

OSU PHYSICS DEPARTMENT
COMPREHENSIVE EXAMINATION #108

March 29 and 30, 2010

Spring 2010 Comprehensive Examination

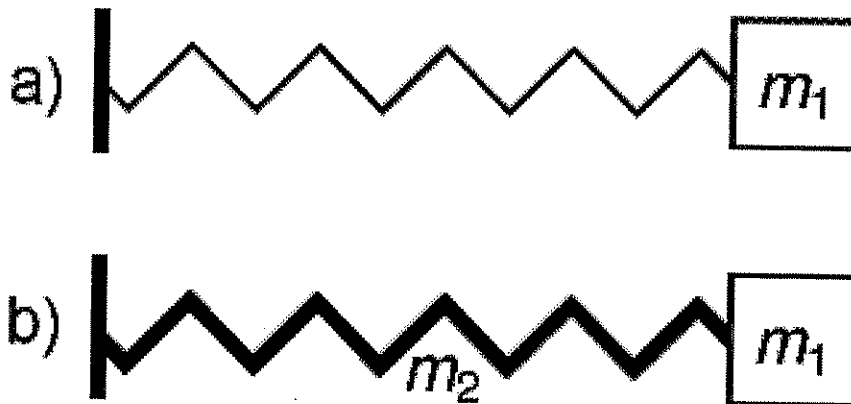
PART 1, Monday, March 29, 9:00am

General Instructions

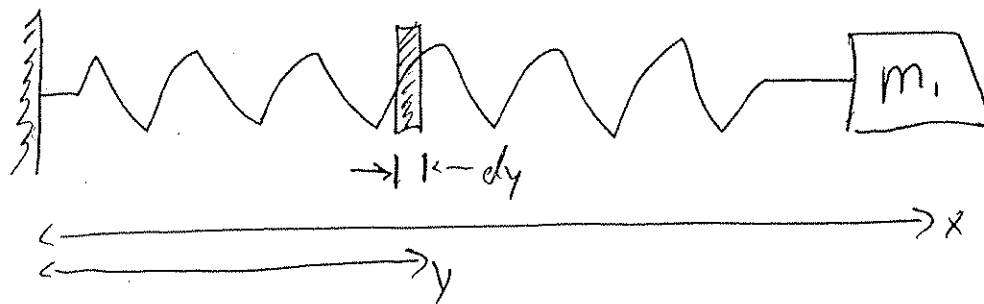
This Spring 2010 Comprehensive Examination consists of eight problems of equal weight (20 points each). It has four parts. The first part (Problems 1-2) is handed out at 9:00 am on Monday, March 29, and lasts three hours. The second part (Problems 3-4) will be handed out at 1:00 pm on the same day and will also last three hours. The third and fourth parts will be administered on Tuesday, March 30, at 9:00 am and 1:00 pm, respectively. Work carefully, indicate your reasoning, and display your work clearly. Even if you do not complete a problem, it might be possible to obtain partial credit—especially if your understanding is manifest. Use no scratch paper; do all work in the bluebooks, work each problem in its own numbered bluebook, and be certain that your chosen student letter (but not your name) is inside the back cover of every booklet. Be sure to make note of your student letter for use in the remaining parts of the examination.

If something is omitted from the statement of the problem or you feel there are ambiguities, please get up and ask your question quietly and privately, so as not to disturb the others. Put all materials, books, and papers on the floor, except the exam, bluebooks and the collection of formulas and data distributed with the exam. Calculators are not allowed except when a numerical answer is required—calculators will then be provided by the person proctoring the exam. Please return all bluebooks and formula sheets at the end of the exam. Use the last pages of your bluebooks for “scratch” work, separated by at least one empty page from your solutions. “Scratch” work will not be graded.

Consider a one-dimensional undamped oscillator of mass m_1 and spring constant k , as illustrated in Fig. (a), where the spring is fixed to a wall at left. In the standard analysis, the spring is assumed to be massless and the resulting motion of the mass is simple harmonic motion. For this problem, assume that the spring has a mass m_2 , as illustrated in Fig. (b). Assume that the spring is uniform and that it stretches uniformly. The potential energy of this massive spring is $kx^2/2$ (the same as the massless spring in Fig. (a)), but the kinetic energy of the massive spring must now be included in the analysis. Use the Lagrange method to find the motion of this new system (Fig. (b)) and show that the system undergoes simple harmonic motion with a frequency different from the massless spring case (Fig. (a)). Find this new frequency.



Solutions of Problem #1



$\frac{y}{x} = f$ fractional position

Spring KE: $dT_s = \frac{1}{2} \rho dy \dot{y}^2$ $\rho = \frac{m_2}{x}$

$dT_s = \frac{1}{2} \left(\frac{m_2}{x}\right) f^2 \dot{x}^2 x df$

$T_s = \int dT = \int_0^1 \frac{1}{2} m_2 \dot{x}^2 f^2 df$

$= \frac{m_2}{2} \dot{x}^2 \left[\frac{f^3}{3} \right]_0^1$

$T_s = \frac{1}{6} m_2 \dot{x}^2$

$\mathcal{L} = T - U = \frac{1}{2} m_1 \dot{x}^2 + \frac{1}{6} m_2 \dot{x}^2 - \frac{1}{2} k x^2$
 $= \frac{1}{2} \dot{x}^2 (m_1 + \frac{1}{3} m_2) - \frac{1}{2} k x^2$

$\frac{\partial \mathcal{L}}{\partial x} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}}$ $\frac{\partial \mathcal{L}}{\partial x} = -kx$; $\frac{\partial \mathcal{L}}{\partial \dot{x}} = \dot{x} (m_1 + \frac{1}{3} m_2)$

$\Rightarrow -kx = \ddot{x} (m_1 + \frac{1}{3} m_2) \Rightarrow \ddot{x} = -\frac{k}{m_1 + \frac{1}{3} m_2} x$

\Rightarrow SHO

ω

$\omega = \sqrt{\frac{k}{m_1 + \frac{1}{3} m_2}}$

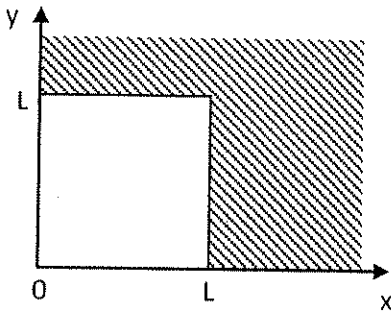
QM

Problem #2

Consider a particle with mass M in a two-dimensional square box of length L (see Figure below). The system is perturbed by a weak potential $V'(x, y) = V_0 L^2 \delta(x - x_0) \delta(y - y_0)$, with $V_0 > 0$.

- 1) Write down energies and eigenfunctions of the unperturbed system.
- 2) What is the unperturbed energy of the ground state? Find a first-order correction to the energy of the ground state. Also find a first-order correction to the wave function of the ground state.
- 3) What is the unperturbed energy of the first excited state? Find a first-order correction to the energy of the first excited state.
- 4) Sketch unperturbed energy levels of the ground and first excited state and what happens to them upon perturbation for the cases: (i) $x_0 = y_0 = L/4$ and (ii) $x_0 = y_0 = L/2$. Discuss.

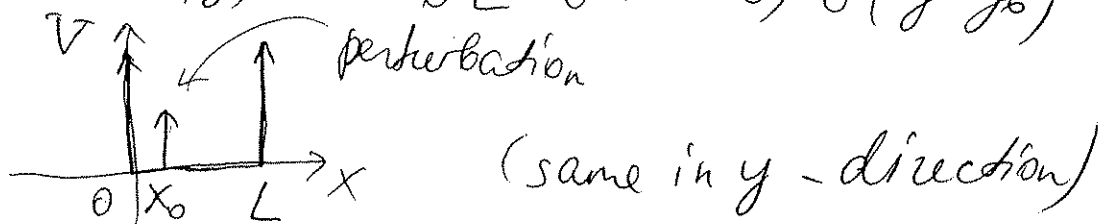
Hint: First-order correction to the l -th state is $|\varphi_l^{(1)}\rangle = \sum_{n \neq l} \frac{\langle \varphi_n | V' | \varphi_l \rangle}{E_l^{(0)} - E_n^{(0)}} |\varphi_n\rangle$



Solution of Problem # 2

(1)

$$V'(x, y) = V_0 L^2 \delta(x - x_0) \delta(y - y_0)$$



1) The eigenfunctions and energies of the unperturbed states are:

$$\psi_{nm}^{(0)}(x, y) = \frac{2}{L} \sin\left(\frac{j\pi x}{L}\right) \sin\left(\frac{j\pi y}{L}\right)$$

particle in 2D box

$$E_{nm}^{(0)} = \frac{j^2 \hbar^2}{2ML^2} (n^2 + m^2)$$

← mass of the particle

2) Ground state: $n = m = 1 \Rightarrow E_{11}^{(0)} = \frac{j^2 \hbar^2}{ML^2}$

First-order energy correction:

$$E_{11}^{(1)} = \langle \psi_{11}^{(0)} | V' | \psi_{11}^{(0)} \rangle = \frac{4}{L^2} V_0 L^2 \int_0^L \int_0^L \sin^2\left(\frac{j\pi x}{L}\right) \sin^2\left(\frac{j\pi y}{L}\right) \delta(x - x_0) \delta(y - y_0) dx dy = 4V_0 \sin^2\left(\frac{j\pi x_0}{L}\right)$$

$n=1$

First-order state vector correction:

(C)

$$|\psi_{11}^{(1)}\rangle = \sum_{n,m \neq 1,1} \frac{\langle \psi_{nm}^{(0)} | V' | \psi_{11}^{(0)} \rangle}{E_{11}^{(0)} - E_{nm}^{(0)}} |\psi_{nm}^{(0)}\rangle$$
$$= \sum_{n,m \neq 1,1} \frac{4V_0 \int_0^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi n x}{L}\right) \delta(x-x_0) dx \int_0^L \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi m y}{L}\right) dy}{E_{11}^{(0)} - E_{nm}^{(0)}}$$

• $\delta(y-y_0) dy$

$$\cdot \frac{2}{L} \sin\left(\frac{\pi n x}{L}\right) \sin\left(\frac{\pi m y}{L}\right) =$$

$$= \frac{16V_0 ML}{\pi^2 \hbar^2} \sum_{n,m \neq 1,1} \frac{\sin\left(\frac{\pi x_0}{L}\right) \sin\left(\frac{\pi y_0}{L}\right) \sin\left(\frac{\pi n x_0}{L}\right) \sin\left(\frac{\pi m y_0}{L}\right)}{2 - n^2 - m^2}$$

$$\uparrow \quad E_{11}^{(0)} - E_{nm}^{(0)} = \frac{\pi^2 \hbar^2}{2ML^2} (2 - n^2 - m^2)$$

$$\cdot \sin\left(\frac{\pi n x}{L}\right) \sin\left(\frac{\pi m y}{L}\right)$$

3) First excited state energy $E_{12}^{(0)} = E_{21}^{(0)} =$
 $= \frac{\pi^2 \hbar^2}{2ML^2} \cdot 5$ double-degenerate

(C)

Use degenerate perturbation theory: (3)

$$|\Psi_{12}^{(0)}\rangle \Rightarrow \frac{2}{L} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right)$$

$$|\Psi_{21}^{(0)}\rangle \Rightarrow \frac{2}{L} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right)$$

Compose 2×2 matrix:

$$\begin{bmatrix} \langle \Psi_{12}^{(0)} | \mathcal{V}' | \Psi_{12}^{(0)} \rangle & \langle \Psi_{12}^{(0)} | \mathcal{V}' | \Psi_{21}^{(0)} \rangle \\ \langle \Psi_{21}^{(0)} | \mathcal{V}' | \Psi_{12}^{(0)} \rangle & \langle \Psi_{21}^{(0)} | \mathcal{V}' | \Psi_{21}^{(0)} \rangle \end{bmatrix} \equiv$$

$$\equiv \begin{bmatrix} \mathcal{V}'_{12,12} & \mathcal{V}'_{12,21} \\ \mathcal{V}'_{21,12} & \mathcal{V}'_{21,21} \end{bmatrix}$$

Now,
$$\begin{vmatrix} \mathcal{V}'_{12,12} - E_{12}^{(1)} & \mathcal{V}'_{12,21} \\ \mathcal{V}'_{21,12} & \mathcal{V}'_{21,21} - E_{12}^{(1)} \end{vmatrix} = 0 \Rightarrow$$

$$\mathcal{V}'_{12,21} = \mathcal{V}_0 \int_0^L \int_0^L \frac{4}{L^2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi x}{L}\right) \delta(x-x_0) \sin\left(\frac{\pi y}{L}\right)$$

$$\cdot \sin\left(\frac{2\pi y}{L}\right) \delta(y-y_0) dx dy = 4\mathcal{V}_0 \sin\left(\frac{\pi x_0}{L}\right) \sin\left(\frac{2\pi x_0}{L}\right)$$

$$\sin\left(\frac{\pi y_0}{L}\right) \sin\left(\frac{2\pi y_0}{L}\right) = \mathcal{V}'_{21,12}$$

$$\sum_0, \quad (\bar{V}_{12,12}^1 - E_{12}^{(1)}) (\bar{V}_{21,21}^1 - E_{12}^{(1)}) - (\bar{V}_{12,21}^1)^2 = 0 \quad (4)$$

$$(E_{12}^{(1)})^2 - E_{12}^{(1)} (\bar{V}_{12,12}^1 + \bar{V}_{21,21}^1) + \bar{V}_{12,12}^1 \bar{V}_{21,21}^1 - (\bar{V}_{12,21}^1)^2 = 0;$$

$$\begin{aligned} \mathcal{D} &= (\bar{V}_{12,12}^1 + \bar{V}_{21,21}^1)^2 - 4 (\bar{V}_{12,12}^1 \bar{V}_{21,21}^1 - (\bar{V}_{12,21}^1)^2) \\ &= (\bar{V}_{12,12}^1 - \bar{V}_{21,21}^1)^2 + 4 (\bar{V}_{12,21}^1)^2 = (\bar{V}_{12,12}^1 + \bar{V}_{21,21}^1)^2 \end{aligned}$$

$$E_{12}^{(1)} = \frac{\bar{V}_{12,12}^1 + \bar{V}_{21,21}^1}{2} \pm \frac{\sqrt{\mathcal{D}}}{2} = 0; \quad \bar{V}_{12,12}^1 + \bar{V}_{21,21}^1$$

$$\bar{V}_{12,12}^1 = \frac{4}{L^2} \bar{V}_0 L^2 \sin^2\left(\frac{\pi x_0}{L}\right) \sin^2\left(\frac{2\pi y_0}{L}\right)$$

$$\bar{V}_{21,21}^1 = 4\bar{V}_0 \sin^2\left(\frac{2\pi x_0}{L}\right) \sin^2\left(\frac{\pi y_0}{L}\right)$$

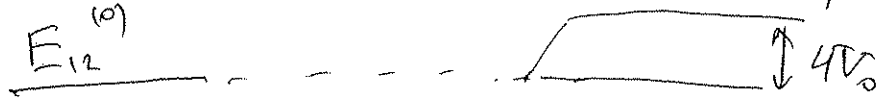
$$4) \quad x_0 = \frac{L}{4}, \quad y_0 = \frac{L}{4} \Rightarrow$$

$$E_{11}^{(1)} = 4\bar{V}_0 \cdot \left(\frac{\sqrt{2}}{2}\right)^4 = \bar{V}_0$$

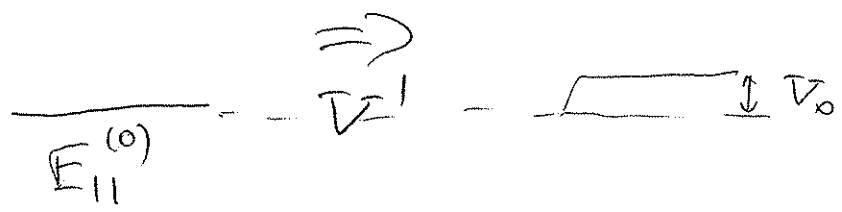
(5)

$$E_{12}^{(1)} = 2V_0 \pm 2V_0 = \begin{cases} 4V_0 \\ 0 \end{cases}$$

$$V_{12,12}^1 = 4V_0 \frac{1}{2} = 2V_0; \quad V_{21,21}^1 = 2V_0; \quad V_{12,21}^1 = 2V_0$$



← degeneracy removed



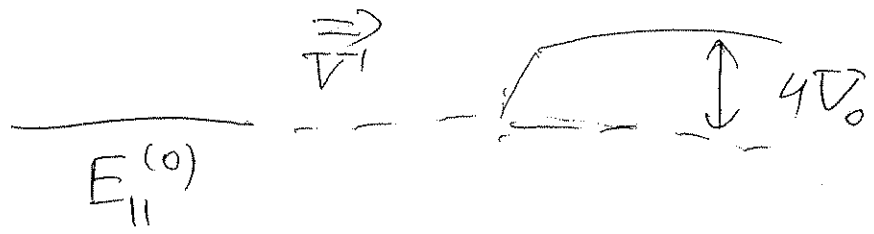
$$x_0 = \frac{L}{2}, \quad y_0 = \frac{L}{2} \Rightarrow E_{11}^{(1)} = 4V_0$$

$$E_{12}^{(1)} = 0$$

$$V_{12,12}^1 = 0, \quad V_{21,21}^1 = 0, \quad V_{12,21}^1 = 0$$



← degeneracy is not removed



$$\psi_{12}^{(0)} \text{ or } \psi_{21}^{(0)}$$

not surprising, since wave function (unperturbed) vanishes at $x=y=\frac{L}{2}$ whether there is a δ -function perturbation at that spot

Due to a cooking mistake, you discover that a particular black rock, when heated, turns orange in a reversible way. After careful investigation, you establish that this is a bona fide phase transition. Through careful measurements, you establish that the phase transition occurs at temperature T_c , when the pressure is p_0 .

- (a) You measure the volume change when the rock changes color, and find that the volume increases by an amount ΔV when the rock is heated to turn orange at temperature T_c at constant pressure p_0 . How much work is done during this process?

Solution:

At constant pressure, a change of ΔV gives a work done *by* the rock when it turns orange of

$$W = p_0 \Delta V \quad (1)$$

which is positive.

- (b) You measure the heat required to turn the rock orange, and find a result L (which is positive), for the same process in which the rock starts and ends at T_c , at constant pressure p_0 . What is the change in entropy of the rock when it changes from black to orange? Is the entropy of the rock greater when it is orange or when it is black?

Solution:

The change in entropy for any reversible process is

$$\Delta S = \int \frac{dQ_{\text{reversible}}}{T} \quad (2)$$

For a reversible, isothermal process, this integral is trivial, and we find that

$$\Delta S = \frac{L}{T_c} \quad (3)$$

Which tells us that since L is positive, the entropy of the rock is greater when it is orange than when it is black.

- (c) What is the change in the rock's internal energy under this transformation? Which color rock has a greater internal energy?

Solution:

We can just use the first law, and see that

$$\Delta U = Q - W \quad (4)$$

$$= L - p_0 \Delta V \quad (5)$$

We don't know if this is positive or negative, that depends on the relative values of L and ΔV .

- (d) What is the criterion for a pressure and temperature at which the black and orange phases may coexist?

Solution:

The coexistence criterion for fixed pressure and temperature is that the Gibbs free energy of the two phases must be the same.

We can derive (although you were not required to do so) this from the second law, by recognizing that if the two phases can coexist, we must be able to reversibly transform between them. So the entropy of system plus surroundings must not change when the phase transition happens.

$$\Delta S_{\text{rock}} + \Delta S_{\text{surroundings}} = 0 \quad (6)$$

So now we have to figure out how much the entropy of the surroundings when the rock transforms. One part of that is the latent heat, but we're also doing work on the surroundings by changing our volume. Let's go back to the thermodynamic identity...

$$dU_{\text{surroundings}} = TdS_{\text{surroundings}} - pdV_{\text{surroundings}} \quad (7)$$

$$dS_{\text{surroundings}} = \frac{dU_{\text{surroundings}}}{T} + \frac{pdV_{\text{surroundings}}}{T} \quad (8)$$

$$= -\frac{dU_{\text{rock}}}{T} - \frac{pdV_{\text{rock}}}{T} \quad (9)$$

where, in the last line, we took advantage of the fact that the change in volume and internal energy of the rock and its surroundings must be equal and opposite (by conservation).

$$0 = \Delta S_{\text{rock}} + \Delta S_{\text{surroundings}} \quad (10)$$

$$= \Delta S_{\text{rock}} - \frac{\Delta U_{\text{rock}}}{T} - \frac{p\Delta V_{\text{rock}}}{T} \quad (11)$$

$$0 = \frac{\Delta U_{\text{rock}}}{T} + \frac{p\Delta V_{\text{rock}}}{T} + -\Delta S_{\text{rock}} \quad (12)$$

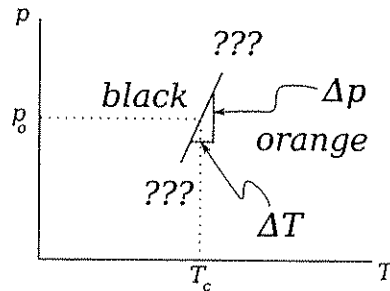
$$0 = \Delta U_{\text{rock}} + p\Delta V_{\text{rock}} - T\Delta S_{\text{rock}} \quad (13)$$

$$= \Delta(U + pV - TS) \quad (14)$$

$$= \Delta G_{\text{rock}} \quad (15)$$

where in the last step we take advantage of the fact that the phase change we're looking at is a constant-pressure, constant-temperature process, since we're talking about coexistence at a given pressure and temperature.

- (e) Suppose you'd like to sketch a phase diagram of the rock, but aren't easily able to change the pressure. You start sketching the phase diagram as shown below, but need to figure out the slope at T_c . What is the slope of this coexistence line, $\frac{\Delta p}{\Delta T}$?¹



Solution:

Given the answer to the previous question, this one is pretty simple. Our coexistence condition is that

$$G_{\text{orange}}(p, T) = G_{\text{black}}(p, T) \quad (16)$$

Since we only have data at p_0, T_c , we must expand about that point:

$$G_{\text{orange}}(p_0, T_c) + \Delta G_{\text{orange}} = G_{\text{black}}(p, T) + \Delta G_{\text{black}} \quad (17)$$

$$G_{\text{orange}}(p_0, T_c) + V_{\text{orange}}\Delta p - S_{\text{orange}}\Delta T = G_{\text{black}}(p, T) + V_{\text{black}}\Delta p - S_{\text{black}}\Delta T \quad (18)$$

$$G_{\text{orange}}(p_0, T_c) + V_{\text{orange}}(p - p_0) - S_{\text{orange}}(T - T_c) = G_{\text{black}}(p, T) + V_{\text{black}}(p - p_0) - S_{\text{black}}(T - T_c) \quad (19)$$

$$V_{\text{orange}}(p - p_0) - S_{\text{orange}}(T - T_c) = V_{\text{black}}(p - p_0) - S_{\text{black}}(T - T_c) \quad (20)$$

$$(V_{\text{orange}} - V_{\text{black}})(p - p_0) = (S_{\text{orange}} - S_{\text{black}})(T - T_c) \quad (21)$$

$$\frac{p - p_0}{T - T_c} = \frac{S_{\text{orange}} - S_{\text{black}}}{V_{\text{orange}} - V_{\text{black}}} \quad (22)$$

$$\frac{p - p_0}{T - T_c} = \frac{\Delta S}{\Delta V} \quad (23)$$

$$\frac{\Delta p}{\Delta T} = \frac{\Delta S}{\Delta V} \quad (24)$$

$$\frac{\Delta p}{\Delta T} = \frac{L}{T\Delta V} \quad (25)$$

¹Yes, you can find this based on the information already given...

- (f) Is this slope positive or negative? Under what circumstance would the slope have a different sign?

Solution:

This slope is positive, since L , ΔV and T are all positive. In order for the slope to be negative, we'd need for ΔV and L to have opposite signs, which means when you heat the rock up, it would have to shrink, like ice does when you melt it.

This problem deals with the time-dependent potentials and fields arising from a single moving charge q in the Lorentz Gauge.

- a. What is the Lorentz condition?
- b. Write the wave equations for the potentials Φ and \vec{A} in this gauge.
- c. What is the appropriate Green function $G(\vec{r}, \vec{r}', t, t')$?
- d. The charge q moves along the trajectory $\vec{r}'(t)$ at constant velocity \vec{v} . Show that scalar and vector potentials measured at the origin are

$$\Phi(t) = \frac{1}{4\pi\epsilon_0} \frac{q}{r + \vec{r}' \cdot \vec{v}/c} \quad \text{and} \quad \vec{A}(t) = \frac{\mu_0}{4\pi} \frac{q\vec{v}}{r + \vec{r}' \cdot \vec{v}/c}.$$

- e. Find the electric and magnetic fields at the origin.
- f. Find the momentum density of the electromagnetic field due to this moving charge.

Moving Charge Potentials

$$a) \vec{B} = \vec{v} \times \vec{A} \quad \text{and} \quad \vec{v} \times \vec{B} = -\frac{\partial \vec{B}}{\partial t} = \vec{v} \times \left(\vec{v} \times \vec{A} - \frac{\partial \vec{A}}{\partial t} \right)$$

$$\vec{v} \cdot \vec{B} = \rho / \epsilon_0 \Rightarrow \nabla^2 \Phi + \frac{\partial}{\partial t} \vec{v} \cdot \vec{A} = -\rho / \epsilon_0$$

$$\vec{v} \times \vec{B} = \mu_0 \vec{J} + \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} = \mu_0 \vec{J} + \mu_0 \epsilon_0 \left(-\nabla \Phi - \frac{\partial \vec{A}}{\partial t} - \nabla (\vec{v} \cdot \vec{A}) + \frac{\partial^2 \Phi}{c^2 \partial t^2} \right)$$

$$\text{Lorentz gauge: } \nabla \cdot \vec{A} + \frac{1}{c^2} \frac{\partial \Phi}{\partial t} = 0$$

$$b) \nabla^2 \vec{A} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} = -\mu_0 \vec{J}$$

$$\nabla^2 \Phi - \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} = -\rho / \epsilon_0$$

$$c) \nabla^2 G - \frac{1}{c^2} \frac{\partial^2 G}{\partial t^2} = -4\pi \delta(\vec{r} - \vec{r}') \delta(t - t')$$

$$G(\vec{r}, \vec{r}', t, t') = \frac{\delta(t - t' - |\vec{r} - \vec{r}'|/c)}{|\vec{r} - \vec{r}'|}$$

$$d) \Phi(\vec{x}, t) = \int dt' d^3x' \frac{g(\vec{x}', t') \delta(t' - t + |\vec{x} - \vec{x}'|/c)}{|\vec{x} - \vec{x}'|}$$

$$g(\vec{x}, t) = q \delta(\vec{x} - \vec{r}_0(t))$$

$$\Phi(\vec{x}, t) = \int dt' q \frac{\delta(t' - t + |\vec{x} - \vec{r}_0(t')|/c)}{|\vec{x} - \vec{r}_0(t')|}$$

Using $\vec{r}(\vec{x}, t) = \vec{x} - \vec{r}_0(t)$, and $t' + \frac{r(\vec{x}, t')}{c} = t$

for fixed \vec{x} , $(1 - \hat{n} \cdot \vec{v}/c) \frac{\partial t'}{\partial r} = 1$, $\hat{n} = \frac{\vec{r}(\vec{x}, t')}{r(\vec{x}, t')}$

and $\vec{v} = \dot{\vec{r}}_0(t')$

$$\text{So } \Phi(\vec{x}, t) = \frac{1}{4\pi\epsilon_0} \frac{q}{r - \vec{r} \cdot \vec{v}/c}$$

For \vec{A} , use $\vec{J}(\vec{x}, t) = q(\vec{x}, t) \vec{v}(t) = q \delta(\vec{x} - \vec{r}_0(t)) \dot{\vec{r}}_0(t)$

$$\text{then } \vec{A}(\vec{x}, t) = \frac{\mu_0}{4\pi} \frac{e\vec{v}}{r - \vec{r} \cdot \vec{v}/c}$$

If $\vec{x} = \text{origin}$, then $\vec{r} = -\vec{r}_0$

$$e) \vec{v} = \dot{\vec{r}}_0 = \text{constant}$$

$$\vec{E} = \frac{e}{4\pi\epsilon_0} \frac{1 - v^2/c^2}{r^2 (1 - \hat{n} \cdot \vec{v}/c)^3} (\hat{n} - \vec{v}/c)$$

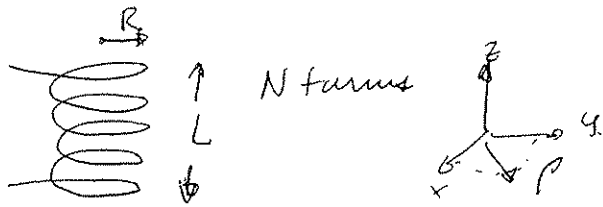
$$\text{and } \vec{B} = \frac{1}{c} \hat{n} \times \vec{E}$$

$$f) \vec{g} = \vec{S}/c^2 = \frac{\vec{E} \times \vec{B}}{\mu_0 c^2}$$

A solenoid of length L and radius R has N total turns and is subjected to a current $I(t) = I_0 e^{-i\omega t}$. Assume that $L \gg R$. The center of the solenoid is at the origin of your coordinate system, and it is oriented along the z axis.

- a. Find the leading term in the electric field within the solenoid.
- b. Find the leading term in the electric field at position \vec{r} when $r \gg L$.
- c. Determine the Poynting vector and explain the physical significance in both regions.

Solenoid and $I(t)$ problem.



$$I(t) = I_0 e^{-i\omega t}$$

Slowly varying.

a) $\vec{\nabla} \times \vec{B} = \mu_0 \vec{J} \Rightarrow \oint \vec{B} \cdot d\vec{l} = \mu_0 N I$ for loop path \perp loops.
 Assume $\vec{B}_{\text{outside}} = 0$. Then $B_{\text{inside}} L = \mu_0 N I(t)$.

$$\text{or } \vec{B} \approx \mu_0 \frac{N}{L} I(t) \hat{z} \text{ inside}$$

Now use $\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$ to find $\vec{E}(t)$,

path with $\rho < R$. $\oint \vec{E} \cdot d\vec{l} = -\frac{\partial}{\partial t} \int \vec{B} \cdot d\vec{l}$

$$E(t) 2\pi r = -\frac{\partial}{\partial t} \pi r^2 \mu_0 n I(t) \text{ with } n = N/L$$

$$\text{So } \vec{E}(t) = \frac{i\omega r \mu_0 n}{2} I(t) \hat{\phi} \text{ note the phase!}$$

No other components of \vec{E} arising from $I(t)$ are possible by symmetry since $(\vec{\nabla} \times \vec{E})_z = \frac{\partial}{\partial r} E_\phi - \frac{1}{r} \frac{\partial}{\partial \phi} E_r$

$$\text{and } \frac{\partial}{\partial \phi} E_r = 0$$

b) Far outside the solenoid, \vec{B} arises from a point magnetic dipole $\vec{m} = I A N \hat{z}$ where $A = \pi R^2$.

Slowly-varying field: $\vec{B} = -\vec{\nabla} \Phi_m = \frac{\mu_0}{4\pi} \frac{3\vec{r}(\vec{m} \cdot \vec{r}) - \vec{m}r^2}{r^3}$

$$\vec{B}(\vec{r}) = \frac{\mu_0}{4\pi} \left[\frac{2m \cos \theta \vec{r}}{r^3} - \frac{m \sin^2 \theta \hat{\theta}}{r^3} \right] \text{ This is not the radiative field!}$$

Consider $\theta = \pi/2$ then $(\vec{\nabla} \times \vec{E})_\theta = -\frac{\partial}{\partial r} E_\phi = -\frac{\partial}{\partial t} B_\theta$ by symmetry

c) Inside: $\vec{S} = \frac{\vec{E} \times \vec{B}}{\mu_0} = \frac{\mu_0 n^2 I_0^2 \omega r \hat{\rho}}{2} e^{-i\omega t} e^{-i(\omega t - \pi/2)}$

Time average $\langle \vec{S} \rangle = \phi$.

Outside: Since \vec{E} differs by phase factor $e^{i\pi/2}$, $\langle \vec{S} \rangle = 0$

QM

Problem #1

Consider coherent states $|z\rangle$ of a simple harmonic oscillator given by $|z\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle$ in terms of the complex number z .

- 1) Show that states $|z\rangle$ are normalized and are eigenstates of the annihilation operator a .
- 2) Find the expectation value of the number operator N in the coherent state $|z\rangle$.
- 3) Suppose that the oscillator is initially (i.e. at $t = 0$) in the state $|z\rangle$. Calculate the probability of finding the oscillator in the same state $|z\rangle$ at a later time $t > 0$.
- 4) Is the time-evolved state still an eigenstate of the annihilation operator a ?
- 5) Calculate the expectation value of the number operator N in the time-evolved state. Discuss.

Solution of Problem #5

(1)

$$\begin{aligned} 1) \langle z|z \rangle &= e^{-|z|^2} \sum_{m,n=0}^{\infty} \frac{(z^*)^m z^n}{\sqrt{m!n!}} \underbrace{\langle m|n \rangle}_{\delta_{mn}} \\ &= e^{-|z|^2} \sum_{n=0}^{\infty} \frac{|z|^{2n}}{n!} = 1 \end{aligned}$$

" $e^{|z|^2}$

$$\underbrace{a|z\rangle}_{\substack{\text{"} \\ \sqrt{n}|n-1\rangle}} = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} \underbrace{|n\rangle}_{\substack{\text{"} \\ \sqrt{n}|n-1\rangle}} =$$

$$= e^{-|z|^2/2} z \sum_{n=1}^{\infty} \frac{z^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle = z|z\rangle$$

$|z\rangle$ is an eigenstate of \hat{a} with eigenvalue z .

$$2) \langle N \rangle = \langle z| \hat{a}^\dagger \hat{a} |z\rangle = |z|^2$$

↑
part 1)

3) Time-evolved state

(2)

$$|\Psi(t)\rangle = \sum_{n=0}^{\infty} C_n e^{-\frac{i}{\hbar} E_n t} |n\rangle =$$

$$C_n = e^{-|z|^2/2} \frac{z^n}{\sqrt{n!}}$$

$$E_n = \hbar \omega (n + \frac{1}{2})$$

$$= e^{-i\omega t/2} e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{(ze^{-i\omega t})^n}{\sqrt{n!}} |n\rangle$$

The probability amplitude for being in the initial state $|z\rangle$ at time t :

$$\langle z | \Psi(t) \rangle = e^{-i\omega t/2} e^{-|z|^2} \underbrace{\sum_{n=0}^{\infty} \frac{|z|^{2n} e^{-i\omega t n}}{n!}}_{"}$$

$$= e^{-i\omega t/2} e^{-|z|^2} e^{|z|^2 e^{-i\omega t}} = e^{-i\omega t/2} e^{-|z|^2 (1 - e^{-i\omega t})}$$

$$= e^{-i\omega t/2} e^{-|z|^2} e^{|z|^2 \cos \omega t} e^{-|z|^2 i \sin \omega t}$$

The probability

(3)

$$P = |\langle z | \Psi(t) \rangle|^2 = |e^{-i\omega t/2} e^{-|z|^2} \cdot e^{|z|^2 \cos \omega t} e^{-i|z|^2 \sin \omega t}|^2 = e^{-2|z|^2(1 - \cos \omega t)} = e^{-4|z|^2 \sin^2 \frac{\omega t}{2}}$$

4) Time-evolved state is $|\Psi(t)\rangle \stackrel{\text{part 3)}}{=} e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-|z|^2/2} \frac{z^n}{\sqrt{n!}} e^{-i\omega(n+1/2)t} |n\rangle$

$$a|\Psi(t)\rangle = e^{-|z|^2/2} e^{-i\omega t/2} \sum_{n=1}^{\infty} \frac{z^n e^{-i\omega n t}}{\sqrt{(n-1)!}} |n-1\rangle = z e^{i\omega t} e^{-|z|^2/2} e^{-i\omega t/2} \sum_{n=1}^{\infty} \frac{z^{n-1} e^{-i\omega(n-1)t}}{\sqrt{(n-1)!}} |n-1\rangle \stackrel{\text{"}}{=} |\Psi(t)\rangle$$

So, $|\Psi(t)\rangle$ is an eigenstate of a with eigenvalue

$$\langle N \rangle = \langle \Psi(t) | a^\dagger a | \Psi(t) \rangle = |z|^2 e^{i\omega t}$$

Consider a one-dimensional damped oscillator of mass m , spring constant k , and resistive damping force $f_r = -bv$. The oscillator is subject to an external driving force $F(t) = F_0 \cos(\omega t)$, where ω is a variable angular frequency.

- (a) Solve Newton's equation of motion to find the amplitude of motion in the steady state. In your solution, identify the "natural" angular frequency of the system and the "damping constant" (with dimensions of angular frequency) of the system.
- (b) Find the relative phase of the oscillator motion with respect to the driving force. Discuss the behavior of the phase for angular frequencies above, below and equal to the "natural" angular frequency of the system.
- (c) Show that the amplitude of motion of this driven, damped system has a maximum response at an angular frequency that is shifted with respect to the natural angular frequency of the system.
- (d) Find the average power that the external force delivers to the system. Show that the delivered power is a maximum when the driving angular frequency equals the natural angular frequency of the system.

Consider a diatomic molecule such as H_2 , with a bond length a , a molecular mass M and a vibrational frequency ω_0 . The low-energy eigenstates of a single such molecule are well approximated by

$$E_{\mathbf{k},n,l,m} = \frac{\hbar^2 k^2}{2M} + \left(n + \frac{1}{2}\right) \hbar \omega_0 + \frac{\hbar^2 l(l+1)}{2Ma^2}$$

You may assume that interactions between molecules are negligible.

- (a) Write down a partition function describing a gas of N noninteracting molecules at temperature T . Throughout this problem, you may assume that the temperature is sufficiently high that you can safely treat the translational degrees of freedom classically. *At this stage, you need not eliminate all summations from the partition function.*

Solution:

$$Z \equiv \sum_i^{\text{all states}} e^{-\beta E_i} \quad (26)$$

$$\beta \equiv \frac{1}{k_B T} \quad (27)$$

since these are non-interacting particles, the energy separates. And the energy of a single molecule also separates, in the approximation provided.

$$Z = \frac{1}{N!} \sum_{\vec{k}_1, n_1, l_1, m_1} \sum_{\vec{k}_2, n_2, l_2, m_2} \cdots \sum_{\vec{k}_N, n_N, l_N, m_N} e^{-\beta (E_{\vec{k}_1, n_1, l_1, m_1} + E_{\vec{k}_2, n_2, l_2, m_2} + \cdots + E_{\vec{k}_N, n_N, l_N, m_N})} \quad (28)$$

$$= \frac{1}{N!} \left(\sum_{\vec{k}nlm} e^{-\beta E_{\vec{k}nlm}} \right)^N \quad (29)$$

$$= \frac{1}{N!} Z_1^N \quad (30)$$

$$a) F = ma$$

$$F(t) - kx - b\dot{x} = m\ddot{x}$$

$$\ddot{x} + \frac{b}{m}\dot{x} + \frac{k}{m}x = \frac{F_0}{m}\cos\omega t = \operatorname{Re}\left[\frac{F_0}{m}e^{i\omega t}\right]$$

$$\frac{b}{2m} \equiv \beta = \text{damping constant}$$

$$\sqrt{\frac{k}{m}} \equiv \omega_0 = \text{natural frequency}$$

$$\ddot{x} + 2\beta\dot{x} + \omega_0^2 x = \frac{F_0}{m}e^{i\omega t}$$

$$x = Ce^{i\omega t}$$

$$(-\omega^2 + 2i\beta\omega + \omega_0^2)Ce^{i\omega t} = \frac{F_0}{m}e^{i\omega t}$$

$$\Rightarrow C = \frac{F_0/m}{\omega_0^2 - \omega^2 + 2i\beta\omega} = \frac{F_0/m(\omega_0^2 - \omega^2 - 2i\beta\omega)}{(\omega_0^2 - \omega^2)^2 + 4\beta^2\omega^2}$$

$$x = A\cos(\omega t - \delta) = \operatorname{Re}[Ce^{i\omega t}]$$

$$A\cos\delta\cos\omega t + A\sin\delta\sin\omega t = \operatorname{Re}[C\cos\omega t + iC\sin\omega t]$$

$$= \frac{F_0}{m}\left[\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + 4\beta^2\omega^2}\cos\omega t + \frac{2\beta\omega}{(\omega_0^2 - \omega^2)^2 + 4\beta^2\omega^2}\sin\omega t\right]$$

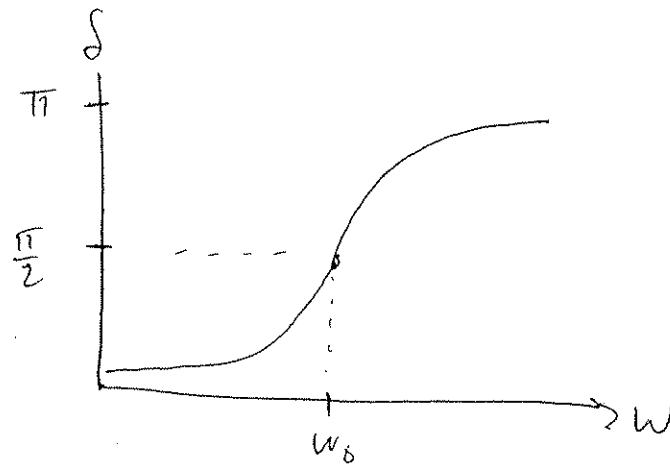
$$\Rightarrow A = \frac{F_0/m}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\beta^2\omega^2}}$$

(a)

$$\delta = \tan^{-1}\left(\frac{2\beta\omega}{\omega_0^2 - \omega^2}\right)$$

(b)

b) phase



$$\omega \ll \omega_0 : \delta \rightarrow 0$$

$$\omega = \omega_0 : \delta = \pi/2$$

$$\omega \gg \omega_0 : \delta \rightarrow \pi$$

c) max amp @ $\frac{\partial A}{\partial \omega} = 0$

$$\frac{\partial A}{\partial \omega} = \frac{F_0/m}{[(\omega_0^2 - \omega^2)^2 + 4\beta^2\omega^2]^{3/2}} \cdot \left(-\frac{1}{2}\right) (2(\omega_0^2 - \omega^2)(-2\omega) + 8\beta^2\omega)$$

$$\Rightarrow 8\beta^2\omega - 4\omega(\omega_0^2 - \omega^2) = 0$$

$$\omega [8\beta^2 - 4\omega_0^2 + 4\omega^2] = 0$$

$$\Rightarrow \omega = \sqrt{\omega_0^2 - 2\beta^2}$$

$$\approx \omega_0 \text{ for } \beta \rightarrow 0$$

$$d) \text{ Power} = F \cdot v$$

$$v = \dot{x} = -Aw \sin(\omega t - \delta)$$

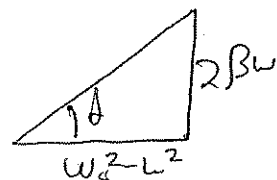
$$P = F_0 \cos \omega t (-Aw \sin(\omega t - \delta))$$

$$= -Aw F_0 \cos \omega t [\sin \omega t \cos \delta - \cos \omega t \sin \delta]$$

$$\langle \cos \omega t \sin \omega t \rangle = 0, \quad \langle \cos \omega t \cos \omega t \rangle = \frac{1}{2}$$

$$\Rightarrow \langle P \rangle = \frac{1}{2} Aw F_0 \sin \delta$$

$$= \frac{w F_0}{2} \sin \delta \frac{F_0/m}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\beta^2 \omega^2}}$$



$$\sin \delta = \frac{2\beta\omega}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4\beta^2 \omega^2}}$$

$$\langle P \rangle = \frac{F_0^2 \beta}{m} \frac{\omega^2}{(\omega_0^2 - \omega^2)^2 + 4\beta^2 \omega^2}$$

$$\text{Power max @ } \frac{d\langle P \rangle}{d\omega} = 0$$

$$\frac{d\langle P \rangle}{d\omega} = \frac{F_0^2 \beta}{m} \left[\frac{2\omega}{(\omega_0^2 - \omega^2)^2 + 4\beta^2 \omega^2} - \frac{\omega^2 (2(\omega_0^2 - \omega^2)(-2\omega) + 8\beta^2 \omega)}{[(\omega_0^2 - \omega^2)^2 + 4\beta^2 \omega^2]^2} \right]$$

$$\Rightarrow 2\omega(\omega_0^2 - \omega^2)^2 + 8\beta^2 \omega^3 + 4\omega^3(\omega_0^2 - \omega^2) - 8\beta^2 \omega^3 = 0$$

$$(\omega_0^2 - \omega^2) [2\omega\omega_0^2 - 2\omega^3 + 4\omega^3] = 0$$

$$(\omega_0^2 - \omega^2) \omega 2(\omega_0^2 + \omega^2) = 0$$

$$\Rightarrow \boxed{\omega = \omega_0}$$

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$$= \frac{1}{N!} \left(\sum_{\vec{k}nlm} e^{-\beta E_{\vec{k}nlm}} \right)^N \quad (29)$$

$$= \frac{1}{N!} Z_1^N \quad (30)$$

where the $N!$ comes from avoiding overcounting identical states, since the molecules are indistinguishable.

$$Z_1 \equiv \sum_{\vec{k}nlm} e^{-\beta E_{\vec{k}nlm}} \quad (31)$$

$$= \sum_{\vec{k}} \sum_{n=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l e^{-\beta(E_{\vec{k}} + E_n + E_l)} \quad (32)$$

$$= \left(\sum_{\vec{k}} e^{-\beta E_{\vec{k}}} \right) \left(\sum_{n=0}^{\infty} e^{-\beta E_n} \right) \left(\sum_{l=0}^{\infty} \sum_{m=-l}^l e^{-\beta E_l} \right) \quad (33)$$

$$= \left(\sum_{\vec{k}} e^{-\beta \frac{\hbar^2 k^2}{2m}} \right) \left(\sum_{n=0}^{\infty} e^{-\beta \hbar \omega_0 (n + \frac{1}{2})} \right) \left(\sum_{l=0}^{\infty} (2l+1) e^{-\beta \frac{\hbar^2}{2M\alpha^2} l(l+1)} \right) \quad (34)$$

$$= Z_{\text{trans}} Z_{\text{vib}} Z_{\text{rot}} \quad (35)$$

While I'm here, since it's easy to solve, I'll solve for Z_{vib} . This is just a harmonic sum:

$$Z_{\text{vib}} = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega_0 (n + \frac{1}{2})} \quad (36)$$

$$= C \sum_{n=0}^{\infty} X^n \quad (37)$$

$$X Z_{\text{vib}} = X C \sum_{n=0}^{\infty} X^n \quad (38)$$

$$= C \sum_{n=1}^{\infty} X^n \quad (39)$$

$$= -C + \sum_{n=0}^{\infty} X^n \quad (40)$$

$$= Z_{\text{vib}} - C \quad (41)$$

$$Z_{\text{vib}}(1 - X) = X \quad (42)$$

$$Z_{\text{vib}} = \frac{C}{1 - X} \quad (43)$$

$$= \frac{e^{-\beta \frac{\hbar \omega_0}{2}}}{1 - e^{-\beta \hbar \omega_0}} \quad (44)$$

- (b) What fraction of the molecules will be in the vibrational ground state, $n = 0$? Derive this as a simple expression containing no explicit summations.

Solution:

The probability of any single-molecule state is

$$P_{\bar{k}nlm} = \frac{e^{-\beta E_{\bar{k}nlm}}}{Z_1} \quad (45)$$

but we want the probability of a molecule being in any state with $n = 0$, so we need to sum over the other degrees of freedom:

$$P_{n=0} = \sum_{\bar{k}} \sum_l \sum_m \frac{e^{-\beta E_{\bar{k}nlm}}}{Z_1} \quad (46)$$

You can quickly see that the sums over other degrees of freedom just cancel out their respective partition functions, so we get

$$P_{n=0} = \frac{e^{-\beta \hbar \omega_0 \frac{1}{2}}}{Z_{\text{vib}}} \quad (47)$$

In fact, this is also where Equation 45 came from, although in that case we had to look at the many-body probability.

$$P_{n=0} = e^{-\beta \hbar \omega_0 \frac{1}{2}} \frac{1 - e^{-\beta \hbar \omega_0}}{e^{-\beta \hbar \omega_0 \frac{1}{2}}} \quad (48)$$

$$= 1 - e^{-\beta \hbar \omega_0} \quad (49)$$

This looks right. In the low-temperature limit, it approaches one, and in the high temperature limit, it goes to zero.

- (c) What fraction of the molecules will be in the rotational ground state, $l = 0$, in the limiting case

$$k_B T \ll \frac{\hbar^2}{M a^2}$$

Please keep the first two non-zero terms!

Solution:

$$P_{l=0} = \frac{1}{Z_{\text{rot}}} \quad (50)$$

So we just need to approximate Z_{rot} .

$$Z_{\text{rot}} = \sum_{l=0}^{\infty} (2l+1) e^{-\beta \frac{\hbar^2}{2M a^2} l(l+1)} \quad (51)$$

$$= 1 + 3e^{-\beta \frac{\hbar^2}{M a^2}} + \dots \quad (52)$$

Since the dimensionless number $\frac{\beta\hbar^2}{Ma^2}$ is large, these exponentials are increasingly small, and we can just take the first two terms:

$$Z_{\text{rot}} \approx 1 + 3e^{-\frac{\beta\hbar^2}{Ma^2}} \quad (53)$$

$$P_{l=0} \approx 1 - 3e^{-\frac{\beta\hbar^2}{Ma^2}} \quad (54)$$

This looks correct: at very low temperatures, the fraction in the ground state gets very close to zero.

- (d) What fraction of the molecules will be in the rotational ground state, $l = 0$, in the limiting case

$$\frac{\hbar^2}{Ma^2} \ll k_B T$$

In this case, you need only keep the first non-zero term.

Solution:

Here, we can't just keep the first few terms of the sum, since $e^{-\beta\frac{\hbar^2}{Ma^2}}$ is very close to one. Instead, let's see about turning the summation into an integral.

$$Z_{\text{rot}} = \sum_{l=0}^{\infty} (2l+1) e^{-\beta\frac{\hbar^2}{2Ma^2}l(l+1)} \quad (55)$$

$$= \sum_{l=0}^{\infty} \left(-\frac{2Ma^2}{\hbar^2} \right) \frac{d}{dl} e^{-\beta\frac{\hbar^2}{2Ma^2}l(l+1)} \quad (56)$$

$$= -\frac{2Ma^2}{\hbar^2} \sum_{l=0}^{\infty} \frac{d}{dl} e^{-\beta\frac{\hbar^2}{2Ma^2}l(l+1)} \quad (57)$$

$$\approx -\frac{2Ma^2}{\beta\hbar^2} \int_0^{\infty} dl \frac{d}{dl} e^{-\beta\frac{\hbar^2}{2Ma^2}l(l+1)} \quad (58)$$

$$= -\frac{2Ma^2}{\beta\hbar^2} e^{-\beta\frac{\hbar^2}{2Ma^2}l(l+1)} \Big|_0^{\infty} \quad (59)$$

$$= \frac{2Ma^2}{\beta\hbar^2} \quad (60)$$

$$P_{l=0} \approx \frac{\beta\hbar^2}{2Ma^2} \quad (61)$$

- (e) What is the internal energy and heat capacity C_V at temperatures

$$k_B T \ll \frac{\hbar^2}{Ma^2} \ll \hbar\omega_0$$

Solution:

The internal energy is given by

$$U = \sum_i E_i P_i \quad (62)$$

$$= -\frac{\partial}{\partial \beta} \ln Z \quad (63)$$

$$= -\frac{\frac{\partial Z}{\partial \beta}}{Z} \quad (64)$$

When the system separates, so the partition function is a product, its log is a sum, and the internal energy separates (as it must) into

$$U = -\frac{\frac{\partial Z_A}{\partial \beta}}{Z_A} - \frac{\frac{\partial Z_B}{\partial \beta}}{Z_B} - \dots \quad (65)$$

In our case, the energy separates into translational, rotational and vibrational components.

$$U = -\frac{\frac{\partial Z_{\text{trans}}}{\partial \beta}}{Z_{\text{trans}}} - \frac{\frac{\partial Z_{\text{vib}}}{\partial \beta}}{Z_{\text{vib}}} - \frac{\frac{\partial Z_{\text{rot}}}{\partial \beta}}{Z_{\text{rot}}} \quad (66)$$

so I'll calculate these three terms, one at a time. The translational internal energy we can just get from equipartition, since we're in the classical limit as far as these degrees of freedom are concerned, so

$$U_{\text{trans}} = \frac{3}{2} N k_B T \quad (67)$$

Moving to the vibrational energy, we can compute this analytically, and it is

$$U_{\text{vib}} = -N \frac{\frac{\partial Z_{\text{vib}}}{\partial \beta}}{Z_{\text{vib}}} \quad (68)$$

$$= -N \frac{1}{Z_{\text{vib}}} \left(\frac{-\frac{\hbar\omega_0}{2} e^{-\frac{\beta\hbar\omega_0}{2}}}{1 - e^{-\beta\hbar\omega_0}} - \frac{e^{-\frac{\beta\hbar\omega_0}{2}}}{(1 - e^{-\beta\hbar\omega_0})^2} \hbar\omega_0 e^{-\beta\hbar\omega_0} \right) \quad (69)$$

$$= N\hbar\omega_0 \left(\frac{1}{2} + \frac{e^{-\beta\hbar\omega_0}}{1 - e^{-\beta\hbar\omega_0}} \right) \quad (70)$$

$$= N\hbar\omega_0 \left(\frac{1}{e^{\beta\hbar\omega_0} - 1} + \frac{1}{2} \right) \quad (71)$$

I haven't yet assumed the low-temperature limit that this problem requests, since I didn't want to have to re-do this value in the next to sections. At low temperatures, $\beta \rightarrow \infty$, so we can simplify things a bit, and the Bose-Einstein distribution reduces to the Boltzmann distribution. In particular, $e^{\beta\hbar\omega_0} \gg 1$, so we can take

$$U_{\text{vib}} \approx N\hbar\omega_0 \left(e^{-\beta\hbar\omega_0} + \frac{1}{2} \right) \quad (72)$$

Finally, we have the rotational energy.

$$U_{\text{rot}} = N \frac{-\frac{\partial Z_{\text{rot}}}{\partial \beta}}{Z_{\text{rot}}} \quad (73)$$

$$= N \frac{\sum_{l=0}^{\infty} (2l+1) \left(\frac{\hbar^2}{2ma^2} l(l+1) \right) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}}{\sum_{l=0}^{\infty} (2l+1) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}} \quad (74)$$

This looks pretty yucky. But we must persevere, and had best make use of the fact that $k_B T \ll \frac{\hbar^2}{ma^2}$, which means that the Boltzmann factors are all very small (since β is big). Except, of course, for the $l=0$ contribution, for which the Boltzmann factor is 1. So we can drop all but the first contribution, taking the sum up to just $l=1$, and then we get...

$$U_{\text{rot}} = N \frac{\sum_{l=0}^{\infty} (2l+1) \left(\frac{\hbar^2}{2ma^2} l(l+1) \right) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}}{\sum_{l=0}^{\infty} (2l+1) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}} \quad (75)$$

$$\approx N \frac{3 \frac{\hbar^2}{ma^2} e^{-\frac{\beta \hbar^2}{ma^2}}}{1 + 3e^{-\frac{\beta \hbar^2}{ma^2}}} \quad (76)$$

$$\approx 3N \frac{\hbar^2}{ma^2} e^{-\frac{\beta \hbar^2}{ma^2}} \quad (77)$$

So our total internal energy in this limit comes out to

$$U = \frac{3}{2} N k_B T + 3N \frac{\hbar^2}{ma^2} e^{-\frac{\beta \hbar^2}{ma^2}} + N \hbar \omega_0 \left(e^{-\beta \hbar \omega_0} + \frac{1}{2} \right) \quad (78)$$

From this, we can find the heat capacity C_V just by

$$C_V = N \left(\frac{\partial U}{\partial T} \right)_V \quad (79)$$

$$= \left(\frac{3}{2} + 3 \left(\frac{\beta \hbar^2}{ma^2} \right)^2 e^{-\frac{\beta \hbar^2}{ma^2}} + (\beta \hbar \omega_0)^2 e^{-\beta \hbar \omega_0} \right) N k_B \quad (80)$$

(f) What is the internal energy and heat capacity C_V at temperatures

$$\frac{\hbar^2}{Ma^2} \ll k_B T \ll \hbar \omega_0$$

Solution:

The translational and vibrational internal energies will be the same in this limit as they were in the last, with the only difference being the vibrational energy. The easy way to find the vibrational energy (which earns full credit) is to recognize that equipartition applies in this case, so

there will be $k_B T$ internal rotational energy, since there are two rotational degrees of freedom.

I'll now go ahead to demonstrate the hard way, since it's not *that* hard, and is worth a look at how to take the classical limit.

$$U_{\text{rot}} = N \frac{\sum_{l=0}^{\infty} (2l+1) \left(\frac{\hbar^2}{2ma^2} l(l+1) \right) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}}{\sum_{l=0}^{\infty} (2l+1) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}} \quad (81)$$

In this high-temperature limit, the Boltzmann factors are all very small, so very high l values become important. Thus it is reasonable to convert this summation into an integral, and to replace $l+1$ with l .

$$U_{\text{rot}} = N \frac{\sum_{l=0}^{\infty} (2l+1) \left(\frac{\hbar^2}{2ma^2} l(l+1) \right) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}}{\sum_{l=0}^{\infty} (2l+1) e^{-\frac{\beta \hbar^2 l(l+1)}{2ma^2}}} \quad (82)$$

$$\approx N \frac{\int_0^{\infty} \frac{\hbar^2}{ma^2} l^3 e^{-\frac{\beta \hbar^2 l^2}{2ma^2}} dl}{\int_0^{\infty} 2l e^{-\frac{\beta \hbar^2 l^2}{2ma^2}} dl} \quad (83)$$

$$u \equiv N \frac{\beta \hbar^2 l^2}{2ma^2} \quad (84)$$

$$du = N \frac{\beta \hbar^2 l}{ma^2} dl \quad (85)$$

$$U_{\text{rot}} = N \frac{k_B T \frac{2ma^2}{\beta \hbar^2} \int_0^{\infty} u e^{-u} du}{\frac{2ma^2}{\beta \hbar^2} \int_0^{\infty} e^{-u} du} \quad (86)$$

$$= N k_B T \quad (87)$$

The integrals above are easy to remember:

$$\int_0^{\infty} u^n e^{-u} du = n! \quad (88)$$

They're also not hard to do by hand, just use integration by parts. So the final answer is the same as the one we get using the easy approach (i.e. equipartition). Yay. So our final answer is a bit easier than the last time:

$$U = \frac{5}{2} N k_B T + N \hbar \omega_0 \left(e^{-\beta \hbar \omega_0} + \frac{1}{2} \right) \quad (89)$$

The heat capacity C_V is now a bit simpler

$$C_V = N \left(\frac{\partial U}{\partial T} \right)_V \quad (90)$$

$$= \left(\frac{5}{2} + (\beta \hbar \omega_0)^2 e^{-\beta \hbar \omega_0} \right) N k_B \quad (91)$$

Hopefully these $\frac{3}{2}$ and $\frac{5}{2}$ look a bit familiar...

- (g) What is the internal energy and heat capacity C_V at temperatures

$$\frac{\hbar^2}{Ma^2} \ll \hbar\omega_0 \ll k_B T$$

Solution:

This one you should be able to get, even if you missed the other two, just by using equipartition. There are two vibrational degrees of freedom, one kinetic and one potential, so we expect another $k_B T$ of internal energy, plus the zero-point energy, of course.

Once again, I'll take the limit by hand, just to demonstrate how the classical limit arises from the quantum mechanical solution. It's easier than the rotational case, since we were already able to solve for the internal energy exactly, so all we need do is look at the limiting case.

$$U_{\text{vib}} = N\hbar\omega_0 \left(\frac{1}{e^{\beta\hbar\omega_0} - 1} + \frac{1}{2} \right) \quad (92)$$

This time around, $\beta\hbar\omega_0 \ll 1$, so the Boltzmann factor is very close to one.

$$U_{\text{vib}} = N\hbar\omega_0 \left(\frac{1}{e^{\beta\hbar\omega_0} - 1} + \frac{1}{2} \right) \quad (93)$$

$$\approx N\hbar\omega_0 \left(\frac{1}{(1 + \beta\hbar\omega_0) - 1} + \frac{1}{2} \right) \quad (94)$$

$$= N\hbar\omega_0 \left(\frac{1}{\beta\hbar\omega_0} + \frac{1}{2} \right) \quad (95)$$

$$= Nk_B T + \frac{1}{2} N\hbar\omega_0 \quad (96)$$

So there we have it. Putting everything together, we find that

$$U = \frac{7}{2} Nk_B T + \frac{1}{2} N\hbar\omega_0 \quad (97)$$

$$C_V = \frac{7}{2} Nk_B \quad (98)$$

- (h) Please sketch the heat capacity C_V as a function of temperature.

Solution:

Since we've already computed all three limiting cases (well, leaving out the Bose-Einstein condensate or Fermi liquid at *very* low temperatures), this is quite easy to plot.

At the lowest temperatures, both the rotational and vibrational degrees of freedom are frozen out and the heat capacity starts at $\frac{3}{2}k_B$, rising exponentially. Once the rotational motion is classical, the heat capacity is

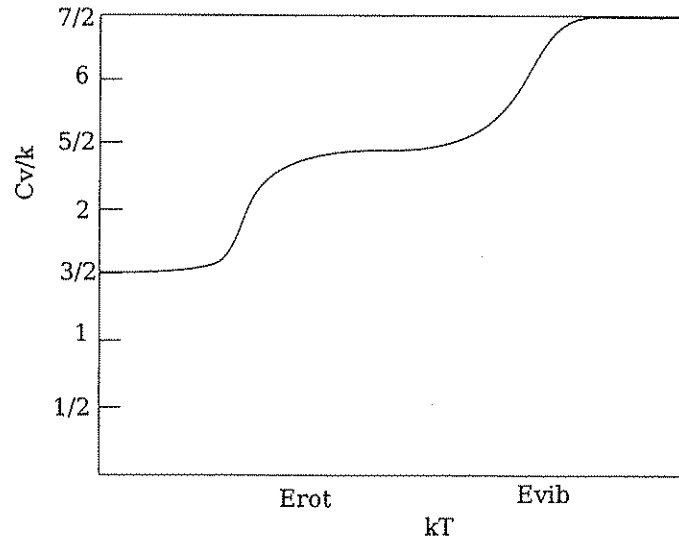


Figure 1: Plot of C_V/N versus $k_B T$ where $E_{\text{rot}} \equiv \frac{\hbar^2}{ma^2}$ and $E_{\text{vib}} \equiv \hbar\omega_0$. The important features

close to $\frac{5}{2}k_B$, with the vibrational contribution exponentially small. And finally the heat capacity rises to $\frac{7}{2}k_B$.

Interestingly, if we were to increase the energy yet further, we might be able to dissociate the atoms, lowering the heat capacity to $3k_B$. But that ignores electronic degrees of freedom, which would probably have a net effect of raising the heat capacity even more. For the solution, see Figure 1.