can find the statistical average of the squared amplitude in the n^{th} mode,

$$\langle A_n^2 \rangle = \frac{4L}{\pi^2 n^2 \sigma}\frac{\varepsilon_n}{e^{\varepsilon_n/T}-1} \approx \frac{4LT}{\pi^2 n^2 \sigma}\,. \tag{11}$$

Note that only the odd modes will contribute to the midpoint: for example, in the y direction,

$$\langle \overline{y^2} \rangle_{x=L/2} = \sum_{n=1}^{\infty} \langle A_n^2 \rangle \sin^2 \frac{\pi n}{2} \overline{\cos^2(\omega_n t)} = \sum_{n\ \text{odd}}^{\infty} \frac{1}{2}\langle A_n^2 \rangle\,. \tag{12}$$

Taking into account also the z direction, we get the total mean squared transverse deviation (fluctuation),

$$\langle \overline{y^2 + z^2} \rangle_{x=L/2} = 2 \sum_{n\ \text{odd}} \frac{1}{2}\frac{4LT}{\pi^2 n^2 \sigma} = \frac{4LT}{\pi^2 \sigma} \cdot \frac{\pi^2}{8} = \frac{LT}{2\sigma}\,. \tag{13}$$

Note that in this case one cannot replace summation with integration, because the integral would diverge at the lower limit ($\omega_n \to 0$). The physical meaning of this is that most of the transverse fluctuation is due to the lowest modes, while the contributions of higher modes decrease rapidly with the number of nodes $(n-1)$.

(E) [4pt] The velocity of the string's midpoint can be computed similarly, except that now all *active* modes contribute approximately equally due to the equipartitioning theorem, and these thermal excitations must be computed using the exact statistics of quantum harmonic oscillators,

$$\langle \overline{K_n} \rangle = \frac{1}{8}\rho L \omega_n^2 \langle A_n^2 \rangle = \frac{1}{2}\langle \varepsilon_n \rangle = \frac{1}{2}\frac{\hbar\omega_n}{e^{\hbar\omega_n/T}-1} \quad \Longrightarrow \quad \omega_n^2 \langle A_n^2 \rangle = \frac{4}{\rho L}\frac{\varepsilon_n}{e^{\varepsilon_n/T}-1}\,. \tag{14}$$

In this cas, the summation *should* be approximated with the integration to get an analytic result,

$$\langle\overline{\dot{y}^2+\dot{z}^2}\rangle_{x=L/2} = 2\sum_{n\ \text{odd}}\frac{1}{2}\,\omega_n^2\langle A_n^2\rangle \approx 2\cdot\frac{1}{2}\int\frac{d\varepsilon}{\hbar\omega_0}\,\frac{2}{\rho L}\,\frac{\varepsilon}{e^{\varepsilon/T}-1} = \frac{2T^2}{\rho L\hbar\omega_0}\,\frac{\pi^2}{6} = \frac{\pi^2T^2}{3\rho L\hbar\omega_0} = \frac{E}{\rho L} \tag{15}$$

The same answer can be obtained by observing that exactly half of the string's energy is kinetic, of which only approximately half is given by the *odd* modes. Finally, at the midpoint, the mean squared velocity is twice its average over the length of the string. With careful tracking of all the factors, the same result can be reproduced.

Statistical Mechanics 2

Landau Diamagnetism

In a uniform magnetic field $\vec{H} = H\hat{z}$, the energy of electron motion in the (xy) plane is quantized:

$$\varepsilon(n, p_z) = \frac{e\hbar|H|}{m_e c}\big(n + \frac{1}{2}\big) + \frac{p_z^2}{2m_e}\,, \quad n = 0, 1, \dots\,, \tag{1}$$

which is known as Landau levels, while the motion along the magnetic field direction is unaffected. Assuming that the electron is confined into a box $L_x \times L_y \times L_z$, each Landau level n has degeneracy

$$g_{xy} = L_x L_y \,\frac{e|H|}{2\pi\hbar c} = \frac{L_x L_y}{\phi_e/|H|}\,, \quad \phi_e = \frac{2\pi\hbar c}{e}\,, \tag{2}$$

where ϕ_e is a quantum of magnetic flux. Apart from the degeneracy $g_e = 2$, *the intrinsic spin of electrons is neglected in this problem.* Electromagnetic interactions between electrons are also neglected.

(A) (4pt) Write expression for the grand potential $\Omega(T, \mu, V, H)$ for the ensemble of electrons in magnetic field (1), without evaluating it.

(B) (2pt) What is the condition on μ and T for the system to be nondegenerate, i.e. the probability for each level to be occupied by an electron $p_{\rm occ}(\varepsilon) \ll 1$?

(C) (4pt) Assuming that the system is nondegenerate as in part(B), calculate the approximate grand potential $\Omega(T, \mu, V, H)$.

(D) (4pt) Compute the density of electrons N/V. How does the chemical potential μ depend on magnetic field at constant temperature T and density N/V? Compare to the case of an ideal gas.

(E) (6pt) Assuming that the magnetic field is weak ($|H| \ll \frac{m_e c T}{e\hbar}$), compute the magnetization of the gas $M_z = -\big(\frac{\partial\Omega}{\partial H}\big)_{T,\mu,V}$ and its diamagnetic susceptibility $\chi_{\rm dia} = \big(\frac{\partial M_z}{\partial H}\big)_{T,N,V}$. Explain qualitatively the negative sign of $\chi_{\rm dia}$.

Landau Diamagnetism: Solutions

(A) [4pt] Each electron state in the system is characterized by its spin, Landau level number, and the momentum component along the $\hat{z}$ axis, and can have zero or one electron occupying it. The grand canonical partition function is a product over all independent electron states, which can be empty or filled,

$$Z_G(T,\mu,V,H) = \prod_{p_z}\prod_{n=0}^{\infty}\left[1+e^{\frac{\mu-\varepsilon(n,p_z)}{T}}\right]^{g_{xy}g_e}, \tag{3}$$

where the power $g_{xy}g_e$ takes into account the Landau level and the spin degeneracies (the energy of electron magnetic dipole moments are neglected in this problem). The momentum p_z in the product is quantized with increments of $\frac{2\pi\hbar}{L_z}$ due to the finite size of the sample. The grand potential is then

$$\begin{aligned}\Omega(T,\mu,V,H) = -T\ln Z_G(T,\mu,V,H) &= (-T)g_{xy}g_e\int_{-\infty}^{+\infty}\frac{dz\,dp_z}{2\pi\hbar}\sum_{n=0}^{\infty}\ln\left[1+e^{\frac{\mu-\varepsilon(n,p_z)}{T}}\right] \\ &= (-T)\frac{g_eL_xL_yL_z}{\phi_e/|H|}\int_{-\infty}^{+\infty}\frac{dp_z}{2\pi\hbar}\sum_{n=0}^{\infty}\ln\left[1+e^{\frac{\mu-\varepsilon(n,p_z)}{T}}\right],\end{aligned} \tag{4}$$

where the sum over quantized momentum p_z has been replaced with an integral.

(B) [2pt] The quantum system is nondegenerate if the probability for all the levels function to be occupied are negligible compared to the probability to be empty. For the grand partition function in part (A), it means that for all n and p_z

$$e^{\frac{\mu-\varepsilon(n,p_z)}{T}} \ll 1 \tag{5}$$

Since it must hold for all levels $\varepsilon(n,p_z) > 0$, this condition is equivalent to $e^{\mu/T} \ll 1$, or $\mu < 0$ and $|\mu| \gg T$.

(C) [4pt] If the system is nondegenerate, then the logarithm in the expression for the grand potential can be approximated with the first term in the Taylor expansion,

$$\begin{aligned}\Omega(T,\mu,V,H) &\approx (-T)\frac{g_eL_xL_yL_z}{\phi_e/|H|}\int_{-\infty}^{+\infty}\frac{dp_z}{2\pi\hbar}\sum_{n=0}^{\infty}e^{\frac{\mu-\varepsilon(n,p_z)}{T}} \\ &= (-T)\frac{g_eL_xL_yL_z}{\phi_e/|H|}\int_{-\infty}^{+\infty}\frac{dp_z}{2\pi\hbar}e^{-\frac{p_z^2}{2m_eT}}\sum_{n=0}^{\infty}e^{-\frac{e\hbar|H|}{m_ecT}(n+\frac{1}{2})} \\ &= (-T)\frac{g_eL_xL_yL_z\,e^{\mu/T}}{\lambda_T\phi_e/|H|}\frac{e^{-\frac{e\hbar|H|}{2m_ecT}}}{1-e^{-\frac{e\hbar|H|}{m_ecT}}} = (-T)\frac{g_eV\,e^{\mu/T}}{\lambda_T\phi_e/|H|}\frac{1}{2\sinh\frac{e\hbar|H|}{2m_ecT}}\end{aligned} \tag{6}$$

where $\lambda_T = \sqrt{\frac{2\pi\hbar^2}{m_eT}}$ is the electron thermal wavelength and $V = L_xL_yL_z$ is the total volume.

(D) [4pt] Computing the number density of electrons is straightforward from the grand potential,

$$n = \frac{N}{V} = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V,H} = \frac{g_e\,e^{\mu/T}}{\lambda_T\phi_e/|H|}\frac{1}{2\sinh\frac{e\hbar|H|}{2m_ecT}}. \tag{7}$$

To explore the magnetic field dependence, it is convenient to introduce a new variable $\xi = \frac{e\hbar|H|}{2m_e cT}$,

$$\frac{N}{V} = \frac{g_e\, e^{\mu/T}}{\lambda_T \phi_e}\, \frac{m_e cT}{e\hbar}\, \frac{\xi}{\sinh\xi} = \frac{g_e\, e^{\mu/T}}{\lambda_T^3}\, \frac{\xi}{\sinh\xi}\,, \tag{8}$$

so that the entire dependence on $|H|$ is expressed in the last factor, which is equal to 1 in the $|H| = 0$ limit so that the density is equal to that of the ideal gas. Solving for the chemical potential, one obtains

$$\mu = T \log\Big[\frac{N\lambda_T^3}{g_e V}\, \frac{\sinh\xi}{\xi}\Big]\,. \tag{9}$$

In the case of small magnetic field ($H \ll \frac{m_e cT}{e\hbar}$), $\xi \ll 1$, and the ratio $\frac{\sinh\xi}{\xi} = 1 + \frac{\xi^2}{6} + O(\xi^4)$, so that the chemical potential gets an additive contribution quadratic in $|H|$ compared to the ideal gas case,

$$\mu = T\log\frac{N\lambda_T^3}{g_e V} + T\log\frac{\sinh\xi}{\xi} \approx \mu^{\rm ideal} + \frac{T}{6}\xi^2 = \mu^{\rm ideal} + \frac{e^2\hbar^2}{24 m_e^2 c^2 T} H^2\,. \tag{10}$$

In the case of large magnetic field, the chemical potential has contribution from the energy of the lowest Landau level ($n = 0$) that grows linearly with $|H|$,

$$\mu = \mu^{\rm ideal} - T\log 2\xi + \frac{e\hbar}{2m_e c}|H|\,. \tag{11}$$

The second term $(-T\log 2\xi) = T\log T + const$ compensates for the two translational degrees of freedom in the (xy) plane that are "frozen out" due to Landau level quantization, so that

$$\mu^{\rm ideal} - T\log 2\xi = -\frac{1}{2} T\log T + const\,, \tag{12}$$

is effectively the 1-dimensional ideal gas chemical potential with corresponding heat capacity $c = \frac{1}{2}$ per electron.

(E) [6pt] Computing magnetization is straightforward with the representation used above,

$$\begin{aligned} M_z = -\left(\frac{\partial\Omega}{\partial H}\right)_{T,\mu,V} &= \frac{g_e V T e^{\mu/T}}{\lambda_T^3}\, \frac{e\hbar}{2m_e cT}\, \frac{d}{d\xi}\frac{\xi}{\sinh\xi} \\ &\approx \frac{g_e V e^{\mu/T}}{\lambda_T^3}\, \frac{e\hbar}{2m_e c}\,\big(-\frac{\xi}{3}\big) \approx -\frac{N}{12}\Big(\frac{e\hbar}{m_e c}\Big)^2 H\,. \end{aligned} \tag{13}$$

In the last step, the combination of constants was replaced with the number of electrons approximately equal to that of the ideal gas, since the difference between them is only $O(\xi^2)$. Note also that this can only be done *after* computing the partial derivative $\partial/\partial H$ that must be taken with $\mu = const$.

Finally, the magnetic susceptibility is

$$\chi = \left(\frac{\partial M_z}{\partial H}\right)_{T,N,V} \approx -\frac{N}{12}\Big(\frac{e\hbar}{m_e c}\Big)^2\,. \tag{14}$$

In contrast to the paramagnetic case, the internal energy of the electron gas in magnetic field is increased due to the fact that the electron motion is constrained to the Landau levels. This is especially evident in the limit of large magnetic field H, when all the electrons accumulate in the lowest highly-degenerate Landau level and have the energy $\varepsilon(H \to \infty) = \frac{1}{2}\hbar\omega_c = \frac{e\hbar|H|}{2m_e c}$. Therefore, the gas response is opposite to the paramagnetic case, and the corresponding diamagnetic susceptibility $\chi \propto (-\frac{\partial^2 \varepsilon}{\partial H^2})$ must be negative.

Statistical Mechanics 3

Hydrogen and Deuterium molecules

Deuterium (D) is a heavy isotope of hydrogen (H) with the a proton and neutron nucleus, $d = pn$. This nucleus is a boson with spin 1 and is approximately two times heavier compared to the hydrogen nucleus, the proton with spin-$\frac{1}{2}$. To a good approximation, the electronic state energies and wave functions are the same in the three molecules H_2, D_2, HD, and *will be assumed identical* in this problem.

(A) (1point) Assuming that r.m.s. distance between atoms in all three cases is the same, $R = 7.4 \times 10^{-11}$ m, express the moments of inertia of HD and D_2 in unints of $I_0 = I_{H_2}$.

In the HD molecule, the two nuclei p and d are not identical and there are no constraints on its rotational wave function.

(B) (3 points) Show that the spin-rotational of HD is given by the formula

$$Z\text{spin-rot}_{HD} = (2 \cdot 3) \sum_{L=0}^{\infty} (2L+1) \exp\Big(- \frac{\hbar^2 L(L+1)}{2 I_{HD} T} \Big) \tag{1}$$

(explain the integer factors in front of the sum) and compute it for high temperature $T \gg \hbar^2 / I_{HD}$.

However, the rotational partition functions for H_2 and D_2 are different due to the particle statistics of the nuclei. Depending on the combined spin of the nuclei S (not counting electrons), their orbital angular momenta (OAM) L is constrained to be $L = 0, 2, 4, \ldots$(even) or $L = 1, 3, 5 \ldots$(odd):

	spin-symmetric	spin-antisymmetric
H_2	$S = 1$, $L = odd$	$S = 0$, $L = even$
D_2	$S = 0$ or 2, $L = even$	$S = 1$, $L = odd$

(C) (3 points) Explain the constraints on OAM in the table and count the number of combined nuclear spin S orientations for each case.

Hint: for the nucleus made of identical fermions, the total (spin $\times$ rotational) wave function must be antisymmetric, while for the nucleons made of identical bosons it must be symmetric.

(D) (4 points) With these constraints, calculate the spin-rotational partition functions $Z^{\text{spin-rot}}$ for H_2 and D_2 gases at high temperature $T \gg \hbar^2 / I_0$:

$$Z^{\text{spin-rot}}_{HH} = N^{\text{spin}}_{HH,L=odd} \sum_{L=odd} (...) + N^{\text{spin}}_{HH,L=even} \sum_{L=even} (...) \,, \tag{2}$$

$$Z^{\text{spin-rot}}_{DD} = N^{\text{spin}}_{DD,L=odd} \sum_{L=odd} (...) + N^{\text{spin}}_{DD,L=even} \sum_{L=even} (...) \tag{3}$$

Now consider the equilibrium in the mixed gas of diatomic molecules $H_2 + D_2 \leftrightarrow 2HD$.

(E) (4 points) Show that the relation between molecular densities is

$$\frac{(N_{HD})^2}{N_{H_2}\,N_{D_2}} = \frac{(Z_{HD})^2}{Z_{H_2}\,Z_{D_2}} = \Big[\frac{(Z_{HD}^{\text{trans}})^2}{Z_{H_2}^{\text{trans}} Z_{D_2}^{\text{trans}}}\Big] \cdot \Big[\frac{(Z_{HD}^{\text{spin-rot}})^2}{Z_{H_2}^{\text{spin-rot}} Z_{D_2}^{\text{spin-rot}}}\Big] \cdot \Big[\frac{(Z_{HD}^{\text{osc}})^2}{Z_{H_2}^{\text{osc}} Z_{D_2}^{\text{osc}}}\Big] \tag{4}$$

where the factors in the r.h.s. correspond to translational, rotational and oscillational motions of the molecules.

(F) (5 points) Compute the translational partition functions of the gases and estimate the ratio of $N_{HD}^2/\big(N_{H_2} N_{D_2}\big)$ at room temperature $T \approx 300\,\text{K}$ *ignoring oscillations.* Are the formulas for spin-rotational partition functions derived above applicable at this temperature?

Solution

(a) Computing moments of inertia around the center of mass, one easily gets $I_{H_2} = I_0 = \frac{1}{2}m_pR^2$, $I_{HD} = \frac{4}{3}I_0$, $I_{D_2} = 2I_0$. Another option is to compute the moment of inertia around one of the nuclei but use the reduced mass $m_{HH}^{\rm red} = \frac{1}{2}m_p$, $m_{DD}^{\rm red} = m_p$, $m_{HD}^{\rm red} = \frac{2}{3}m_p$.

(b) The spin-rotational partition function is given by summation over all the values of OAM, counting the degeneracies of each $N_L = 2L + 1$. In addition to that, spins of p and d are 2- and 3-degenerate due to the $2S + 1$ factor, so

$$Z_{HD}^{\text{spin-rot}} = (2S_p+1)(2S_d+1)\sum_{L=0,1,\ldots}^{\infty}(2L+1)e^{-E_{L)/T}} = 2\cdot 3\cdot\sum_{L}^{\infty}(2L+1)e^{-\hbar^2L(L+1)/2I_{HD}T} \quad (5)$$

If $T \gg \hbar^2/I_0$, the summation can be replaced by integration $\sum_{L=0}^{\infty} \longrightarrow \int_0^{\infty} dL$, and

$$Z_{HD}^{\text{spin-rot}} \approx 6\int_0^{\infty} dL\,(2L+1)e^{-\hbar^2L(L+1)/2I_{HD}T} = \frac{12I_{HD}T}{\hbar^2} \quad (6)$$

(c) The combined spin of two spin-$\frac{1}{2}$ particles is either $S = 0$ (antisymmetric spin combination) or $S = 1$ (symmetric spin combination). The numbers of spin orientations are $(2S + 1) = 1$ and 3, respectively. The total wave function has to be antisymmetric for fermions. Spatial inversion of the coordinate wave function is equivalent to the exchange of the two particles, and results in the sign $\propto (-1)^L$ that depends on the OAM. Thus, the coordinate wave function of the H_2 nucleus is spatially symmetric with $L = 0, 2, 4, \ldots$ and antisymmetric with $L = 1, 3, 5, \ldots$, respectively, for $S = 0$ and $S = 1$.

Analogously, the combined spin of two spin-1 particles can be $S = 0$ and $S = 2$ (symmetric spin wave function) or $S = 1$ (antisymmetric spin wave function), with the numbers of spin orientations $1 + 5 = 6$ and 3, respectively. The total number of spin states $6 + 3 = 9$ matches the total number of the spin states of individual deuterons $3 \cdot 3 = 9$, as it should. Since the total wave function for bosons must be symmetric, the spatial wave function of D_2 nucleus is symmetric with $L = 0, 2, 4, \ldots$ and antisymmetric with $L = 1, 3, 5, \ldots$.

(d) Solution not supplied by author.

(e) Solution not supplied by author.

(f)

In order to check the applicability of the approximations for the spin-rotational partition functions, one has to estimate the ratio $(\hbar^2/I_0)$.

$$I_0 = \frac{1}{2}m_pR^2 \approx \frac{1}{2}1.67\cdot 10^{-27}\ \text{kg}\ \cdot(7.4\cdot 10^{-11}\ \text{m})^2 \approx 4.57\cdot 10^{-48}\,, \quad (7)$$

$$\hbar^2/I_0 \approx (1.054\cdot 10^{-34}\text{J}\cdot s)^2/(4.57\cdot 10^{-48}) \approx 2.43\cdot 10^{-21}\ \text{J} \approx 0.0152\ \text{eV} \approx 176\ \text{K}\,, \quad (8)$$

i.e., $(\hbar^2/2I_0)$ is equivalent to temperature 88 K, so the approximations made above must be valid at $T \approx 300$ K.