Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

January 2017 (in 4 separate parts: CM, EM, QM, SM)

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

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

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

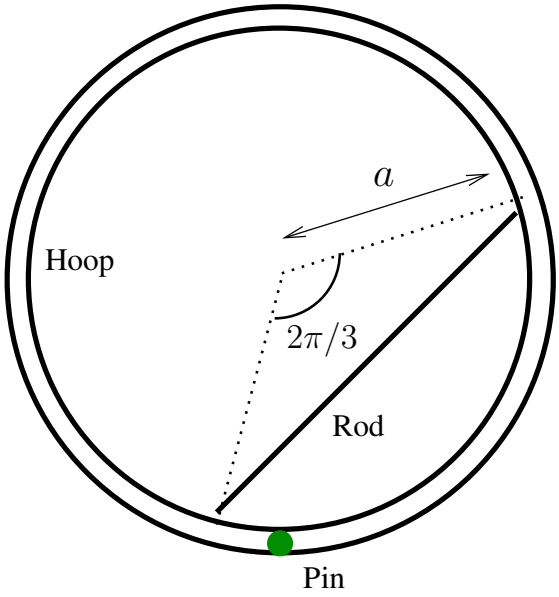
Write your ID number (not your name!) on the exam booklet.

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

Classical Mechanics 1

A rod in a ring

A rod slides without friction in a hoop of inner radius a experiencing earths gravitational acceleration, g. The hoop is fixed to the floor by a small pin that does not influence the motion. The rod subtends an angle of 120^o (or $2\pi/3$ radians) as shown below.



(a) (9 points) Write down the Lagrangian of the system and solve for the frequency of small oscillations.

(b) (3 points) For small oscillations with a maximum angle of θ_o, what is the maximum force on the pin? Draw a sketch (or sketches) showing the position of the rod and the direction of the force on the pin when the magnitude of the force is maximal.

(c) (6 points) Now assume that the maximum oscillation angle θ_o is small, but large enough that the first non-linear corrections become important. Determine the period of oscillation including the first dependence on θ_0. (Hint: note the identity $\cos(3x) = 4\cos(x)^3 - 3\cos(x)$.)

(d) (2 points) For the non-linear oscillations described in the last item, the motion is periodic with period τ but it is not sinusoidal. The angle as a function of time can be expanded as a Fourier series

$$\frac{\theta(t)}{\theta_o} = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi n(t/\tau)} \tag{1}$$

Qualitatively sketch the power spectrum (i.e. $|c_n|^2$ as a function of n) for oscillations in the linear and weakly non-linear regimes.

Solution

(a) The moment of inertia around the center of mass of the rod is given

$$I_{\rm cm} = \frac{m}{L}\int_{-L/2}^{L/2} dx x^2 = \frac{1}{12}mL^2 \tag{2}$$

Here $L = 2a\sin(60^o) = 2a\,(\sqrt{3}/2) = a\sqrt{3}$ is the length of the rod. Then $I_{\rm cm} = \frac{1}{4}ma^2$. Then using the parallel axis theorm

$$\begin{aligned} I &= I_{cm} + md^2 && (3)\\ &= \frac{1}{4}ma^2 + \frac{1}{4}ma^2 && (4)\\ &= \frac{1}{2}ma^2 && (5)\end{aligned}$$

where we have identified $d \equiv a\cos(60^o) = (a/2)$, as the distance from the center of mass of the rod to the center of the circle.

The Lagrangian of the system is

$$\begin{aligned} L =& \frac{1}{2}I\dot{\phi}^2 - mgd(1-\cos\phi)\,, && (6)\\ =& \frac{1}{2}I\dot{\phi}^2 - \frac{1}{2}mga(1-\cos\phi)\,. && (7)\end{aligned}$$

The equation of motion is

$$-\partial_t\left(\frac{\partial L}{\partial\dot{\phi}}\right) + \frac{\partial L}{\partial\phi} = 0\,, \tag{8}$$

or

$$I\ddot{\phi} = -\tfrac{1}{2}mga\sin\phi\,. \tag{9}$$

Then for small oscillations we have

$$\ddot{\phi} = -\frac{mga}{2I}\phi\,, \tag{10}$$

yielding the resonance frequency

$$\omega_o^2 = \frac{mga}{2I} = \frac{g}{a}\,. \tag{11}$$

(b) The center of mass moves with trajectory

$$\boldsymbol{x} = (d\sin\phi(t), -d\cos\phi(t))\,, \tag{12}$$

where we have taken the origin to be the center of the circle. Differentiating twice, we find acceleration of the center of mass

$$m\ddot{\boldsymbol{x}} \simeq m\,(d\ddot{\phi}, 0) = -md\omega_o^2\,(\phi(t),\,0)\,. \tag{13}$$

The (mass × acceleration) of the center of mass in the x direction is the external force *by* the pin on the rod-hoop system. The force *on* the pin is minus this,

$$F^x_{\rm max} = md\omega_o^2\theta_0\,. \tag{14}$$

Thus, taking positive angle as counter-clockwise, the force points in the positive x direction when the angle has reached its maximum.

The maximum force is

$$F^x_{\rm max} = m\left(\frac{a}{2}\right)\left(\frac{g}{a}\right)\theta_o = \frac{mg\theta_o}{2}\,. \tag{15}$$

(c) Returning to

$$\ddot{\phi} = -\omega_o^2\sin\phi\,, \tag{16}$$

We expand $\sin\phi = \phi - \phi^3/6$ and we aim to solve

$$\ddot{\phi} = -\omega_o^2\phi + \frac{\omega_o^2}{6}\phi^3\,. \tag{17}$$

To this end we substitute a solution of the form

$$\phi = (\theta_o - \delta)\cos(\Omega t) + \delta\cos(3\Omega t)\,, \tag{18}$$

into Eq. (17). Here δ is a small parameter. We find

$$\begin{aligned} -\Omega^2(\theta_o-\delta)\cos(\omega t) - \delta(3\Omega)^2\cos(3\Omega t) = -\omega_o^2\left[(\theta_o-\delta)\cos(\Omega t) + \delta\cos(3\Omega t)\right] \\ + \frac{\omega_o^2}{6}((\theta_o-\delta)\cos(\Omega t))^3\,, \end{aligned} \tag{19}$$

where we have approximated the last term by its lowest harmonic only. Using

$$\cos(3x) = 4\cos(x)^3 - 3\cos(x) \qquad \text{or} \qquad \cos(x)^3 = \frac{1}{4}\cos(3x) + \frac{3}{4}\cos(x)\,, \tag{20}$$

we find from the first harmonic in Eq. (19) that

$$-\Omega^2 = -\omega_o^2 + \frac{\omega_o^2}{6}\left(\frac{3}{4}\theta_o^2\right)\,. \tag{21}$$

Thus, the angular frequency of oscillation is

$$\Omega \simeq \omega_o\left(1 - \frac{\theta_o^2}{16}\right)\,, \tag{22}$$

and the period is

$$\tau = \frac{2\pi}{\Omega} \simeq \frac{2\pi}{\omega}\left(1 + \frac{\theta_o^2}{16} + \ldots\right)\,. \tag{23}$$

(d) The amplitude of the third harmonic is significantly smaller. From the third harmonic in Eq. (19) we find

$$-9\omega_o^2\delta = -\omega_o^2\delta + \frac{\omega_o^2}{6}\,\frac{1}{4}\theta_o^3\,, \tag{24}$$

yielding

$$\delta = -\frac{\theta_o^3}{6\cdot 4\cdot 8} = -\frac{1}{3}\left(\frac{\theta_o}{4}\right)^3\,. \tag{25}$$

Qualitatively, the power spectrum is shown in Fig. 1.

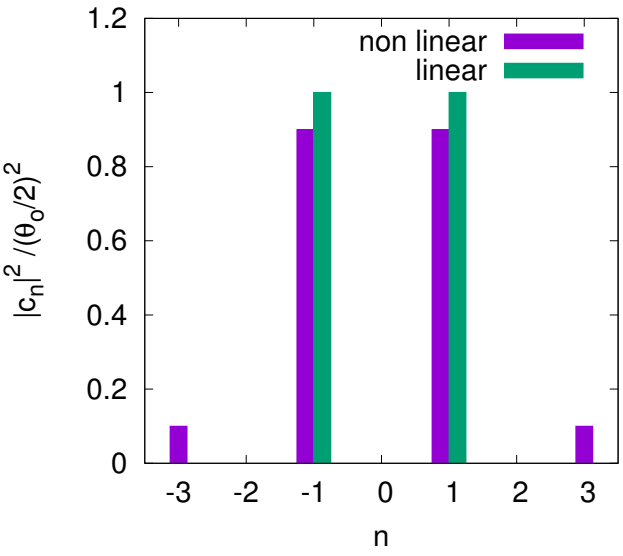
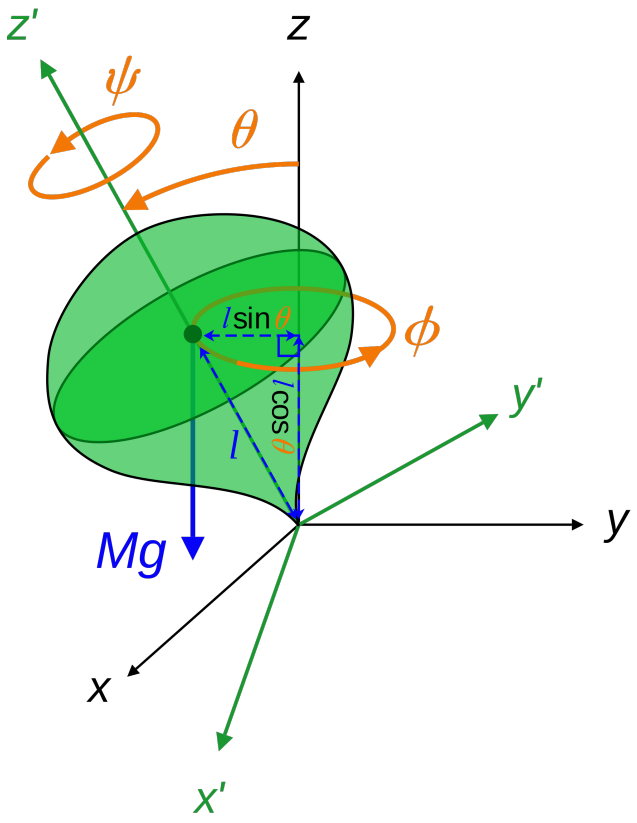


Figure 1: Qualitative power spectrum $|c_n|^2$. For the linear oscillator $\phi(t) = (\theta_0/2)\,(e^{-i\omega_o t} + e^{+i\omega_o t})$, so we have normalized the $(\theta_0/2)^2$.

Classical Mechanics 2

Stability of a symmetric top



The Lagrangian of a symmetric top rotating around its fixed lowest point on the axis of symmetry can be expressed in terms of the Euler's angles ϕ, θ, ψ as

$$\mathcal{L} = \frac{I}{2}\left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right) + \frac{I_\parallel}{2}\left(\dot{\psi} + \dot{\phi}\cos\theta\right)^2 - Mgl\cos\theta\,,$$

where M is the mass of the top, $I = I_\perp + Ml^2$, with l being the distance between the rotation center and the center of mass above it; $I_\parallel$, $I_\perp$ – the two principal moments of inertia of the symmetric top, for the rotation, respectively, along the axis of symmetry and an axis orthogonal to it, and the axis z used in the definition of the Euler's angles points vertically up.

(a) (6 points) Find expressions for the two integrals of motion (besides the energy E) and identify the physical nature of these integrals. Briefly (in one sentence for each) state explicit physical reason for their conservation.

(b) (6 points) With the two integrals of motion from part (a), the problem reduces effectively to a problem with one degree of freedom. Derive an expression for the energy of this one-dimensional problem using the integrals of motion.

(c) (8 points) Assume that the top rotates around its axis with the angular velocity Ω. Using the result of (b), find the condition on Ω which ensures that a rotating top in the vertical position (i.e. $\theta \simeq 0$) is stable.

Solution

(a) The two of the Euler's angles ϕ and ψ do not enter the Lagrangian. The corresponding Lagrange equations imply then that their generalized momenta are conserved:

$$\frac{\partial \mathcal{L}}{\partial \dot{\phi}} = I\dot{\phi}\sin^2\theta + I_\parallel\big(\dot{\psi} + \dot{\phi}\cos\theta\big)\cos\theta \equiv L_z\,,$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\psi}} = I_\parallel\big(\dot{\psi} + \dot{\phi}\cos\theta\big) \equiv L_\parallel\,.$$

The first of these quantities, L_z, has the meaning of the projection of the angular momentum on the z axis and, physically, is conserved because the system is symmetric with respect to rotation around this axis. The second quantity, $L_\parallel$, is the projection of the angular momentum on the symmetry axis of the top and is conserved because the torque created by the gravity force is orthogonal to this axis for any orientation of the top.

(b) The total energy E of the top is

$$E = T + U = \frac{I}{2}\big(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta\big) + \frac{I_\parallel}{2}\big(\dot{\psi} + \dot{\phi}\cos\theta\big)^2 + Mgl\cos\theta\,.$$

Equations for the integrals of motion, L_z and $L_\parallel$, allow us to express angular velocities $\dot{\phi}$ and $\dot{\psi}$ in the expression for E in terms of θ,

$$\dot{\phi} = \frac{L_z - L_\parallel\cos\theta}{I\sin^2\theta}\,, \qquad \dot{\psi} = \frac{L_\parallel}{I_\parallel} - \frac{L_z - L_\parallel\cos\theta}{I\sin^2\theta}\cos\theta\,,$$

and obtain the energy $E(\theta)$ for the dynamics of θ:

$$E(\theta) = \frac{I}{2}\dot{\theta}^2 + \frac{\big(L_z - L_\parallel\cos\theta\big)^2}{2I\sin^2\theta} + Mgl\cos\theta + \frac{L_\parallel^2}{2I_\parallel}\,.$$

(c) To analyze the stability of the vertical position of the top, $\theta \simeq 0$, one needs to examine the behavior of the effective potential $U_{eff}(\theta)$ in the energy $E(\theta)$ at the point $\theta = 0$.

$$U_{eff}(\theta) = \frac{\big(L_z - L_\parallel\cos\theta\big)^2}{2I\sin^2\theta} + Mgl\cos\theta\,.$$

For vertical orientation of the top, $L_z = L_\parallel \equiv L$, and

$$U_{eff}(\theta)\Big|_{\theta\simeq 0} = \frac{L^2\theta^2}{8I} - Mgl\frac{\theta^2}{2} + \text{const}\,.$$

We see that the potential has a minimum at $\theta = 0$, i.e. the vertical position of the top is stable is

$$\frac{L^2}{4I} > Mgl\,, \quad \text{i.e.} \quad \Omega > 2\frac{(IMgl)^{1/2}}{I_\parallel}\,.$$

Classical Mechanics 3

Time as a canonical variable

In special relativity, space and time are treated on equal footing. In this problem we reformulate classical mechanics in this way. We parametrize both the space coordinates q^i of a point particle, but also the time t, as functions of a new time variable θ, so $q^i = q^i(\theta)$ and $t = t(\theta)$. Thus θ parametrizes the space-time path $x^\mu(\theta) = (ct(\theta), q^i(\theta))$ of the point particle.

(a) (2 points) If $L(q^i, \dot{q}^i, t)$ is the Lagrangian of a system with coordinates $q^i = q^i(t)$, show that the Lagrangian L_θ for the corresponding system with θ as the time variable is given by

$$L_\theta(q(\theta), t(\theta), q'(\theta), t'(\theta)) = t' L(q, q'/t', t)$$

where $t'(\theta) = dt/d\theta$ and $q'(\theta) = dq/d\theta$.

(b) (2 points) Show that the momentum conjugate to t in the new formulation is given by $p_t = -H$ where $H = H(p, q, t)$ is the ordinary Hamiltonian. Show that the momentum conjugate to q is unchanged in the new formulation. So now, phase space is $4 + 4$ instead of $3 + 3$ dimensional.

(c) (2 points) Derive the two Euler-Lagrange equations of motion for L_θ. Show that they are equivalent to the equation of motion for L.

(d) Consider a nonrelativistic point particle in ordinary classical mechanics with Lagrangian $L = T - V$ and a potential V that does not explicitly depend on time t.

  (i) (3 points) Derive the Noether charge for time translational invariance.

  (ii) (3 points) Now consider the corresponding Lagrangian L_θ. Is there a corresponding Noether charge for θ-translational invariance?

(e) Now consider the Lagrangian for a relativistic point particle with mass m and electric charge e, coupled to ordinary electromagnetic fields $A_\mu(q, t)$.

  (i) (4 points) Construct the Hamiltonian H of ordinary classical mechanics with $A_\mu(q(t), t)$.

  (ii) (4 points) Construct the Hamiltonian H_θ with $A_\mu(x(\theta))$ with $x^\mu = (ct(\theta), q(\theta))$.

Time as a canonical variable

In special relativity, space and time are treated on equal footing. In this problem we reformulate classical mechanics in this way. We parametrize both the space coordinates q^i of a point particle, but also the time t, as functions of a new time variable θ, so $q^i = q^i(\theta)$ and $t = t(\theta)$.

(a) If $L(q^i, \dot{q}^i, t)$ is the Lagrangian of a system with coordinates $q^i = q^i(t)$, show that the Lagrangian L_θ for the corresponding system with θ as the time variable is given by

$$L_\theta = t' L(q, q'/t', t)$$

where $t' = dt/d\theta$ and $q' = dq/d\theta$.

Solution: The equations of motion follow from the Euler-Lagrange variation of the action. Hence

$$S = \int L\, dt = \int L_\theta\, d\theta.$$

It follows that $L_\theta = t'L$, where $t' = dt/d\theta$. The variables in L_θ are $q(\theta)$ and $t(\theta)$, so we must replace $\dot{q} = dq/dt$ by $q'/t' = (dq/d\theta)/(dt/d\theta)$. So altogether

$$L_\theta(q(\theta), t(\theta), q'(\theta), t'(\theta), \theta) = t'(\theta) L\left(q(\theta), q'(\theta)/t'(\theta), t(\theta)\right).$$

Note that there is no explicit dependence on θ.

(b) Show that the momentum conjugate to t in the new formulation is given by $p_t = -H$ where $H = H(p, q, t)$ is the ordinary Hamiltonian. Show that the momentum conjugate to q is unchanged in the new formulation. So now, phase space is $4+4$ instead of $3+3$ dimensional.

Solution: The momentum conjugate to $t(\theta)$ is

$$\begin{aligned}
p_t =& \frac{\partial}{\partial t'} L_\theta = \frac{\partial}{\partial t'}(t' L(q, q'/t', t)) \\
=& L(q, q'/t', t) + t' \frac{\partial}{\partial t'} L(q, q'/t', t) \\
=& L(q, q'/t', t) - q' \frac{\partial}{\partial q'} L \\
=& L - \dot{q} \frac{\partial}{\partial \dot{q}} L = L - \dot{q} p \\
=& -H(p, q, t) \qquad\qquad \text{where } p = p\left(q(t(\theta)), q'(\theta)/t'(\theta), t(\theta)\right).
\end{aligned}$$

We used that $q' \frac{\partial}{\partial q'} L = \dot{q} \frac{\partial}{\partial \dot{q}} L$ because $q' \frac{\partial}{\partial q'}$ counts the number of q' in L, and $\dot{q} \frac{\partial}{\partial \dot{q}}$ counts the number of $\dot{q}$ in L. They are clearly equal.

The momentum conjugate to $q(\theta)$ is

$$\begin{aligned} p_q =& \frac{\partial}{\partial q'} L_\theta = \frac{\partial}{\partial q'}(t' L(q, q'/t', t)) \\ =& t' \frac{\partial}{\partial q'} L(q, q'/t', t) \\ =& t' \left(\frac{1}{t'} \frac{\partial}{\partial \dot{q}} L(q, \dot{q}, t) \right) \\ =& \frac{\partial}{\partial \dot{q}} L(q, \dot{q}, t) \end{aligned}$$

where $\dot{q}$ in the last term stands for q'/t'.

(c) Derive the two Euler-Lagrange equations of motion for L_θ. Show that they are equivalent to the equation of motion for L.

Solution: The Euler-Lagrange equation for $t(\theta)$ reads

$$\begin{aligned} 0 =& \frac{d}{d\theta} \frac{\partial L_\theta}{\partial t'} - \frac{\partial L_\theta}{\partial t} \\ =& \frac{d}{d\theta} \frac{\partial}{\partial t'}(t' L) - \frac{\partial}{\partial t}(t' L) \\ =& \frac{d}{d\theta} \left(L - \dot{q} \frac{\partial}{\partial \dot{q}} L \right) - t' \frac{\partial}{\partial t} L \\ =& \frac{d}{d\theta} \left(-H(p, q, t) \right) - t' \frac{\partial}{\partial t} L \\ =& t' \frac{d}{dt}(-H) - t' \frac{\partial}{\partial t} L. \end{aligned}$$

We used the chain rule to replace $d/d\theta$ by $t' d/dt$. This vanishes in Lagrangian dynamics where $dH/dt = \partial H/\partial t = -\partial L/\partial t$.

The Euler-Lagrange equation of motion for $q(\theta)$ reads

$$\begin{aligned} 0 =& \frac{d}{d\theta} \frac{\partial}{\partial q'} L_\theta - \frac{\partial}{\partial q} L_\theta \\ =& \frac{d}{d\theta} \frac{\partial}{\partial q'}(t' L) - \frac{\partial}{\partial q}(t' L) \\ =& \frac{d}{d\theta} \left(t' \frac{\partial}{\partial q'} L \right) - t' \frac{\partial}{\partial q} L \\ =& \frac{d}{d\theta} \frac{\partial}{\partial \dot{q}} L - t' \frac{\partial}{\partial q} L \\ =& t' \left(\frac{d}{dt} \frac{\partial}{\partial \dot{q}} L - \frac{\partial}{\partial q} L \right). \end{aligned}$$

After dividing by t', this is the equation of motion for $q(t)$ and L.

(d) Consider a nonrelativistic point particle in ordinary classical mechanics with Lagrangian $L = T - V$ and a potential V that does not explicitly depend on time t. Derive the Noether charge for time translational invariance. Now consider the corresponding Lagrangian L_θ. Is there a corresponding Noether charge for θ-translational invariance?

Solution: Under time translations, each particle transforms as $\delta x(t) = \frac{d}{dt}x(t)$. Then $\delta L = \frac{d}{dt}L$, and the Noether charge becomes

$$\frac{\partial L}{\partial \frac{dx}{dt}}\frac{dx}{dt} - L = p\dot{x} - L = H.$$

So the Hamiltonian is the generator of time translations.

The Lagrangian L_θ does not depend explicitly on θ. Hence under θ-translations, $\delta x = x' = \frac{dx}{d\theta}$ and $\delta L_\theta = \frac{d}{d\theta}L_\theta$. Then the Noether charge for θ translation is (with $x^\mu = (ct, q)$)

$$\frac{\partial L_\theta}{\partial \frac{dx^\mu}{d\theta}}\frac{dx^\mu}{d\theta} - L_\theta = p^\mu \frac{dx^\mu}{d\theta} - L_\theta = H_\theta.$$

(e) Now consider the Lagrangian for a relativistic point particle with mass m and electric charge e, coupled to ordinary electromagnetic fields $A_\mu(q, t)$. Construct first the Hamiltonian H of ordinary classical mechanics, and then the Hamiltonian H_θ.

Solution: $L = -mc^2\sqrt{1 - \frac{v^2}{c^2}} + \frac{e}{c}A_\mu\frac{dx^\mu}{dt}$, with $x^0 = ct$.

(As a check on signs, note that $L = T - V$ and $V = -\frac{e}{c}A_0\frac{dx^0}{dt} = -eA_0 = e\phi$ which is correct.)

The Hamiltonian H is given by $\vec{p}\dot{\vec{x}} - L$ where

$$\vec{p} = \frac{m\dot{\vec{x}}}{\sqrt{1 - \frac{v^2}{c^2}}} + \frac{e}{c}\vec{A}.$$

Then

$$\begin{aligned} H =& \frac{mv^2}{\sqrt{1 - \frac{v^2}{c^2}}} + mc^2\sqrt{1 - \frac{v^2}{c^2}} - eA_0 \\ =& \sqrt{(mc^2)^2 + (\vec{p}c - e\vec{A})^2} - e\phi_0. \end{aligned}$$

On the other hand, L_θ is given by

$$\begin{aligned} L_\theta =& t'L = -mc\sqrt{c^2\left(\frac{dt}{d\theta}\right)^2 - \left(\frac{d\vec{x}}{d\theta}\right)^2} + \frac{e}{c}A_\mu\frac{dx^\mu}{d\theta} \\ =& -mc\sqrt{-\left(\frac{dx^\mu}{d\theta}\right)^2} + \frac{e}{c}A_\mu\frac{dx^\mu}{d\theta} \end{aligned}$$

Then

$$p_\mu = \frac{\partial}{\partial(dx^\mu/d\theta)} L_\theta = \frac{mc}{\sqrt{-(dx^\mu/d\theta)^2}} \frac{dx_\mu}{d\theta} + \frac{e}{c} A_\mu$$

$$\begin{aligned} H_\theta =& p_\mu \frac{dx^\mu}{d\theta} - L_\theta \\ =& \frac{mc \frac{dx^\mu}{d\theta} \frac{dx_\mu}{d\theta}}{\sqrt{-\left(\frac{dx^\mu}{d\theta}\right)^2}} + \frac{e}{c} A_\mu \frac{dx^\mu}{d\theta} + mc \sqrt{-\left(\frac{dx^\mu}{d\theta}\right)^2} - \frac{e}{c} A_\mu \frac{dx^\mu}{d\theta} = 0. \end{aligned}$$

Hence the Hamiltonian for a system in which time is a canonical variable vanishes! This is, in fact, true for any system, relativistic or not.

Going back to the definition of the momenta

$$p^\mu - \frac{e}{c} A^\mu = mc \frac{\frac{dx^\mu}{d\theta}}{\left|\frac{dx^\mu}{d\theta}\right|}$$

where $\left|\frac{dx^\mu}{d\theta}\right| = \sqrt{-\left(\frac{dx^\mu}{d\theta}\right)^2}$, we see that the momenta are not all independent, but satisfy a constraint

$$\left(p^\mu - \frac{e}{c} A^\mu\right)\left(p_\mu - \frac{e}{c} A_\mu\right) = -(mc)^2.$$

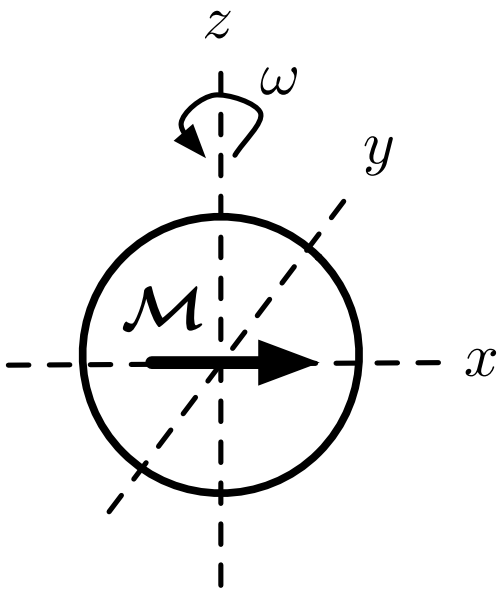
There is an extension of the canonical formalism, by Dirac, for constrained Hamiltonian systems. It explains that the constraint on the momenta generates a gauge invariance of the action $\int L_\theta \, d\theta$.

Electromagnetism 1

Magnetic field on the surface of a star

A star (roughly modeled on the Crab Pulsar) has mass M of $1.4\,M_\odot$ (or $1.4\times 2\times 10^{30}\,\mathrm{kg}$) and radius R of 10 km. It rotates (non-relativistically) with a period $\tau = 2\pi/\omega$ of 33 milliseconds. The period slowly decreases due to the emission of electromgnetic radiation. The change in period per time is, $|\dot{\tau}| = 4.0\times 10^{-13}$.

Model the star as a uniformly magnetized sphere spinning around the z-axis, with a magnetization $\boldsymbol{\mathcal{M}}$ lying in the $x-y$ plane.



(a) (7 points) Determine the total magnetic dipole moment of the star $m_o = \mathcal{M}\,\frac{4}{3}\pi R^3$ in terms of $\dot{\tau}$.

(b) (6 points) Determine the magnitude of the magnetic field at the north pole of the star. Check that your expression is dimensionally correct, and make a rough order of magnitude estimate for the magnetic field in Tesla.

Parts (c) and (d) are indpendent of parts (a) and (b); refer to the solution of part (a) as m_o.

(c) (5 points) Determine the electric field at the north pole of the star as a function of time. (Neglect the slow decrease of the rotational period with time.) Hint: what is the vector potential of the star?

(d) (2 points) Numerically estimate the ratio of the energy density in the magnetic field to the energy density in the electric field at the north pole of the star.

Solution

(a) The decrease in rotational energy of the star is the result of magnetic dipole radiation

$$-\frac{d}{dt}\left(\frac{1}{2}I\omega^2\right) = \overline{P} \tag{1}$$

Here P is

$$P = \frac{1}{4\pi c^3}\frac{2}{3}\ddot{\boldsymbol{m}}^2 \tag{2}$$

is the energy lost due to magnetic dipole radiation.

Now $\boldsymbol{m}$ is harmonic

$$\boldsymbol{m}(t) = m_o(\cos(\omega t)\hat{\boldsymbol{x}} + \sin(\omega t)\hat{\boldsymbol{y}})\,, \tag{3}$$

$$= m_o\,\mathrm{Re}\,e^{-i\omega t}(\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}})\,, \tag{4}$$

and we find after time averaging

$$\overline{P} = \frac{1}{4\pi c^3}\frac{1}{3}\omega^4 m_o^2|\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}|^2\,. \tag{5}$$

With $\dot{\omega}^2 = -\omega^3\dot{\tau}/\pi$ (which follows from $\omega = 2\pi/\tau$ and the moment of inertia of a sphere $I = (2/5)MR^2$, we find

$$\frac{1}{2}\left(\frac{2}{5}MR^2\right)\frac{\omega^3|\dot{\tau}|}{\pi} = P \tag{6}$$

Solving for m_o we find

$$m_o = \sqrt{\frac{6}{5}}R\left(\frac{Mc^3\dot{\tau}}{\omega}\right)^{1/2} \tag{7}$$

(b) Outside of the sphere and in the radiation zone, the magnetic field at the north pole is just that of a time dependent magnetic dipole:

$$\boldsymbol{B}(t) = \frac{3\boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{m}(t)) - \boldsymbol{m}(t)}{4\pi r^3}\,. \tag{8}$$

On the north pole of the star $\boldsymbol{n} = \hat{\boldsymbol{z}}$ and $\boldsymbol{n}\cdot\boldsymbol{m}(t)$ is zero. Thus

$$|\boldsymbol{B}(t)| = \frac{|-\boldsymbol{m}(t)|}{4\pi R^3} \tag{9}$$

$$= \frac{m_o}{4\pi R^3} \tag{10}$$

Substituting the magnetic moment from part (a), and converting to SI units, $B_{HL} = B_{SI}/\sqrt{\mu_o}$, we find

$$B = \frac{1}{4\pi}\sqrt{\frac{6}{5}}\left(\frac{\mu_o Mc^2}{R^3}\right)^{1/2}\left(\frac{c\tau}{R(2\pi)}\right)^{1/2}(\dot{\tau})^{1/2} \tag{11}$$

The factor

$$\sqrt{\frac{\mu_o M c^2}{R^3}} \tag{12}$$

has units of Tesla, since $[\mu_o] = T^2\mathrm{m}^3/\mathrm{J}$ and Mc^2/R^3 has dimension of J/m^3. The remaining factors are dimensionless. Substituting numbers

$$M = 2.8 \times 10^{30}\,\mathrm{kg} \qquad \mu = \frac{4\pi}{10} \times 10^{-6} T^2\,\mathrm{m}^3/\mathrm{J} \tag{13}$$

$$\tau = 3.3 \times 10^{-2}\,\mathrm{s} \qquad R = 1.0 \times 10^4\,\mathrm{m} \tag{14}$$

$$\dot{\tau} = 4.0 \times 10^{-13} \qquad c = 3 \times 10^8\,\mathrm{m/s} \tag{15}$$

we find

$$B = 3.9 \times 10^8\,\mathrm{T} \tag{16}$$

A rough estimate is found by keeping powers of 10 in Eq. (11)

$$B \sim \left(\frac{10^{-6} \times 10^{30} \times (10^8)^2}{(10^4)^3} \times \frac{10^8 \times 10^{-2}}{10^4} \times 10^{-14} \right)^{1/2} \text{Tesla} \sim \sqrt{10} \times 10^8\,\text{Tesla} \tag{17}$$

(c) The vector potential of the magnetized sphere is

$$\boldsymbol{A} = \frac{\boldsymbol{m}(t) \times \hat{\boldsymbol{r}}}{4\pi r^2} \tag{18}$$

The electric field is

$$\boldsymbol{E} = -\frac{1}{c}\partial_t \boldsymbol{A} \tag{19}$$

The dipole moment and its derivative are

$$\boldsymbol{m}(t) = m_o e^{-i\omega t}(\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}})\,, \tag{20}$$

$$\dot{\boldsymbol{m}}(t) = \omega m_o e^{-i\omega t}(-i\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})\,. \tag{21}$$

Then for $\hat{\boldsymbol{r}} = \hat{\boldsymbol{z}}$ (i.e. at the north pole of the star), and $r = R$ we find

$$\boldsymbol{E}(t) = -\frac{\omega m_o}{4\pi R^2 c}\, e^{-i\omega t}(-i\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \times \hat{\boldsymbol{z}} \tag{22}$$

Working out the elementary cross products (i.e. $\hat{\boldsymbol{x}} \times \hat{\boldsymbol{z}} = -\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{y}} \times \hat{\boldsymbol{z}} = \hat{\boldsymbol{x}}$) and taking the real part we find

$$\boldsymbol{E}(t) = -\frac{\omega m_o}{4\pi R^2 c} e^{-i\omega t}(-i\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \times \hat{\boldsymbol{z}} \tag{23}$$

$$= -\frac{\omega m_o}{4\pi R^2 c} \left[\sin(\omega t)\hat{\boldsymbol{y}} + \cos(\omega t)\hat{\boldsymbol{x}}\right] \tag{24}$$

(d) We can estimate the ratio of energy densities by noting that

$$E \sim \frac{\omega R}{c} B\,. \tag{25}$$

as expected on general grounds in the near field, quasi-static, regime. The dimensionless factor is small, and controls the quasi-static approximation

$$\frac{\omega R}{c} \sim 6 \times 10^{-3} \,. \tag{26}$$

The ratio of energy densities is

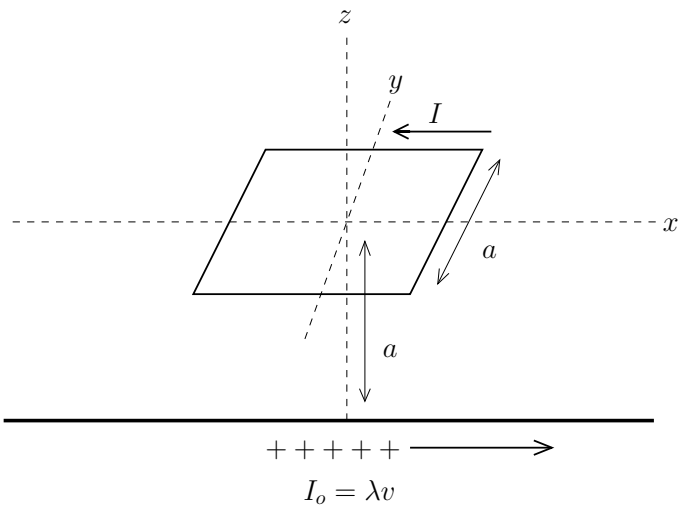
$$\frac{u_M}{u_E} = \frac{B^2}{E^2} \sim \left(\frac{c}{\omega R}\right)^2 \sim 2.5 \times 10^4 \tag{27}$$

Electromagnetism 2

Torques in Relativity

After the Michelson-Morley experiment of 1887, there was another experiment to measure the velocity of the earth through the aether: the Trouton-Noble experiment of 1903. It seemed to show that Maxwell's theory of electromagnetism is inconsistent. In this problem we will study a simplified version of this experiment and show how special relativity removes this inconsistency.

A neutral square loop of wire with sides of length a carries a current I. The square lies flat in the xy plane and is centered at the origin. Directly below the square is an infinite line of positive charge with charge per length λ_o. The line is parallel to the x-axis, but is displaced by a distance a below the origin in the negative z direction (see below). The positive charges in the infinite line move to the right with velocity v, producing a net current $I_o = \lambda_o v$. The neutral square can rotate around the x-axis



(a) (4 points) Calculate the net torque on the square due to the line of charge.

(b) (6 points) An observer moving to the right along the x-axis with velocity v measures a charge density in the square loop. Determine the charge per length in all four legs of the square loop. Make a sketch illustrating the distribution of charges in each leg.

(c) (3 points) Qualitatively explain the origin of the net torque according the right moving observer of part (b).

(d) (3 points) Determine the torque according to the right moving observer of part (b).

(e) (4 points) Compare the torques computed in parts (a) and (d). Are they equal? How does the Lorentz force per volume (i.e. $\boldsymbol{f} = \rho\boldsymbol{E} + \frac{\boldsymbol{J}}{c} \times \boldsymbol{B}$) transform under Lorentz transformation. Transform the Lorentz forces per volume in part (a) to explain results of part (d).

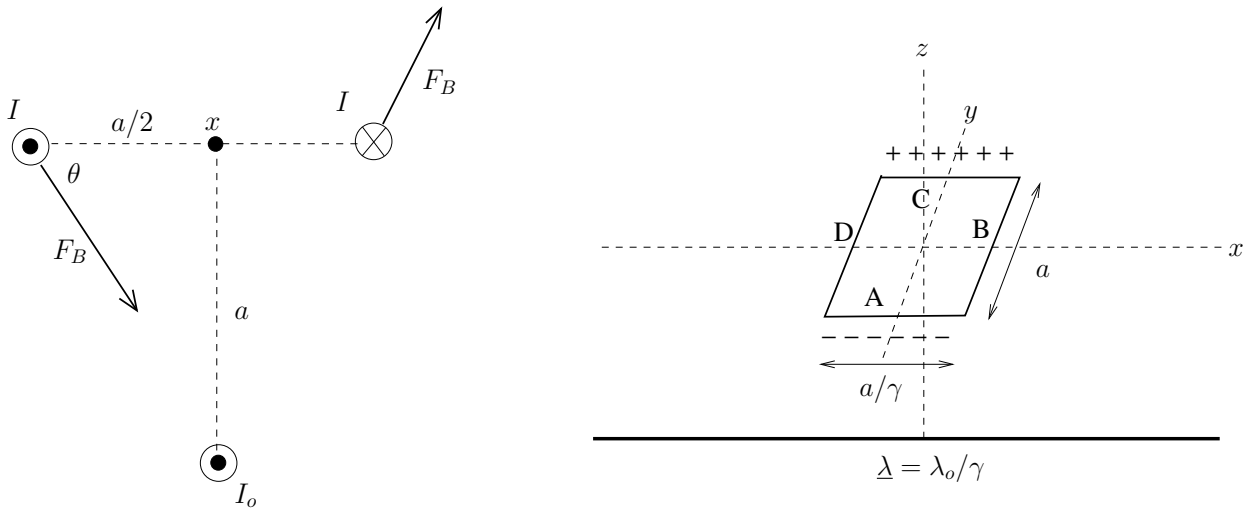


Figure 1: (a) The magnetic forces and geometry in the lab frame. The x-axis comes out of the page. (b) The geometry of the square in the boosted frame, together with the charge density in each wire.

Solution

(a) Fig. 1(a) shows a head-on view of the square loop of wire with the x-axis coming out of the page. The magnetic field from the line of moving charge (with current I_o) is

$$B_\phi = \frac{I_o/c}{2\pi\rho}\,, \tag{1}$$

which is later evaluated at

$$\rho_o \equiv \sqrt{(a)^2 + (a/2)^2} = \sqrt{(5/4)}\,a\,. \tag{2}$$

There are two torques around the x-axis due to the magnetic forces F_B on the legs of the square (leg A and C as shown in Fig. 1). The net torque is directed along the x-axis and has magnitude

$$\begin{aligned}
\tau =& 2rF_B\sin(\theta) && (3)\\
=& 2\left(\frac{a}{2}\right)\left(\frac{I}{c}\ell B\right)\sin(\theta)\,, && (4)\\
=& 2\left(\frac{a}{2}\right)\left(\frac{I}{c}a\,\frac{(I_o/c)}{2\pi\rho_o}\right)\,\frac{a}{\rho_o}\,, && (5)\\
=& \frac{II_o}{c^2}\frac{a^3}{2\pi\rho_o^2}\,. && (6)
\end{aligned}$$

(b) There are four legs of the square A, B, C, D as shown in Fig. 1. The four-current in the rest frame of the square takes the form

$$J^\mu = (c\rho, \boldsymbol{j}) = (0, \boldsymbol{j})\,. \tag{7}$$

since the square is neutral in the rest frame, $\rho = 0$. Making a boost

$$\underline{J}^\mu = L^\mu_{\ \nu} J^\nu \,. \tag{8}$$

with $L^0_3 = -\gamma\beta$

$$c\underline{\rho} = -\gamma\beta j^z \,. \tag{9}$$

For a current carrying wire the current per area is $j^z = I^z/A$, and we will quote the charge per length $\underline{\lambda} = \underline{\rho}\underline{A}$. Thus

$$\underline{\lambda} = -\gamma\beta(I^z/c) \tag{10}$$

In the four cases we find

- Wire A:

$$I^z = I \qquad \underline{\lambda}_A = -\gamma\beta(I/c) \tag{11}$$

- Wire B:

$$I^z = 0 \qquad \underline{\lambda}_B = 0 \tag{12}$$

- Wire C:

$$I^z = -I \qquad \underline{\lambda}_C = +\gamma\beta(I/c) \tag{13}$$

- Wire D:

$$I^z = 0 \qquad \underline{\lambda}_D = 0 \tag{14}$$

(c) In the boosted frame the torque arises because of the electrostatic attraction and repulsion of the wires A and C which are now charged. In particular there is an attractive coulomb force between wire A and the line of charge, and a repulsive coulomb force between wire C and the line of charge.

(d) To compute the torque in the moving frame we also need the linear charge density of the infinitely long wire. In this case the wire is not electrically neutral and $J^0 = c\lambda_o/A$, and $J^z = I_o v/A$ Then

$$A\underline{J}^0 = \gamma A J^0 - \gamma\beta A J^z \,, \tag{15}$$

and thus

$$\begin{aligned} \underline{\lambda}_o =& \gamma\lambda_o - \gamma\beta(I_o/c) \,, & (16)\\ =& \gamma\lambda_o - \gamma\beta^2\lambda \,, & (17)\\ =& \frac{\lambda_o}{\gamma} \,. & (18) \end{aligned}$$

The charge per length is modified by a factor of $1/\gamma$, which reflects the length contraction of the infinite wire. The electric field from a line of charge is

$$\underline{E}_\rho = \frac{\underline{\lambda}_o}{2\pi\rho} \tag{19}$$

Then, since transverse distances are not changed under boosts, the torque on wire A is

$$\tau_A = rF\sin(\theta) \tag{20}$$

$$= \frac{a}{2}\left[\frac{|Q_A|\underline{\lambda}_o}{2\pi\rho_o}\right]\frac{a}{\rho_o} \tag{21}$$

where Q_A is the magnitude of the charge in leg A. Remembering that a square of length a is length contracted under boost – see Fig. 1

$$Q_A = \underline{\lambda}_A\left(\frac{a}{\gamma}\right) = -\beta a(I/c) \tag{22}$$

and thus

$$\tau_A = \frac{a}{2}\left[\frac{(\beta(I/c)a)(\lambda_o/\gamma)}{2\pi\rho_o}\right]\frac{a}{\rho_o} \tag{23}$$

Multiplying by a factor of two to account for wire C and recalling that $\beta\lambda_o = I_o/c$ the total torque is

$$\tau_A = \frac{II_o}{2\pi c^2}\frac{a^3}{\gamma\rho_o^2} \tag{24}$$

(e) The torques in parts (a) and (d) are not equal. The Lorentz force per volume transforms as part of a four vector

$$f^\mu = F^\mu{}_\nu\frac{J^\nu}{c} \tag{25}$$

The four-force is

$$f^\mu = (f^0, \boldsymbol{f}) = (\boldsymbol{E}\cdot\boldsymbol{J}/c,\ \rho\boldsymbol{E} + \frac{\boldsymbol{J}}{c}\times\boldsymbol{B}) \tag{26}$$

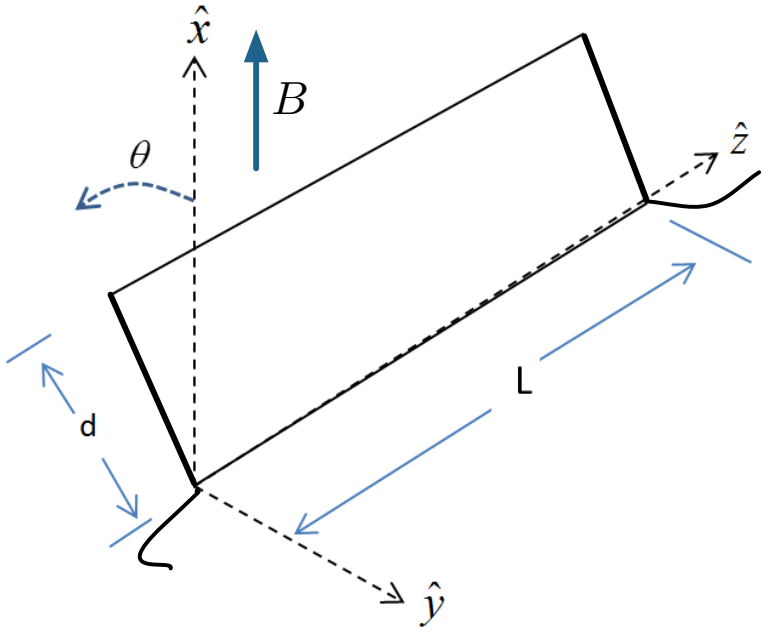
In this case the forces per volume in part (a) (the magnetic forces per volume shown in Fig. 1(a)) are transverse to the x-axis, and are therefore unmodified by a boost along the x-axis. However the square is length contracted by a factor of γ, and therefore the net force (not the force per volume) is reduced by a factor of γ in legs A and C.

The torque is similarly reduced by a factor of γ. The moment arms involved in computing the torque are transverse to the x-axis and are therefore unmodified by the boost. Only the reduction of the net force reduces the net torque.

Electromagnetism 3

A conducting plate in a magnetic field

A thin rectangular nonmagnetic metal plate with dimensions $L \times d \times t$ has mass density ρ, and conductivity σ. The bottom edge of the plate is held fixed, but the plate is free to rotate around the z-axis (see below). Charge can flow on and off the plate through two leads of negligble resistance at either end of the plate. The plate sits in a constant magnetic field directed along the x-axis ($\mathbf{B} = B\,\hat{\boldsymbol{x}}$), and experiences the Earth's gravitational pull ($\mathbf{g} = -g\,\hat{\boldsymbol{x}}$) as shown below. For the analysis below assume that the length L is very large, so that the plate is essentially infinitely long. Also assume that the thickness t is very small, so that the plate is essentially two dimensional.



(a) (5 points) Assume plate rotates in a counter-clockwise fashion around the z axis (increasing θ as shown in the figure): (i) sketch how the current flows in the plate. Explain your reasoning. (ii) sketch a free body diagram showing the magnetic and gravitational forces on the plate.

(b) (8 points) Find an equation for the plate's angle $\theta(t)$ as a function of time.

(c) (3 points) Specialize this equation to the case $\theta \ll 1$ and find the small angle solution for $\theta(t)$, given the initial conditions $\theta(0) = \theta_0 \ll 1$ and $\dot{\theta}(0) = 0$.

(d) (4 points) For the typical values given below, show that the angle increases approximately as $e^{\gamma t}$ after an initial transient. Calculate the time constant $1/\gamma$ in seconds. Assume that $d = 1\,\mathrm{m}$, $\rho = 10^4\,\mathrm{kg/m^3}$, $\sigma = 10^8\,(\Omega\,\mathrm{m})^{-1}$, $B = 1\,\mathrm{T}$, and $g = 10\,\mathrm{m/s^2}$, and $\epsilon_o = 8.85 \times 10^{-12}\,\mathrm{Nm^2/C^2}$

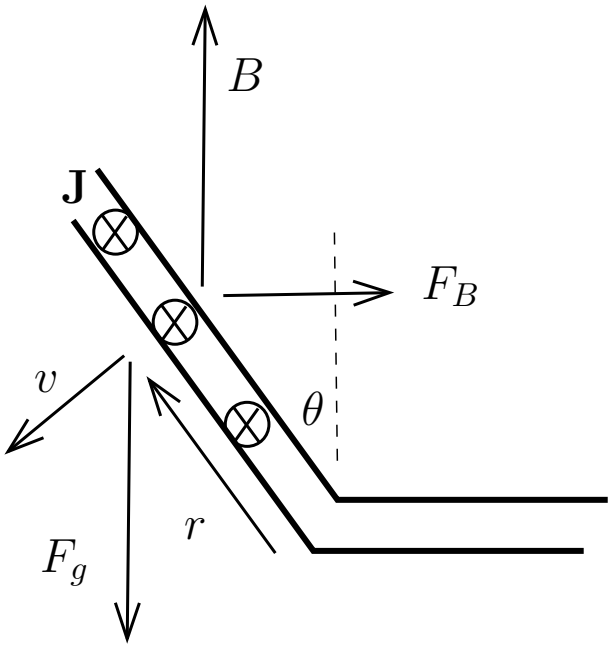


Figure 1: A free body diagram showing the magnetic and gravitational forces as well as other vectors.

Solution

(a) This solution uses MKS units. If the plate rotates with increasing θ, the current which is given by

$$\mathbf{J} = \sigma \mathbf{v} \times \mathbf{B} \tag{1}$$

is directed along the z axis (into the page in Fig. 1). The magnetic force F_B is, by the right hand rule, directed in the y-direction. The gravitational force points directly downward in Fig. 1. The

(b) The current is

$$\mathbf{J} = \sigma \mathbf{E}' = \sigma(\mathbf{v} \times \mathbf{B}) = \sigma r \dot{\theta} B \cos(\theta)\ \hat{\boldsymbol{z}}\,.$$

Then the force follows

$$d\mathbf{F} = \mathbf{J} d^3x \times \mathbf{B} = \sigma r \dot{\theta} B^2 \cos(\theta) d^3x\ \hat{\boldsymbol{y}}\,.$$

The torque due to the magnetic force is

$$\boldsymbol{\tau}_{EM} = \int \mathbf{r} \times d\mathbf{F} = Lt\,\hat{\boldsymbol{z}} \int \sigma r^2 \dot{\theta} B^2 \cos^2(\theta)\ dr = \sigma \dot{\theta} B^2 (d^3/3) Lt \cos^2(\theta)\ \hat{\boldsymbol{z}}\,.$$

The gravitational torque is

$$\boldsymbol{\tau}_g = (d/2) Mg \sin(\theta)(-\hat{\boldsymbol{z}}) = -\rho g (d^2/2) Lt \sin(\theta)\ \hat{\boldsymbol{z}}\,.$$

Taking torques positive in the $-\hat{z}$ direction for increasing θ we find the equation of motion

$$\rho g(d^2/2)Lt\sin(\theta) - \sigma\dot{\theta}B^2(d^3/3)Lt\cos(\theta) = I\ddot{\theta}\,,$$

where

$$I = \int \rho r^2 d^3x = \rho(d^3/3)Lt\,,$$

is the moment of inertia. So the equation of motion is

$$\ddot{\theta} + \frac{\sigma B^2}{\rho}\cos^2(\theta)\;\dot{\theta} - \frac{3g}{2d}\sin(\theta) = 0\,. \tag{2}$$

(c) Restricting the motion to small θ, the equation of motion becomes

$$\ddot{\theta} + b\dot{\theta} + c\theta = 0$$

where

$$b = \frac{\sigma B^2}{\rho} \qquad \text{and} \qquad c = -\frac{3g}{2d}$$

Assuming exponential solutions of the form $\theta = Ae^{\gamma t}$, we solve the quadratic equation

$$\gamma^2 + b\gamma + c = 0$$

to find the two homogeneous solutions of the differential equation

$$\gamma = -\frac{b}{2} \pm \frac{b}{2}\Big[1 - \frac{4c}{b^2}\Big]^{\frac{1}{2}}\,.$$

From the initial conditions, we find

$$\theta = \frac{\theta_0}{1 - \frac{\gamma_2}{\gamma_1}}\Big[e^{\gamma_2 t} - \frac{\gamma_2}{\gamma_1}e^{\gamma_1 t}\Big]\,. \tag{3}$$

(d) Substituting the numerical values for the parameters, we find

$$b = \frac{\sigma B^2}{\rho} = 10^4 s^{-1} \qquad and \qquad c = -\frac{3g}{2d} = -15 s^{-2} \qquad .$$

Since $4c/b^2 = -6\times 10^{-7}$, we amy expand the square root and find to a good approximation

$$\gamma_1 = -b = -10^4 s^{-1} \qquad \text{and} \qquad \gamma_2 = -\frac{c}{b} = +1.5\times 10^{-3} s^{-1}\,.$$

Examining the signs of γ_1 and γ_2, we see that the second solution $e^{\gamma_2 t}$ is increasing in time, while the first solution $e^{\gamma_1 t}$ is (rapidly) decreasing in time. Further $\gamma_2 \ll |\gamma_1|$, and therefore the second term in Eq. (3) is a tiny transient. Thus, we may approximate Eq. (3)

$$\theta = \frac{\theta_0}{1 - \frac{\gamma_2}{\gamma_1}}\Big[e^{\gamma_2 t} - \frac{\gamma_2}{\gamma_1}e^{\gamma_1 t}\Big] \simeq \theta_0 e^{\gamma_2 t}\,. \tag{4}$$

The time constant for the motion is $\frac{1}{\gamma_2} = 667 s$, about 10 minutes.

Quantum Mechanics 1

Quantum mechanics of a charged rod

A rod of length l and uniform mass distribution rotates around its center in the xy-plane. The rod has mass M. Two charge $+Q$ and $-Q$ are fixed at the end of the rod.

(a) (5 points) Describe this system quantum mechanically by finding its eigenfunctions and eigenvalues. Is the spectrum degenerate and why?

(b) (5 points) A constant weak electric field $\mathbf{E} = E\hat{\mathbf{x}}$ lying in the plane of rotation is applied. Find the new energies and eigenfunctions.

(c) (5 points) For a constant but strong electric field $\mathbf{E} = E\hat{\mathbf{x}}$, find an approximate wave function and energy for the ground state.

(d) (5 points) If at time $t = 0$ a weak time dependent electric field is applied $\mathbf{E}(t) = 2\cos(\omega t)\mathbf{E}$, find the probability for the transition from the ground state to any excited state.

Solution: I. Zahed

a. In the xy-plane, the eigenvalue problem in polar coordinates is

$$-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\theta^2}\varphi^0_m(\theta)=E^0_m\varphi^0_m(\theta) \tag{1}$$

with the moment of inertial for a fixed length rod $I=Ml^2/12$. This is a free motion on S^1, with $\varphi_m(2\pi+\theta)=\varphi_m(\theta)$. Thus, the spectrum

$$\varphi^0_m(\theta)=\frac{e^{im\theta}}{\sqrt{2\pi}} \qquad\qquad E^0_m=\frac{\hbar^2m^2}{2I} \tag{2}$$

with $m=0,\pm1,....$ Each state is doubly degenerate due to the invariance of the Hamiltonian under time reversal symmetry.

b. The Hamiltonian (1) is changed to

$$H=-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\theta^2}-QlE\cos(\theta) \tag{3}$$

Although $\varphi_\pm(\theta)$ are degenerate, the dipole interaction is still diagonal in this subspace since

$$\langle -m|V(\theta)|+m\rangle=\int_0^{2\pi}(-QlE)\cos(\theta)\frac{e^{2im\theta}}{2\pi}=0 \tag{4}$$

and we can use standard non-degenerate perturbation theory. To first order the energies do not shift

$$E^1_m=\langle m|V(\theta)|m\rangle=\int_0^{2\pi}(-QlE)\cos(\theta)=0 \tag{5}$$

but the wavefunctions shift

$$\varphi^1_m(\theta)=\sum_{n\neq m}\frac{\langle n|V(\theta)|m\rangle}{E^0_m-E^0_n}\varphi^0_n(\theta) \tag{6}$$

The dipole matrix elements are

$$\langle n|V(\theta)|m\rangle=-\frac{1}{2\pi}QlE\left(\delta_{m-n+1}+\delta_{m-n-1,0}\right) \tag{7}$$

and therefore to first order

$$\begin{aligned}E_m&=E^0_m+0\\ \varphi_m&=\varphi^0_m+\frac{IlQE}{\hbar^2\sqrt{2\pi}}\left(\frac{e^{i(m+1)\theta}}{1+2m}+\frac{e^{i(m-1)\theta}}{1-2m}\right)\end{aligned} \tag{8}$$

c. For a strong electric field, the dipole is close to its classical limit of total alignment. Thus, (3) can be expanded around $\theta = 0$,

$$H \approx -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\theta^2} - QlE\left(1 - \frac{\theta^2}{2}\right) \tag{9}$$

The spectrum is harmonic with $\omega_0 = lQE/I$. The ground state is

$$\begin{aligned} E_0 &= \frac{1}{2}\hbar\omega_0 \\ \varphi_0(\theta) &= \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-a\theta^2/2} \end{aligned} \tag{10}$$

with $a^2 = I^2\omega_0$.

d. For a weak interaction, we can use first order time-dependent perturbation theory. The transition probability amplitude from the ground state to any excited state is

$$A_{0\to n} = \frac{1}{i\hbar}\left(\int_0^\infty \langle n|V(\theta)|0\rangle\, e^{i\omega t}dt + \text{c.c.}\right) \tag{11}$$

Using (7) and keeping only the absorption part (the emission part does not contribute) we have for the probability

$$P_{0\to n} = |A_{0\to n}|^2 = \left(\frac{lQE}{2\pi}\frac{1}{\hbar\omega - \hbar^2/2I}\right)^2 \delta_{n,\pm 1} \tag{12}$$

Quantum Mechanics 2

Approximations of an anharmonic oscillator

The purpose of this problem is to compare various estimates for the ground state energy of the anharmonic oscillator. For that, consider the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x^4 \equiv H_\omega + \lambda x^4 \tag{13}$$

a. (3 points) For a weakly anharmonic oscillator use dimensional and physical reasoning to estimate (i) the typical size of the ground state wave function and (ii) the shift in the ground state energy due to the anharmonic term. Explain your reasoning.
b. (3 points) Use first order perturbation theory to determine the ground state energy of the weakly anharmonic oscillator.
c. (6 points) If Ψ_ω denotes the ground state wavefunction of the harmonic oscillator Hamiltonian H_ω (see eq. (13)), use Ψ_Ω as a variational ansatz to determine the optimal variational frequency $\Omega(m, \omega, \lambda)$ and corresponding variational energy $\mathcal{E}(m, \omega, \lambda)$ for the ground state of the anharmonic Hamiltonian. Compare to the results in **b.**
d. (3 points) Write the classical equation of motion corresponding to the anharmonic potential in (13), and approximately solve the equation with a single harmonic ansatz, $x(t) = A\cos(\Omega t)$, i.e. determine the oscillation frequency Ω as a function of A. For what value of A does classical oscillation frequency equal the variational frequency Ω in **c.**? Compare your result to the estimate of part **a**.
e. (5 points) Use the WKB approximation to evaluate the energy of the ground state of the anharmonic oscillator to first order in λ. How does your result compare to the results in **b, c** and why?

Solution:

a. The typical size x_0 of the ground state of a harmonic oscillator is found by comparing the kinetic and potential terms

$$\frac{\hbar^2}{2mx_0^2} \sim \frac{1}{2}m\omega^2 x_0^2 \tag{14}$$

or

$$x_0 \sim \sqrt{\frac{\hbar}{m\omega}} \tag{15}$$

This is just an estimate. It can be made more precise by noting that for the harmonic oscillator the virial theorem says that $\langle KE\rangle = \langle PE\rangle$, which is a statement that the ground state is a minimal uncertainty wave packet. Recalling that the ground state energy is $\frac{1}{2}\hbar\omega$, we can find

$$\left\langle \frac{1}{2}m\omega^2 x^2 \right\rangle = \frac{\hbar\omega}{4}\,, \tag{16}$$

and the variance in position is therefore

$$\sigma^2 = \left\langle x^2 \right\rangle = \frac{1}{2}x_0^2\,. \tag{17}$$

The correction to the energy is of order

$$\Delta E \sim \lambda x_0^4\,. \tag{18}$$

b. The canonical units are $e_0 = \hbar\omega$ and $x_0 = \sqrt{\hbar/m\omega}$. The ground state energy and wavefunctions are

$$E_0^0 = \frac{e_0}{2} \qquad\qquad \Psi_0(x) = \left(\frac{1}{\pi x_0^2}\right)^{\frac{1}{4}} e^{-\frac{x^2}{2x_0^2}}\,. \tag{19}$$

This can be remembered by recalling that the ground state wave function squared is a normalized Gaussian with variance of σ^2

$$|\Psi_0(x)|^2 = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}\,. \tag{20}$$

The first order shift in the energy is

$$E_0^1 = E_0 + \left\langle 0|\lambda x^4|0\right\rangle = \frac{\hbar\omega}{2} + \frac{3}{4}\lambda x_0^4 \tag{21}$$

c. The variational energy can be obtained from

$$E(\Omega) = \left\langle \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x^4 \right\rangle$$
$$= \frac{\hbar\Omega}{2} + \frac{m}{4}(\omega^2 - \Omega^2)x_\Omega^2 + \frac{3\lambda}{4}x_\Omega^4 \tag{22}$$

and minimized through $dE/d\Omega = 0$ fixes Ω through

$$\Omega^2 - \omega^2 - \frac{6\lambda\hbar}{m^2\Omega} = 0 \tag{23}$$

with a solution to first order in λ

$$\Omega = \left(\omega^2 + \frac{6\lambda\hbar}{m^2\Omega}\right)^{\frac{1}{2}} \approx \omega + \frac{3\lambda\hbar}{m^2\omega^2} \tag{24}$$

Inserting this value back into (22) gives the variational ground state energy

$$\mathcal{E}(m, \omega, \lambda) \approx \frac{\hbar\omega}{2} + \frac{3}{4}\lambda x_0^4 \tag{25}$$

The variational estimate is identical with the result in **a.** which is exactly the lower bound of the variational analysis.

d. The classical anaharmonic equation is

$$\dot{\dot{x}} + \omega^2 x = -\frac{4\lambda}{m}x^3 \tag{26}$$

Using the single harmonic ansatz $x(t) = A\cos(\Omega t)$ the solution reads

$$(\omega^2 - \Omega^2)\, A\cos(\Omega t) = -\frac{\lambda A^3}{m}\left(3\cos(\Omega t) + \cos(3\Omega t)\right) \approx -\frac{3\lambda}{m}A^3\cos(\Omega t) \tag{27}$$

which in the single harmonic approximation valid to leading order in λ we have

$$\Omega \approx \omega + \frac{3\lambda}{2m\omega}A^2 \tag{28}$$

By choosing $A = \sqrt{2\hbar/m\omega}$ in (28) the optimal variational frequency in (24) equals the classical oscillation frequency in (28). In this way, the quantum state Ψ_Ω for the anaharmonic oscillator estimate corresponds to classical harmonic motion with fixed amplitude. We also note that this value of A (i.e. $\sqrt{2\hbar/m\omega}$) is of order the estimate of the harmonic oscillator length of part **a.**

d. The energy levels in the WKB approximation are fixed by

$$\int_{x_-}^{x_+} p(x)dx = \left(n + \frac{1}{2}\right) h \tag{29}$$

The turning points are fixed by the condition $p(x_\pm) = 0$ with

$$p(x) = (2m(E - V(x)))^{\frac{1}{2}} \tag{30}$$

Using the canonical units defined in **a** we re-write (29) as

$$\int_0^{X(\lambda)} dx\, Q(x,\lambda) \equiv \int_0^{\frac{x_+(\lambda)}{x_0}} dx \left(\epsilon_n(\lambda) - x^2 - \lambda\alpha x^4\right)^{\frac{1}{2}} = \left(n + \frac{1}{2}\right) \frac{\pi\hbar}{2} \tag{31}$$

with $\alpha = 2x_0^4/e_0$, $x_+(0)/x_0 = 1$ and $\epsilon_n(\lambda) = E_n(\lambda)/e_0/2$. To first order in λ we have

$$\int_0^{X(0)} dx\, Q(x,0) + X'(0)Q(X(0),0) + \lambda \int_0^{X(0)} Q'(x,0) \approx \left(n + \frac{1}{2}\right) \frac{\pi\hbar}{2} \tag{32}$$

The second contribution vanishes since $Q(X(0),0) = 0$ and can be dropped. The first contribution can be rescaled to give precisely the right hand side through

$$\frac{E_n^0}{E_0^0} \int_0^1 (1 - x^2)^{\frac{1}{2}} = \left(n + \frac{1}{2}\right) \frac{\pi\hbar}{2} \tag{33}$$

The third contribution can be rescaled to give the first order WKB correction

$$\frac{E_n^1}{E_0^0} = \alpha \left(\frac{E_n^0}{E_0^0}\right)^2 \frac{\int_0^1 x^4/\sqrt{1-x^2}}{\int_0^1 1/\sqrt{1-x^2}} \tag{34}$$

which gives the WKB spectrum to leading λ

$$E_n \approx E_n^0 + E_n^1 \approx \left(n + \frac{1}{2}\right) \hbar\omega + \frac{3}{8}\lambda x_0^4 \left(4n^2 + 4n + 1\right) \tag{35}$$

For the ground state

$$E_0 \approx \frac{\hbar\omega}{2} + \frac{3}{8}\lambda x_0^4 \tag{36}$$

which is exact in leading order and below the perturbative ground state **a**.

Quantum Mechanics 3

Cyclic quantum evolution and Berry phases

Consider a Hamiltonian $\hat{H}'(\lambda(t))$ that depends on time through a slowly varying parameter $\lambda(t)$. (For example H' could describe the spin Hamiltonian of a neutron in a time dependent magnetic field.) The eigenstates $|\epsilon_n(\lambda)\rangle$ and eigenvalues $\epsilon_n(\lambda)$ of H' are all slow functions of time through the parameter $\lambda(t)$. Any state of the system $|\Psi(t)\rangle$ can be expanded in terms of the instantaneous eigenstates of $\hat{H}'$, i.e. $|\Psi(t)\rangle = \sum \varphi_n(t)\,|\epsilon_n(\lambda)\rangle$.

(a) (6 points) Assume that the system starts in $|\epsilon_0(\lambda)\rangle$ and subsequently evolves in a single eigenstate, i.e. $|\Psi(t)\rangle = \varphi(t)\,|\epsilon_0(\lambda)\rangle$. The parameter $\lambda(t)$ is cyclically varied over a time T so that $\lambda(T) = \lambda(0)$:

(i) Determine the final state $|\Psi(T)\rangle$ of the system given its initial condition $|\Psi(0)\rangle$.

(ii) Show that $|\Psi(T)\rangle$ contains a nonvanishing phase ϕ (known as the *Berry phase*) that is independent of the period T. Express the Berry phase in terms of the *Berry connection*, $A \equiv i\hbar\langle\epsilon|\frac{d}{d\lambda}|\epsilon\rangle$.

Now consider a quantum mechanical particle. A time independent Hamiltonian $\hat{H}'(\mathbf{r})$ describes the internal degrees of freedom of the particle (e.g. its spin state). Now $\hat{H}'$ varies slowly in space, but does not vary in time. Its eigenstates $|\epsilon_n(\mathbf{r})\rangle$ and eigenvalues $\epsilon_n(\mathbf{r})$ also vary slowly in space, but not in time.

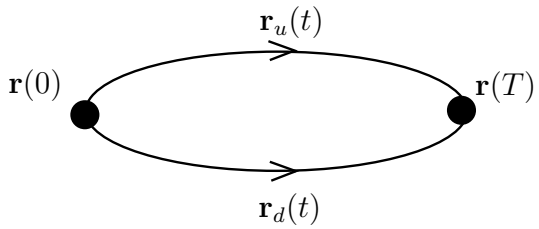
(b) (6 points) Assume that the full wave function in coordinate and "spin" space takes the form $|\Psi(\mathbf{r},t)\rangle = \varphi(\mathbf{r},t) \otimes |\epsilon_0(\mathbf{r})\rangle$ at all times. Analyze the time evolution of $|\Psi(\mathbf{r},t)\rangle$ under the full Hamiltonian $\hat{H} = \hat{\mathbf{p}}^2/2m + \hat{H}'$ and show that the Schrödinger equation for $\varphi(\boldsymbol{r},t)$ involves the effective Hamiltonian

$$\hat{H}_\varphi = \frac{1}{2m}\left[\hat{\mathbf{p}} - \mathbf{A}(\mathbf{r})\right]^2 + V(\mathbf{r}) + \epsilon_0(\mathbf{r}),$$

where $V(\boldsymbol{r}) = \sum_{n\neq 0} |\langle\epsilon_n|\boldsymbol{\nabla}\epsilon_0\rangle|^2$ is a scalar function of no further interest, and $\boldsymbol{A}(\mathbf{r}) \equiv i\hbar\langle\epsilon_0(\mathbf{r})|\nabla\epsilon_0(\mathbf{r})\rangle$ is the Berry connection in this case.

The Hamiltonian $\hat{H}_\varphi$ is analogous to the motion of a charged particle in a magnetic field. The "magnetic field" in this case is known as the *Berry curvature*, $\mathbf{B} = \nabla \times \mathbf{A}$. Now consider a wave packet in the set-up of part (b). The packet is localized at a central position $\mathbf{r}(t)$, which slowly changes in time. At $\mathbf{r}(0)$ the wave packet is split into two, $\varphi_{\rm u}(\mathbf{r}_u(t))$ and $\varphi_d(\mathbf{r}_d(t))$, and the two waves propagate along opposites sides of the contour (up and down as shown below) to finally interfere at $\mathbf{r}(T)$.

(c) (2 points) Use the results of part (a) (with $\boldsymbol{r}(t)$ as the adiabatic parameters) to determine the interference $\varphi_u^*\varphi_d$ at $\mathbf{r}(T)$ in terms of the "magnetic flux" through the contour and the wave functions φ_u and φ_d at $\mathbf{r}(0)$.



(d) (3 points) The eigenfunctions $|\epsilon_n(\mathbf{r})\rangle$ of H' are defined only up to an overall $\mathbf{r}$-dependent phase. If the kets are rotated by a function $\chi(\mathbf{r})$, $|\epsilon_n(\mathbf{r})\rangle \to e^{i\chi(\mathbf{r})}\,|\epsilon_n(\mathbf{r})\rangle$, how does the Berry connection $\mathbf{A}(\mathbf{r})$ and interference of part (c) change? Explain.

The analysis in parts (a) and (c) was for a single non-degenerate eigenstate $|\epsilon_0(\mathbf{r}(t))\rangle$ with a slowly varying parameter $\mathbf{r}(t)$. Now repeat the analysis of parts (a) and (c) but assume that at each point there are two degenerate eigenstates, $|\epsilon_0(\mathbf{r}(t))\rangle$ and $|\epsilon_1(\mathbf{r}(t))\rangle$, depending on the parameter $\boldsymbol{r}(t)$. Assume that the full wave function lies in their span, $|\Psi(t)\rangle = \varphi_0(t)\,|\epsilon_0(\mathbf{r}(t))\rangle + \varphi_1(t)\,|\epsilon_1(\mathbf{r}(t))\rangle$.

(e) (3 points) Derive an equation of motion and effective Hamiltonian for the pair of functions $(\varphi_0(t), \varphi_1(t))$ involving an appropriate Berry connection, $\mathbf{A}_{ab}(\boldsymbol{r}(t)) = i\hbar\langle\epsilon_a|\nabla\epsilon_b\rangle$ (where a, b=0, 1). Is adiabatic evolution possible? Explain.

Note that the Berry connection does not commute in this case. This is called non-abelian behavior.

Solution

(a) Starting with the Schrödinger equation $\hat{H}' |\Psi(t)\rangle = i\hbar \frac{d}{dt} |\Psi(t)\rangle$ and inserting $|\Psi\rangle = \varphi(t) |\epsilon_0(\lambda)\rangle$ yields

$$\epsilon_0 \varphi(t) |\epsilon_0\rangle = i\hbar \left(\dot{\varphi} |\epsilon_0\rangle + \varphi \tfrac{d}{d\lambda} |\epsilon_0\rangle \dot{\lambda} \right) . \tag{37}$$

After left multiplication with $\langle \epsilon_0|$ we find

$$i\hbar \dot{\varphi} = \left(\epsilon_0(\lambda) - i\hbar \langle \epsilon_0| \frac{d}{d\lambda} |\epsilon_0\rangle \dot{\lambda} \right) \varphi \, . \tag{38}$$

The formal solution of this equation, using the definition for $A = i\hbar \langle \epsilon_0| \frac{d}{d\lambda} |\epsilon_0\rangle$, is

$$\varphi(T) = \varphi(0) \exp\left[\frac{-i}{\hbar} \int_0^T \epsilon_0(\lambda(t)) dt \right] \exp\left[\frac{i}{\hbar} \int_0^T A(\lambda(t)) \, \dot{\lambda}(t) \, dt \right] . \tag{39}$$

The phase in the second exponential

$$\frac{1}{\hbar} \int_0^T A(\lambda) \cdot \dot{\lambda} \, dt = \frac{1}{\hbar} \oint A(\lambda) \cdot d\lambda \, , \tag{40}$$

is time-independent but depends on the contour.

(b) Inserting the state $|\Psi\rangle = \varphi(\mathbf{r}, t) \otimes |\epsilon_0(\mathbf{r})\rangle$ into the Schrödinger equation, using $\hat{\mathbf{p}} = -i\hbar\nabla$, and left multiplication with $\langle \epsilon_0|$ yields the equation

$$i\hbar \dot{\varphi} = -\frac{\hbar^2}{2m} \left[\nabla^2 + 2 \langle \epsilon_0| \boldsymbol{\nabla} |\epsilon_o\rangle \cdot \boldsymbol{\nabla} + \langle \epsilon_0| \nabla^2 |\epsilon_0\rangle \right] \varphi + \epsilon_0 \varphi \tag{41}$$

The term $\langle \epsilon_0| \nabla^2 |\epsilon_0\rangle$ can be re-written as

$$\begin{aligned} \langle \epsilon_0| \nabla^2 |\epsilon_0\rangle &= \langle \epsilon_0| \boldsymbol{\nabla} \cdot \left(\sum_n |\epsilon_n\rangle \langle \epsilon_n| \right) \boldsymbol{\nabla} |\epsilon_0\rangle & (42) \\ &= \sum_n \langle \epsilon_0| \boldsymbol{\nabla} |\epsilon_n\rangle \cdot \langle \epsilon_n| \boldsymbol{\nabla} |\epsilon_0\rangle & (43) \\ &= \langle \epsilon_0| \boldsymbol{\nabla} |\epsilon_0\rangle^2 + \sum_{n \neq 0} | \langle \epsilon_n| \boldsymbol{\nabla} |\epsilon_0\rangle |^2 & (44) \end{aligned}$$

such that

$$i\hbar \dot{\varphi} = \left[\frac{1}{2m} \left(\hat{\mathbf{p}}^2 - 2i\hbar \langle \epsilon_0| \boldsymbol{\nabla} |\epsilon_0\rangle \cdot \hat{\mathbf{p}} - \hbar^2 \langle \epsilon_0| \boldsymbol{\nabla} |\epsilon_0\rangle^2 \right) + \sum_{n \neq 0} | \langle \epsilon_n| \boldsymbol{\nabla} |\epsilon_0\rangle |^2 \right] \varphi_0 + \epsilon_0 \varphi, \tag{45}$$

or

$$i\hbar \, \dot{\varphi}(\mathbf{r}, t) = \left[\frac{1}{2m} \left(\hat{\mathbf{p}} - \mathbf{A}(\mathbf{r}) \right)^2 + V(\mathbf{r}) + \epsilon_0(\mathbf{r}) \right] \varphi(\mathbf{r}, t) \tag{46}$$

(c) Following the upper (lower) half of the contour from the origin to $\mathbf{r}'$, the wave functions at this point are given by

$$\varphi_{(u,d)}(\mathbf{r}) = \varphi_{(u,d)}(0) \exp\left[\frac{i}{\hbar}\int_{0(u,d)}^{\mathbf{r}(T)} \mathbf{A}\cdot d\mathbf{r}\right] \tag{47}$$

This means that the interference term $\varphi_u^*\varphi_d$ is given by

$$\begin{aligned}
\varphi_u(\mathbf{r}(T))^*\varphi_d(\mathbf{r}(T)) &= \varphi_u(0)^*\varphi_d(0)\exp\left[\frac{-i}{\hbar}\int_{0(u)}^{\mathbf{r}(T)}\mathbf{A}\cdot d\mathbf{r}\right]\exp\left[\frac{i}{\hbar}\int_{0(d)}^{\mathbf{r}(T)}\mathbf{A}\cdot d\mathbf{r}\right] &(48)\\
&= \varphi_u(0)^*\varphi_d(0)\exp\left[\frac{i}{\hbar}\int_{\mathbf{r}(T)(u)}^{0}\mathbf{A}\cdot d\mathbf{r}\right]\exp\left[\frac{i}{\hbar}\int_{0(d)}^{\mathbf{r}(T)}\mathbf{A}\cdot d\mathbf{r}\right] &(49)\\
&= \varphi_u(0)^*\varphi_d(0)\exp\left[\frac{i}{\hbar}\oint\mathbf{A}\cdot d\mathbf{r}\right] &(50)\\
&= \varphi_u(0)^*\varphi_d(0)\exp\left[\frac{i}{\hbar}\Phi\right] &(51)
\end{aligned}$$

where Φ is the magnetic flux, $\int \mathbf{B}\cdot \mathrm{d}\boldsymbol{S}$, through the surface outline by the closed contour.

(d) The transformation changes the Berry connection $\mathbf{A}' = \mathbf{A} - \boldsymbol{\nabla}\chi(\mathbf{r})$. However, this does not affect the results in (c) since $\boldsymbol{\nabla}\times\mathbf{A}' = \boldsymbol{\nabla}\times\mathbf{A} - \boldsymbol{\nabla}\times\boldsymbol{\nabla}\chi = \boldsymbol{\nabla}\times\mathbf{A} = \mathbf{B}$, and the magnetic flux is the same.

(e) Following the approach in (a), but now using $|\Psi(t)\rangle = \varphi_0(t)\,|\epsilon_0(\mathbf{r}(t))\rangle + \varphi_1(t)\,|\epsilon_1(\mathbf{r}(t))\rangle$ leads to the equation

$$\begin{aligned}
i\hbar\begin{pmatrix}\dot\varphi_0\\ \dot\varphi_1\end{pmatrix} =& \epsilon_0(\mathbf{r}(t))\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\varphi_0\\\varphi_1\end{pmatrix} - i\hbar\begin{pmatrix}\langle\epsilon_0|\boldsymbol{\nabla}|\epsilon_0\rangle & \langle\epsilon_0|\boldsymbol{\nabla}|\epsilon_1\rangle\\ \langle\epsilon_1|\boldsymbol{\nabla}|\epsilon_0\rangle & \langle\epsilon_1|\boldsymbol{\nabla}|\epsilon_1\rangle\end{pmatrix}\cdot\begin{pmatrix}\varphi_0\\\varphi_1\end{pmatrix} &(52)\\
=& \epsilon_0(\boldsymbol{r}(t))\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}\varphi_0\\\varphi_1\end{pmatrix} - \mathbf{A}\cdot\begin{pmatrix}\varphi_0\\\varphi_1\end{pmatrix} &(53)
\end{aligned}$$

The dynamics is just that of a coupled two-level system, where overlap between the internal states in the off-diagonal elements lead to coherent transitions between the external wavefunctions. The evolution can only remain adiabatic in the set of the two states, but not for the individual states within the set.

The solution to Eq. (52) is

$$\varphi_a(t) = e^{-\frac{i}{\hbar}\int_0^t \epsilon_0(\boldsymbol{r}(t))dt}\,U_{ab}(\boldsymbol{r}(t))\varphi_b \tag{54}$$

where U_{ab} is the time-ordered exponential

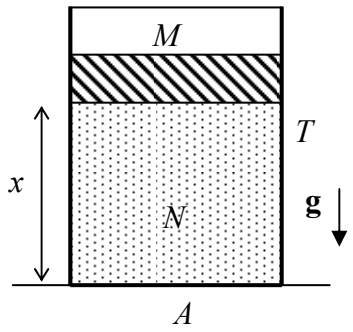
$$U_{ab} = \left[T\exp\left(\frac{i}{\hbar}\int_0^t \mathrm{d}t\frac{\mathrm{d}\mathbf{r}(t)}{\mathrm{d}t}\cdot\mathbf{A}(\boldsymbol{r}(t))\right)\right]_{ab} \tag{55}$$

known as a non-abelian Wilson line.

Statistical Mechanics 1

Heavy piston

A vertically positioned cylinder, whose walls are kept at constant temperature T, is closed with a very heavy piston of mass M (see Fig. on the right), and contains $N >> 1$ molecules of an ideal gas. Neglecting the external pressure, and the friction between the piston and the cylinder's walls, calculate:



A (1 point) the equilibrium position x_0 of the piston;

B (2 points) the frequency of small oscillations of the piston near x_0;

C (3 points) the r.m.s. value δx of the piston's thermal fluctuations.

D (4 points) Now let the piston, moving with velocity u, also experience a drag force with the statistical average $\langle F \rangle = -\eta u$. Use this relation and the fluctuation-dissipation theorem to re-derive the answer to question C.

E (6 points) The drag force, mentioned in question D, may arise due to the molecules reflecting from the moving piston. Assuming that the velocity u of the piston is much lower than the typical molecular velocity, use the elementary kinetics and statistics of the ideal gas to calculate the drag coefficient η.

F (2 points) Formulate quantitatively the conditions of validity of your results. In particular, what is the condition that the oscillation process is isothermal?

Solution

A (1 point). With the equation of state of the ideal gas,

$$PV = NT\,, \tag{1}$$

where $T \equiv k_B T_{Kelvin}$ is temperature in energy units, and the evident relation $V = xA$ (where A is the cylinder's base area), the equation of piston's mechanical equilibrium,

$$PA = Mg\,,$$

gives the result independent of A:

$$x_0 = \frac{NT}{Mg}\,, \tag{2}$$

B (2 points). If the piston is very heavy, the piston's oscillations near the equilibrium are very slow, so that the gas temperature always have time to adjust to that of the walls. As a result, the oscillation process is isothermal, and Eq. (1) may be used even in dynamics, giving the following equation of piston's motion:

$$M\ddot{x} = PA - Mg = \frac{NT}{x} - Mg = \frac{NT}{x_0 + \tilde{x}} - Mg\,, \tag{3}$$

where $\tilde{x} \equiv x - x_0$ is the deviation from the equilibrium position. For small oscillations ($|\tilde{x}| << x_0$) we may Taylor-expand the right-hand part of this equation, keep only the two leading terms, and then use Eq. (2) to obtain

$$M\ddot{x} \equiv M\ddot{\tilde{x}} = \frac{NT}{x_0\left(1 + \tilde{x}/x_0\right)} - Mg \approx \frac{NT}{x_0}\left(1 - \frac{\tilde{x}}{x_0}\right) - Mg = -k\tilde{x}\,.$$

where the effective spring constant

$$k \equiv \frac{NT}{x_0^2} = \frac{M^2 g^2}{NT}\,.$$

From here, the frequency of small oscillations is

$$\omega_0 = \left(\frac{k}{M}\right)^{1/2} \equiv \left(\frac{M}{NT}\right)^{1/2} g\,. \tag{4}$$

Note two curious facts. First, with N and T fixed, the oscillation frequency *grows* with the mass M of the piston (because of a faster growth of the effective spring constant k.) Second, with Eq. (2) for x_0, Eq. (4) may be rewritten in the form,

$$\omega_0 = \left(\frac{g}{x_0}\right)^{1/2}\,,$$

which coincides with the well-known expression for the frequency of small oscillations of a point-mass ("mathematical") pendulum of length x_0, in the same gravity field.

C (3 points). The simplest way to calculate r.m.s. value δx (i.e. the square root of the variance) of the thermal fluctuations is to apply, to the average potential energy U of these classical fluctuations, the equipartition theorem:

$$\langle U \rangle = \frac{k}{2}\langle \tilde{x}^2 \rangle \equiv \frac{k}{2}(\delta x)^2 = \frac{T}{2}.$$

From here,

$$\delta x = \left(\frac{T}{k}\right)^{1/2} = \frac{N^{1/2}T}{Mg}. \tag{5}$$

Comparing this expression with Eq. (2), we see that the relative r.m.s. fluctuation obeys the well-known equality

$$\frac{\delta x}{x_0} = \frac{1}{N^{1/2}} << 1,$$

following from the independence of the individual molecules in an ideal gas.

D (4 points). Adding the viscosity term $-\eta u$ to the right-hand part of Eq. (3),

$$M\ddot{x} = \frac{NT}{x} - \eta\dot{x} - Mg,$$

and linearizing in small $\tilde{x} \equiv x - x_0$ just as in Task B, we get the following linear differential equation:[1]

$$M\ddot{x} + \eta\dot{x} + kx = 0. \tag{6}$$

The fluctuation-dissipation theorem, in its classical limit, gives the following relation,

$$S_F(\omega) = \frac{\chi''(\omega)}{\pi\omega} T, \tag{7}$$

between the spectral density S_F of the Langevin force, which should be placed into the right-hand part of Eq. (6) for the description of molecular hit randomness,

$$M\ddot{\tilde{x}} + \eta\dot{\tilde{x}} + k\tilde{x} = \tilde{F}(t), \qquad \text{where } \tilde{F}(t) \equiv F(t) - \langle F \rangle(t), \tag{8}$$

and the imaginary part of the complex generalized susceptibility of the system's environment:

[1] Note that this equation neglects the random ("Langevin") force $F(t) - \langle F \rangle$, describing the randomness of individual molecular hits, and is valid only if $|x| << \delta x$, where δx is the scale of piston's fluctuations, given by Eq. (4) – see the discussion below.

$$\chi(\omega) \equiv \frac{\langle F_\omega \rangle}{x_\omega},$$

where the lower index denotes the Fourier component of the corresponding function of time, and $x(t)$ is considered as a given function of time.

In our case, for small oscillations, the average molecular force is

$$\langle F \rangle - \langle F(x_0) \rangle = -k\tilde{x} - \eta\dot{\tilde{x}},$$

so that the relation between the Fourier components of the force and displacement is

$$F_\omega = (-k + i\omega\eta)x_\omega.$$

Hence

$$\chi''(\omega) \equiv \mathrm{Im}\,\chi(\omega) = \mathrm{Im}(-k + i\omega\eta) = \omega\eta,$$

and Eq. (7) is reduced to

$$S_F(\omega) = \frac{\eta}{\pi}T\,.$$

Now writing Eq. (8) in the Fourier representation,

$$(-M\omega^2 - i\omega\eta + k)x_\omega = \tilde{F}_\omega,$$

and taking into account that the spectral density of any function $f(t)$ is proportional to $|f_\omega|^2$, we get

$$S_x(\omega) = \frac{S_F(\omega)}{\left|-M\omega^2 - i\omega\eta + k\right|^2} = \frac{\eta}{\pi}T\frac{1}{M^2\left(\omega_0^2 - \omega^2\right)^2 + (\omega\eta)^2}.$$

The variance of random fluctuations of a function of time, in our case of the piston displacement x, is just the integral of its spectral density over all frequencies:

$$\langle \tilde{x}^2 \rangle \equiv (\delta x)^2 = \int_{-\infty}^{+\infty} S_x(\omega)d\omega = 2\frac{\eta}{\pi}T\int_0^{\infty}\frac{d\omega}{M^2\left(\omega_0^2 - \omega^2\right)^2 + (\omega\eta)^2}.$$

This integral may be readily worked out in our current case of a sufficiently low viscosity η, when the function under the integral has a sharp, narrow resonance peak at $\omega \approx \omega_0$, which gives the dominating contribution to the integral. Near this peak, i.e. at frequencies with $|\omega - \omega_0| << \omega_0$, we may take $\omega^2 - \omega_0^2 \approx 2\omega_0(\omega - \omega_0)$, and $\omega\eta/M \approx \omega_0\eta/M$, so that

$$(\delta x)^2 = 2\frac{\eta}{\pi}T\int_{\omega\approx\omega_0}\frac{d\omega}{4M^2\omega_0^2(\omega - \omega_0)^2 + (\omega_0\eta)^2} = 2\frac{\eta}{\pi}T\frac{1}{2M\omega_0^2\eta}\int_{-\infty}^{+\infty}\frac{d\xi}{\xi^2 + 1},$$

where $\xi \equiv 2M(\omega - \omega_0)/\eta$. This is a well-known table integral, equal to π, so that we finally get

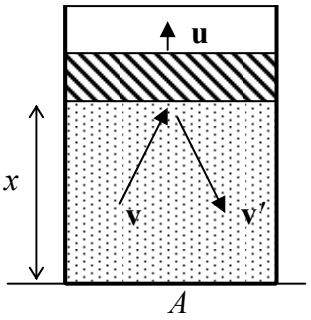
$$(\delta x)^2 = 2\frac{\eta}{\pi}T\frac{1}{2M\omega_0^2\eta}\pi = \frac{T}{M\omega_0^2} = \frac{T}{k},$$

thus returning to Eq. (5).

Note that this result is independent of the particular expression for the viscosity η, provided that it is sufficiently low:

$$\frac{\eta}{M} << \omega_0 . \tag{9}$$

E (6 points). Let the piston move with a low velocity u. Consider a molecule hitting the piston, with the initial horizontal velocity $v_x > 0$ (in the lab reference frame) - see Fig. on the right. In the reference frame connected to the piston, this component is $(v_x - u)$. At an elastic collision, in piston's reference frame the component's modulus is conserved, so that after the collision it is $-(v_x - u) = -v_x + u$, and in the lab frame it is $v'_x = (-v_x + u) + u = -(v_x - 2u)$. Hence the momentum transferred to the piston is $-\Delta(mv_x) = -m[(-v_x - 2u) - v_x] = 2m(v_x - u)$, where m is the mass of the molecule.



The time interval Δt between the previous collision and the analyzed one (at moment t) may be found from the evident kinematic equation: $v_x\Delta t = x(t) + x(t - \Delta t) = 2x(t) - u\Delta t$, giving $\Delta t = 2x(t)/(v_x + u)$. A similar analysis of the next time interval $\Delta t'$ is $v'_x\Delta t' = x(t + \Delta t') + x(t) = 2x(t) + u\Delta t'$, so that $\Delta t' = 2x(t)/(v'_x - u)$. Using the v'_x calculated above, this gives $\Delta t' = 2x(t)/(v_x - 3u)$. The momentum $2m(v_x - u)$ given to the piston by the collision at time t has to be attributed equally to both these time intervals, so that it is equivalent to the following average force:

$$\overline{F}_m = \left(\frac{2m(v_x - u)}{\Delta t}\right)_{\text{ave}} = \frac{1}{2}\left(\frac{2m(v_x - u)}{\Delta t} + \frac{2m(v_x - u)}{\Delta t'}\right)$$

$$= \frac{m}{x}(v_x - u)\left[(v_x + u) + (v_x - 3u)\right] = \frac{m}{x}(v_x - u)^2 \approx \frac{m}{x}\left(v_x^2 - 2uv_x\right),$$

with the last transition valid if $u^2 << v^2_x$.

Since a particle moving initially in the opposite direction but the same $|v_x|$ will exert on the piston the similar average force, we can generalize this result as follows:

$$\overline{F}_m \approx \frac{m}{x}(v_x^2 - 2u|v_x|),$$

Now this force should be averaged over the 1D Maxwell distribution

$$dW = \frac{1}{\sqrt{2\pi}\sigma}\exp\left\{-\frac{v_x^2}{2\sigma^2}\right\}dv_x, \quad \text{with } \sigma^2 \equiv \left\langle v_x^2 \right\rangle = \frac{T}{m}.$$

The resulting average force from N molecules is

$$\left\langle F \right\rangle \equiv N\left\langle \overline{F}_m \right\rangle = \frac{Nm}{x}\left\langle v_x^2 \right\rangle - 2\frac{Nm}{x}\left\langle |v_x| \right\rangle u = \frac{NT}{x} - \eta u , \tag{9}$$

where

$$\eta \equiv 2\frac{Nm}{x}\left\langle \left| v_x \right| \right\rangle = 2\frac{Nm}{x}\frac{1}{\sqrt{2\pi}\sigma}2\int_0^\infty v_x \exp\left\{-\frac{v_x^2}{2\sigma^2}\right\}dv_x = \left(\frac{8mT}{\pi}\right)^{1/2}\frac{N}{x}.$$

The first term in the right-hand part of Eq. (9) is the usual (static) pressure force of the ideal classical gas (also given by Eq. (1) above), while the second term represents the damping force, always directed against piston's velocity. Hence η is the required viscosity coefficient; near the equilibrium position of the piston,

$$\eta = \left(\frac{8mT}{\pi}\right)^{1/2}\frac{N}{x_0} = \left(\frac{8m}{\pi T}\right)^{1/2} Mg\ .$$

F (2 points). First, from the last result for η, and Eq. (4) for ω_0, the condition (9) of low damping becomes simply

$$M_{\text{gas}} \equiv Nm << M\ .$$

Actually, this condition was already implied at writing Eqs. (3), (6) and (7) of piston's motion, where the gas' inertia was neglected.

Second, these equations of motion are valid only for an isothermal process (T = const), so that the oscillation frequency ω_0 has to be much lower than $1/\tau$, where τ is the time of thermal relaxation of the gas in the cylinder.[2]) According to the equation of diffusion,

$$\frac{\partial T}{\partial t} = D\nabla^2 T\ ,$$

the reciprocal time $1/\tau$ is of the order of D/a^2, where a is the smallest linear dimension of the cylinder (not necessarily x_0). For a nearly-ideal gas, with a relatively large mean free path $l >> (V/N)^{1/3}$, the diffusion coefficient D is of the order of $lv_{\text{rms}} = l(T/m)^{1/2}$, so that the condition is frequency smallness becomes[3]

$$\omega_0 << \frac{l}{a^2}\left(\frac{T}{m}\right)^{1/2}\ .$$

Finally, the given condition $N >> 1$ was repeatedly used throughout the solution.

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[2] In the opposite limit, the process is adiabatic, with a different effective spring constant.

[3] This estimate has to be altered for extremely low gas densities, when l becomes comparable with a. In this case, the condition depends of the character (diffusive vs. specular) of molecule's reflection from cylinder's walls.

Statistical Mechanics 2

Gas condensation

A closed container of volume V with a classical gas of $N >> 1$ indistinguishable particles. The inner surfaces of the container's walls have $N_S >> 1$ similar traps (potential wells of small size). Each trap can hold only one particle, in one of g_S degenerate states; energy $\Delta > 0$ is required to free the particle from the trap.

A (3 points). Assuming that the chemical potential μ of the system is known, calculate the number N_g of particles in the gas phase (i.e. in the volume of the container). What condition should be imposed on N_g for the gas to behave classically?

B (4 points). Again assuming that the chemical potential is known, calculate the probability of each trap to be filled, and the full number of filled traps (i.e. of condensed particles), as functions of μ.

C (4 points). Use the results obtained in A and B to derive the equation for the chemical potential of the system in equilibrium.

D (4 points). Solve the equation analytically in the limit of $N/N_S >> 1$, and analyze the solution; in particular, calculate the gas pressure.

E (4 points). Solve the equation for the chemical potential in the opposite limit, $N/N_S << 1$, and calculate the gas pressure in this case.

F (1 point). Summarizing your results, spell out the conditions at which the gas pressure is significantly affected by particle condensation in the traps.

Solutions

A (3 points). For a classical gas, the probability for a particle to occupy a certain quantum state of energy ε_n is given by the Boltzmann distribution:

$$W_n = \exp\left\{\frac{\mu - \varepsilon_n}{T}\right\},$$

where $T \equiv k_B T_K$ is the temperature in energy units. For a free particle, $\varepsilon_n = p_n^2/2m$, so that the total number of gas particles may be calculated as

$$N_g = g_V \sum_n W_n = g_V \sum_n \exp\left\{-\frac{p_n^2}{2mT}\right\},$$

where g_V is the orbital state degeneracy (e.g., due to particle's spin). Using the standard replacement of summation over the continuous-spectrum states by integration, we get

$$N_g = \frac{g_V V}{(2\pi\hbar)^3}\int \exp\left\{-\frac{p^2}{2mT}\right\} d^3p = \frac{g_V V}{(2\pi\hbar)^3} 4\pi \int_0^\infty \exp\left\{-\frac{p^2}{2mT}\right\} p^2 dp = \frac{g_V V}{(2\pi\hbar)^3} 4\pi (2mT)^{3/2} \int_0^\infty \exp\{-\xi^2\}\xi^2 d\xi .$$

This is the standard Gaussian integral, equal to $\pi^{1/2}/4$, and we finally get

$$N_g = N_V(T)\exp\left\{\frac{\mu}{T}\right\}, \qquad \text{where } N_V(T) \equiv \frac{g_V V}{\hbar^3}\left(\frac{mT}{2\pi}\right)^{3/2}. \tag{1}$$

For the Boltzmann distribution to be valid, all probabilities W_n, including the largest one (with $\varepsilon_n = 0$), have to be much smaller than 1, giving the condition $-\mu >> T$. According to Eq. (1), this means that N_g has to be much less than $N_V(T)$ – which is, physically, the number of gas-phase states available at temperature T.

B (4 points). Let us apply the grand canonical distribution

$$W_{m,N} = \frac{1}{Z_G}\exp\left\{\frac{\mu N - \varepsilon_{m,N}}{T}\right\}, \qquad Z_G = \sum_{m,N}\exp\left\{\frac{\mu N - \varepsilon_{m,N}}{T}\right\},$$

to a statistical ensemble of single traps, with $(1 + g_S)$ different states: one empty-trap state ($N = 0$), of certain (inconsequential) energy ε_0, and g_S different possible states with one trapped particle ($N = 1$), with energy $(\varepsilon_0 - \Delta)$:

$$W_0 = \frac{1}{Z_G}\exp\left\{-\frac{\varepsilon_0}{T}\right\}, \qquad W_1 = \frac{1}{Z_G}\exp\left\{\frac{\mu + \Delta - \varepsilon_0}{T}\right\}, \qquad Z_G = \exp\left\{-\frac{\varepsilon_0}{T}\right\} + g_S \exp\left\{\frac{\mu + \Delta - \varepsilon_0}{T}\right\},$$

so that the average number of filled traps (regardless of the quantum state of the trapped particle) is

$$N_c = N_S g_S W_1 = N_S \frac{g_S \exp\{(\mu + \Delta)/T\}}{1 + g_S \exp\{(\mu + \Delta)/T\}} \equiv \frac{N_S}{g_S^{-1}\exp\{-(\mu + \Delta)/T\} + 1}. \tag{2}$$

Note that this formula is similar to, but (if $g_S \neq 1$) still different from the Fermi-Dirac distribution for energy $(-\Delta)$.[1]

C (4 points). The total number of particles, N, has to equal the sum of the number N_g of the particles thermally activated into the gas phase, which is given by Eq. (1), and the number N_c of condensed particles, localized at the surface traps, given by Eq. (2). In the equilibrium, the values of μ and T in all these expressions are equal, so that the particle number balance, $N_g + N_c = N$, gives the following equation:

$$N_V(T)\exp\left\{\frac{\mu}{T}\right\} + \frac{N_S}{g_S^{-1}\exp\{-(\Delta+\mu)/T\}+1} = N. \qquad (3)$$

This transcendent equation for μ defies an exact analytical solution in the general case, but may be readily solved in the limits of low and high values of the N/N_S ratio.

D (4 points). Since N_c cannot be larger than N_S, in the limit $N >> N_S$ most particles have to be in the gas phase, so that in the 0^{th} approximation the second term in Eq. (3) may be ignored, and this equation is reduced to that of the ideal classical gas of N particles, giving

$$\mu = -T\ln\frac{N}{N_V(T)}, \qquad P = \frac{N_g T}{V} = \frac{NT}{V} \propto T.$$

(*Remark*: If necessary, we may use the last value of μ to calculate the (relatively small) number of condensed particles:

$$N_c = \frac{N_S}{g_S^{-1}[N_V(T)/N]\exp\{-\Delta/T\}+1} << N. \qquad (4)$$

As was discussed above, the ratio $N_V(T)/N$ has to be much larger than 1 to keep the gas classical. However, since the exponent is such a steep function, the ratio N_c/N_S depends mostly on the condensation energy Δ: if it is much larger than the *crossover value*[2]

$$\Delta_c \equiv T\ln\frac{N_V(T)}{g_S N}, \qquad (5)$$

the first term in the denominator is negligibly small, and $N_c \approx N_S$. In the opposite limit, $\Delta << \Delta_c$, the ratio N_c/N_S is exponentially small. Now Eq. (4) may be plugged into Eq. (3) to obtain the 1^{st} order corrections to μ and P, etc.)

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[1] Note also that Eq. (2) is valid in the (practically very important) case of donor dopants in semiconductors, with the ground state energy lower, by Δ, then the conduction band edge. (With the opposite sign under the exponent, it is also valid for acceptor dopants, with the ground state energy higher, by Δ, than the valence band edge.)

[2] The term "crossover" rather than "critical" is used to emphasize that the transition from one regime to another one is a smooth transition ("crossover") rather than a genuine (sharp) phase transition.

E (4 points). In the opposite limit of a relatively small number of particles, $N << N_S$, Eq. (3) may be satisfied only if the second term in its left-hand part is much less than N_S, i.e. at $\exp\{-(\Delta + \mu)/T\} >> g_S \sim 1$, so that the equation is reduced to

$$N_V(T)\exp\left\{\frac{\mu}{T}\right\} + N_S g_S \exp\left\{\frac{\Delta+\mu}{T}\right\} = N ,$$

and may be readily solved for μ:

$$\exp\left\{\frac{\mu}{T}\right\} = \frac{N}{N_V(T) + N_S g_S \exp\{\Delta/T\}}, \quad \text{so that } \mu = -T\ln\left(\frac{N_V(T)}{N} + \frac{N_S g_S}{N}\exp\left\{\frac{\Delta}{T}\right\}\right),$$

giving

$$N_g = N_V(T)\exp\left\{\frac{\mu}{T}\right\} = \frac{N}{1 + [N_S g_S / N_V(T)]\exp\{\Delta/T\}}, \qquad P = \frac{N_g T}{V} = \frac{T}{V}\frac{N}{1 + [N_S g_S / N_V(T)]\exp\{\Delta/T\}}.$$

Again, the ratio $N_V(T)/N$ has to be large for the gas to stay classical. However, since in our limit the ratio N_S/N is also large, and $\exp\{\Delta/T\}$ is a very steep function, the gas pressure depends mostly on the condensation energy Δ. If the energy is much larger than the crossover value Δ_c given by Eq. (5), the number of particles in the gas phase is exponentially small,

$$N_g = N_V(T)\frac{N}{N_S g_S}\exp\left\{-\frac{\Delta}{T}\right\} \propto T^{3/2}\exp\left\{-\frac{\Delta}{T}\right\}$$

(because virtually all particles are condensed on the surface traps), and so is its pressure:

$$P = \frac{T}{V}\frac{N_V(T)N}{N_S g_S}\exp\left\{-\frac{\Delta}{T}\right\} \propto NT^{5/2}\exp\left\{-\frac{\Delta}{T}\right\} .$$

Evidently, this result is very much different from the equation of state of a classical gas with a fixed number of particles. Note also a very natural trend, $P \propto 1/N_S$, though the condition $N_S >> N$ used for the derivation of this result does not allow using it to follow the no-trap limit $N_S \to 0$.

In the opposite limit of low condensation energy $\Delta << \Delta_c$, our result is again reduced to the pressure of an ideal classical gas of N particles, $P = NT/V$. This is natural, because in this limit virtually all particles are thermally activated into the gas phase.

F (1 point). Summarizing the above analysis, the particle condensation on the surface affects the gas properties substantially only if:

- the number N_S of traps is of the order of the N (or higher), *and*

- the condensation energy is larger than the crossover value (5).

Statistical Mechanics 3

The 1D Potts model

In the so-called Potts model, a uniform 1D chain of N classical spins (in the absence of an external magnetic field) is described by the following interaction Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\eta_i, \eta_j} \ , \text{with } J > 0 \ , \tag{1}$$

where J is a positive coupling constant, η_i is the classical spin variable at the site i, describing the spin state, which may take integer values in the set $\{1, ..., q\}$, $\delta_{a,b}$ is the Kronecker delta symbol; and the summation is over all pairs of adjacent spins. Consider the model with $q = 3$ in thermal equilibrium at temperature T.

Do parts parts (a), (b), and (c) for finite N, and then take the limit $N \to \infty$ for parts (d), (e), and (f). For parts (c), (d), (e), and (f), you should give an explicit closed-form expression, not an abstract expression involving a summation.

(a) (1 pts.) Write the general expression for the statistical sum (= partition function) Z of the system.

(b) (2 pts.) Assuming periodic boundary conditions, express Z via the appropriate transfer matrix.

(c) (4 pts.) Use this expression to calculate Z. (Check your work as all subsequent parts depend on this result.)

Take $N \to \infty$ for the remainder of the problem:

(d) (3 pts.) Calculate the free energy per site, F, and the average energy per site, E.

(e) (3 pts.) Calculate the specific heat capacity per site, C, and the entropy per site, S.

(f) (5 pts.) Calculate the values of E, C, and S in the limits $T \to 0$ and $T \to \infty$. Physically and quantitatively explain your results for E and S in both limits.

(g) (2 pts.) Does this system have a symmetry-breaking phase transition at finite temperature? Prove your answer.

Solution

(a) (1 pt.) Write the general expression for the statistical sum (= partition function) Z of the system. Ans. Let $\beta = 1/(k_B T)$, where k_B is the Boltzmann constant. In general, the partition function of a statistical system in thermal equilibrium at temperature T is

$$Z = \sum_{var.} e^{-\beta \mathcal{H}} \tag{2}$$

where the sum is over the values of all of the dynamical variables in the system. Let $K = \beta J$. Then here

$$Z = \sum_{\{\eta_r\}} e^{K \sum_{\langle ij \rangle} \delta_{\eta_i, \eta_j}} \tag{3}$$

where $\{\eta_r\}$ denotes the set of all variables η_r with r denoting a site on the lattice. Each of these variables η_r can take on values in the set $\{1,\ 2,\ 3\}$.

(b) (2 pts.) Assuming periodic boundary conditions, express Z via the appropriate transfer matrix. Ans. Denote the transfer matrix as $\mathcal{T}$, with matrix elements $\langle \eta_i | \mathcal{T} | \eta_j \rangle$. Given the periodic boundary conditions (BC),

$$Z = \mathrm{Tr}(\mathcal{T}^N) \tag{4}$$

(c) (4 pts.) Use this expression to calculate Z. Ans. Let $y = e^K$. Then in the basis of states (1,2,3), the transfer matrix is

$$\begin{pmatrix} y & 1 & 1 \\ 1 & y & 1 \\ 1 & 1 & y \end{pmatrix} \tag{5}$$

This is a real symmetric matrix, so it can be diagonalized by an orthogonal transformation R (with $R^T = R^{-1}$):

$$R \mathcal{T} R^{-1} = \mathcal{T}_d \equiv \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \tag{6}$$

where, as indicated, $\mathcal{T}_d$ is a diagonal matrix, and λ_p, $p = 1, 2, 3$ are the eigenvalues of $\mathcal{T}$. Thus, $\mathcal{T} = R^{-1} \mathcal{T}_d R$. Solving the indicial equation, we find these to be $\lambda_1 = y + 2$ and $\lambda_2 = \lambda_3 = y - 1$. Using the cyclic property of the trace, $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$, we have

$$\begin{aligned} \mathrm{Tr}(\mathcal{T}^N) &= \mathrm{Tr}[(R^{-1} \mathcal{T}_d R) \cdots (R^{-1} \mathcal{T}_d R)] \\ &= \mathrm{Tr}(\mathcal{T}_d^N) = (\lambda_1)^N + 2(\lambda_2)^N \\ &= (y+2)^N + 2(y-1)^N \end{aligned} \tag{7}$$

(where the $\cdots$ in the first line indicate an N-fold product). Hence,

$$Z = (y+2)^N + 2(y-1)^N \tag{8}$$

(d) (3 pts.) Calculate the Gibbs free energy per site, G, and the internal energy per site, E. The Gibbs free energy per site is $G = -k_B T f$, where the dimensionless function f is

$$\begin{aligned} f &= \lim_{N\to\infty} \frac{1}{N} \ln Z \\ &= \ln(y+2) \end{aligned} \tag{9}$$

so

$$G = -k_B T \ln(y+2) \tag{10}$$

Note that only the dominant eigenvalue contributes in this limit. The internal (configurational) energy per site E is given by

$$E = -\frac{\partial f}{\partial \beta} = -J\frac{\partial f}{\partial K} \tag{11}$$

Now $\partial/\partial K = (\partial y/\partial K)\partial/\partial y$ and $(\partial y/\partial K) = y$, so

$$E = -Jy\frac{\partial f}{\partial y} = -\frac{Jy}{y+2} \tag{12}$$

(e) (3 pts.) Calculate the specific heat capacity per site, C, and the entropy per site, S. Ans. The specific heat $C = dU/dT$ here. Now $dU/dT = -k_B(K^2/J)dU/dK$, so

$$C = k_B K^2 y \frac{\partial}{\partial y}\Big(\frac{y}{y+2}\Big) = \frac{2k_B K^2 y}{(y+2)^2} \tag{13}$$

The entropy S can be calculated from the relation $G = E - TS$, i.e., $S = (E-G)/T = k_B\beta(E-G)$. Subsituting our results for G and E, we have

$$S = k_B\Big[-\frac{Ky}{y+2} + \ln(y+2)\Big] \tag{14}$$

(f) (5 pts.) Calculate the values of E, C, and S in the low-temperature limit $T \to 0$ and the high-temperature limit $T \to \infty$. Ans. The limit $T \to \infty$ is $\beta \to 0$, i.e., $y \to 1$. In this limit,

$$E = -\frac{J}{3}, \quad C = 0, \quad S = k_B \ln 3 \quad \text{for } \beta \to 0 \tag{15}$$

The limit $T \to 0$ with $J > 0$ is $\beta \to \infty$ and $K \to \infty$. In this limit

$$E = -J, \quad C = 0, \quad S = 0 \quad \text{for } T \to 0 \tag{16}$$

These results can be understood physically. In the high-temperature limit the interaction is negligible compared to the temperature. The spins can be in any of the three states with equal probability, $1/3$. The entropy per site is then simply $S = k_B \ln 3$. Since the neighboring spins are random, the average energy per site is just the interaction energy between neighboring spins, times the probability that the two neighboring spins are in the

same state. There are three such same-state configurations out of the nine possible states of neighboring spins, and thus the energy per site is $-J/3$. As the temperature approaches 0, there is local ordering of the spins, so the energy per site approaches the interaction energy per site, $-J$. At $T = 0$ (but not at any finite temperature, regardless of how small), all of the spins are in one of the three states and the entropy per site is therefore zero. Although the entropy per site approaches zero continuously as $T \to 0$, the magnetization is identically zero for any finite temperature, regardless of how small, and jumps discontinuously to 1 at $T = 0$.

(g) (2 pts.) Does this system have a symmetry-breaking phase transition at finite temperature? Prove your answer. Ans. No, this system does not have a symmetry-breaking phase transition at finite temperature. The proof, using what is known as the Peierls argument, goes as follows. To simplify the proof, use the fact that the boundary conditions have no effect in the thermodynamic limit and hence use free boundary conditions. Assume that there is an incipient ordering, with a nonzero order parameter, i.e., magnetization, $\langle \eta_i \rangle = 1$ for all i. Clearly, this would break the symmetry of the theory, under which any of the three values of η_i is equally likely. We show that this incipient symmetry-breaking long-range order is not stable under a change that minimizes the Gibbs free energy $G = E - TS$. We can destabilize this incipient ordering by flipping the value of η_i to another value, say 2, for the interval $i \geq \ell$, where $1 \leq \ell \leq N$. The cost in energy is $\Delta E = J$ but since we can choose ℓ in any of N ways, the gain in entropy is $\Delta S = k_B \ln N$, so the total change in the Gibbs free energy is $\Delta G = J - k_B T \ln N$. Since $T > 0$, this is always negative as $N \to \infty$. So an incipient ordered state is not thermodynamically stable. Therefore, there is no symmetry-breaking phase transition of this system at finite temperature. (There is, in fact, a symmetry-breaking phase transition at zero temperature.) Another proof that is accepted is to observe that all of the thermodynamic functions are analytic for all $T > 0$, thereby precluding any phase transition, since the latter involves nonanalyticity of thermodynamic functions.