OSU Physics Department
Comprehensive Examination #131

Monday, April 2 and Tuesday, April 3, 2018

Spring 2018 Comprehensive Examination

PART 1, Monday, April 2, 9:00am
PART 2, Monday, April 2, 1:00pm
PART 3, Tuesday, April 3, 9:00am
PART 4, Tuesday, April 3, 1:00pm

General Instructions

This Spring 2018 Comprehensive Examination consists of four separate parts of two problems each. Each problem caries equal weight (20 points each) and lasts three hours. 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 on the provided pages, work each problem in its own labeled pages, and be certain that your chosen student letter (but not your name) is on the header of each page of your exam, including any unused pages. If you need additional paper for your work, use the blank pages provided. Each page of work should include the problem number, a page number, your chosen student letter, and the total number of pages actually used. 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 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 exams and formula sheets at the end of the exam.

The Hamiltonian of an one dimensional harmonic oscillator

$$H_x = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

satisfies the eigenvalue equation,

$$H_x|n\rangle = E_n|n\rangle, \text{ where } E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{for } n = 0, 1, 2, \cdots$$

Now we consider a two-dimensional isotropic harmonic oscillator, whose Hamiltonian is expressed as

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2\right)$$

(a) Write down the eigenvalues and eigenstates of the Hamiltonian, H. How many states are degenerate for an energy eigenvalue?

Assume that the oscillator is initially in an arbitrary state, a superposition of many energy eigenstates, and you make a measurement on its energy. What is the most general form of the resulting state after the measurement?

(b) We consider a perturbation

$$V = gxy,$$

where $g(\ll m\omega^2)$ is a positive constant.

(i) Calculate the energy eigenvalue of the ground state up to the second order and eigenstate up to the first order.

(ii) Calculate the energy eigenvalue and eigenstate of the first excited state up to the first order.

The Hamiltonian of an one dimensional harmonic oscillator

$$H_x = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

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Now we consider a two-dimensional isotropic harmonic oscillator, whose Hamiltonian is expressed as

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2\right)$$

(a) Write down the eigenvalues and eigenstates of the Hamiltonian, H. How many states are degenerate for an energy eigenvalue?

Assume that the oscillator is initially in an arbitrary state, a superposition of many energy eigenstates, and you make a measurement on its energy. What is the most general form of the resulting state after the measurement?

Solution:
The 2D SHO Hamiltonian can be written as a sum of two 1D Hamiltonian, $H = H_x + H_y$. Therefore, a direct product of the eigenstates of H_x and H_y is an eigenstate of H:

$$|n_x n_y\rangle = |n_x\rangle \otimes |n_y\rangle \quad \text{for } n_x, n_y = 0, 1, 2, \cdots$$

and the corresponding eigenvalue is

$$E_{n_x n_y} = E_{n_x} + E_{n_y} = (n_x + n_y + 1)\hbar\omega = (N+1)\hbar\omega, \text{ where } N = 0, 1, 2, \cdots$$

For a given $N = n_x + n_y$, n_x runs from 0 to N while $n_y = N - n_x$. Thus, the number of degeneracy for the energy eigenvalue $E_N = (N+1)\hbar\omega$ is $N + 1$.

The result of the measurement must be an energy eigenvalue, E_N, and the resulting state must be a superposition of the degenerate states, $\{|n_x N - n_x\rangle\}$ for $n_x = 0, 1, \cdots, N$,

$$|N\rangle = \sum_{n_x=0}^{N} C_{n_x}|n_x N - n_x\rangle,$$

where C_{n_x} is an arbitrary constant satisfying the normalization condition, $\sum_{n_x=1}^{n} |C_{n_x}|^2 = 1$.

(b) We consider a perturbation

$$V = gxy,$$

where $g(\ll m\omega^2)$ is a positive constant.

(i) Calculate the energy eigenvalue of the ground state up to the second order and eigenstate up to the first order.

(ii) Calculate the energy eigenvalue and eigenstate of the first excited state up to the first order.

Solution:
The perturbation can be expressed in terms of a and $a^\dagger$,

$$V = gxy = g\left(\frac{\hbar}{2m\omega}\right)(a_x + a_x^\dagger)(a_y + a_y^\dagger)$$

(i) The unperturbed ground state is $|00\rangle$ and its energy is $E_{00}^{(0)} = \hbar\omega$. The first order energy correction is

$$E_0^{(1)} = \langle 00|V|00\rangle = g\left(\frac{\hbar}{2m\omega}\right)\langle 00|11\rangle = 0$$

and the second order energy correction is

$$\begin{aligned} E_0^{(2)} &= \sum_{n_x n_y} \frac{|\langle n_x n_y|V|00\rangle|^2}{E_{00}^{(0)} - E_{n_x n_y}^{(0)}} = \left|\frac{g\hbar}{2m\omega}\right|^2 \sum_{n_x n_y} \frac{|\langle n_x n_y|11\rangle|^2}{E_{00}^{(0)} - E_{n_x n_y}^{(0)}} \\ &= \frac{\left|\frac{g\hbar}{2m\omega}\right|^2}{E_{00}^{(0)} - E_{11}^{(0)}} = \frac{g^2\hbar^2}{(2m\omega)^2(-2\hbar\omega)} = -\frac{\hbar g^2}{8m^2\omega^3} \end{aligned}$$

Therefore, the ground state energy up to the second order is

$$E_0 \cong \hbar\omega\left(1 - \frac{g^2}{8m^2\omega^4}\right)$$

The ground state up to the first order is

$$|0\rangle \cong |00\rangle + \sum_{n_x n_y} \frac{\langle n_x n_y|V|00\rangle}{E_{00}^{(0)} - E_{n_x n_y}^{(0)}}|n_x n_y\rangle = |00\rangle + \frac{g\left(\frac{\hbar}{2m\omega}\right)}{-2\hbar\omega}|11\rangle = |00\rangle - \frac{g}{4m\omega^2}|11\rangle$$

(ii) The unperturbed first excited states, $|10\rangle$ and $|01\rangle$, are degenerate. In the subspace with the two basis vectors,

$$|10\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |01\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

the perturbation is represented by a 2×2 matrix,

$$V \doteq \begin{pmatrix} \langle 10|V|10\rangle & \langle 10|V|01\rangle \\ \langle 01|V|10\rangle & \langle 01|V|01\rangle \end{pmatrix} = \begin{pmatrix} 0 & \frac{g\hbar}{m\omega} \\ \frac{g\hbar}{m\omega} & 0 \end{pmatrix}$$

The first order energy correction of the degenerate states is obtained by diagonalizing the matrix:

$$E_\pm^{(1)} = \pm\frac{g\hbar}{2m\omega}$$

Thus the energies of the first excited states up to the first order are

$$E_\pm = 2\hbar\omega\left(1 \pm \frac{g}{4m\omega^2}\right)$$

The corresponding eigenstates are

$$|1\rangle_{\pm} \cong \frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle)$$

The first excited states up to the first order are

$$|1\rangle_{\pm} \cong \frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle) + \sum_{n_x n_y} \frac{\langle n_x n_y | V \frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle)}{E^{(0)}_{00} - E^{(0)}_{n_x n_y}} |n_x n_y\rangle$$

where

$$\begin{aligned} V\frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle) &= g\left(\frac{\hbar}{2m\omega}\right)(a_x + a_x^\dagger)(a_y + a_y^\dagger)\frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle) \\ &= g\left(\frac{\hbar}{2m\omega}\right)\frac{1}{\sqrt{2}}(\sqrt{2}|21\rangle \pm \sqrt{2}|12\rangle) = \left(\frac{g\hbar}{2m\omega}\right)(|21\rangle \pm |12\rangle) \end{aligned}$$

Thus,

$$|1\rangle_{\pm} \cong \frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle) + \frac{g\left(\frac{\hbar}{2m\omega}\right)}{-2\hbar\omega}(|21\rangle \pm |12\rangle) = \frac{1}{\sqrt{2}}(|10\rangle \pm |01\rangle) - \frac{g}{4m\omega^2}(|21\rangle \pm |12\rangle)$$

An electron is subject to a uniform, time-independent magnetic field of strength B in the positive z-direction. The Hamiltonian of the system is expressed as

$$H = -\gamma B S_z = \omega_0 S_z$$

Find the energy and the expectation value of the spin angular momentum of the electron at t and sketch the time evolution of the spin angular momentum,

(a) when the expectation value of the spin angular momentum at $t = 0$ is given as

$$\langle S_x \rangle = \frac{\hbar}{2}, \quad \langle S_y \rangle = \langle S_z \rangle = 0$$

(b) and when the expectation value of the spin angular momentum at $t = 0$ is given as

$$\langle S_x \rangle = 0, \quad \langle S_y \rangle = \langle S_z \rangle > 0$$

An electron is subject to a uniform, time-independent magnetic field of strength B in the positive z-direction. The Hamiltonian of the system is expressed as

$$H = -\gamma B S_z = \omega_0 S_z$$

Find the energy and the expectation value of the spin angular momentum of the electron at t and sketch the time evolution of the spin angular momentum,

Solution:
An electron spin in a uniform magnetic field precesses around the the direction of the magnetic field. We use the Ehrenfest's Theorem to obtain the temporal evolution of the expectation value of the spin angular momenum:

$$\frac{d}{dt}\langle S_i\rangle = \frac{i}{\hbar}\langle [H, S_i]\rangle, \quad i = x, y, z,$$

which leads to

$$\begin{aligned}
\frac{d}{dt}\langle S_x\rangle &= \frac{i\omega_0}{\hbar}\langle [S_z, S_x]\rangle = \frac{i\omega_0}{\hbar}\langle i\hbar S_y\rangle = -\omega_0\langle S_y\rangle \\
\frac{d}{dt}\langle S_y\rangle &= \frac{i\omega_0}{\hbar}\langle [S_z, S_y]\rangle = \frac{i\omega_0}{\hbar}\langle -i\hbar S_x\rangle = \omega_0\langle S_x\rangle \\
\frac{d}{dt}\langle S_z\rangle &= \frac{i\omega_0}{\hbar}\langle [S_z, S_z]\rangle = 0
\end{aligned}$$

Here we have the equation of motion of the spin angular momentum,

$$\begin{aligned}
\frac{d^2}{dt^2}\langle S_x\rangle &= -\omega_0\frac{d}{dt}\langle S_y\rangle = -\omega_0^2\langle S_x\rangle \\
\frac{d^2}{dt^2}\langle S_y\rangle &= \omega_0\frac{d}{dt}\langle S_x\rangle = -\omega_0^2\langle S_y\rangle \\
\frac{d}{dt}\langle S_z\rangle &= 0
\end{aligned}$$

The solution of the equation of motion is

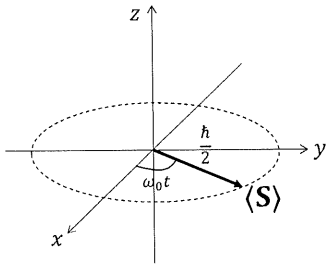
$$\begin{aligned}
\langle S_x\rangle(t) &= \langle S_x\rangle(0)\cos\omega_0 t - \langle S_y\rangle(0)\sin\omega_0 t \\
\langle S_y\rangle(t) &= \langle S_x\rangle(0)\sin\omega_0 t + \langle S_y\rangle(0)\cos\omega_0 t \\
\langle S_z\rangle(t) &= \langle S_z\rangle(0)
\end{aligned}$$

(a) when the expectation value of the spin angular momentum at $t = 0$ is given as

$$\langle S_x\rangle = \frac{\hbar}{2}, \quad \langle S_y\rangle = \langle S_z\rangle = 0$$

Solution:
Using the initial condition, we get

$$\begin{aligned}
\langle S_x\rangle(t) &= \frac{\hbar}{2}\cos\omega_0 t \\
\langle S_y\rangle(t) &= \frac{\hbar}{2}\sin\omega_0 t \\
\langle S_z\rangle(t) &= 0
\end{aligned}$$



The energy is independent of time: $E = \langle H \rangle = \omega_0 \langle S_z \rangle (t) = 0$

(b) and when the expectation value of the spin angular momentum at $t = 0$ is given as

$$\langle S_x \rangle = 0, \quad \langle S_y \rangle = \langle S_z \rangle > 0$$

Solution:
An arbitrary spin state is actually a spin-up state of S_n on a certain axis n with the eigenvalue $\hbar/2$, which leads to

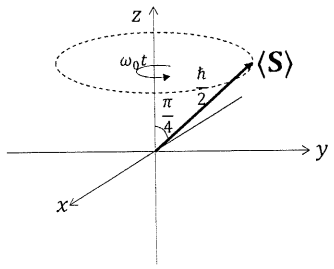
$$|\langle \mathbf{S} \rangle| = \sqrt{\langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2} = \frac{\hbar}{2}$$

Therefore,

$$\langle S_y \rangle = \langle S_z \rangle = \frac{\hbar}{2\sqrt{2}}$$

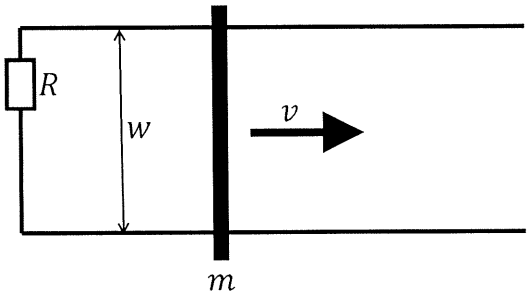
Using the initial condition, we get

$$\begin{aligned} \langle S_x \rangle (t) &= -\frac{\hbar}{2\sqrt{2}} \sin \omega_0 t \\ \langle S_y \rangle (t) &= \frac{\hbar}{2\sqrt{2}} \cos \omega_0 t \\ \langle S_z \rangle (t) &= \frac{\hbar}{2\sqrt{2}} \end{aligned}$$



The energy is independent of time: $E = \langle H \rangle = \omega_0 \langle S_z \rangle (t) = \frac{\hbar \omega_0}{2\sqrt{2}}$

A metal bar of mass m slides frictionlessly on two parallel conducting rails a distance w apart (see figure). A resistor R is connected across the rails and a uniform magnetic field $\vec{B}$, pointing into the page, fills the entire region.



(a) If the bar moves to the right at speed v, what is the current in the resistor? In what direction does it flow?

(b) What is the magnetic force on the bar? In what direction?

(c) If the bar starts out with speed v_0 at time $t = 0$, and is left to slide, what is its speed at a later time t?

(d) Verify by explicit calculation that in the process described in the previous part the energy delivered to the resistor is exactly $\frac{1}{2}mv_0^2$.

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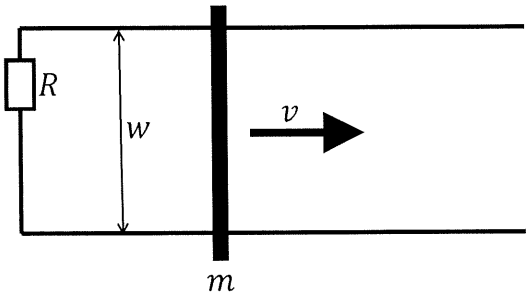

(a) If the bar moves to the right at speed v, what is the current in the resistor? In what direction does it flow?

Solution:
The magnitude of the motional emf is given by

$$\mathcal{E} = \left| -\frac{d\phi}{dt} \right| = \frac{d(B \cdot A)}{dt} = B\frac{dA}{dt} = Bwv \tag{1}$$

The direction of the current is counterclockwise through the loop formed by the bar, rails and the resistor and the current is

$$I = \frac{|\mathcal{E}|}{R} = \frac{Bwv}{R} \tag{2}$$

(b) What is the magnetic force on the bar? In what direction?

Solution:
The force on a current carrying section of wire $d\vec{w}$ follows from the force on a moving charge in a magnetic field

$$d\vec{F} = q\vec{v} \times \vec{B} = q\frac{d\vec{w}}{dt} \times \vec{B} = Id\vec{w} \times \vec{B}\,, \tag{3}$$

and the force on the bar is in the opposite direction of $\vec{v}$ (Lenz law) with magnitude

$$F = IwB = \frac{vw^2B^2}{R} \tag{4}$$

(c) If the bar starts out with speed v_0 at time $t = 0$, and is left to slide, what is its speed at a later time t?

Solution:

$$\frac{d\vec{v}}{dt} = \frac{1}{m}\vec{F} = -\frac{w^2B^2}{mR}\vec{v}, \tag{5}$$

and

$$v(t) = v_0 e^{-t/\tau}, \quad \tau = \frac{mR}{w^2B^2} \tag{6}$$

(d) Verify by explicit calculation that in the process described in the previous part the energy delivered to the resistor is exactly $\frac{1}{2}mv_0^2$.

Solution:

$$\int_0^\infty P_{\text{joule}}(t)dt = \int_0^\infty \frac{\mathcal{E}(t)^2}{R}dt = \frac{w^2B^2}{R}v_0^2\int_0^\infty e^{-2t/\tau}dt = \frac{w^2B^2}{R}v_0^2\frac{\tau}{2} = \frac{1}{2}mv_0^2 \tag{7}$$

A homogeneous dielectric sphere (dielectric permittivity ϵ) of radius R is placed in a uniform electric field $\vec{E} = E_0 \hat{e}_z$.

(a) Calculate the electric potential everywhere, i.e inside and outside the sphere.

(b) Calculate the electric field inside and outside the sphere. Show that the electric field outside the sphere is the sum of the orignal uniform electric field and the field due to an induced electric dipole and determine the strength of the induced electric dipole.

A homogeneous dielectric sphere (dielectric permittivity ϵ) of radius R is placed in a uniform electric field $\vec{E} = E_0 \hat{e}_z$.

(a) Calculate the electric potential everywhere, i.e inside and outside the sphere.

Solution:
The problem has axial symmetry and the potential satisfies Laplace's equation, which can be solved using an expansion in Legendre polynomials in 2 separate regions:

$$\begin{aligned} 1: \quad & r \leq R \\ 2: \quad & r > R \end{aligned}$$

The contribution from the external field and from the polarized sphere must be included separately. The expansion in Legendre polynominals in the general case is (formula sheet)

$$\phi(r,\theta) = \sum_{l=0}^{\infty} \left(a_l r^l + \frac{b_l}{r^{l+1}} \right) P_l(\cos\theta) \,.$$

and the potential for the external field is

$$\phi_0 = -E_0 z = -E_0 r \cos\theta = -E_0 P_1(\cos\theta)$$

where P_1 is given on the formula sheet.

For our problem, note that in region 1 terms $\sim \frac{b_l}{r^{l+1}}$ must vanish ($b_l = 0$) to avoid divergences at the origin and in region 2 terms $\sim a_l r^l$ must vanish ($a_l = 0$) to avoid divergences at ∞. We get:

$$\phi_1(r,\theta) = \sum_l a_l r^l P_l(\cos\theta) - E_0 r P_1(\cos\theta), \qquad r \leq R \tag{8}$$

$$\phi_2(r,\theta) = \sum_l \frac{b_l}{r^{l+1}} P_l(\cos\theta) - E_0 r P_1(\cos\theta), \qquad r > R. \tag{9}$$

The remaining coefficients a_l and b_l are determinded by the boundary conditions for ϕ and $\mathbf{D}$ at the surface of the sphere, $r = R$. Uniqueness of the Legendre polynomial expansion allows us to equate terms for each l seperately. The continuity of ϕ at $r = R$ gives

$$a_l R^l = \frac{b_l}{R^{l+1}}, \tag{10}$$

$$b_l = a_l R^{2l+1}. \tag{11}$$

The continuity of D_n at $r = R$ written in terms of the potential ϕ is

$$\epsilon \left.\frac{\partial \phi_1(r,\theta)}{\partial r}\right|_{r=R} = \epsilon_0 \left.\frac{\partial \phi_2(r,\theta)}{\partial r}\right|_{r=R}. \tag{12}$$

This gives

$$\sum_l \epsilon_r l a_l R^{l-1} P_l(\cos\theta) - \epsilon_r E_0 P_1(\cos\theta) = \sum_l \frac{-(l+1)b_l}{R^{l+2}} P_l(\cos\theta) - E_0 P_1(\cos\theta)$$

and using (4)

$$= -\sum_l (l+1) a_l R^{l-1} P_l(\cos\theta) - E_0 P_1(\cos\theta) \tag{13}$$

Because the expansion in the P_l is unique, Eqn. (13) must hold for each l seperately, and all a_l must be zero except for a_1:

$$a_1 = \frac{\epsilon_r - 1}{\epsilon_r + 2} E_0 . \tag{14}$$

The potential is given by

$$\phi_1(r,\theta) = -\frac{3E_0 r\cos\theta}{\epsilon_r + 2}, \qquad r \le R \tag{15}$$

$$\phi_2(r,\theta) = \frac{\epsilon_r - 1}{\epsilon_r + 2}\frac{E_0 R^3}{r^2}\cos\theta - E_0 r\cos\theta, \qquad r > R. \tag{16}$$

(b) Calculate the electric field inside and outside the sphere. Show that the electric field outside the sphere is the sum of the original uniform electric field and the field due to an induced electric dipole and determine the strength of the induced electric dipole.

Solution:
The electric field inside the sphere is uniform and given by

$$\vec{E}_1 = \frac{3}{\epsilon_r + 2}\vec{E}_0 . \tag{17}$$

The electric potential outside the sphere consists of two terms, of which the second can be readily identified as the external field. The first term of the potential is proportional to $1/4\pi\epsilon_0 r^2\cos\theta$ which is the well known form of a dipole potential. Hence the electric dipole moment is given by

$$p = 4\pi\epsilon_0 \frac{\epsilon_r - 1}{\epsilon_r + 2} E_0 R^3 \tag{18}$$

and the electric field outside the sphere is

$$\vec{E}_2(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{3\hat{r}(\hat{r}\cdot\vec{p}) - \vec{p}}{r^3} + \vec{E}_0 . \tag{19}$$

Alice measures the tension τ of a Bungee cord over a range of temperatures T and extension L, where the first law is formulated $dU = TdS + \tau dL$. She finds the data can be well approximated by

$$\tau = (a - be^{-T/T_0})L$$

where a, b, and T_0 are positive constants.

(a) Find the change of free energy $F = U - TS$

$$\Delta F = F(T, L) - F(T, 0)$$

(b) Find the change of entropy $\Delta S = S(T, L) - S(T, 0)$.

Hint: consider using Maxwell relation to simplify your calculation.

(c) Find the change of internal energy $\Delta U = U(T, L) - U(T, 0)$.

(d) Explain the physics of the tension-extension relation, $\tau = (a - be^{-T/T_0})L$. Why would the tension depends on temperature?

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$$\tau = (a - be^{-T/T_0})L$$

where a, b, and T_0 are positive constants.

(a) Find the change of free energy $F = U - TS$

$$\Delta F = F(T, L) - F(T, 0)$$

Solution:
from $dF = -SdT + \tau dL$, we have

$$\begin{aligned} \Delta F &= \int_0^L (a - be^{-T/T_0})LdL \\ &= \frac{1}{2}(a - be^{-T/T_0})L^2 \end{aligned}$$

(b) Find the change of entropy $\Delta S = S(T, L) - S(T, 0)$.
Hint: consider using Maxwell relation to simplify your calculation.

Solution:
from $dF = -SdT + \tau dL$, we have

$$(\frac{\partial S}{\partial L})_T = -(\frac{\partial \tau}{\partial T})_L$$

Therefore

$$\begin{aligned} \Delta S &= \int dL(\frac{\partial S}{\partial L})_T \\ &= \int dL[-(\frac{\partial \tau}{\partial T})_L] \\ &= -\frac{b}{2T_0}e^{-T/T_0}L^2 \end{aligned}$$

(c) Find the change of internal energy $\Delta U = U(T, L) - U(T, 0)$.

Solution:
$\Delta U = \Delta F + T\Delta S = \frac{1}{2}(a - be^{-T/T_0})L^2 - \frac{bT}{2T_0}e^{-T/T_0}L^2$.

(d) Explain the physics of the tension-extension relation, $\tau = (a - be^{-T/T_0})L$. Why would the tension depends on temperature?

Solution:
When we straighten the cable, its entropy decreases (less room for wiggling). Therefore part of the tension comes from the **entropic effect**. At a fixed extension, increasing temperature makes the cable to be more relaxed/stretched, thereby reducing the tension.

Motivation: One way to generate a vacuum is to make the wall of a gas container sticky. In other words, gas molecules want to adhere to the container wall (surface states) to reduce energy. As a result, there will be fewer molecules freely moving in the container (bulk states). However, this process cannot be 100% efficient. Because there are more bulk states than surface states, gas molecules will also want to stay in the bulk to maximize the entropy. In the following problem, we devise a simple model to understand the interplay between energy and entropy.

Problem: Assuming our container has N_b bulk sites, and N_s surface sites. When a molecule occupies a bulk site, its energy is ϵ_b. When a molecule occupies a surface site, its energy is ϵ_s. Assume the container is in contact with a heat bath of temperature T.

There are N distinguishable molecules, which can be partitioned to occupy either surface or bulk sites. No sites can be occupied by more than one molecule. We will consider the case where $N \ll N_s \ll N_b$.

(a) Calculate the partition function of the system.

(b) Calculate the internal energy and entropy of the equilibrium state.

(c) Calculate the fraction γ of molecules in the surface state.

(d) Sketch and explain how γ depends on $\frac{N_s}{N_b}$.

Motivation: One way to generate a vacuum is to make the wall of a gas container sticky. In other words, gas molecules want to adhere to the container wall (surface states) to reduce energy. As a result, there will be fewer molecules freely moving in the container (bulk states). However, this process cannot be 100% efficient. Because there are more bulk states than surface states, gas molecules will also want to stay in the bulk to maximize the entropy. In the following problem, we devise a simple model to understand the interplay between energy and entropy.

Problem: Assuming our container has N_b bulk sites, and N_s surface sites. When a molecule occupies a bulk site, its energy is ϵ_b. When a molecule occupies a surface site, its energy is ϵ_s. Assume the container is in contact with a heat bath of temperature T.

There are N distinguishable molecules, which can be partitioned to occupy either surface or bulk sites. No sites can be occupied by more than one molecule. We will consider the case where $N \ll N_s \ll N_b$.

(a) Calculate the partition function of the system.

Solution:
The partition function is

$$Z = (e^{-\beta\epsilon_s}N_s + e^{-\beta\epsilon_b}N_b)^N = B^N$$

where B is the single particle partition function.

(b) Calculate the internal energy and entropy of the equilibrium state.

Solution:
Knowing the partition function, we can use the following standard formulas to calculate the entropy and energy.

$$\begin{aligned} S &= \frac{\partial(k_B T \ln Z)}{\partial T} \\ &= Nk_B[\ln B + \frac{\beta\epsilon_a N_S e^{-\beta\epsilon_a} + \beta\epsilon_b N_b e^{-\beta\epsilon_b}}{B}] \\ U &= -\partial_\beta \ln Z \\ &= N\frac{\epsilon_a N_s e^{-\beta\epsilon_a} + \epsilon_b N_b e^{-\beta\epsilon_b}}{B} \end{aligned}$$

(c) Calculate the fraction γ of molecules in the surface state.

Solution:
Note that the internal energy U of the system equals to $U = N\gamma\epsilon_s + N(1-\gamma)\epsilon_b$. Using the solution of (2) we can find $\gamma = \frac{N_s e^{-\beta\epsilon_a}}{N_s e^{-\beta\epsilon_a} + N_b e^{-\beta\epsilon_b}}$.

(d) Sketch and explain how γ depends on $\frac{N_s}{N_b}$.

Solution:
If we define $q = \frac{N_a}{N_b}$, we can rewrite $\gamma = \frac{e^{-\beta\epsilon_a}}{e^{-\beta\epsilon_a} + \frac{1}{q}e^{-\beta\epsilon_b}}$. As the system size increases, q decreases, and γ decreases. When N is large, $\gamma \sim qe^{-\beta(\epsilon_a - \epsilon_a)}$.

A mass m is constrained to move along a frictionless track that defines the x-axis of a coordinate system. The mass is also attached to a massless spring of spring constant K, with equilibrium length L. The other end of the spring is nailed to a fixed point $(x = 0, y = d)$. In other words, d is the perpendicular distance from the track to the fixed point. Start the problem, assume that $d > L$, i.e. that the spring is always stretched. The mass is set into motion by releasing it from some position away from its equilibrium position.

- Gravity is not relevant in this problem - for example, if gravity acts in the z direction, you can imagine the whole setup on a horizontal table in the xy plane.
- Assume that the spring is ideal and obeys Hooke's law.
- Assume no frictional or other energy loss mechanisms.

(a) Find $U(x)$, the potential energy of the mass as a function of its position.

(b) Show that $x = 0$ is a point of stable equilibrium if $d > L$.

(c) Show that, for small oscillations about equilibrium, the system can be treated as a mass on an ideal spring with an effective spring constant. Derive the effective spring constant and hence identify the oscillation frequency.

(d) If, instead, $d < L$, then $x = 0$ is a point of unstable equilibrium. Give a physical justification for this statement (no calculation) and draw a qualitative sketch of the potential energy U(x) in this situation.

Comprehensive Exam, Winter 2018, Undergraduate CM Solution

A mass m is constrained to move along a frictionless track that defines the x-axis of a coordinate system. The mass is also attached to a massless spring of spring constant K, with equilibrium length L_0. The other end of the spring is nailed to a fixed point ($x = 0, y = d$). In other words, d is the perpendicular distance from the track to the fixed point. To start the problem, assume that $d > L_0$, *i.e.* that the spring is always stretched. The mass is set into motion by releasing it from some position away from its equilibrium position.

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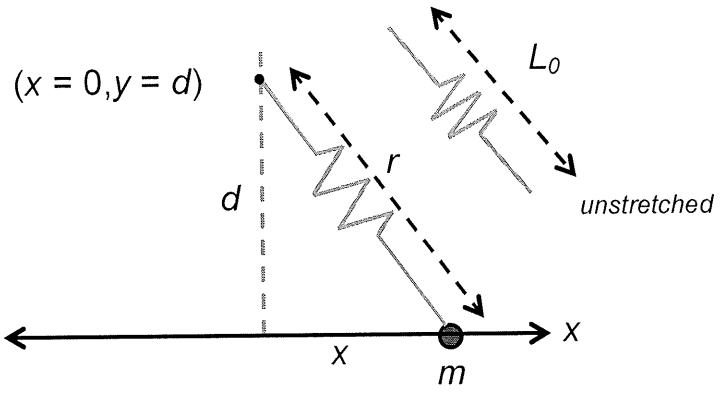
(d) If, instead, $d < L_0$, then $x = 0$ is a point of unstable equilibrium. Give a physical justification for this statement (no calculation) and draw a qualitative sketch of the potential energy $U(x)$ in this situation.

(a) Establish the coordinate system. Let r be the position of the mass, with its position along the track denoted by x. The length of the stretched spring is r; the unstretched length is L_0.



Let the position of the mass be $r = \sqrt{x^2 + d^2}$

Ideal spring has restoring force $\vec{F} = -K(r - L_0)\hat{r}$ (where unit vector points from pivot point to mass) or potential energy $U = \frac{1}{2}K(r - L_0)^2$

Substitute expression for r to find $U(x)$:

$$\boxed{U(x) = \frac{1}{2}K\left(\sqrt{x^2 + d^2} - L_0\right)^2}$$

(b) Equilibrium is a minimum in the potential (derivative is zero) and it is stable if the second derivative is positive (like the bottom of a parabola).

$$\frac{dU(x)}{dx} = \frac{d}{dx}\left(\frac{1}{2}K\left(\left(x^2+d^2\right)^{1/2} - L_0\right)^2\right)$$

Eqm:
$$= \frac{2}{2}K\left(\left(x^2+d^2\right)^{1/2} - L_0\right)\left(\frac{1}{2}\right)\left(x^2+d^2\right)^{-1/2} 2x$$

$$= K\left(1 - \frac{L_0}{\left(x^2+d^2\right)^{1/2}}\right)x$$

This is zero at $x = 0$, so $x = 0$ is an equilibrium point.

Stable?

$$\frac{d^2U(x)}{dx^2} = \frac{d}{dx}K\left(1 - \frac{L_0}{\left(x^2+d^2\right)^{1/2}}\right)x$$

$$= K\left(1 - \frac{L_0}{\left(x^2+d^2\right)^{1/2}}\right) + Kx\left(-\frac{(-1/2)2xL_0}{\left(x^2+d^2\right)^{3/2}}\right)$$

$$= K\left(1 - \frac{L_0}{\left(x^2+d^2\right)^{1/2}}\right) + K\left(\frac{x^2L_0}{\left(x^2+d^2\right)^{3/2}}\right)$$

$$= K\left(1 - \frac{L_0}{\left(x^2+d^2\right)^{1/2}} + \frac{x^2L_0}{\left(x^2+d^2\right)^{3/2}}\right)$$

$$= K\left(1 + \frac{-L_0\left(x^2+d^2\right) + x^2L_0}{\left(x^2+d^2\right)^{3/2}}\right)$$

$$= K\left(1 + \frac{-L_0d^2}{\left(x^2+d^2\right)^{3/2}}\right) \xrightarrow{x=0} K\left(1 - \frac{L_0}{d}\right)$$

Evaluated at the equilibrium point, the second derivative is positive if $d > L_0$ and the equilibrium is indeed stable. (Can also easily second derivative is negative and equilibrium is unstable if $d < L_0$ which is part of (d)).

(c) For small oscillations, x is not too different from its equilibrium value of zero, so expand the potential in a Taylor series about its value at $x = 0$. Noting that the first derivative is zero at equilibrium, we get, to second order:

$$U(x) = U_0 + x\left.\frac{dU}{dx}\right|_{x=0} + \frac{x^2}{2}\left.\frac{d^2U}{dx^2}\right|_{x=0} + \ldots$$

$$U(x) = U_0 + \underbrace{\frac{x^2}{2}\left.\frac{d^2U}{dx^2}\right|_{x=0}}_{\text{effective } K}$$

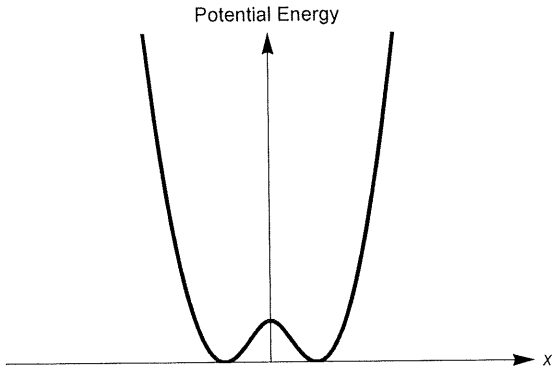
So the second derivative of U is just an effective spring constant. (The finite value of U_0 is just an offset that does not affect the motion.)

$$K_{eff} = K\left(1 - \frac{L_0}{d}\right)$$

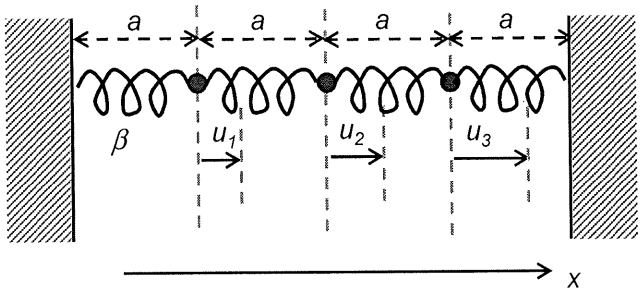
We can identify a frequency of oscillation

$$\omega = \sqrt{\frac{K_{eff}}{m}} = \sqrt{\frac{K}{m}\left(1 - \frac{L_0}{d}\right)}$$

(d) As we saw in (b) the equilibrium is unstable if $d < L_0$. Physically, it means the spring has to be compressed at $x = 0$, which means it stores energy. There must be <u>two</u> positions (one on either side, where the spring can assumes its equilibrium length, and this would be a lower energy state. As x becomes larger, either positive or negative, the spring is stretched again and once more stores energy. At very large stretching, the contribution from the "d" part of the displacement is negligible and the parabolic potential energy is that of the spring constant K. So $U(x)$ looks like this:



A useful model of vibrations of atoms in a periodic solid is to model atoms in the solid as point masses m coupled to neighboring atoms by ideal springs with spring constant β. As the very simplest model, consider just 3 "atoms" with equilibrium spacing a as shown below with the first and third coupled to rigid walls. An atom displacement from equilibrium is u, as shown below. For ease of computation, you can assume that all motion is along the line joining the atoms and that only nearest-neighbor coupling is significant.



(a) Set up the equations of motion for this system.

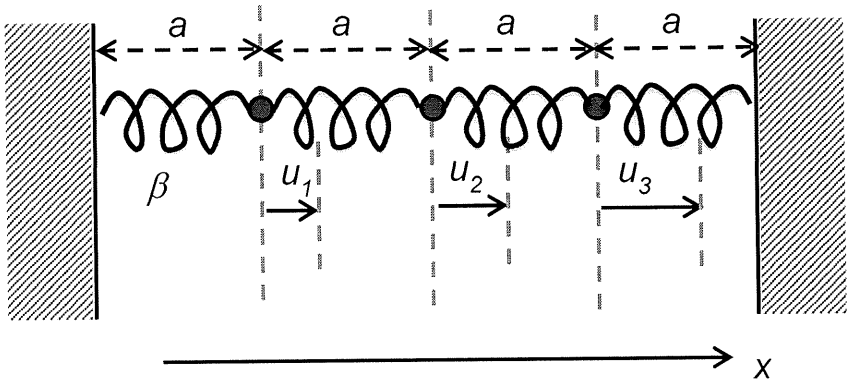
(b) Explain what normal modes are.

(c) Find normal mode solutions to the equations of motion of the atoms.

(d) Sketch the normal modes (arrows indicate the relative directions of motion; arrow length roughly gives the amplitude; a dot if the atom is stationary), indicating the ordering of the frequencies of the modes, with a brief physical explanation.

Comprehensive Exam, Spring 2018 CM Grad (Solution)

A useful model of vibrations of atoms in a periodic solid is to model atoms in the solid as point masses m coupled to neighboring atoms by ideal springs with spring constant β. As the very simplest model, consider just 3 "atoms" with equilibrium spacing a as shown below with the first and third coupled to rigid walls. An atom displacement from equilibrium is u, as shown below. For ease of computation, you can assume that all motion is along the line joining the atoms and that only nearest-neighbor coupling is significant.



a) Set up the equations of motion for this system.
Label the particles 1, 2, 3 starting from the left. Let u_n be the displacement of each particle from it equilibrium position (positive u means in the direction of +ve x). Each mass is subject to two spring forces proportional to the extension of the spring.

$$m\ddot{x}_1 = F_1 = -\beta u_1 - \beta(u_1 - u_2)$$
$$m\ddot{x}_2 = F_2 = -\beta(u_2 - u_1) - \beta(u_2 - u_3)$$
$$m\ddot{x}_3 = F_3 = -\beta u_3 - \beta(u_3 - u_2)$$

You can test that the signs are correct by making one displacement large and checking whether the spring is extended or compressed and if so, which way it pulls on the each mass. Because $x_1 = a + u_1; x_2 = 2a + u_2; x_3 = 3a + u_3$ and a is a constant, $\ddot{x} = \ddot{u}$. Also define $\frac{\beta}{m} \equiv \omega_0^2$, the natural frequency of a single mass-spring system.

$$\ddot{u}_1 = -\frac{\beta}{m}u_1 - \frac{\beta}{m}(u_1 - u_2) = -\omega_0^2 u_1 - \omega_0^2(u_1 - u_2)$$
$$\ddot{u}_2 = -\frac{\beta}{m}(u_2 - u_1) - \frac{\beta}{m}(u_2 - u_3) = -\omega_0^2(u_2 - u_1) - \omega_0^2(u_2 - u_3)$$
$$\ddot{u}_3 = -\frac{\beta}{m}u_3 - \frac{\beta}{m}(u_3 - u_2) = -\omega_0^2 u_3 - \omega_0^2(u_3 - u_2)$$

b) Explain what normal modes are.
Normal modes are those types of motion where all atoms (masses) *oscillate with the same frequency*. Our goal is to find those frequencies (there are N in an N-body problem, so let's call them ω_a, ω_b and ω_c) and the amplitude of oscillation of each atom at each frequency. This set of oscillations decouples the coupled equations above.

c) Find normal modes solutions to the equations of motion of the atoms.

Assume oscillating solutions of the form $\begin{pmatrix} u_{1a} \\ u_{2a} \\ u_{3a} \end{pmatrix} = \begin{pmatrix} A_{1a} \\ A_{2a} \\ A_{3a} \end{pmatrix} e^{i\omega_a t}$

For the a^{th} mode and similar for the b and c modes. We drop the subscript "a" for the moment and substitute a generic form into the coupled equations, which allows us to set up a matrix equation yielding eigenvalues ω_a, ω_b and ω_c, with corresponding eigenvectors as the normal modes.

All the time dependence is in the exponential, and all factors $e^{i\omega_a t}$ cancel (by construction!)

$$-\omega^2 A_1 = -\omega_0^2 A_1 - \omega_0^2 (A_1 - A_2)$$
$$-\omega^2 A_2 = -\omega_0^2 (A_2 - A_1) - \omega_0^2 (A_2 - A_3)$$
$$-\omega^2 A_3 = -\omega_0^2 A_3 - \omega_0^2 (A_3 - A_2)$$

So we get:

$$-\omega^2 A_1 = -2\omega_0^2 A_1 + \omega_0^2 A_2$$
$$-\omega^2 A_2 = \omega_0^2 A_1 - 2\omega_0^2 A_2 + \omega_0^2 A_3$$
$$-\omega^2 A_3 = \omega_0^2 A_2 - 2\omega_0^2 A_3$$

which can be rewritten in matrix form

$$\begin{pmatrix} -\omega^2 + 2\omega_0^2 & -\omega_0^2 & 0 \\ -\omega_0^2 & -\omega^2 + 2\omega_0^2 & -\omega_0^2 \\ 0 & -\omega_0^2 & -\omega^2 + 2\omega_0^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

The set of equations has a solution if the determinant is zero.

$$\begin{vmatrix} -\omega^2 + 2\omega_0^2 & -\omega_0^2 & 0 \\ -\omega_0^2 & -\omega^2 + 2\omega_0^2 & -\omega_0^2 \\ 0 & -\omega_0^2 & -\omega^2 + 2\omega_0^2 \end{vmatrix} = 0$$

Expand by the first row to find the determinant:

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

Common factor:

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

which gives

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

The roots are:

$\omega_b^2=2\omega_0^2$ (the label "b" is arbitrary, but it turns out to be the intermediate frequency).

and

$$\omega^4-4\omega_0^2\omega^2+2\omega_0^4=0\Rightarrow$$

$$\omega_c^2=2\omega_0^2+\sqrt{4\omega_0^4-2\omega_0^4}=\left(2+\sqrt{2}\right)\omega_0^2$$

$$\omega_a^2=2\omega_0^2-\sqrt{4\omega_0^4-2\omega_0^4}\,\omega_c^2=\left(2-\sqrt{2}\right)\omega_0^2$$

Plug these back into the matrix equation to get:

Normal mode (b) $\omega_b^2=2\omega_0^2$

$$\begin{pmatrix}0&-\omega_0^2&0\\-\omega_0^2&0&-\omega_0^2\\0&-\omega_0^2&0\end{pmatrix}\begin{pmatrix}A_{1b}\\A_{2b}\\A_{3b}\end{pmatrix}=\begin{pmatrix}0\\0\\0\end{pmatrix}\text{ which gives }A_{2b}=0;A_{1b}=-A_{3b}$$

$$\begin{pmatrix}u_{1b}\\u_{2b}\\u_{3b}\end{pmatrix}=\begin{pmatrix}1\\0\\-1\end{pmatrix}e^{i\sqrt{2}\omega_0 t}\text{ (up to a normalization constant)}$$

Normal mode (a) $\omega_a^2=\left(2-\sqrt{2}\right)\omega_0^2$

$$\begin{pmatrix}\sqrt{2}\omega_0^2&-\omega_0^2&0\\-\omega_0^2&\sqrt{2}\omega_0^2&-\omega_0^2\\0&-\omega_0^2&\sqrt{2}\omega_0^2\end{pmatrix}\begin{pmatrix}A_{1a}\\A_{2a}\\A_{3a}\end{pmatrix}=\begin{pmatrix}0\\0\\0\end{pmatrix}\text{ which gives }A_{1b}=A_{3b}=\frac{1}{\sqrt{2}}A_{1b}$$

$$\begin{pmatrix}u_{1a}\\u_{2a}\\u_{3a}\end{pmatrix}=\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}e^{i\left(2-\sqrt{2}\right)^{1/2}\omega_0 t}\text{ (up to a normalization constant)}$$

Normal mode (c) $\omega_c^2 = \left(2+\sqrt{2}\right)\omega_0^2$

$$\begin{pmatrix} -\sqrt{2}\omega_0^2 & -\omega_0^2 & 0 \\ -\omega_0^2 & -\sqrt{2}\omega_0^2 & -\omega_0^2 \\ 0 & -\omega_0^2 & -\sqrt{2}\omega_0^2 \end{pmatrix}\begin{pmatrix} A_{1c} \\ A_{2c} \\ A_{3c} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \text{ which gives } A_{1b} = A_{3b} = -\frac{1}{\sqrt{2}}A_{1b}$$

$$\begin{pmatrix} u_{1a} \\ u_{2a} \\ u_{3a} \end{pmatrix} = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} e^{i\left(2+\sqrt{2}\right)^{1/2}\omega_0 t} \text{ (up to a normalization constant)}$$

d) Sketch the normal modes (arrows indicate the relative directions of motion; arrow length roughly gives the amplitude; a dot if the atom is stationary), indicating the ordering of the frequencies of the modes, with a brief physical explanation.

If all atoms move in phase, then at least a few springs are minimally stretched, so this must be the lowest energy, or lowest frequency mode. If adjacent atoms move in antiphase, then all springs are guaranteed to be stretched or compressed, so this is the highest frequency mode. The mode with the stationary atom is intermediate. This mode, with atom #2 stationary, has atoms #1 and #3 oscillating under the influence of 2 springs each with frequency ω_0, so an effective frequency of 2 ω_0.