OSU PHYSICS DEPARTMENT
COMPREHENSIVE EXAMINATION #104

March 31 and April 1, 2008

Comprehensive examination for Spring 2008

PART 1, Monday March 31, 9:00 am

General Instructions

This Comprehensive Examination for Spring 2008 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 31, and lasts three hours. The second part (Problems 3-4) will be handed out at 1:30 pm on the same day and will also last three hours. The third and fourth parts will be administered on Tuesday, April 1, at 9:00 am and 1:30 pm.

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. 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.

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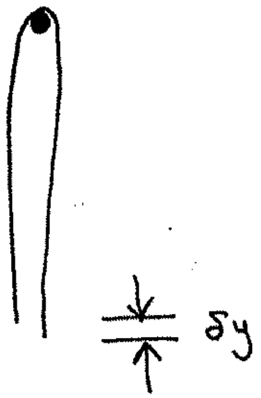
Problem 1

A uniform rope of length L is hanging over a nail with the ends even. One end is pulled downward a very small distance δy and the rope slides slowly off the nail. Assume that the rope is prevented from lifting off the nail and neglect any friction between the rope and the nail.



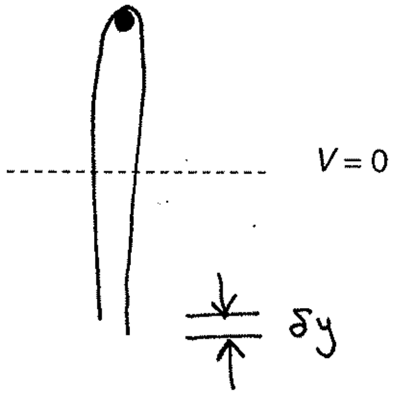
(a) Find an expression for the velocity of the rope after the end of the rope has moved a distance y.

(b) What is the time required for the rope to slide completely off the nail?

Classical Mechanics – Undergraduate

Solution

A uniform rope of length L is hanging over a nail with the ends even. One end is pulled downward a very small distance δy and the rope slides slowly off the nail. Assume that the rope is prevented from lifting off the nail and neglect any friction between the rope and the nail.



(a) Find an expression for the velocity of the rope after the end of the rope has moved a distance y.

First set up the Lagrangian. It is easiest to define the zero of potential energy at the midpoint of the rope when the ends are even. Then, for a displacement of the right-hand rope end downward a distance y, the potential energy is

$$V = m_l g h_l + m_r g h_r = \left(\frac{L}{2} - y\right)\rho g\left(\frac{y}{2}\right) + \left(\frac{L}{2} + y\right)\rho g\left(-\frac{y}{2}\right) = -\rho g y^2$$

where m_l and m_r are, respectively, the masses of the left- and right-hand portions of the rope and h_l and h_r are, respectively, the heights of the center of masses of the two portions. The linear density of the rope is ρ.

The kinetic energy is $T = \frac{1}{2}\rho L\dot{y}^2$ so the Lagrangian is $L = \frac{1}{2}\rho L\dot{y}^2 + \rho g y^2$.

The Lagrangian equation of motion, $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) - \frac{\partial L}{\partial y} = 0$ gives $\rho L\frac{d}{dt}(\dot{y}) = \rho L\frac{dv}{dt} = 2\rho g y$.

Then write

$$\frac{dv}{dt} = \frac{dv}{dy}\frac{dy}{dt} = v\frac{dv}{dy} = \frac{2g}{L}y$$

$$v\,dv = \frac{2g}{L}\,y\,dy$$

$$\int_0^v v'dv' = \frac{2g}{L}\int_0^y y'dy'$$

Integrate:

$$\frac{1}{2}v^2 = \frac{2g}{L}\frac{1}{2}y^2$$

$$v = \sqrt{\frac{g}{2L}}y$$

(b) What is the time required for the rope to slide completely off the nail?

$$2\varrho gy = \rho L\frac{dv}{dt} \Longrightarrow \frac{dv}{dt} = \frac{d^2y}{dt^2} = \frac{2g}{L}y$$

$$\frac{d^2y}{dt^2} - \frac{2g}{L}y = 0$$

Solution: $y(t) = y(0)e^{\sqrt{\frac{2g}{L}}t} = \delta y\, e^{\sqrt{\frac{2g}{L}}t}$

Solve for t: $t = \sqrt{\frac{L}{2g}}\,ln\left(\frac{y}{\delta y}\right)$

When rope is about to slide completely off the nail, $y = \frac{L}{2}$ and $t = \sqrt{\frac{L}{2g}}\,ln\left(\frac{L}{2\,\delta y}\right)$.

Problem 2

Consider a particle of mass m placed in a one-dimensional delta function potential

$$V(x) = -\alpha\delta(x),$$

where α characterizes the strength of the attractive well ($\alpha > 0$).

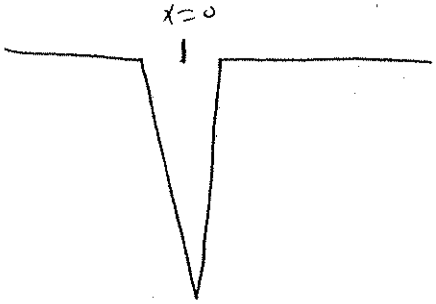
a) Find the energies and wave functions of the allowed bound states of the system.

b) For the ground state of the system, calculate the uncertainties in position and momentum and show that the uncertainty principle is obeyed.

The following integral may be useful:

$$\int_0^\infty \frac{x^2}{\left(1+x^2\right)^2}\,dx = \frac{\pi}{4}$$

$$V(x) = -\alpha\,\delta(x)$$



$$H\psi = E\psi$$

$$H = T + V = \frac{p^2}{2m} + V(x)$$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\,\delta(x)$$

ψ is continuous at $x=0$, but ψ' is not

Find discontinuity by integrating Sch eqn.

$$\int_{-\epsilon}^{\epsilon}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\,\delta(x)\,\psi\right]dx = \int_{-\epsilon}^{\epsilon} E\psi\,dx$$

$$-\frac{\hbar^2}{2m}\left[\left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon}\right] - \alpha\,\psi(0) = E\int_{-\epsilon}^{\epsilon}\psi(x)\,dx$$

as $\epsilon \to 0$ r.h.s. $\to 0$

$$\Rightarrow \left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon} = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

To be normalizable, $\psi(x)$ must be decaying exponential since $-\frac{\hbar^3}{2m}\frac{d^2\psi}{dx^2} = E\psi$ for $x \neq 0$

$$\Rightarrow \psi(x) = \begin{cases} A_1\,e^{+Kx} & x<0 \\ A_2\,e^{-Kx} & x>0 \end{cases} \qquad K = \sqrt{\frac{-2mE}{\hbar^2}}$$

Bound. cond: @ $x=0$

ψ: $A_1 = A_2 \equiv A$

ψ': $-KA - (KA) = -\frac{2m\alpha}{\hbar^2} A$

$$\Rightarrow A\left[2K - \frac{2m\alpha}{\hbar^2}\right] = 0$$

$\Rightarrow K = \frac{m\alpha}{\hbar^2}$ only 1 soln.

get A from normalization

$$\int_{-\infty}^{\infty} |\psi(x)|^2 = 1 = A^2\left[\int_{-\infty}^{0} e^{2Kx}\,dx + \int_0^{\infty} e^{-2Kx}\,dx\right]$$

$$= A^2\left(\frac{1}{2K} + \frac{1}{2K}\right)$$

$$\Rightarrow A = \sqrt{K} = \sqrt{\frac{m\alpha}{\hbar^2}}$$

$$\Rightarrow E = \frac{-\hbar^2 K^2}{2m} = -\frac{\hbar^2}{2m}\frac{m^2\alpha^2}{\hbar^4}$$

$\boxed{E = -\frac{m\alpha^2}{2\hbar^2}}$ is only bound state

$$\psi(x) = \left\{\begin{array}{ll} \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{\frac{m\alpha}{\hbar^2}x} & x < 0 \\ \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{-\frac{m\alpha}{\hbar^2}x} & x > 0 \end{array}\right\}$$

b) $\Delta x = \sqrt{\langle (x - \langle x\rangle)^2 \rangle} = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$

symmetry of state $\Rightarrow$ $\langle x\rangle = 0$

$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2 |\psi^2| \, dx$$

$$= 2 \frac{m\alpha}{\hbar^2} \int_0^\infty x^2 e^{-2\frac{m\alpha}{\hbar^2}x} dx$$

let $z = \frac{2m\alpha}{\hbar^2} x$

$$\langle x^2\rangle = 2 \frac{m\alpha}{\hbar^2} \left(\frac{\hbar^2}{2m\alpha}\right)^3 \int_0^\infty z^2 e^{-z} dz$$

$$= 2 \left(\frac{\hbar^2}{m\alpha}\right)^2 \cdot \frac{1}{8} \cdot 2!$$

$$\Rightarrow \boxed{\Delta x = \frac{1}{\sqrt{2}} \frac{\hbar^2}{m\alpha}}$$

$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$ $\qquad$ $\langle p\rangle = 0$ by symmetry

$$\langle p^2\rangle = \int_{-\infty}^{\infty} \psi^* \left(-\hbar^2 \frac{d^2\psi}{dx^2}\right) dx$$

but $\frac{d^2\psi}{dx^2}$ has infinity at zero.

Either integrate by parts or use energy expectation values:

$$\frac{p^2}{2m} = T \Rightarrow \langle p^2 \rangle = 2m \langle T \rangle$$

$$H = T + V \Rightarrow \langle T \rangle = \langle H \rangle - \langle V \rangle$$

$$\langle H \rangle = E = -\frac{m\alpha^2}{2\hbar^2}$$

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(-\alpha\, \delta(x)\right) \psi(x)\, dx$$

$$= -\alpha\, |\psi(0)|^2 = -\alpha \frac{m\alpha}{\hbar^2}$$

$$\Rightarrow \langle T \rangle = -\frac{m\alpha^2}{2\hbar^2} - \left(-\frac{m\alpha^2}{\hbar^2}\right) = \frac{m\alpha^2}{2\hbar^2}$$

$$\Rightarrow \langle p^2 \rangle = 2m \frac{m\alpha^2}{2\hbar^2} = \left(\frac{m\alpha}{\hbar}\right)^2$$

$$\Rightarrow \boxed{\Delta p = \frac{m\alpha}{\hbar}}$$

$$\Delta x\, \Delta p = \frac{1}{\sqrt{2}} \frac{\hbar^2}{m\alpha} \cdot \frac{m\alpha}{\hbar} = \frac{\hbar}{\sqrt{2}}$$

Heis. unc. princ: $\Delta x\, \Delta p \geq \frac{\hbar}{2}$

$\frac{\hbar}{\sqrt{2}} > \frac{\hbar}{2}$ so satisfied!

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Problem 3

A point dipole (dipole moment $\vec{p}$ is placed at the center of dielectric sphere (radius R, relative permittivity ϵ) surrounded by vacuum. Find the potential inside and outside the sphere

The potential inside the sphere is a sum of potential of a dipole and of homogeneous field; the potential outside the sphere is that of a dipole:

$$V_{in} = \frac{1}{4\pi\epsilon}\left(-B\, r\cos\theta + \frac{p}{r^2}\cos\theta\right)$$

$$V_{out} = \frac{1}{4\pi\epsilon_0}\frac{C}{r^2}\cos\theta$$

Boundary conditions:

$$\begin{cases} V_{in}\Big|_{r=R} = V_{out}\Big|_{r=R} \\ \epsilon_{in}\frac{\partial V_{in}}{\partial r}\Big|_{r=R} = \epsilon_0 \frac{\partial V_{out}}{\partial r}\Big|_{r=R} \end{cases}$$

$$\begin{cases} \left(-BR + \frac{p}{R^2}\right)\frac{1}{\epsilon_{in}} = \frac{1}{\epsilon_0}\frac{C}{R^2} \\ \left(-B - \frac{2p}{R^3}\right) = -\frac{2C}{R^3} \end{cases}$$

$$\begin{cases} -B + \frac{p}{R^3} = \frac{C}{R^3}\frac{\epsilon_{in}}{\epsilon_0} \\ B + \frac{2p}{R^3} = \frac{2C}{R^3} \end{cases} \quad \begin{cases} C = \frac{3p\epsilon_0}{2\epsilon_0 + \epsilon_{in}} \\ B = \frac{2p}{R^3}\frac{\epsilon_0 - \epsilon_{in}}{2\epsilon_0 + \epsilon_{in}} \end{cases}$$

$$V_{in} = \frac{p\cos\theta}{4\pi\epsilon r^2}\left[1 - \frac{2r^3}{R^3}\frac{\epsilon_0 - \epsilon_{in}}{2\epsilon_0 + \epsilon_{in}}\right]$$

$$V_{out} = \frac{3p\cos\theta}{4\pi r^2}\cdot\frac{1}{2\epsilon_0 + \epsilon_{in}}$$

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Problem 4

Consider an n-type semiconductor whose donor levels lie $E_{\rm D}$ below the bottom of the conduction band. Let's use the following symbols:

$N_{\rm D}$ – the number of donor levels per unit volume;

$n_{\rm D}$ – the number of electrons in the donor levels per unit volume;

n – the number of electrons in the conduction band per unit volume.

Assume that the possible microscopic states of a donor level are: (a) an empty state, (b) a state occupied by a single "spin up" electron, or (c) a state occupied by a single "spin down" electron. Also, assume that the (b) and (c) states may occur with the same probability.

The semiconductor is in the state of thermal equilibrium at finite temperature T.

I. Find the entropy of the sub-system of electrons in the donor levels (*Hint:* You may want to use the Stirling approximation $\ln N! \approx N \ln N - N$);

II. Find the Helmholtz free energy F of this system;

III. Find the chemical potential μ of the electrons in the donor levels;

IV. Assuming that the system of electrons in the conduction band is not degenerate and obeys the ideal gas laws, with

$$\mu = kT \ln\left(\frac{n}{n_{\rm Q}}\right) \quad \text{where} \quad n_{\rm Q} = 2\left(\frac{mkT}{\hbar^2}\right)^{3/2}$$

show that the following relation is valid:

$$\frac{n(N_{\rm D} - n_{\rm D})}{n_{\rm D}} = \frac{1}{2} n_{\rm Q} \exp\left(-\frac{E_{\rm D}}{kT}\right)$$

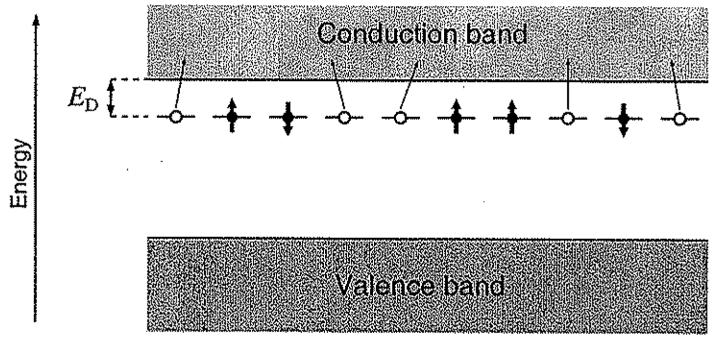

Figure 1: A diagram showing the valence band and the conduction band in a semiconductor with an energy gap in between – and donor levels located below the bottom of the conduction band. Each state may be occupied by a *single* "spin-up" or "spin-down" electron (up and down-pointing arrows in the plot) – or it may be "empty" (open circles), if the electon is excited to the conduction band. The electrons in the conduction band can be treated as a non-degenerate gas of spin $\frac{1}{2}$ particles obeying the Maxwell-Boltzmann statistics (the valence band is shown in the figure only for completeness, but the electrons in the valence band do not play any relevant role in the present problem).

I. The number of ways in which n_{D} spinless particles can be distributed among N_{D} donor levels is $N_{\mathrm{D}}!/[(N_{\mathrm{D}}-n_{\mathrm{D}})!n_{\mathrm{D}}!]$. In the case of $\frac{1}{2}$ particles, each of the n_{D} can be in two different states, so that number should be additionally multiplied by $2^{n_{\mathrm{D}}}$, so that the total multiplicity factor becomes:

$$g(n_{\mathrm{D}}) = 2^{n_{\mathrm{D}}} \times \frac{N_{\mathrm{D}}!}{(N_{\mathrm{D}}-n_{\mathrm{D}})!n_{\mathrm{D}}!}$$

Now, the entropy is $S(n_{\mathrm{D}}) = k \ln g(n_{\mathrm{D}})$. With the help of Stirling approximation, one obtains:

$$S = k\left[n_{\mathrm{D}}\ln 2 - n_{\mathrm{D}}\ln\frac{n_{\mathrm{D}}}{N_{\mathrm{D}}} - (N_{\mathrm{D}}-n_{\mathrm{D}})\ln\frac{N_{\mathrm{D}}-n_{\mathrm{D}}}{N_{\mathrm{D}}}\right]$$

II. The Helmholtz free energy is $F = U - TS$, end the energy of the n_{D} electrons with energy $-E_{\mathrm{D}}$ each is obviously $-n_{\mathrm{D}}E_{\mathrm{D}}$, so we get:

$$F = -n_{\mathrm{D}}E_{\mathrm{D}} - kT\left[n_{\mathrm{D}}\ln 2 - n_{\mathrm{D}}\ln\frac{n_{\mathrm{D}}}{N_{\mathrm{D}}} - (N_{\mathrm{D}}-n_{\mathrm{D}})\ln\frac{N_{\mathrm{D}}-n_{\mathrm{D}}}{N_{\mathrm{D}}}\right]$$

III. The chemical potential can be obtained from F in a straightforward manner:

$$\mu = \frac{\partial F}{n_{\mathrm{D}}} = -E_{\mathrm{D}} - kT\left[\ln 2 - \ln\frac{n_{\mathrm{D}}}{N_{\mathrm{D}}-n_{\mathrm{D}}}\right]$$

IV. In the state of equilibrium, the chemical potentials of the sub-systems comprising the the total system must all be equal. By equating the above equation with that for the chemical potential of a non-degenerate gas of electrons given in the problem statement, one can readily obtain the result that has to be derived.

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Problem 5

A planar waveguide is formed by a slab of glass extending between $-\frac{a}{2} < x < \frac{a}{2}$ (relative permittivity ϵ) surrounded by air (relative permittivity 1), Fig.1. Your task is to analyze the behavior of first two Transverse-Electric (TE) modes of this structure

1. Assuming that the modes propagate along z coordinate of Cartesian coordinate system (see Fig.1), derive the dispersion relation for first symmetric and first anti-symmetric TE modes in the system.
2. Analyze the behavior of dispersion relations when waveguide is very thin (in the limit $a \to 0$). Derive the analytical expressions for $k_z(\omega)$ for the modes that exist in this limit.
3. Explain why the existence of the modes does not violate diffraction limit that prohibits confinement of electromagnetic wave in sub-wavelength space. Hint: analyze field profiles of the existing modes in the limit $a \to 0$.

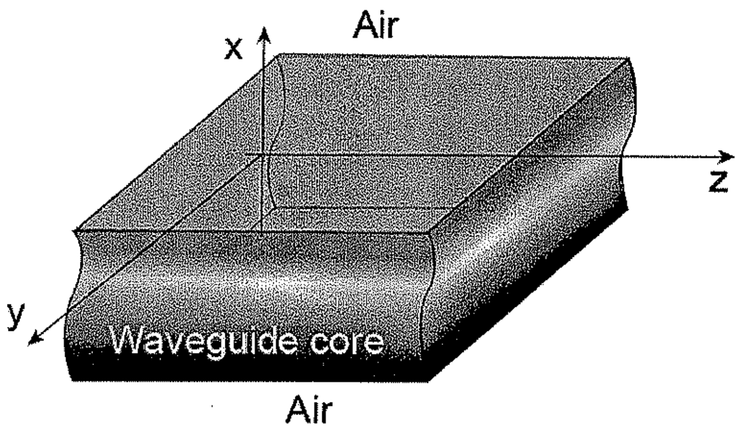

Fig.1

① We represent all components of the fields via z-component of magnetic field

TE modes:

$$\begin{cases} E_x = \dfrac{i\omega}{c\varkappa^2}\dfrac{\partial H_z}{\partial y} \\ E_y = -\dfrac{i\omega}{c\varkappa^2}\dfrac{\partial H_z}{\partial x} \\ H_x = \dfrac{ik_z}{\varkappa^2}\dfrac{\partial H_z}{\partial x} \\ H_y = \dfrac{ik_z}{\varkappa^2}\dfrac{\partial H_z}{\partial y} \end{cases}$$

where $\varkappa^2 = \epsilon\frac{\omega^2}{c^2} - k_z^2$

for waves propagating along z direction:

$$H_z \propto \begin{cases} \beta e^{i\varkappa_0 x + ik_z z} & x > \frac{a}{2} \\ \alpha_1 \sin(\varkappa x) e^{ik_z z} + \alpha_2 \cos(\varkappa x) e^{ik_z z}, & x < \frac{a}{2} \end{cases}$$

The dispersion relation connecting k_z and ω is obtained from boundary conditions for symmetric E_x, H_z must be anti-symmetric; so we obtain:

Anti-symmetric H_z:

$$\begin{cases} H_z\Big|_{x=a} = \text{const} & \alpha \sin\left(\varkappa_{in}\frac{a}{2}\right) = \beta e^{+i\varkappa_0\frac{a}{2}} \\ H_x\Big|_{x=a} = \text{const} & \frac{i\alpha}{\varkappa_{in}}\cos\left(\varkappa_{in}\frac{a}{2}\right) = \frac{-\beta}{\varkappa_0} e^{i\varkappa_0\frac{a}{2}} \end{cases}$$

$$\boxed{\varkappa_{in}\tan\left(\varkappa_{in}\frac{a}{2}\right) = -i\varkappa_0}$$

② when $\varkappa a \ll 1$:

$$\varkappa_{in}\left(\varkappa_{in}\frac{a}{2}\right) = -i\varkappa_0$$

$$\frac{a}{2}\left(\epsilon\frac{\omega^2}{c^2}-k_z^2\right) = -i\sqrt{\frac{\omega^2}{c^2}-k_z^2} = +\sqrt{k_z^2-\frac{\omega^2}{c^2}}$$

Introducing $k_z^2-\frac{\omega^2}{c^2}=\xi^2$, obtain:

$$a\xi^2+2\xi-a(\epsilon-1)\frac{\omega^2}{c^2}=0$$

$$D_1 = 1+a^2(\epsilon-1)\frac{\omega^2}{c^2} \; ; \; \sqrt{D_1}\simeq 1+\frac{a^2}{2}(\epsilon-1)\frac{\omega^2}{c^2} \geq 1$$

$$\xi \simeq \frac{1}{a}\left(\frac{a^2}{2}(\epsilon-1)\frac{\omega^2}{c^2}\right) = \frac{a}{2}(\epsilon-1)\frac{\omega^2}{c^2} \ll \frac{\omega}{c}$$

$$k_z \simeq \sqrt{\frac{\omega^2}{c^2}+\xi^2} \simeq \frac{\omega}{c}+\frac{a^2}{8}(\epsilon-1)^2\frac{\omega^3}{c^3}$$

③ In the limit $a \to 0$ the mode expands and becomes plane wave

① Symmetric H_z:

$$\begin{cases} H_z\big|_{x=a} = \text{const} & \alpha\cos\left(\varkappa_{in}\frac{a}{2}\right) = \beta e^{+i\varkappa_0\frac{a}{2}} \\ H_x\big|_{x=a} = \text{const} & -\frac{i\alpha}{\varkappa_{in}}\sin\left(\varkappa_{in}\frac{a}{2}\right) = \frac{-\beta}{\varkappa_0} e^{i\varkappa_0\frac{a}{2}} \end{cases}$$

$$\tan\left(\varkappa_{in}\frac{a}{2}\right) = \frac{i\varkappa_{in}}{\varkappa_0}$$

@ $\varkappa_{in} a \ll 1$:

$$\varkappa_{in} a = \frac{i\varkappa_{in}}{\varkappa_0}$$

$$\frac{a\varkappa_0}{i} = 1$$

Note that $\varkappa_0 \sim \varkappa_i \to$ solution $\varkappa_0 = \frac{i}{a}$ does not satisfy requirement $\varkappa_i a \ll 1 \to$

② The solution does not exist.

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Problem 6

Consider a body whose internal energy dependence on temperature is described by a simple relation $U = CT$, with a constant C.

I. What is the change ΔS in the body's entropy when its temperature changes from T_i to T_f?

In Tasks II-IV you are expected to use the result from Task I rather than to perform more integration.

II. Suppose that two identical bodies characterized by the $U = CT$ relation are put in an adiabatic container. Initially, their temperatures are T_1 and T_2, and there is no thermal contact between them.

Next, the bodies are brought into direct thermal contact. Heat starts flowing, and after some time thermal equilibrium is reached – now the temperature of each body has the same value of T_f. Find T_f, and then find the change ΔS in the total entropy of the two-body system resulting from the heat transfer process.

By analyzing the expression you have obtained, show that ΔS is *intrinsically positive*, meaning that such a process of direct heat transfer between the two bodies *always* leads to entropy *increase* – and explain what are the fundamental reasons that ΔS can never be zero in such a process.

III. Sketch the thermodynamic cycle of a Carnot engine using an ideal gas. Make one plot in (V, p) coordinates, and another in (S, T) coordinates. Briefly describe the lines in each diagram on the plot field.

IV. Consider another possible way of bringing the two bodies to a common final temperature. As in **II.**, their initial temperatures are T_1 and T_2. But now instead of bringing them to a direct contact, we connect them to a Carnot engine. The body of higher temperature acts now as a "hot source", and the body of lower T acts as a "heat sink". The engine operation results in a transfer of thermal energy from the "hot source" to the "sink", and mechanical work is delivered. The process lasts until the two bodies are brought to a common final temperature T_f'. What is the final temperature T_f'? Is it higher, or lower than the T_f you found in **II.**? What is the total mechanical work delivered by the Carnot engine?

Problem 1 - "undergraduate":

I. $U = CT$

$$dS = \frac{đQ}{T} \quad \text{but} \quad đQ = dU = C\,dT$$

so that $dS = C\frac{dT}{T}$

$$\Delta S = \int_{T_i}^{T_f} dS = C\int_{T_i}^{T_f}\frac{dT}{T} = C\ln\frac{T_f}{T_i}$$

II. Initial internal energies are $U_1 = CT_1$ and $U_2 = CT_2$

The energy of each body after equilibrium is reached is $U_f = CT_f$

From energy conservation: $U_1 + U_2 = 2U_f$

So: $CT_1 + CT_2 = 2CT_f$

Ergo: $T_f = \frac{T_1 + T_2}{2}$

The change of entropy of body 1 is

$\Delta S_1 = C\ln\frac{T_f}{T_1}$; of body 2 is $\Delta S_2 = C\ln\frac{T_f}{T_2}$

Total change in entropy is $\Delta S_{TOT} = \Delta S_1 + \Delta S_2$

$$= C\ln\frac{T_f}{T_1} + C\ln\frac{T_f}{T_2} = C\ln\frac{T_f^2}{T_1T_2}$$

Inserting T_f:

$$\Delta S_{TOT} = C\ln\frac{(T_1+T_2)^2}{4T_1T_2}$$

Let's check the argument:

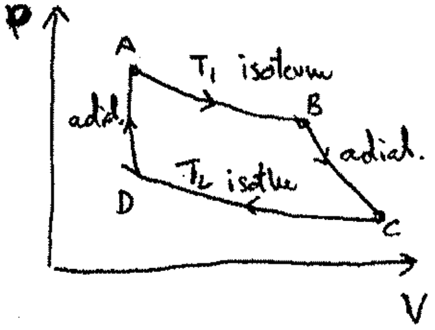
$$\frac{(T_1+T_2)^2}{4T_1T_2} = \frac{T_1^2+T_2^2+2T_1T_2}{4T_1T_2} = \frac{T_1^2+T_2^2-2T_1T_2+4T_1T_2}{4T_1T_2}$$

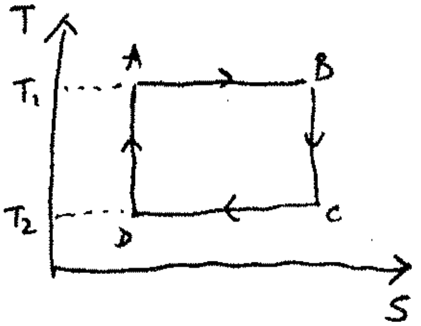
$$= 1+\frac{(T_1-T_2)^2}{4T_1T_2} >$$ always! $\frac{(T_1-T_2)^2}{4T_1T_2} > 0$, for any $T_1 \neq T_2$

So, $C \ln \frac{(T_1+T_2)^2}{4T_1T_2} > 0$ QED

Heat flow from a hotter body to a cooler body is an irreversible process, so that the entropy must increase.

III





IV. As illustrated clearly by the (S, T) diagram, the entropy transferred from the hot source to the engine in the A → B part of the cycle is equal to the entropy transferred to the "sink" in the C → D part. So, the sum of the entropies of the two bodies remain constant in the process!

So: $\Delta S_{TOT} = C \ln \frac{T_f'}{T_1} + C \ln \frac{T_f'}{T_2} = 0$

$$C \ln \frac{T_f'^2}{T_1 T_2} = 0 \Rightarrow \frac{T_f'^2}{T_1 T_2} = 1$$

$$T_f' = \sqrt{T_1 T_2}$$

Mechanical work output can be obtained by calculating the change in energy:

$$W = \Delta U_{TOT} = CT_1 + CT_2 - 2CT_f' = C(T_1 + T_2 - 2\sqrt{T_1 T_2})$$

$T_f' < T_f$:

$$T_f^2 = \frac{(T_1+T_2)^2}{4} = \frac{T_1^2 + T_2^2 + 2T_1T_2}{4} = \frac{T_1^2 + T_2^2 - 2T_1T_2 + 4T_1T_2}{4}$$

$$= T_1 T_2 + \underbrace{\frac{(T_1 - T_2)^2}{4}}_{\text{always positive}}$$

So, $T_f^2 > T_1 T_2 \Rightarrow T_f > \sqrt{T_1 T_2} \Rightarrow T_f > T_f'$

Work was delivered, so less energy remained in the system.

OSU Physics Comp Exam, Spring 2008
Problem 7

Consider a system of two distinguishable spin-1/2 particles. For times $t < 0$, the Hamiltonian is zero. At time $t = 0$, an interaction Hamiltonian $H' = \frac{4A}{\hbar^2}\vec{\mathbf{S}}_1 \cdot \vec{\mathbf{S}}_2$ is turned on. The system is in the state $|+-\rangle \equiv \left|m_1 = +\frac{\hbar}{2},\ m_2 = -\frac{\hbar}{2}\right\rangle$ at time $t = 0$. Calculate the probability for the system at a later time t to be found in each of the four states $|++\rangle$, $|+-\rangle$, $|-+\rangle$, and $|--\rangle$.

a) First solve for the four probabilities exactly.

b) Then solve for the four probabilities using first-order time-dependent perturbation theory.

c) Under what conditions does perturbation theory give the correct results?

Recall the main result from first-order time-dependent perturbation theory:

$$c_n(t) = \frac{1}{i\hbar}\int_0^t \langle n|H'(t')|i\rangle e^{i\frac{E_n - E_i}{\hbar}t'}\, dt'$$

c) To solve exactly need eigenenergies:

$$H' = \frac{4A}{\hbar^2} \vec{S}_1 \cdot \vec{S}_2$$

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

$$\vec{S}^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

$$\Rightarrow \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\right)$$

$$= \frac{1}{2}\left[S(S+1)\hbar^2 - \frac{3}{4}\hbar^2 - \frac{3}{4}\hbar^2\right]$$

$$\Rightarrow \boxed{H' = A\left[2S(S+1) - 3\right]}$$

$S_1 = \frac{1}{2}, S_2 = \frac{1}{2} \Rightarrow S = 0, 1$

eigenstates are coupled spin states $|SM\rangle$

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left[|+-\rangle - |-+\rangle\right] \rightarrow E_0 = -3A$$

$$\left.\begin{aligned} |1,1\rangle &= |++\rangle \\ |1,0\rangle &= \frac{1}{\sqrt{2}}\left[|+-\rangle + |-+\rangle\right] \\ |1,-1\rangle &= |--\rangle \end{aligned}\right\} \rightarrow E_1 = A$$

$$|\psi(0)\rangle = |+-\rangle = \frac{1}{\sqrt{2}}\left[|0,0\rangle + |1,0\rangle\right]$$

$$\Rightarrow |\psi(t)\rangle = \sum_i a_i e^{-i\frac{E_i t}{\hbar}} |E_i\rangle$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left[|0,0\rangle e^{\frac{3iA}{\hbar}t} + |1,0\rangle e^{-\frac{iA}{\hbar}t}\right]$$

$$P_{m,m_2}(t) = \left| \langle m, m_2 | \psi(t) \rangle \right|^2$$

$$= \frac{1}{2} \left| \langle m, m_2 | 0,0 \rangle e^{\frac{3iA}{\hbar}t} + \langle m, m_2 | 1,0 \rangle e^{-\frac{iA}{\hbar}t} \right|^2$$

$$= \frac{1}{2} \left| e^{\frac{iAt}{\hbar}} \right|^2 \left| \langle m, m_2 | 0,0 \rangle e^{\frac{2iA}{\hbar}t} + \langle m, m_2 | 1 0 \rangle e^{-i\frac{2A}{\hbar}t} \right|^2$$

$$\langle ++ | 0,0 \rangle = \langle ++ | 1,0 \rangle = 0$$

$$\langle -- | 0,0 \rangle = \langle -- | 1,0 \rangle = 0$$

$$\langle +- | 0,0 \rangle = \frac{1}{\sqrt{2}}$$

$$\langle +- | 1,0 \rangle = \frac{1}{\sqrt{2}}$$

$$\langle -+ | 0,0 \rangle = -\frac{1}{\sqrt{2}}$$

$$\langle -+ | 1,0 \rangle = \frac{1}{\sqrt{2}}$$

$$\Rightarrow P_{++} = P_{--} = 0$$

$$P_{+-} = \frac{1}{2} \left| \frac{1}{\sqrt{2}} \left(e^{\frac{2iA}{\hbar}t} + e^{-\frac{2iA}{\hbar}t} \right) \right|^2$$

$$P_{+-} = \cos^2\left(\frac{2A}{\hbar}t\right)$$

$$P_{-+} = \sin^2\left(\frac{2A}{\hbar}t\right)$$

③

b) $C_n(t) = \frac{1}{i\hbar}\int_0^t \langle n|H'(t')|i\rangle e^{i\frac{E_n-E_i}{\hbar}t'}dt'$ $n\neq i$

assumes $C_i(0)=1$

$\quad$ & $|C_i(t)|=1 \Rightarrow$ no change

$\Rightarrow \mathcal{P}_{+-} = 1$ at this level of approx

H' is diagonal in $|S,m\rangle$

but not in $|m_1 m_2\rangle$

but form of H' tells us it only couples

$|+-\rangle$ to $|-+\rangle$

i.e. $\langle ++|H'|+-\rangle = 0$

$\langle --|H'|+-\rangle = 0$

$$\Rightarrow \mathcal{P}_{++} = \mathcal{P}_{--} = 0$$

$$\langle -+|H'|+-\rangle = \frac{1}{\sqrt{2}}\left[\langle 1,0| - \langle 0,0|\right]A\left(2S(S+1)-3\right)\frac{1}{\sqrt{2}}\left[|1,0\rangle+|0,0\rangle\right]$$

$$= \frac{1}{2}\left[A - (-3A)\right] = 2A$$

$\Rightarrow C_{-+}(t) = \frac{1}{i\hbar}\int_0^t 2A\, e^{i0t'}dt'$ since $E_n=0$ before H' turned on.

$$\Rightarrow c_{-+}(t) = \frac{2A}{i\hbar}\int_0^t dt'$$

$$= \frac{2At}{i\hbar}$$

$$\Rightarrow P_{-+}(t) = \left|\frac{2At}{i\hbar}\right|^2$$

$$\boxed{P_{-+}(t) = \frac{4A^2t^2}{\hbar^2}}$$

c) Pert th assumes prob $\ll 1$

$$\Rightarrow \frac{4A^2t^3}{\hbar^2} \ll 1$$

under this condition exact results are

$$P_{-+} = \sin^2\left(\frac{2A}{\hbar}t\right) \simeq \left(\frac{2At}{\hbar}\right)^2 = \frac{4A^2t^2}{\hbar^2}$$

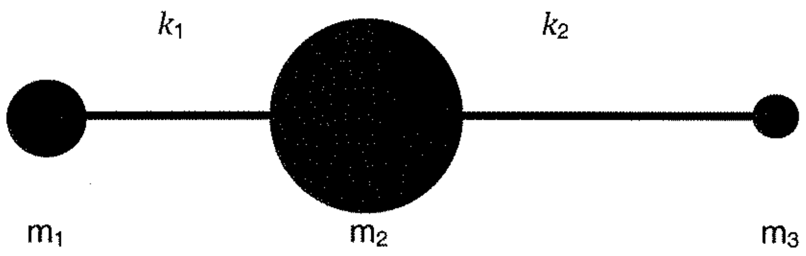
<u>so they agree</u>

$$P_{+-} = \cos^2\left(\frac{2A}{\hbar}t\right) \simeq 1 \quad \text{for small argument}$$

OSU Physics Comp Exam, Spring 2008

Problem 8

Consider an asymmetric triatomic molecule of the form shown below:



The atomic masses $m_1 \neq m_2 \neq m_3$ and the “spring constants” $k_1 \neq k_2$.

(1) Considering only motion along the direction of the molecular axis, obtain expressions for the frequencies of the normal modes of molecular vibrations in terms of the given parameters.

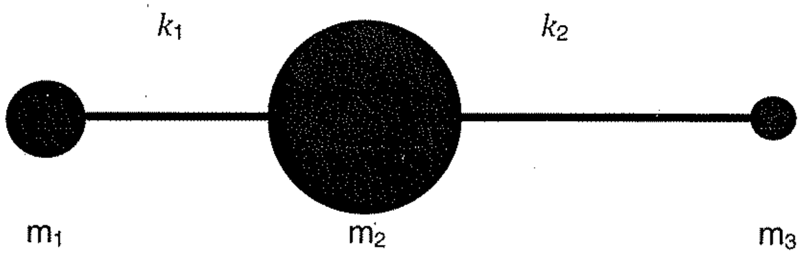
(2) Using your intuition (do not try to calculate), draw a diagram illustrating the atomic motions of the normal modes.

(3) Given a gas of such molecules, how would you actually measure the frequencies of these molecular vibrations?

Classical Mechanics – Graduate

Solution

Consider an asymmetric triatomic molecule of the form shown below:



The atomic masses $m_1 \neq m_2 \neq m_3$ and the "spring constants" $k_1 \neq k_2$.

(1) Considering only motion along the direction of the molecular axis, obtain expressions for the frequencies of the normal modes of molecular vibrations in terms of the given parameters.

Let $\dot{x}_i$ be the displacement from equilibrium of the i^{th} mass. Then the kinetic energy is

$$T = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2$$

and the potential energy is

$$V = \frac{1}{2}k_1(x_1 - x_2)^2 + \frac{1}{2}k_2(x_2 - x_3)^2$$

The Euler-Lagrange equation separates into terms involving only the kinetic and potential energies, respectively:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) - \frac{\partial L}{\partial x_i} = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}_i}\right) + \frac{\partial V}{\partial x_i} = 0 \qquad i = 1, 2, 3$$

Then

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{x}_i}\right) = m_i\ddot{x}_i \quad i = 1, 2, 3$$

and

$$\frac{\partial V}{\partial x_1} = k_1x_1 - k_1x_2 \quad \frac{\partial V}{\partial x_2} = (k_1+k_2)x_2 \; - k_1x_1 \; - k_2x_3 \quad \frac{\partial V}{\partial x_1} = k_2x_3 - k_2x_2$$

The equations of motion giving by the Euler-Lagrange equation are

$$m_1\ddot{x}_1 + \; k_1x_1 - k_1x_2 \; = \; 0$$

$$m_2\ddot{x}_2 - \; k_1x_1 + (k_1+k_2)x_2 - \; k_2x_3 \; = \; 0$$

$$m_3\ddot{x}_3 + \; k_2x_3 - k_2x_2 \; = \; 0$$

Now, to get the normal mode frequencies, assume oscillatory solutions of the form

$$x_i = a_i e^{i\omega t} \quad \Rightarrow \quad \ddot{x}_i \; = \; -\omega^2 a_i$$

Substitute in the equations of motion and cancel the exponentials to get the set of linear equations for the amplitudes:

$$\begin{aligned} (k_1 \; - \; \omega^2 m_1)a_1 \quad - \quad k_1a_2 \qquad\qquad &= \; 0 \\ -k_1a_1 \; + \; [(k_1+k_2) - \omega^2 m_2]a_2 \; - \; k_2\,a_3 \; &= \; 0 \\ -k_2a_2 \; + \; (k_2 \; - \; \omega^2 m_3)a_3 \; &= \; 0 \end{aligned}$$

The secular determinant is

$$\begin{vmatrix} k_1-\omega^2m_1 & -k_1 & 0 \\ -k_1 & k_1+k_2-\omega^2m_2 & -k_2 \\ 0 & -k_2 & k_2-\omega^2m_3 \end{vmatrix} \; = \; 0$$

Evaluating the determinant:

$$(k_1-\omega^2m_1)[(k_1+k_2-\omega^2m_2)(k_2-\omega^2m_3) - k_2^2] + k_1[-k_1(k_2-\omega^2m_3)] = 0$$

Multiply out and collect powers of ω:

$$-\omega^6(m_1m_2m_3) + \omega^4[m_2m_3k_1 + m_1m_3(k_1+k_2) + m_1m_2k_2] \\ + \omega^2[-m_3k_1(k_1+k_2) - m_2k_1k_2 + m_3k_1^2 - m_1k_2(k_1+k_2) + m_1k_2^2] = 0$$

Simplify the ω^2 term:

$$-\cancel{m_3k_1^2} - m_3k_1k_2 - m_2k_1k_2 + \cancel{m_3k_1^2} - m_1k_1k_2 - \cancel{m_1k_2^2} + \cancel{m_1k_2^2} = -k_1k_2M$$

where $M \equiv m_1 + m_2 + m_3$ is the total molecular mass.

Simplify the ω^2 term:

$$[m_2m_3k_1 + m_1m_3(k_1+k_2) + m_1m_2k_2] = m_3(m_1+m_2)k_1 + m_1(m_2+m_3)k_2.$$

Factoring ω^2 gives one solution $\omega = 0$, which corresponds to uniform translation of the whole molecule (no vibration).

We are left with a quadratic in ω^2:

$$(m_1m_2m_3)\omega^4 - [m_3(m_1+m_2)k_1 + m_1(m_2+m_3)k_2]\omega^2 + Mk_1k_2 = 0.$$

The solutions are

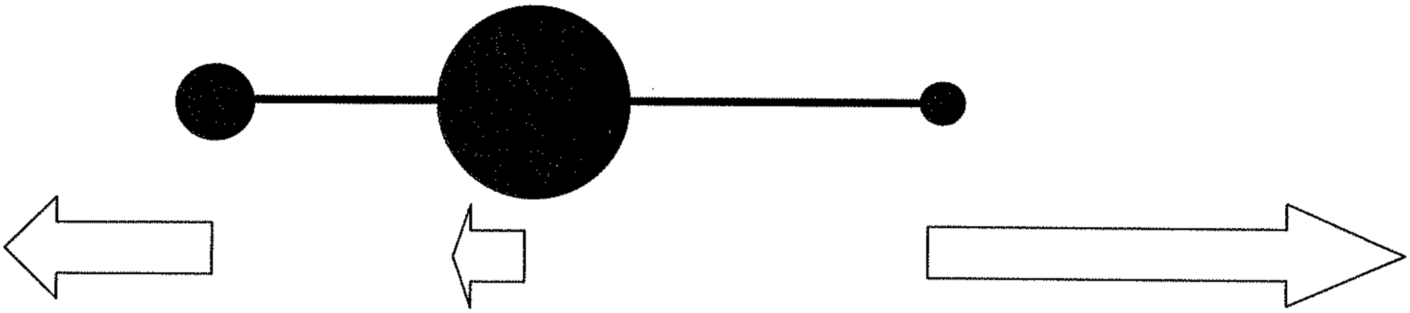
$$\omega^2 = \left[\frac{1}{2(m_1m_2m_3)}\right]\Big\{[m_3(m_1+m_2)k_1 + m_1(m_2+m_3)k_2] \\ \pm \sqrt{[m_3(m_1+m_2)k_1 + m_1(m_2+m_3)k_2]^2 - 4(m_1m_2m_3)Mk_1k_2}\Big\}$$

Dividing through by $(m_1m_2m_3)$, we can express the result in terms of various frequencies $\omega_{ij}^2 = \frac{k_i}{m_j}$:

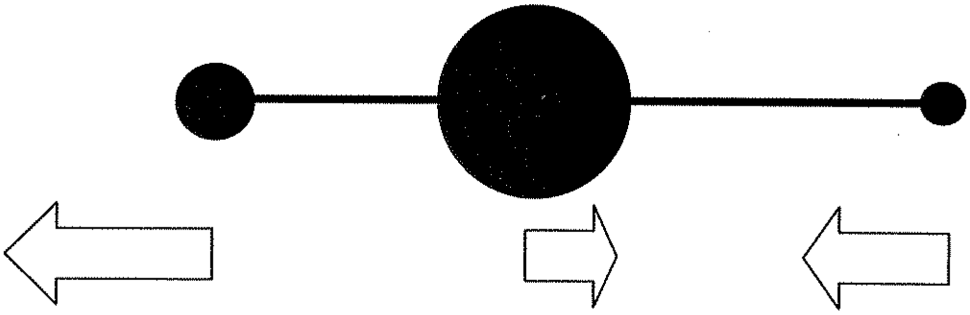
$$\omega^2 = \frac{1}{2}(\omega_{11}^2 + \omega_{12}^2 + \omega_{22}^2 + \omega_{23}^2) \pm \frac{1}{2}\sqrt{(\omega_{11}^2 + \omega_{12}^2 + \omega_{22}^2 + \omega_{23}^2)^2 - \frac{4M}{m_3}\omega_{11}^2\omega_{22}^2}.$$

(2) Using your intuition (do not try to calculate), draw a diagram illustrating the atomic motions of the normal modes.

The lower frequency (obtained by taking the minus sign with the radical) will correspond to a more symmetric motion with the outer atoms moving in opposite directions:



The higher frequency (obtained by taking the plus sign with the radical) will correspond to motion with the outer atoms moving in the same directions:



In order to conserve linear momentum (no motion of the center of mass), the displacements must be such that, at all times,

$$m_1x_1 + m_2x_2 + m_3x_3 = 0$$

(3) Given a gas of such molecules, how would you actually measure the frequencies of these molecular vibrations?

In a real molecule containing atoms of different masses (different chemical elements), the atoms will carry effective electric charges, some positive and some negative. Therefore, the vibrating molecule is essentially an oscillating electric dipole that can interact strongly with electromagnetic radiation. The frequencies of the vibrational modes can be detected by optical absorption spectra, typically in the infra-red.