Spring 2010

DEPARTMENT OF PHYSICS

Ph.D. CANDIDACY EXAMINATION

Day 1

March 24, 2010

(Problems 1 - 6)

Work all six problems. Please write clearly and show all the steps of your work. Define any symbols that you introduce. Credit will be given only for significant progress toward a solution. Use clear diagrams wherever appropriate.

NO NAMES SHOULD APPEAR ON ANYTHING YOU SUBMIT; USE YOUR CODE NUMBER ONLY.

1. Coaxial Cable

Calculate the self-inductance L of a coaxial cable whose solid inner conductor has radius a, and whose outer conducting shell is at radius b.

Solution

If the cable has inductance per unit length L, then the stored energy per unit length is $LI^2/2$ We can also calculate the total stored energy, which is the energy per unit length times the length from the magnetic field density: $W = \frac{1}{2\mu_0} \int B^2 da$ where the integral is over the cross-sectional area of the cable. Equating these two expressions for W gives:

$$L = \frac{1}{\mu_0 I^2} \int B^2 da.$$

We get the magnetic field at a radius r within the solid inner conductor from Amperes Law

$$\oint B \cdot d\ell = \mu_0 \mathcal{I}.$$

$$B = \frac{\mu_0 I}{2\pi} \begin{cases} r/a^2 & 0 < r < a, \\ 1/r & a < r < b, \\ 0 & b < r \end{cases}$$

The inductance per unit length is thus

$$L = \frac{\mu_0}{2\pi} \left[\frac{1}{a^4} \int_0^a r^3 dr + \int_a^b \frac{dr}{r} \right] = \frac{\mu_0}{2\pi} \left[\frac{1}{4} + \log \frac{b}{a} \right]$$

2. A Well and a Barrier

A quantum particle moves in the one-dimensional potential which consists of a delta-function well and a delta-function barrier, separated by a distance a. Assume that the amplitudes of the well and the barrier $-W < 0$ and $W > 0$ are the same.

1. Find incident particle energies such that the potential is reflectionless (this means that a particle approaching from infinity does not experience a reflection).

2. How many bound states exist in this system, if any? If there are bound states, what are the energies of these states?

A Well and a Barrier - Solution

(1) First let us recall the transfer-matrix of the delta-function potential. Let k is a wave-vector of the particle and $t(k) = mW/(\hbar^2 k)$. Then (text-book)

$$T_t = \begin{pmatrix} 1-it & -it \\ it & 1+it \end{pmatrix}. \tag{1}$$

This means that falling and reflecting plane waves represented by a matrix

$$\Psi(x) = \begin{pmatrix} e^{ikx} & 0 \\ 0 & e^{-ikx} \end{pmatrix}$$

to the left of the potential become

$$\begin{pmatrix} 1-it & -it \\ it & 1+it \end{pmatrix} \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}$$

to the right of the potential. Thus, the transfer matrix for this two-delta-function potential is

$$T = T_t \Psi(a) T_{-t} = \begin{pmatrix} 1-it & -it \\ it & 1+it \end{pmatrix} \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix} \begin{pmatrix} 1+it & it \\ -it & 1-it \end{pmatrix}. \tag{2}$$

The transmission probability is $|T_{11}|^{-2}$. It is given by the 11 matrix element of the transfer-matrix. We have

$$|T_{11}|^{-2} = \left|(1+t^2)e^{ika} - t^2 e^{-ika}\right|^{-2} = \frac{1}{1 + 4t^2(t^2+1)\sin^2(ka)}. \tag{3}$$

This transmission probability is 1 if $\sin(ka) = 0$, that is, $k = \pi n/a$ with $n = 1, 2, \ldots$. Energies at which there is no reflection are

$$E^{(n)}_{R=0} = \frac{\hbar^2 \pi^2}{2ma^2} n^2, \quad \text{for } n = 1, 2, \ldots.$$

(2) Bound states correspond to poles of the transmission amplitude

$$1 + 4t^2(t^2+1)\sin^2(ka) = 0.$$

They occur at imaginary $k = i\kappa$ and equal to $E = -\frac{\hbar^2}{2m}\kappa^2$. Let $\kappa_0 = mW/\hbar^2$, then

$$\sinh(\kappa a) = \frac{\kappa^2}{2\kappa_0\sqrt{\kappa_0^2 - \kappa^2}}.$$

To analyze this equation we introduce the dimensionless quantity $x = \kappa/\kappa_0$ and rewrite the above equation as

$$\sinh(\kappa_0 a x) = \frac{x^2}{2\sqrt{1-x^2}}. \tag{4}$$

Both sides of this equation are monotonically growing functions of x. At small x the left hand side is bigger than the right hand side as it grows linearly while the right hand side is $\sim x^2$. At $x \to 1$ the r.h.s. goes to $+\infty$. We conclude that there is only one point of intersection of the curves corresponding to both sides of the equation which will always give the only solution of the equation.

In the case of small W, i.e., $\kappa_0 a \ll 1$ we expect solution at small $x \ll 1$. Expanding (4) we have $\kappa_0 a x \approx x^2/2$, i.e., $x \approx 2\kappa_0 a$ or

$$\kappa_0 a \ll 1, \qquad \kappa \approx \kappa_0(2\kappa_0 a).$$

In this case the energy of the bound state is much closer to 0 than for a single delta-functinal potential well.

At large W ($\kappa_0 a \gg 1$) we expect the solution at $x \approx 1$. Denoting $x = 1 - s$ with $s \ll 1$ and expanding (4) in s we have $\frac{1}{2}e^{\kappa_0 a} = \frac{1}{2\sqrt{2\epsilon}}$ and $s \approx \frac{1}{2}e^{-2\kappa_0 a}$ or

$$\kappa_0 a \gg 1, \qquad \kappa \approx \kappa_0 \left(1 - \frac{1}{2}e^{-2\kappa_0 a}\right).$$

As it is expected, in this case the energy of the bound state is very close to the one of the bound state on a single delta-well with exponentially small corrections due to the presence of the delta-barrier.

3. Thermal Equilibrium of Monomers and Dimers

A container is filled with a gas of monomers (atoms) A and dimers (diatomic molecules) A_2. The only chemical reaction that can occur is $A + A \leftrightarrow A_2$, where the dimer A_2 has a binding energy of E - the energy needed ($E > 0$) or released ($E < 0$) when a dimer is dissociated into two monomers.

1. Suppose in thermal equilibrium there are N_1 atoms and N_2 molecules in the container of volume V at temperature T. Ignoring all internal degrees of freedom of the atoms and dimers, and approximating both A and A_2 as ideal gases, evaluate the partition function Z of the system as an integral over the phase space. What are the conditions for these approximations to be valid?

2. Determine the condition for thermodynamic equilibrium at constant temperature T and total particle number $N = N_1 + 2N_2$, and find the dimer to monomer ratio N_2/N_1 in terms of the binding energy E, temperature T, number of constituents N and volume V. Determine N_2 at large, positive binding energy $E >> k_B T$, and large negative $E << -k_B T$.

The formula you will obtain is a simplified version of the Saha formula which describes the degree of ionization in a plasma.

Formulas:

$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{4} a^{-3/2}$$

$$N! \approx \sqrt{2\pi N} (N/e)^N$$

Thermal Equilibrium of Monomers and Dimers - Solutions

(1) $Z = z^{N_1}(z' \exp[E/kT])^{N_2}/N_1!N_2!$, where z is the partition function

$$z = h^{-3} \int d^3x d^3p \exp(-E/kT) = V/\lambda_{dB}^3$$

of an atom, $z' = 2^{3/2}z$ is that of a molecule, and

$$\lambda_{dB} = h(2\pi m k_B T)^{-1/2}$$

is the atomic thermal de Broglie wavelength.

For this to be valid, one needs to ignore any contributions from the internal degrees of freedom of the monomer and dimer, their interactions, and quantum statistics.

(2) Minimizing the free energy $F = -kT \log Z$ with the particle number constraint $N_1 + 2N_2 = N$, we get $N_2/N_1 = 2^{3/2} N_1 e^{E_b/kT}/z$ or

$$N_2/N_1 = \frac{\sqrt{2^{9/2} e^{E/kT} \lambda_{dB}^3 (N/V) + 1} - 1}{4}.$$

The result is intuitive in the two limits: $E \to \infty$, all atoms are paired $N_2 = N/2$; $E \to -\infty$, all molecules are dissociated $N_2 = 0$.

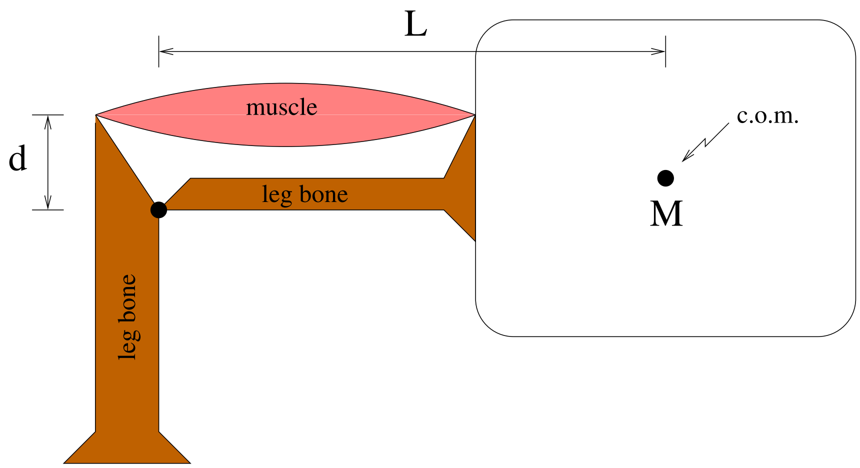

Figure 1: A sketch of a Brontosaurus.

4. The Brontosaurus Limit

Animals as tiny as an ant can lift many times their body weight; animals as large as an elephant have trouble even getting off the ground when lying down. The ability of an animal's muscles to lift its own weight places an approximate upper bound on the size of terrestrial animals.

Consider the simplified model of the figure, where the animal has mass M and center of mass positioned as shown. The muscle acts to lift the animal as it applies a force on the leg bones; treat the knee joint as a frictionless hinge. Assume that muscle can produce a stress of up to 3×10^5 N/m^2. Estimate the typical linear dimensions of the leg muscle on an animal of mass M, and based on this estimate and the given maximum deliverable stress, estimate the maximum mass an animal can attain while still being able to lift its own weight.

The Brontosaurus Limit - Solution

Torque balance yields the equation

$$d \cdot F_m = MgL$$

Let's perform the estimate by scaling up the properties of human-sized mammals, whose mass is approximately 100 kg, and leg muscles have characteristic dimensions of about .1 m $\times$ .1 m $\times$ .5 m. Also take $L \sim .5$ m for humans, and $d \sim .03$ m. Note also that the force delivered by a stress s_m of the muscle is $F_m = s_m A$, where A is the cross-sectional area of the muscle. Then by scaling linearly in all dimensions, the mass will grow as the cube of the linear dimension and one can estimate

$$M_{\max} = \frac{dF_m}{gL} = \frac{ds_m A_m}{gL} = \frac{.03\text{m}(\frac{M_{\max}}{100\text{kg}})^{1/3}\ 3 \cdot 10^5\text{N/m}^2\ (.1\text{m}(\frac{M_{\max}}{100\text{kg}})^{1/3})^2}{10\text{m/s}^2\ .5\text{m}\ (M_{\max}/100\text{kg})^{1/3}}$$

or $M_{\max} \sim 10^6$kg. Indeed, the mass of large dinosaurs has been estimated at about $10^6 - 10^7$kg.

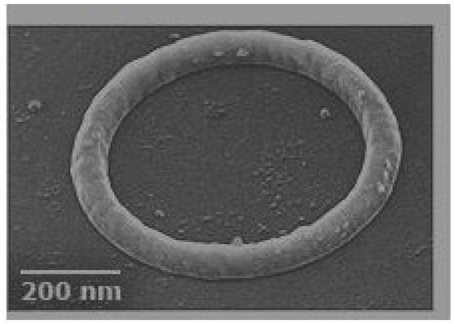

Figure 2: An aluminum ring 200 nm wide in which a persistent current was observed.

5. Persistent Current

A small metal ring is pierced by a magnetic field with a flux Φ. Assume (not realistic) that there is only one electron in the ring. Magnetic flux induces a current in the ring. Find the magnetic moment and the current as a function of the flux.

Currents in mesoscopic devices as in the Figure are called persistent currents. They are tiny, but can run forever (about a week).

Hint: In a mesoscopic (i.e., small) device, energy levels are discrete. The Hamiltonian of a charged particle is $H = \frac{\mathbf{P}^2}{2m}$, where $\mathbf{P} = -i\hbar\nabla - \frac{e}{c}\mathbf{A}$ is the canonical momentum, $\mathbf{A}$ is the vector potential, magnetic flux $\Phi = \int\int \mathbf{B} \cdot d\mathbf{S} = \oint \mathbf{A} \cdot d\mathbf{l}$ (Stokes theorem).

Persistent Current - Solution

The wave function in the presence of a magnetic flux is $\Psi(x) = \Psi_0 e^{i\frac{e\hbar}{c}A_\varphi}$, where A_φ is an azimuth component of vector potential: $\Phi = A_\varphi \cdot 2\pi R$, where R is a radius of the ring, and $\psi_0 = e^{ikR\varphi}$ is the wave function of a free particle without magnetic field. Magnetic flux changes the boundary condition for the wave function:

$$\psi_0(\varphi + 2\pi) = e^{i\Phi}\psi(\varphi)$$

where Φ is measured in units of magnetic flux Φ_0, and R is a radius of the ring. Therefore momentum is quantized as

$$2\pi Rk = \hbar(n + \Phi), \quad n = 0, \pm 1, \pm 2...$$

The energy is

$$E = \frac{k^2}{2m} = \frac{E_0}{2}(n + \Phi)^2, \quad E_0 = \frac{\hbar^2}{(2\pi R)^2 m}$$

If $\Phi < 1/2$ one electron occupies the level $n = 0$. Its energy in units E_0 is $E = \frac{1}{2}\Phi^2$. The current obviously is proportional to the magnetic momen is

$$j = \frac{\Phi_0}{2\pi R} = m, \quad m = \frac{\partial E}{\partial \Phi} = E_0\Phi$$

When $\Phi > 1/2$ the level with $n = -1 \times \mathrm{sign}\Phi$ is occupied. The energy is $E = \frac{E_0}{2}(1 - \Phi)^2$. The current or the moment is

$$m = E_0(\Phi - 1)$$

A saw-like graph: current increases with flux linearly until the flux riches a half-quantum and then abruptly changes the direction. After this decreases with flux and vanishes when the flux riches a flux quantum. Then the pattern repeats periodically.

6. Bouncing Ball

A ball is bouncing vertically and perfectly elastically in a standing elevator. The height of bouncing motion is h_0. The upward acceleration of the elevator changes very slowly from 0 to $g/2$. Find the new height of the bouncing motion.

Bouncing Ball - Solution

The trajectory of the bouncing ball in the phase space is given by parabola $\frac{p^2}{2m} + mgx = E = mgh$ or by $p = m\sqrt{2g(h-x)}$. The adiabatic invariant is the area of the phase space bounded by that trajectory

$$I = \int p\,dx = 2\int_0^h m\sqrt{2g(h-x)}\,dx = \frac{4\sqrt{2}}{3} m g^{1/2} h^{3/2}.$$

In the moving elevator g must be replaced by $a+g$, where a is an acceleration of the elevator. We have

$$I \sim (a+g)^{1/2} h^{3/2} = \text{const.}$$

Comparing adiabatic invariant I with its initial value we obtain $(a+g)^{1/2}h^{3/2} = g^{1/2}h_0^{3/2}$ and

$$h = h_0 \left(\frac{g}{g+a}\right)^{\frac{1}{3}}.$$

We substitute $a = g/2$ and obtain the final result

$$h = h_0 \left(\frac{2}{3}\right)^{\frac{1}{3}}.$$

Spring 2010

DEPARTMENT OF PHYSICS

Ph.D. CANDIDACY EXAMINATION

Day 2

March 25, 2010

(Problems 7 - 12)

Work all six problems. Please write clearly and show all the steps of your work. Define any symbols that you introduce. Credit will be given only for significant progress toward a solution. Use clear diagrams wherever appropriate.

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7. Counting Experiments

1. In a counting experiment, the expected signal-to-background ratio is approximately 3 to 1. You have 10 hours to make a measurement of the signal rate. How much of that time should you spend with the signal source off, i.e. measuring the background rate, so that you get the smallest uncertainty on the signal rate?

2. In another counting experiment, you expect 0.01 counts per second. You turn on the apparatus and record no counts. After how long should you worry that the detector is malfunctioning?

   Assume that both signal and background events are uncorrelated.

Counting Experiments - Solution

(1) Assume we spend time T on the background $B = bT$, and the rest of the time $10 - T$ on the signal $S = (s + b)(10 - T)$, where $s \approx 3b$ and b are the signal and background rates, respectively. We get $s = S/(10 - T) - B/T$.

Based on Poisson statistics and statistical independence the variance is $\sigma^2 \propto S/(10 - T)^2 + B/T^2 = 4b/(10 - T) + b/T$, which is minimized at $T = 10/3$.

(2) Let 3σ be our tolerance, $\sqrt{N} = 3$ gives $N = 9$ or a wait time of $N/0.01 = 900$ seconds.

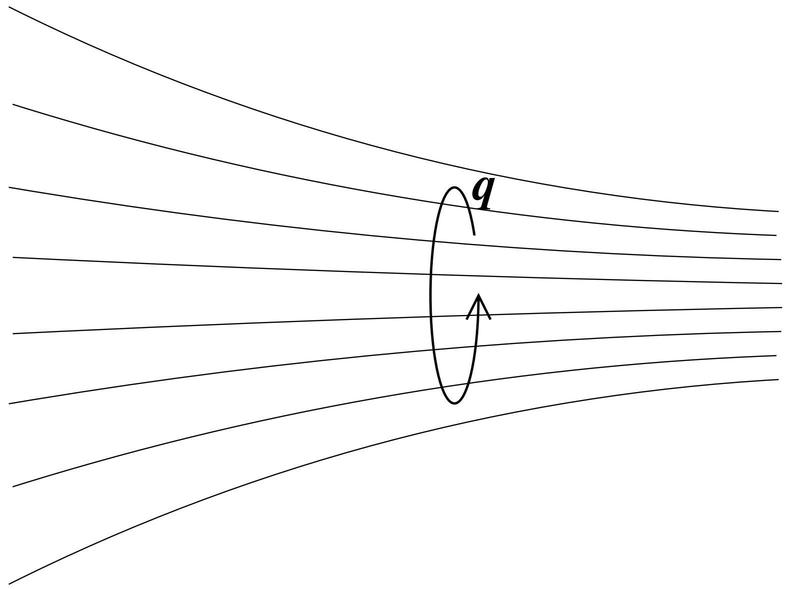

Figure 1: Magnetic lines

8. Magnetic Mirror

(a) A particle of charge q moves in the plane perpendicular to a uniform magnetic field $\mathbf{B}$. Show that if $\mathbf{B}$ changes slowly in time, the magnetic moment produced by the orbital motion of the charge remains constant, and that the magnetic flux through the orbit is constant. These approximate constants of the motion are known as *adiabatic invariants*.

(b) Now suppose that instead, the magnetic field is slightly nonuniform in space but constant in time (see the figure).

Assume that the field has cylindrical symmetry, and varies slowly along the axis of symmetry (call it the z axis). Consider a particle with a velocity v_0 which is mostly in the plane perpendicular to the axis of symmetry, but has a slight component along the axis in the direction of increasing magnetic field. Use the result of part (a) to show that the magnitude of the component of the velocity v_z along the symmetry axis decreases, and find the turning point of the motion as a function of the initial speed v_0, the initial component $v_\perp$ of the velocity in the perpendicular (x-y) plane, and the magnitude of the magnetic field $B(z)$.

Magnetic Mirror - Solution

(a) With constant $\mathbf{B}$, the orbit is circular with radius r and $mv^2/r = qvB/c$, so

$$r = \frac{mcv}{qB}$$

The magnetic moment due to this orbit has magnitude

$$\mu = \frac{\pi r^2 I}{c} = \frac{\pi r^2}{c}\frac{qv}{2\pi r} = \frac{qrv}{2c} = \frac{mv^2}{2B}$$

and is directed opposite to $\mathbf{B}$ according to Lenz's law.

If the field now varies slowly in time, an electric field is induced around the particle's orbit according to Faraday's law

$$\oint \mathbf{E}\cdot d\mathbf{l} = 2\pi r E = -\frac{1}{c}\frac{d}{dt}\int \mathbf{B}\cdot d\mathbf{S} = -\frac{\pi r^2 \dot{B}}{c}$$

Therefore

$$\frac{m\dot{v}}{q} = E = \frac{r\dot{B}}{2c} = \frac{mv\dot{B}}{2qB}$$

and so $v \propto \sqrt{B}$. Thus v^2/B is constant, and μ is constant. The flux linked by the orbit

$$\Phi = \pi r^2 B = \frac{\pi m^2 c^2 v^2}{q^2 B}$$

is also constant. Φ and v^2/B are so-called *adiabatic invariants* of the motion.

(b) The magnetic field experienced by the particle changes in time according to

$$\frac{dB(z(t))}{dt} = \frac{dB}{dz}\,v_z$$

If this change is slow, the analysis of part (a) holds and the particle's motion varies so that $v_\perp^2(z)/B(z)$ remains constant. Therefore

$$v_\perp^2(z) \sim v_\perp^2(0)\frac{B(z)}{B(0)}$$

The magnetic field does no work, therefore $v^2 = v_z^2 + v_\perp^2 = v_0^2$, and so

$$v_z^2(z) = v_0^2 - v_\perp^2(0)\frac{B(z)}{B(0)}$$

and the turning point is where the magnetic field grows to the level that v_z vanishes.

9. Bullet

A bullet of mass m flying horizontally with velocity v_0 hits a block B of mass M. If B is kept fixed in space, the bullet penetrates a distance d_0. If B is allowed to move horizontally, the bullet penetrates a distance d_1. Assuming that inside B the resistance to the bullet's motion depends only on the velocity of the bullet relative to the block, compute the ratio d_1/d_0. How does this ratio depend on the form of the resistance?

Bullet - Solution

If x is the position of the bullet, then the relative velocity of the bullet and the block is $v = \dot{x}$. The resistance (friction) to the bullet motion within B is $-f(v)$. Newton's law reads $m\dot{v} = -f(v)$. A loss of velocity per time dt is $mdv = -f(v)dt$. The loss of velocity per length traveled dx is $mvdv = -f(v)dx$. Thus $dx = -\frac{mvdv}{f(v)}$. Integrating from v_0 to 0, we obtain the penetration length $d_0 = m\int_0^{v_0} \frac{vdv}{f(v)}$.

If the block is allowed to move we have Newton's equations for the bullet $m\dot{v}_b = -f(V)$ and for the block $M\dot{v}_r = f(V)$, which reduce to one equation in the reduced mass $\mu^{-1} = m^{-1} + M^{-1}$ and the relative velocity $V = v_b - v_r$:

$$\mu\dot{V} = -f(V).$$

Therefore $\frac{d_0}{d_1} = \frac{m}{\mu} = 1 + \frac{m}{M}$, which is independent of the functional form of the resistance in the block.

10. Water Droplets in Clouds

In clouds water vapor condenses and forms drops. Drops and vapor are in thermodynamic equilibrium. The vapor pressure saturates due to a surface tension effect of the curved surface of the droplets. Assume that the water vapor is an ideal gas.

1. At constant pressure P and temperature T, write down the free energy of N_v molecules in the water vapor and N_d molecules in a droplet of radius r .

2. In a cloud, water droplets with radius r are in thermal equilibrium with the vapor, determine $P(r)$. Which clouds have larger pressure, those in which the droplets are smaller or larger?

Adopt the notations: P_∞ is the water vapor pressure on a flat water surface; σ is the surface tension; ρ is the density of water liquid (it is much larger than the density of water vapor); g_d is the free energy of water per molecule and g_v is the free energy of vapor per molecule. In an ideal gas, the molecular density is P/kT.

The formula you will obtain is a simplified version of the Kohler theory of cloud formation.

Water Droplets in Clouds - Solution

(1) Let N_d be the number of water molecules in a droplet and N_v the number of molecules in the vapor. The total number is a constant $N_d + N_v$ =const. Free energy of the system has three terms: $G = N_v g_v + N_d g_d + 4\pi r^2 \sigma$, free energy of vapor, free energy of water and the surface tension energy. Here r is the droplet radius.

(2) In equilibrium, the free energy is minimal: $\delta G = \delta N_d (g_d - g_v) + 8\pi r \delta r = 0$. The density of the water is $\rho = N_d m/(4\pi r^3/3)$, where m is the molecular mass. Therefore $m\delta N_d = 4\pi\rho r^2 \delta r$ and $\delta G = \delta N_d (g_d - g_v + 2\sigma m/\rho r) = 0$. We get $g_d - g_v + 2\sigma m/\rho r = 0$.

Thermodynamics gives $v = dg/dP$, where $v = m/\rho$ is the specific volume. Differentiating the equilibrium condition we get $(2\sigma m/\rho) d(1/r)/dP = v_v - v_d \approx v_v = k_B T/P$, where we have assumed water vapor is ideal and the density of water is much higher than of vapor, $v_d << v_v$. The equation, given by $Ad(1/r) = dP/P$ with $A = 2\sigma m/\rho kT$, can be integrated from $r = \infty$ where the pressure is P_∞ to r and yields

$$P(r)/P_\infty = e^{A/r}.$$

This is the Kohler law - a relation between the size of the droplet and the pressure. Smaller droplets require larger pressure.

11. Radar Gun

A radar gun measures the speed of passing cars via the Doppler effect, measuring the beat frequency between the emitted microwave radiation of frequency ν and the returning reflected radiation.

1. Find the beat frequency as a function of the velocity of the car as it approaches the position of the gun. Take the radar gun to lie on the linear trajectory of the car.

2. Estimate the accuracy of the radar gun in determining a car's velocity at typical highway speeds.

Radar Gun - Solution

(a) There are two Doppler shifts to consider. The emitted signal at frequency $\nu = \nu_1$ is a shifted frequency

$$\nu_2 = \frac{\nu_1}{\gamma(1 + \beta\cos[\pi])} = \nu_1\sqrt{\frac{1+\beta}{1-\beta}}$$

as seen by the moving car (for velocity at an angle $\theta = \pi$ with respect to the line of sight). The car reflects this signal with no change in frequency in the car's rest frame, the signal is now moving back toward the radar gun. The radar gun sees in its rest frame a second Doppler shift relative to the reflected signal in the moving frame of the car

$$\nu_3 = \nu_2\sqrt{\frac{1+\beta}{1-\beta}} = \nu_1\frac{1+\beta}{1-\beta}$$

The beat frequency is

$$\nu_3 - \nu_1 = \nu_1(\frac{1+\beta}{1-\beta} - 1) \sim 2\beta\nu_1$$

(b) We have, for microwaves at 10 GHz, and an ability to discriminate beat frequencies to an accuracy of say 10 Hz (due to an observation time of a few tenths of a second), and a car travelling at 30 m/s,

$$\nu_{beat} = 2\beta\nu = 2\ \frac{30\ \text{m/s}}{3 \times 10^8\ \text{m/sec}}\ 10^{10}\ \text{Hz} = 2 \times 10^3\ \text{Hz}$$

A measurement to within 10 Hz is an accuracy of 0.5.

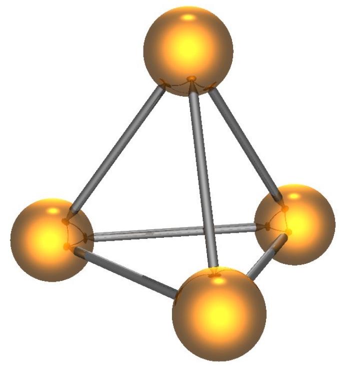

Figure 2: A tetrahedral molecule

12. Tetrahedral Molecule

Consider a tetrahedral molecule. A particle can jump between vertices of the tetrahedron with a transition amplitude per unit time T_1, or can remain where it is with an amplitude T_0. This model is called a *tight-binding approximation.*

1. Write down the Hamiltonian for the particle.

2. What are the symmetries of the Hamiltonian?

3. What is the eigenvalue spectrum of the Hamiltonian and its degeneracy?

4. Initially the particle is located at one given site. What is the probability that it will be found there after a time t? What is the probability that the particle is found at another site at time t?

Tetrahedral Molecule - Solution

(1) The Hamiltonian is a 4x4 matrix

$$H = -T_0\,\mathbf{Id} - T_1 \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}. \tag{1}$$

where **Id** is the 4x4 identity matrix.

(2) The system has tetrahedral symmetry under the symmetric group S_4 of permutations of four elements; $gHg^{-1} = H$ for $g \in S_4$.

(3) The eigenstates will lie in representations of the symmetric group. The simplest representation is the singlet, invariant under permutations; a normalized vector with this property is

$$e_0 = \frac{1}{2}(1,1,1,1)$$

with eigenvalue $-T_0 - 3T_1$. Another symmetry of the tetrahedron interchanges $1 \leftrightarrow 2$, $3 \leftrightarrow 4$. A normalized eigenvector of this symmetry orthogonal to the above eigenvector is

$$e_1 = \frac{1}{\sqrt{2}}(1,-1,0,0),$$

whose Hamiltonian eigenvalue is $-T_0 + T_1$. This eigenstate must lie in a representation of S_4; another element of S_4 fixes 1 and cyclically permutes $(2,3,4)$. This leads to three linearly independent eigenstates with the same eigenvalue; Gram-Schmidt orthogonalization leads to two more normalized eigenvectors with Hamiltonian eigenvalue $-T_0 + T_1$:

$$e_2 = \frac{1}{\sqrt{6}}(1,1,-2,0), \tag{2}$$

$$e_3 = \frac{1}{\sqrt{12}}(1,1,1,-3). \tag{3}$$

(4) Write an initial state $|4\rangle$ $e = (0,0,0,1)$ as

$$e(t=0) = \frac{1}{2}e_0 - \frac{3}{\sqrt{12}}e_3. \tag{4}$$

It evolves as

$$e(t) = e^{-\frac{i}{\hbar}(-3T_1)t}\frac{1}{2}e_0 - e^{-\frac{i}{\hbar}T_1 t}\frac{3}{\sqrt{12}}e_3. \tag{5}$$

where we have ignored the effect of T_0 since it only contributes an overall phase which drops out of transition probabilities. The fourth and the first components of this vector gives

$$\langle 4|\, e(t)\rangle = \frac{1}{4} e^{\frac{i}{\hbar} 3T_1 t} + \frac{3}{4} e^{-\frac{i}{\hbar} T_1 t}, \tag{6}$$

$$\langle 1|\, e(t)\rangle = \frac{1}{4} e^{\frac{i}{\hbar} 3T_1 t} - \frac{1}{4} e^{-\frac{i}{\hbar} T_1 t}. \tag{7}$$

The absolute values squared give correspondent probabilities

$$p_4(t) = |\langle 4|\, e(t)\rangle|^2 = \frac{5}{8} + \frac{3}{8}\cos(4\frac{T_1}{\hbar}t), \tag{8}$$

$$p_1(t) = |\langle 1|\, e(t)\rangle|^2 = \frac{1}{8} - \frac{1}{8}\cos(4\frac{T_1}{\hbar}t). \tag{9}$$

Of course, the second formula can be obtained from the first as $p_1 = (1 - p_4)/3$ due to a permutation symmetry of remaining three states.

Notice that at $t = (2\pi\hbar/T_1)n$, where n is integer, the particle return to its initial state, such that $p_4 = 1$.