

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
DEPARTMENT OF PHYSICS

Academic Programs
Room 4-315

Phone: (617) 253-4851
Fax: (617) 258-8319

DOCTORAL GENERAL EXAMINATION
WRITTEN EXAM - CLASSICAL MECHANICS

January 25, 2016

DURATION: 75 MINUTES

1. This examination has two problems. Read both problems carefully before making your choice. Submit ONLY one problem. IF YOU SUBMIT MORE THAN ONE PROBLEM FROM A SECTION, BOTH WILL BE GRADED, AND THE PROBLEM WITH THE LOWER SCORE WILL BE COUNTED.
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Classical Mechanics 1: Optimal wind power machine

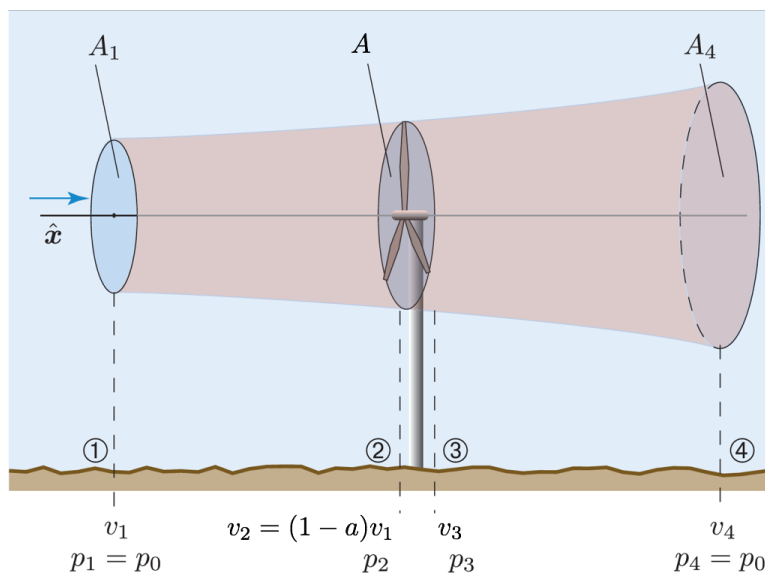
In this problem you will derive an upper limit on the efficiency with which a machine can harvest kinetic energy from a steady wind.

We model the machine as a flat disk of area A that (through unspecified means) removes kinetic energy and momentum from an airstream flowing perpendicular to the disk. The air flow is steady, laminar, and incompressible, with density ρ , with streamlines that are azimuthally symmetric around the disk's symmetry axis.

The figure below shows the flow tube that includes the perimeter of the disk. Far upwind, the flow tube has a cross-sectional area $A_1 < A$, the wind speed is v_1 , and the air pressure is p_0 . Just in front of the turbine, the wind speed has been slowed to $v_2 = (1 - a)v_1$, where $0 < a < 1$ is a parameter characterizing the machine. Just behind the machine, the wind speed is v_3 and the pressure has dropped to p_3 . While the machine is operating, $p_2 > p_3 > p_0$. Far downstream, the flow tube has a cross-sectional area $A_4 > A$, the wind speed has slowed further to v_4 , the pressure is back to the ambient pressure p_0 .

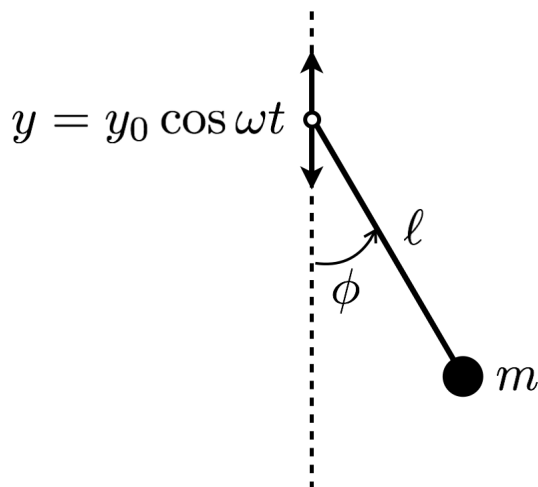
Not all of the quantities defined above are independent. In particular, as you will show, the fraction of wind power extracted by the machine depends solely on a .

- (1 pt) Use conservation of mass and incompressibility of the flow to relate v_2 and v_3 .
- (7 pts) Calculate the power P extracted by the disk, in terms of ρ , A , v_1 , and a .
Hint: consider the differences (if any) in the fluxes of mass, momentum and energy into the flow tube at A_1 and out of the flow tube at A_4 .
- (2 pts) Calculate the efficiency $\eta \equiv P/P_0$, where P_0 is the total rate at which kinetic energy of the air would flow through the area A if the turbine were not present. Your answer should be solely a function of a . Then, calculate the maximum possible efficiency η_{\max} , and value of a for which the maximum is attained.



Classical Mechanics 2: Stabilizing an inverted pendulum

A pendulum has a mass m connected by a rigid rod of length ℓ to a pivot point. An external force causes the pivot point to oscillate vertically, with $y = y_0 \cos \omega t$ and $\omega^2 \gg g/\ell$.



- (a) (1 pt) Write the Lagrangian for the pendulum, in terms of the angular coordinate ϕ .
- (b) (2 pts) Derive the equation of motion for ϕ , which by virtue of a cancellation takes the form $\ddot{\phi} = f(\phi, t)$, as opposed to $f(\phi, \dot{\phi}, t)$.

Next we will find an approximate solution of the form $\phi = \phi_s + \phi_f$. The “slow” component $\phi_s(t)$ is the solution of the equation of motion after time-averaging over the rapid oscillations of the pivot point. The “fast” component $\phi_f(t)$ is a small perturbation ($|\phi_f(t)| \ll 1$), and averages to zero over the rapid oscillations.

- (c) (5 pts) Derive a leading-order equation for ϕ_f . Solve it, and then use the solution to derive a time-averaged equation for ϕ_s of the form

$$\ddot{\phi}_s = A \sin \phi_s + B \sin \phi_s \cos \phi_s, \quad (1)$$

where A and B depend only on the constants g , ℓ , ω , and y_0 .

- (d) (2 pts) Rewrite the preceding equation for ϕ_s in the form $\ddot{\phi}_s = -dU_{\text{eff}}/d\phi_s$, i.e., motion in an effective potential. Then derive a condition on ω and y_0 such that $\phi_s = \pi$ is a stable equilibrium point.

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Classical Mechanics 1: Optimal wind power machine

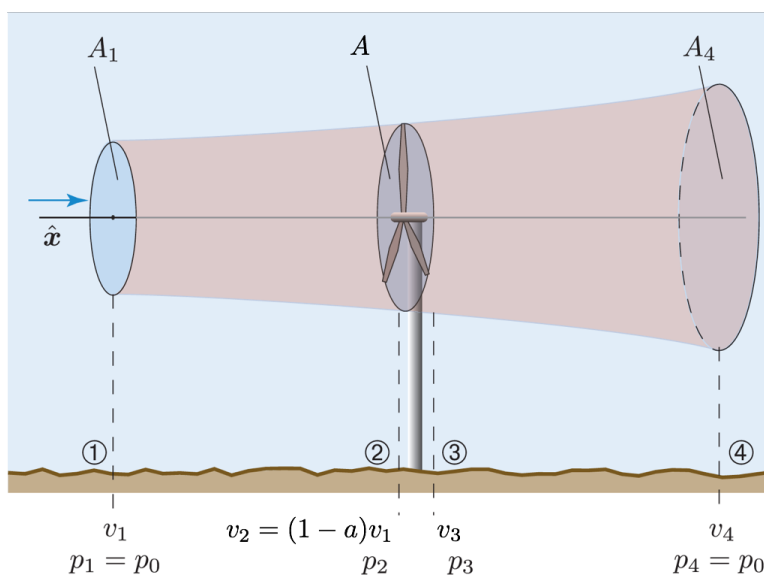
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We model the machine as a flat disk of area A that (through unspecified means) removes kinetic energy and momentum from an airstream flowing perpendicular to the disk. The air flow is steady, laminar, and incompressible, with density ρ , with streamlines that are azimuthally symmetric around the disk's symmetry axis.

The figure below shows the flow tube that includes the perimeter of the disk. Far upwind, the flow tube has a cross-sectional area $A_1 < A$, the wind speed is v_1 , and the air pressure is p_0 . Just in front of the turbine, the wind speed has been slowed to $v_2 = (1 - a)v_1$, where $0 < a < 1$ is a parameter characterizing the machine. Just behind the machine, the wind speed is v_3 and the pressure has dropped to p_3 . While the machine is operating, $p_2 > p_3 > p_0$. Far downstream, the flow tube has a cross-sectional area $A_4 > A$, the wind speed has slowed further to v_4 , the pressure is back to the ambient pressure p_0 .

Not all of the quantities defined above are independent. In particular, as you will show, the fraction of wind power extracted by the machine depends solely on a .

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Hint: consider the differences (if any) in the fluxes of mass, momentum and energy into the flow tube at A_1 and out of the flow tube at A_4 .
- (c) (2 pts) Calculate the efficiency $\eta \equiv P/P_0$, where P_0 is the total rate at which kinetic energy of the air would flow through the area A if the turbine were not present. Your answer should be solely a function of a . Then, calculate the maximum possible efficiency η_{\max} , and value of a for which the maximum is attained.



- Solutions by Josh Winn.

- (a) Consider the flow tube shown in the figure. Conservation of mass requires that $\dot{m} = \rho Av$ be constant across all cross-sections of the tube. Since ρ is itself constant, this requires $Av = \text{constant}$. In particular, $v_2 = v_3$.
- (b) Momentum enters the tube on the upwind face at a rate $\dot{m}v_1$. Since a portion is extracted by the disk, the wind must exert a force F equal to the rate of momentum extraction. The remainder of the momentum departs through the downwind face at a rate $\dot{m}v_4$. Therefore

$$\dot{m}v_1 - F = \dot{m}v_4 \quad (1)$$

$$F = \dot{m}(v_1 - v_4) = \rho Av_2(v_1 - v_4). \quad (2)$$

Next consider energy, which enters the tube on the upwind face at a rate $\dot{m}v_1^2/2$, and exits downwind at a rate $\dot{m}v_4^2/2$. Since the pressure at both locations is p_0 , the difference must be equal to the power absorbed by the disk:

$$\frac{1}{2}\dot{m}(v_1^2 - v_4^2) = P = Fv_2 \quad (3)$$

$$\frac{1}{2}\rho Av_2(v_1^2 - v_4^2) = \rho Av_2^2(v_1 - v_4) \quad (4)$$

$$\frac{1}{2}(v_1 + v_4)(v_1 - v_4) = v_2(v_1 - v_4), \quad (5)$$

leading to the result $v_2 = (v_1 + v_4)/2$, or

$$v_4 = 2v_2 - v_1 = [2(1 - a) - 1]v_1 = (1 - 2a)v_1. \quad (6)$$

Now we can evaluate the power in terms of the desired quantities:

$$P = Fv_2 \quad (7)$$

$$= \rho Av_2^2(v_1 - v_4) \quad (8)$$

$$= \rho A(1 - a)^2 v_1^2 [v_1 - (1 - 2a)v_1] \quad (9)$$

$$= \rho Av_1^3 2a(1 - a)^2. \quad (10)$$

- (c) If the machine were not present, the kinetic energy flux through the area A would be

$$P_0 = \frac{1}{2}\rho v_1^3 A, \quad (11)$$

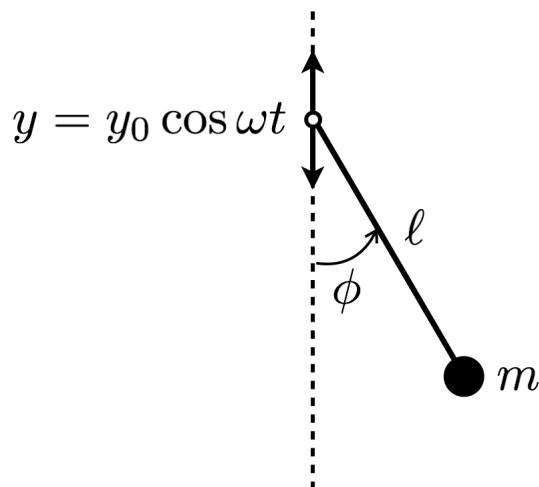
hence

$$\eta = \frac{P}{P_0} = \frac{\rho Av_1^3 2a(1 - a)^2}{\frac{1}{2}\rho v_1^3 A} = 4a(1 - a)^2. \quad (12)$$

By setting $d\eta/da = 0$ we find $\eta_{\max} = 16/27$ for the choice $a = 1/3$. This is known as the *Betz limit*.

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$$\ddot{\phi}_s = A \sin \phi_s + B \sin \phi_s \cos \phi_s, \quad (1)$$

where A and B depend only on the constants g , ℓ , ω , and y_0 .

- (d) (2 pts) Rewrite the preceding equation for ϕ_s in the form $\ddot{\phi}_s = -dU_{\text{eff}}/d\phi_s$, i.e., motion in an effective potential. Then derive a condition on ω and y_0 such that $\phi_s = \pi$ is a stable equilibrium point.

- Solutions by Josh Winn, 2015

(a) Take the origin to be the pivot point at $t = 0$. Then the position of the mass is $x = \ell \sin \phi$ and $y = y_0 \cos \omega t - \ell \cos \phi$. The time derivatives are

$$\dot{x} = \ell \dot{\phi} \cos \phi \quad (2)$$

$$\dot{y} = -y_0 \omega \sin \omega t + \ell \dot{\phi} \sin \phi. \quad (3)$$

The kinetic energy is

$$T = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2) \quad (4)$$

$$= \frac{1}{2} m \left(\ell^2 \dot{\phi}^2 \cos^2 \phi + y_0^2 \omega^2 \sin^2 \omega t - 2y_0 \omega \ell \dot{\phi} \sin \omega t \sin \phi + \ell^2 \dot{\phi}^2 \sin^2 \phi \right) \quad (5)$$

$$= \frac{1}{2} m \left(\ell^2 \dot{\phi}^2 + y_0^2 \omega^2 \sin^2 \omega t - 2y_0 \omega \ell \dot{\phi} \sin \omega t \sin \phi \right). \quad (6)$$

The potential energy is

$$U = mgy = mg(y_0 \cos \omega t - \ell \cos \phi). \quad (7)$$

The Lagrangian is therefore

$$\mathcal{L} = \frac{1}{2} m \left(\ell^2 \dot{\phi}^2 + y_0^2 \omega^2 \sin^2 \omega t - 2y_0 \omega \ell \dot{\phi} \sin \omega t \sin \phi \right) - mg(y_0 \cos \omega t - \ell \cos \phi). \quad (8)$$

(b) The equation of motion is obtained from

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) = \frac{\partial \mathcal{L}}{\partial \phi}. \quad (9)$$

The relevant derivatives of the Lagrangian are

$$\frac{\partial \mathcal{L}}{\partial \phi} = -my_0 \omega \ell \dot{\phi} \sin \omega t \cos \phi - mgl \sin \phi, \quad (10)$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\phi}} = m\ell^2 \dot{\phi} - my_0 \omega \ell \sin \omega t \sin \phi, \quad (11)$$

and

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) = m\ell^2 \ddot{\phi} - my_0 \omega^2 \ell \cos \omega t \sin \phi - my_0 \omega \ell \dot{\phi} \sin \omega t \cos \phi, \quad (12)$$

leading to the equation of motion

$$m\ell^2 \ddot{\phi} - my_0 \omega^2 \ell \cos \omega t \sin \phi - my_0 \omega \ell \dot{\phi} \sin \omega t \cos \phi = -my_0 \omega \ell \dot{\phi} \sin \omega t \cos \phi - mgl \sin \phi. \quad (13)$$

The third term on the left side cancels the first term on the right side. After dividing through by $m\ell^2$ and rearranging we have

$$\ddot{\phi} = -\frac{g}{\ell} \sin \phi + \frac{y_0 \omega^2}{\ell} \sin \phi \cos \omega t. \quad (14)$$

(c) We insert $\phi = \phi_s + \phi_f$ into the equation of motion, and use the first-order approximation

$$\sin \phi = \sin(\phi_s + \phi_f) \approx \sin \phi_s + \phi_f \cos \phi_s, \quad (15)$$

giving

$$\ddot{\phi}_s + \ddot{\phi}_f = -\frac{g}{\ell} \sin \phi_s - \frac{g}{\ell} \phi_f \cos \phi_s + \frac{y_0 \omega^2}{\ell} \sin \phi_s \cos \omega t + \frac{y_0 \omega^2}{\ell} \phi_f \cos \phi_s \cos \omega t. \quad (16)$$

To take advantage of the separation of timescales, we average this equation over the rapid oscillation period. On the left side, $\ddot{\phi}_f$ averages to zero. On the right side, the second and third terms average to zero. (The fourth term generally does *not* average to zero.) Therefore we have

$$\ddot{\phi}_s = -\frac{g}{\ell} \sin \phi_s + \frac{y_0 \omega^2}{\ell} \cos \phi_s \langle \phi_f \cos \omega t \rangle. \quad (17)$$

The task remains to compute the time average $\langle \phi_f \cos \omega t \rangle$. We insert Eqn. (17) back into Eqn. (16), obtaining

$$\ddot{\phi}_f = -\frac{g}{\ell} \phi_f \cos \phi_s + \frac{y_0 \omega^2}{\ell} \sin \phi_s \cos \omega t + \frac{y_0 \omega^2}{\ell} \cos \phi_s (\phi_f \cos \omega t - \langle \phi_f \cos \omega t \rangle). \quad (18)$$

To obtain the leading-order equation we neglect the first term (because $\omega^2 \gg g/\ell$) and the last term (because ϕ_f is a small perturbation), giving

$$\ddot{\phi}_f = \frac{y_0 \omega^2}{\ell} \sin \phi_s \cos \omega t, \quad (19)$$

for which the solution is

$$\phi_f = -\frac{y_0}{\ell} \sin \phi_s \cos \omega t. \quad (20)$$

We may now compute the time average

$$\langle \phi_f \cos \omega t \rangle = -\frac{y_0}{\ell} \sin \phi_s \langle \cos^2 \omega t \rangle = -\frac{y_0}{2\ell} \sin \phi_s. \quad (21)$$

Inserting back into Eqn. (16), we have the desired equation:

$$\ddot{\phi}_s = -\frac{g}{\ell} \sin \phi_s - \frac{\omega^2 y_0^2}{2\ell^2} \sin \phi_s \cos \phi_s. \quad (22)$$

(d) To check on the stability of the equilibrium point $\phi_s = \pi$, we write the equation of motion in the form

$$\ddot{\phi}_s = -\frac{dU_{\text{eff}}}{d\phi_s}, \quad (23)$$

with the effective potential given by

$$U_{\text{eff}} = -\frac{g}{\ell} \cos \phi_s + \frac{\omega^2 y_0^2}{4\ell^2} \sin^2 \phi_s. \quad (24)$$

The second derivative of the effective potential is

$$\frac{d^2 U_{\text{eff}}}{d\phi_s^2} = \frac{g}{\ell} \cos \phi_s + \frac{\omega^2 y_0^2}{2\ell^2} (\cos^2 \phi_s - \sin^2 \phi_s), \quad (25)$$

which evaluates to $-g/\ell + \omega^2 y_0^2/2\ell^2$ at $\phi_s = \pi$. For stability we need the second derivative to be positive, leading to the condition

$$\frac{\omega^2 y_0^2}{2\ell^2} > \frac{g}{\ell}, \quad \frac{\omega^2 y_0^2}{2g\ell} > 1. \quad (26)$$

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DOCTORAL GENERAL EXAMINATION
WRITTEN EXAM - ELECTRICITY AND MAGNETISM

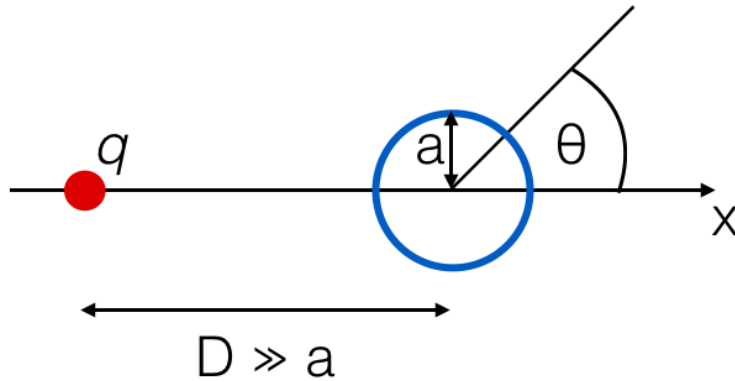
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Electromagnetism 1: Induced Dipole Moment on Conducting Sphere

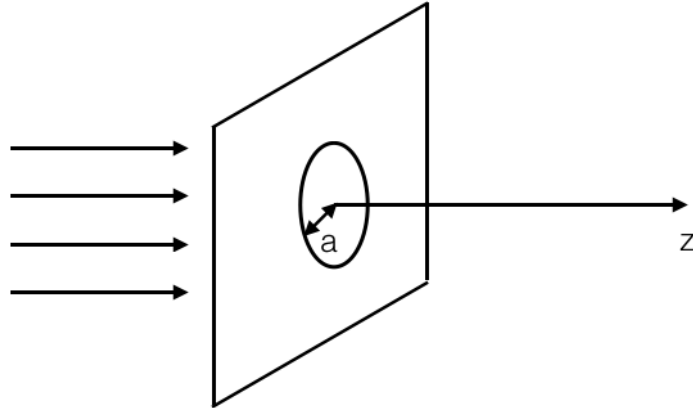
A positive electric point charge $+q$ is placed at a distance D from a conducting sphere of radius a that carries no net charge ($D \gg a$).



- (4 pts) Calculate the induced dipole moment of the sphere. In which direction does it point?
- (3 pts) Determine the induced surface charge density $\sigma(\theta)$ (see figure).
- (3 pts) Determine the force of the sphere (magnitude and direction).

Electromagnetism 2: Light intensity behind circular hole

A circular hole of radius a , cut in a large opaque screen, is illuminated at normal incidence with plane monochromatic radiation of wavelength λ (see figure). You may treat the radiation field as a scalar.



- (5 pts) Calculate the light intensity at a point P lying on the symmetry axis of the aperture as a function of the distance from the aperture z . Assume that $z \gg a$, but that z is comparable to a^2/λ .
- (2 pts) Normalize the light intensity so that, in the absence of a screen and aperture, the intensity is 1. With the screen and aperture in place, and for $a^2/(4\lambda) \leq z \leq 2a^2/\lambda$, what is the maximum intensity and at what value(s) of z does it occur?
- (3 pts) What would be the light intensity distribution on the symmetry axis along z (in the same region as in (a)) if the screen plus hole were replaced by a opaque disk of radius a ?

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WRITTEN EXAM - ELECTRICITY AND MAGNETISM — WITH SOLUTIONS

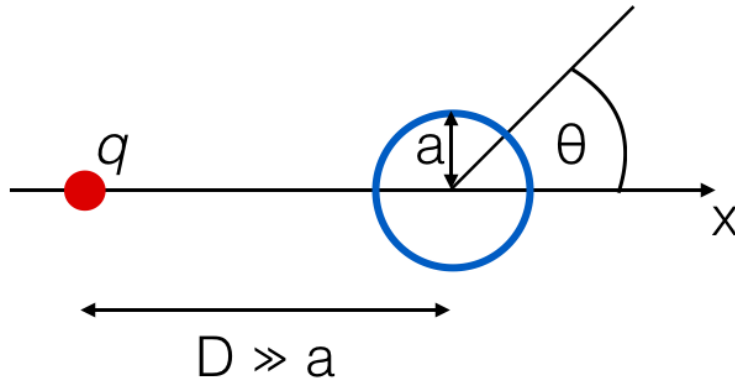
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- (3 pts) Determine the induced surface charge density $\sigma(\theta)$ (see figure).
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- Solutions by Markus Klute (December 2015) An earlier version of this problem also appeared on the Spring 2008 exam.

- (a) By symmetry, the induced dipole moment \vec{d} points along the $\pm x$ axis. Since the point charged q attracts the opposite charges at the surface closer to the point charge, the dipole moment, pointing from the negative to the positive charge, points, along the positive x axis if $q > 0$.

The scalar potential of the dipole field is

$$\phi(r, \theta) = \frac{d \cos \theta}{4\pi\epsilon_0 r^2}, \quad (1)$$

such that the tangential component of the dipole field is given by

$$E_\theta = -\frac{1}{r} \frac{\partial \phi}{\partial \theta} = \frac{d \sin \theta}{4\pi\epsilon_0 r^3}. \quad (2)$$

Since $D \gg a$, we can view the field of the point charged as constant over the sphere,

$$\vec{E}_0 = \frac{q}{4\pi\epsilon_0 D^2} \hat{e}_x, \quad (3)$$

with tangential component $-E_0 \sin \theta$. Since the tangential component of the field must vanish at the surface of the conducting sphere, we obtain

$$\frac{d \sin \theta}{4\pi\epsilon_0 a^3} = \frac{q \sin \theta}{4\pi\epsilon_0 D^2} \quad (4)$$

$$\Rightarrow d = \frac{qa^3}{D^2}. \quad (5)$$

- (b) The surface charge density can be determined from the normal component of the electric field. The radial component of the dipole field is given by

$$E_r = -\frac{\partial \phi}{\partial r} = \frac{d \cos \theta}{2\pi\epsilon_0 r^3} = \frac{qa^3 \cos \theta}{2\pi\epsilon_0 D^2 r^3}, \quad (6)$$

while the radial component of the constant field from the point charge is given by $E_0 \cos \theta$. The total radial field just outside the surface is thus

$$E_1 = \frac{3q}{4\pi D^2}. \quad (7)$$

From Gauss's law for a small area A we find $E_1 A = \sigma A / \epsilon_0$ and

$$\sigma(\theta) = \frac{3q \cos \theta}{4\pi D^2}. \quad (8)$$

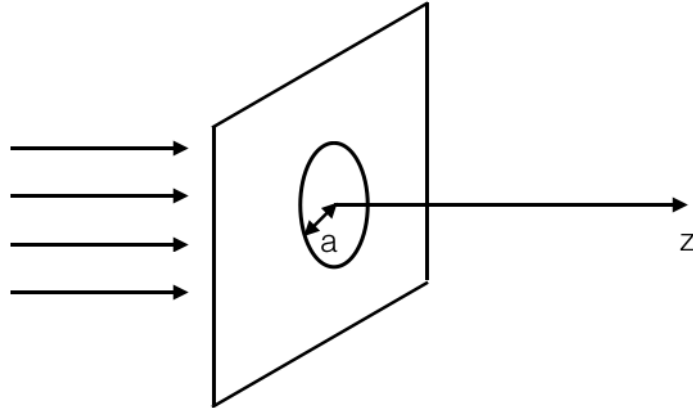
- (c) The energy of the system is $-\vec{d} \cdot \vec{E}_0$. The force is given by

$$\vec{F} = -\vec{\nabla}(-\vec{d} \cdot \vec{E}_0) = \hat{e}_x \frac{\partial}{\partial D} \frac{q^2 a^3}{4\pi\epsilon_0 D^4} = -\frac{q^2 a^3}{\pi\epsilon_0 D^5} \hat{e}_x. \quad (9)$$

An induced dipole is attracted towards regions of increasing field strength.

Electromagnetism 2: Light intensity behind circular hole

A circular hole of radius a , cut in a large opaque screen, is illuminated at normal incidence with plane monochromatic radiation of wavelength λ (see figure). You may treat the radiation field as a scalar.



- (5 pts) Calculate the light intensity at a point P lying on the symmetry axis of the aperture as a function of the distance from the aperture z . Assume that $z \gg a$, but that z is comparable to a^2/λ .
- (2 pts) Normalize the light intensity so that, in the absence of a screen and aperture, the intensity is 1. With the screen and aperture in place, and for $a^2/(4\lambda) \leq z \leq 2a^2/\lambda$, what is the maximum intensity and at what value(s) of z does it occur?
- (3 pts) What would be the light intensity distribution on the symmetry axis along z (in the same region as in (a)) if the screen plus hole were replaced by a opaque disk of radius a ?

- Solutions by Markus Klute (December 2015) An earlier version of this problem also appeared on the Fall 2008 exam.

- (a) According to Huygens' principle, each point in the aperture can be viewed as an emitter of a spherical wave. All emitters oscillate in phase as the incident plane wave has a constant phase over the aperture. The electric field E_{hole} at point P is obtained by summing electric fields from all different point emitters

$$E_{\text{hole}} = A \int_0^a 2\pi\rho d\rho \frac{e^{ik\sqrt{z^2+\rho^2}}}{\sqrt{z^2+\rho^2}}, \quad (1)$$

where A is a normalization factor. Substituting integration variables $y = \sqrt{\rho^2 + z^2}$, $dy = (\rho/y)d\rho$, we have

$$E_{\text{hole}} = 2\pi A \int_z^{\sqrt{z^2+a^2}} e^{iky} dy = \frac{2\pi A}{ik} \left(e^{ik\sqrt{z^2+a^2}} - e^{ikz} \right). \quad (2)$$

Since $z \gg a$ we can expand the first phase as

$$ik\sqrt{z^2+a^2} \approx ikz + i\frac{ka^2}{2z} + O\left(\frac{ka^2}{z} \frac{a^2}{z^2}\right). \quad (3)$$

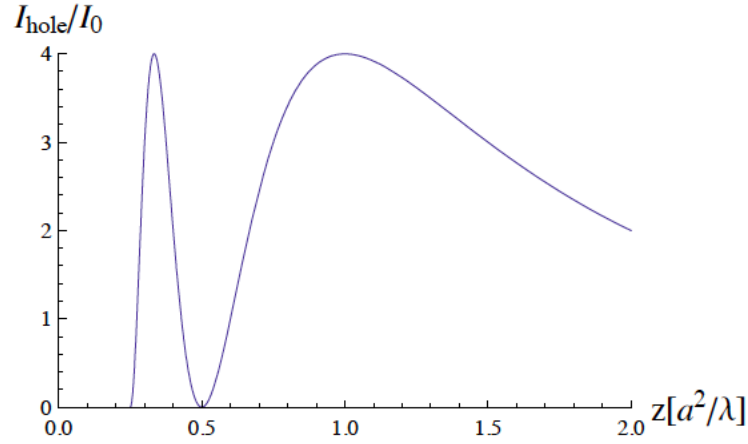
Since $ka^2/z \sim O(1)$ and $a^2/z^2 \ll 1$, the last term can be neglected, and the total field can be written as

$$E_{\text{hole}} \approx \frac{2\pi A}{ik} e^{ikz} \left(e^{ika^2/2z} - 1 \right) = \frac{4\pi A}{k} e^{ikz} e^{ika^2/4z} \sin\left(\frac{ka^2}{4z}\right). \quad (4)$$

Thus the intensity at point P is proportional to

$$I_{\text{hole}} \propto |E_{\text{hole}}|^2 = \left| \frac{4\pi A}{k} \right|^2 \sin^2\left(\frac{ka^2}{4z}\right). \quad (5)$$

- (b) The ratio of normalization factors can be found from Eq. 5 and by letting $a \rightarrow \infty$ in Eq. 3, and asking that we obtain the incident wave. We can set $e^{ika^2/2z}$ to 0 in Eq. (4), or obtain the same result more formally by assuming a smooth envelope for the field that goes to zero as $\rho \rightarrow \infty$, e.g., a Gaussian envelope, integrate, and then let the spatial size of the envelope go to infinity. If the incident plane wave is $E_0 e^{ikz}$, then from Eq. 3 we have $E_0 e^{ikz} = i2\pi A/k e^{ikz}$, or $E_0 = i\frac{2\pi A}{k}$. The maximum of I_{hole}/I_0 is 4, and it occurs at $z = a^2/(3\lambda)$ and $z = a^2/\lambda$ (see figure below).



- (c) According to Babinet's principle, the fields of the screen with hole E_{hole} and of the opaque disk E_{disk} must add to the incident field $E_0 e^{ikz}$. Then the field of the opaque disk is given by

$$E_{\text{disk}} = E_0 e^{ikz} - E_{\text{hole}} = E_0 e^{ikz} - \frac{2\pi A}{ik} e^{ikz} \left(e^{ika^2/2z} - 1 \right) = E_0 e^{ikz} e^{ika^2/2z}. \quad (6)$$

The intensity behind the circular disk on axis is constant and equal to the incident intensity. This is called the Poisson spot.

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Fax: (617) 258-8319

DOCTORAL GENERAL EXAMINATION
WRITTEN EXAM - QUANTUM MECHANICS

January 25, 2016

DURATION: 75 MINUTES

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Quantum Mechanics 1: Harmonic Oscillator Gains Weight over the Holidays

Consider a particle moving in 1-d subject to a harmonic potential, and suppose that the mass is slowly increasing; i.e.

$$H(t) = \frac{p^2}{2m(t)} + \frac{1}{2}m(t)\omega^2x^2, \quad (1)$$

where $m(t) = m_0e^{\nu t}$ for some constants m_0, ν . Suppose that at time $t = 0$ the particle is in the ground state of $H(0)$.

- (a) (3 pts) For small values of ν , the adiabatic theorem guarantees that the particle will remain approximately in the ground state at later times. How small does ν have to be to make this true?
- (b) (2 pts) Suppose that there exists an operator A satisfying

$$[A, p] = \frac{i\nu p}{2} \quad \text{and} \quad [A, x] = \frac{-i\nu x}{2}. \quad (2)$$

Show that this implies that

$$H(t) = e^{iAt}H(0)e^{-iAt}. \quad (3)$$

- (c) (2 pts) Find a Hermitian operator A satisfying Eq. (??). [Hint: consider products of x and p .]
- (d) (3 pts) Let $|\psi(t)\rangle$ be the solution of the Schrödinger equation. It turns out that

$$|\psi(t)\rangle = e^{-iAt}e^{iBt}|\psi(0)\rangle \quad (4)$$

Find B .

Quantum Mechanics 2: Scattering from a Spherical Potential

A spinless non-relativistic particle with momentum $\hbar\mathbf{k}$, represented by a normalized plane wave state $|\mathbf{k}\rangle$, is incident on a region with a (weak) potential $V(r)$. An outgoing scattered particle with momentum $\hbar\mathbf{k}'$ is represented by the plane wave state $|\mathbf{k}'\rangle$. If we observe outgoing particles in a small solid angle $d\Omega$ about the direction of \mathbf{k}' , Fermi's golden rule tells us that the transition rate $\omega_{kk'}$ is given by

$$\omega_{kk'} = \frac{2\pi}{\hbar} g(E_{k'}) |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2, \quad (1)$$

where $g(E)$ is the density of (outgoing) states defined from $dN = g(E_k)dE_{k'}$, where dN is the number of states with energy in the interval dE_k about E_k and direction within $d\Omega$. For normalization work in a large cubic box of volume L^3 .

- (a) (2 pts) Write the normalized wave function $\langle \mathbf{x} | \mathbf{k} \rangle$ for a plane wave state. Calculate $g(E_k)$ in terms of $m, L, k', d\Omega$, and \hbar .
- (b) (2 pts) Compute the probability current density \mathbf{J}_{inc} corresponding to the incident state $|\mathbf{k}\rangle$ [recall: $\mathbf{J} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi)$]. What are the units of J_{inc} ? What are the units of $\omega_{kk'}$?
- (c) (2 pts) Relate \mathbf{J}_{inc} , the differential cross section $d\sigma$, and $\omega_{kk'}$ to obtain a formula for $\frac{d\sigma}{\Omega}$ of the form

$$\frac{d\sigma}{\Omega} = f(m, L, \hbar, k, k') |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2. \quad (2)$$

Give the explicit form of f . Since the scattering is elastic, $k = k'$ may be used to simplify the answer.

- (d) (4 pts) Consider the potential $V(r)$ equal to V_0 for $r < a$ and zero for $r > a$. Let $q \equiv k' - k$ and $q = |q|$. Give q in terms of k and the deflection angle θ ? Calculate $\langle k' | V | k \rangle$ as a function of q, a , and other constants. Find the differential cross section $\frac{d\sigma}{\Omega}$ and its approximate value when $qa \ll 1$.

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DOCTORAL GENERAL EXAMINATION
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January 25, 2016

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$$|\psi(t)\rangle = e^{-iAt}e^{iBt}|\psi(0)\rangle \quad (4)$$

Find B .

- Solutions by Aram Harrow (2015)

(a) First calculate

$$\dot{H} = -\nu \frac{p^2}{2m} + \nu \frac{m\omega^2 x^2}{2}.$$

Recall the standard relations between a and x, p :

$$a \equiv a(t) = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right) \quad x = \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) \quad p = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a).$$

Rewriting \dot{H} in terms of a, a^\dagger we obtain

$$\dot{H} = -\nu \frac{1}{2m} \frac{-\hbar m\omega}{2} (a^\dagger - a)^2 + \nu \frac{m\omega^2}{2} \frac{\hbar}{2m\omega} (a^\dagger + a)^2 \quad (5)$$

$$= \frac{\hbar\omega\nu}{4} (a^\dagger a^\dagger + aa) \quad (6)$$

Let $\{|n\rangle \equiv |n(t)\rangle\}$ denote the instantaneous eigenstates of $H(t)$. If we start in $|0\rangle$ then \dot{H} couples the state only to $|2\rangle$ and the matrix element is $O(\hbar\omega\nu)$.

The adiabatic condition is that this is $\ll g^2/\hbar$, where $g = \hbar\omega$ is the gap. This is equivalent to the condition that $\nu \ll \omega$.

Another way to derive this condition is that there are only two time-scales in this question and they are given by ω and ν .

- (b) Note that $[A, p^2] = i\nu p^2$ and $[A, x^2] = -i\nu x^2$. Now consider Eq. (3). At $t = 0$, Eq. (3) is obviously true. Now we verify that Eq. (1) satisfies Eq. (3). Differentiating the RHS of Eq. (3) we obtain

$$\frac{d}{dt} e^{iAt} H(0) e^{-iAt} = i[A, e^{iAt} H(0) e^{-iAt}] = i[A, H(t)] = -\nu \frac{p^2}{2m} + \nu \frac{m\omega^2 x^2}{2} = \dot{H} \quad (7)$$

Since the derivatives and initial conditions match, we have that Eq. (1) satisfies Eq. (3) for all t .

- (c) Note that $[xp, p] = [x, p]p = i\hbar p$ and $[xp, x] = x[p, x] = -i\hbar x$. Thus xp is proportional to something with the right commutation relations, although it is not Hermitian. We would obtain the same conclusions if we replaced xp with px . To make A Hermitian we should make it proportional to $xp + px$. Specifically we should choose

$$A = \frac{\nu}{4\hbar} (xp + px).$$

- (d) Differentiating Eq. (4) and using the Schrödinger equation we find

$$-\frac{i}{\hbar} H(t) |\psi(t)\rangle = iAe^{iAt} e^{iBt} |\psi(0)\rangle + e^{iAt} iB e^{iBt} |\psi(0)\rangle \quad (8)$$

$$= iA |\psi(t)\rangle + e^{iAt} iB e^{iAt} |\psi(t)\rangle \quad (9)$$

Thus $H(t) = -\hbar A - \hbar e^{iAt} B e^{-iAt}$. Rearranging we have

$$B = e^{-iAt}(H(t) - \hbar A)e^{iAt} \quad (10)$$

$$= e^{-iAt} H(t) e^{iAt} - \hbar A \quad (11)$$

$$= H(0) - \hbar A \quad (12)$$

$$= \frac{p^2}{2m_0} + \frac{1}{2}m_0\omega^2 x^2 - \frac{\nu}{4}(xp + px) \quad (13)$$

Full credit is given for an answer of the form Eq. (12) or anything equivalent.

Quantum Mechanics 2: Scattering from a Spherical Potential

A spinless non-relativistic particle with momentum $\hbar\mathbf{k}$, represented by a normalized plane wave state $|\mathbf{k}\rangle$, is incident on a region with a (weak) potential $V(r)$. An outgoing scattered particle with momentum $\hbar\mathbf{k}'$ is represented by the plane wave state $|\mathbf{k}'\rangle$. If we observe outgoing particles in a small solid angle $d\Omega$ about the direction of \mathbf{k}' , Fermi's golden rule tells us that the transition rate $\omega_{kk'}$ is given by

$$\omega_{kk'} = \frac{2\pi}{\hbar} g(E_{k'}) |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2, \quad (1)$$

where $g(E)$ is the density of (outgoing) states defined from $dN = g(E_k)dE_{k'}$, where dN is the number of states with energy in the interval dE_k about E_k and direction within $d\Omega$. For normalization work in a large cubic box of volume L^3 .

- (a) (2 pts) Write the normalized wave function $\langle \mathbf{x} | \mathbf{k} \rangle$ for a plane wave state. Calculate $g(E_k)$ in terms of $m, L, k', d\Omega$, and \hbar .
- (b) (2 pts) Compute the probability current density \mathbf{J}_{inc} corresponding to the incident state $|\mathbf{k}\rangle$ [recall: $\mathbf{J} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi)$]. What are the units of J_{inc} ? What are the units of $\omega_{kk'}$?
- (c) (2 pts) Relate \mathbf{J}_{inc} , the differential cross section $d\sigma$, and $\omega_{kk'}$ to obtain a formula for $\frac{d\sigma}{\Omega}$ of the form

$$\frac{d\sigma}{\Omega} = f(m, L, \hbar, k, k') |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2. \quad (2)$$

Give the explicit form of f . Since the scattering is elastic, $k = k'$ may be used to simplify the answer.

- (d) (4 pts) Consider the potential $V(r)$ equal to V_0 for $r < a$ and zero for $r > a$. Let $q \equiv k' - k$ and $q = |q|$. Give q in terms of k and the deflection angle θ ? Calculate $\langle k' | V | k \rangle$ as a function of q, a , and other constants. Find the differential cross section $\frac{d\sigma}{\Omega}$ and its approximate value when $qa \ll 1$.

- Solutions by Markus Klute (December 2015) An earlier version of this problem also appeared on the Fall 2005 exam.

(a) We have

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{L^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (3)$$

This is well normalized since

$$\langle \mathbf{k}' | \mathbf{k} \rangle = \int d^3\mathbf{r} \psi_{\mathbf{k}'}^*(\mathbf{r}) \psi_{\mathbf{k}}(\mathbf{r}) = \delta_{\mathbf{k}',\mathbf{k}}. \quad (4)$$

From $k_i L = 2\pi n_i$ we find $d^3k L^3 = (2\pi)^3 dN$. Since we observe states along $d\Omega$, we find

$$d^3k = \frac{d\Omega}{4\pi} 4\pi k^2 dk. \quad (5)$$

Therefore,

$$dN = \frac{d\Omega}{4\pi} 4\pi k^2 dk \frac{L^3}{(2\pi)^3} = \frac{d\Omega}{4\pi} \frac{L^3}{2\pi^2} k(kdk) = \frac{d\Omega}{4\pi} \frac{mL^3}{2\pi^2 \hbar^2} k dE_k, \quad (6)$$

where we used $E_k = \frac{\hbar^2 k^2}{2m}$. It follows that

$$g(E_{k'}) = \frac{d\Omega}{4\pi} \frac{mL^3}{2\pi^2 \hbar^2} k'. \quad (7)$$

(b)

$$\mathbf{J}_{\text{inc}} = \frac{\hbar}{m} \text{Im}(\psi_{\mathbf{k}}^* \nabla \psi_{\mathbf{k}}) = \frac{\hbar}{mL^3} \text{Im}(e^{-i\mathbf{k}\cdot\mathbf{x}} \nabla e^{i\mathbf{k}\cdot\mathbf{x}}) = \frac{\hbar \mathbf{k}}{mL^3}. \quad (8)$$

The units of \mathbf{J}_{inc} are particles (no units) per unit of time per unit of area, of $T^{-1}L^{-2}$. The units of $\omega_{kk'}$ is one over time, or T^{-1} .

(c) The rate $\omega_{kk'}$ is given by the flux times the cross section,

$$\omega_{kk'} = \mathbf{J}_{\text{inc}} d\sigma = \frac{2\pi}{\hbar} g(E_{k'}) |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2. \quad (9)$$

The differential cross section is then

$$\frac{d\sigma}{d\Omega} = \frac{1}{2\hbar} \frac{1}{\mathbf{J}_{\text{inc}}} \frac{mL^3}{2\pi^2 \hbar^2} k' |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2. \quad (10)$$

Using the value of \mathbf{J}_{inc} we find

$$\frac{d\sigma}{d\Omega} = \left(\frac{mL^3}{2\pi^2 \hbar^2} \right)^2 |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2. \quad (11)$$

This determines f .

(d) Since k and k' form the deflection angle θ , we find $q = 2k \sin(\theta/2)$. We have

$$\langle \mathbf{k}' | V | \mathbf{k} \rangle = \frac{1}{L^3} \int d^3 \mathbf{x} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{x}} V(\mathbf{x}) \quad (12)$$

$$= \frac{V_0}{L^3} \int_{|\mathbf{x}| < a} d^3 \mathbf{x} e^{-i\mathbf{q} \cdot \mathbf{x}} \quad (13)$$

$$= \frac{V_0}{L^3} 2\pi \int_0^a r^2 dr \int_{-1}^1 d(\cos \theta') e^{-iq \cos(\theta') r} \quad (14)$$

$$= \frac{V_0}{L^3} 2\pi \int_0^a r^2 dr (-2) \frac{\sin qr}{qr} \quad (15)$$

$$= (-4\pi) \frac{V_0}{q^3 L^3} \int_0^{qa} u du \sin u \quad (16)$$

$$= (-4\pi) \frac{V_0}{q^3 L^3} (\sin qa - qa \cos qa). \quad (17)$$

For small qa we find

$$\sin qa - qa \cos qa \approx qa - \frac{1}{6}(qa)^3 - qa \left(1 - \frac{1}{2}(qa)^2\right) \approx \frac{1}{3}(qa)^3 \quad (18)$$

and can approximate the differential cross section to

$$\frac{d\sigma}{d\Omega} = \left(\frac{2mV_0 a^3}{3\hbar^2} \right)^2. \quad (19)$$

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DOCTORAL GENERAL EXAMINATION
WRITTEN EXAM - STATISTICAL MECHANICS

January 25, 2016

DURATION: 75 MINUTES

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Statistical Mechanics 1: Leaky spacesuit

Suppose that Matt Damon is floating in space, wearing a spacesuit that (for simplicity) contains pure nitrogen gas. The spacesuit also contains a small hole which we assume is much smaller than the mean free path of the gas. Assume further that the escape rate is slow enough that the remaining gas remains in equilibrium by collisions among the gas molecules; neglect any interaction between the gas and Matt Damon. Neglect also the thickness of the spacesuit.

- (a) (*1 pt*) What is the average energy of a gas molecule inside the spacesuit at temperature T ? Treat the rotational modes of the diatomic gas classically, but neglect the vibrational mode which is not excited at room temperature.
- (b) (*4 pts*) What is the average energy, including both kinetic and rotational, per molecule of gas that escapes when the gas inside the spacesuit is at temperature T ?
- (c) (*2 pts*) Suppose the spacesuit initially contains N_0 molecules at temperature T_0 . Once there are only N molecules remaining, what is the temperature T of the remaining gas?
- (d) (*3 pts*) Eventually all of the gas will escape. Assume that Matt Damon does not rotate so that the hole is always pointing in the same direction. What will his momentum be once all the gas is gone ($N = 0$)?

For convenience we include the following formula.

$$\int_0^{\infty} e^{-u} u^n du = \Gamma(n+1) = \begin{cases} n! & \text{if } n \text{ is an integer} \\ \frac{(2n+1)!}{4^{n+1}(n+1/2)!} \sqrt{4\pi} & \text{if } n + 1/2 \text{ is an integer} \end{cases} \quad (1)$$

Statistical Mechanics 2: Atom-Molecule Equilibrium in a Harmonic Trap

In this problem we are analyzing the equilibrium between atoms and molecules trapped in three-dimensional, spherically symmetric harmonic potentials. There are two species of atoms A, B with masses m_A, m_B . Atoms A and B can form a molecule M in a reaction $A + B \leftrightarrow M$, where the molecular binding energy is $-E$ with $E > 0$, i.e., a molecule at rest has less energy than a pair of atoms A, B at rest. We assume that two atoms of the same species do not form molecules, and that there is only one relevant state of the molecule (rotational and vibrational modes are frozen out). The numbers of particles of each species are denoted by N_A, N_B , and N_M . The system is assumed to be in thermal equilibrium at sufficiently high temperature T , such that the fermionic or bosonic character of the particles is irrelevant.

- (a) (1 pt) For each particle, the eigenenergies are given by $E_j = (j + 3/2)\hbar\omega$, with degeneracy g_j , where the same value of ω applies independently of whether the particles are atoms A or B , or molecule M . What is the degeneracy g_j for the energy E_j ? If you do not know how to compute g_j , you may simply leave it in symbolic form and go on to do the rest of the problem.
- (b) (2 pts) Determine the single-particle partition functions Z_α , where $\alpha = A, B, M$. Given particle numbers N_α , what is the condition on Z_α and N_α that allows one to ignore the fermionic or bosonic character of the particles?
- (c) (2 pts) Find the partition function for the complete system of atoms and molecules at fixed particle numbers N_A, N_B , and N_M expressed in terms of the single-particle atomic partition function Z_A .
- (d) (5 pts) Assume that initially there are N_{A_0} and N_{B_0} atoms A, B and no molecules. The system then reaches atom-molecule equilibrium at temperature T with particle number N_α , with $\alpha = A, B, M$. Determine the equilibrium molecule number N_M in terms of N_A, N_B , the single-particle partition functions, and the other quantities given in the problem. Explain why the conversion efficiency of atom pairs into molecules remains small for $E \sim kT$ even though the molecules have less energy. Use Stirling's approximation: $\ln N! \approx N \ln N - N$ to simplify the calculations.

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- Solutions by Aram Harrow: Adapted from Fall 97 SM1

- (a) $\frac{5}{2}kT$ from three momentum degrees of freedom and two rotational degrees of freedom.
- (b) First we compute the velocity distribution. The components v_x, v_y, v_z are independent Gaussians satisfying $\mathbb{E}[v_i] = 0$ and $\mathbb{E}[v_i^2] = kT/m \equiv \sigma^2$. Thus their density is

$$p(v_i) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{v_i^2}{2\sigma^2}\right),$$

and $p(v_1, v_2, v_3) = p(v_1)p(v_2)p(v_3)$. The flux of gas leaving the spacesuit is

$$dN = -n dA dt \int_0^\infty p(v_3)v_3 dv_3.$$

To calculate the change in energy, first note that the energy has contributions from five modes: three from the $p_1, p_2,$ and p_3 components of momentum and two from the rotational modes, which we call ω_1 and ω_2 . The total energy can thus be written as

$$E = E_{p_1} + E_{p_2} + E_{p_3} + E_{\omega_1} + E_{\omega_2}.$$

Of these only $E_{p_3} = \frac{m}{2}v_3^2$ is correlated with v_3 . For the others, the change in energy is directly proportional to the number of molecules leaving the spacesuit, i.e.

$$dE_{p_1} = dE_{p_2} = dE_{\omega_1} = dE_{\omega_2} = \frac{kT}{2}dN.$$

For E_{p_3} the change in energy is

$$dE_3 = -n dA dt \int_0^\infty \frac{mv_3^2}{2}v_3 p(v_3)dv_3 \tag{2}$$

and the ratio is

$$\frac{dE_3}{dN} = \frac{m \int_0^\infty p(v_3)v_3^3 dv_3}{2 \int_0^\infty p(v_3)v_3 dv_3} \tag{3}$$

We will need to calculate

$$\int_0^\infty e^{-\frac{v^2}{2\sigma^2}} v^{2n+1} dv \stackrel{u \equiv \frac{v^2}{2\sigma^2}}{=} \frac{1}{2}(2\sigma^2)^{n+1} \int_0^\infty e^{-u} u^n du = \frac{1}{2}(2\sigma^2)^{n+1} \Gamma(n+1),$$

where $\Gamma(n+1) = n!$ for integer values of n and $\Gamma(n+1) = \frac{(2n+1)!}{4^{n+1}(n+1/2)!} \sqrt{4\pi}$ for half-integer n . Thus we have

$$\frac{\int_0^\infty p(v_3)v_3^3 dv_3}{\int_0^\infty p(v_3)v_3 dv_3} = 2\sigma^2 \frac{\Gamma(2)}{\Gamma(1)} = \frac{2kT}{m}. \tag{4}$$

Substituting into Eq. (3) we find that $dE_3/dN = kT$.

Putting all the contributions together we have that $\frac{dE}{dN} = 3kT$.

- (c) There are effectively 5 degrees of freedom per molecule so $E = \frac{5}{2}NkT$. We calculate dE in two different ways—using the product rule and using (a)—to obtain

$$dE = \frac{5}{2}NkdT + \frac{5}{2}kTdN = 3kTdN.$$

This yields the differential equation

$$\frac{dT}{T} = \frac{1}{5} \frac{dN}{N},$$

which has solution

$$\frac{T}{T_0} = \left(\frac{N}{N_0} \right)^{1/5}.$$

- (d) The average z -momentum of a departing particle is

$$m \frac{\int_0^\infty v_z^2 p(v_z) dv_z}{\int_0^\infty v_z p(v_z) dv_z} = m \sqrt{2\sigma^2} \Gamma(3/2) = \sqrt{\frac{\pi}{2}} \sigma = \sqrt{\frac{\pi}{2} mkT} = \sqrt{\frac{\pi}{2} mkT_0} \frac{N^{1/10}}{N_0^{1/10}} \quad (5)$$

Summing over all the particles we obtain

$$\int_0^{N_0} \sqrt{\frac{\pi}{2} mkT_0} \frac{N^{1/10}}{N_0^{1/10}} dN = \sqrt{\frac{\pi}{2} mkT_0} \frac{N_0^{11/10}}{\frac{11}{10} N_0^{1/10}} = \frac{5\sqrt{2\pi}}{11} \sqrt{mkT_0} N_0 \quad (6)$$

The momentum in the x and y directions is 0 by symmetry.

Note that this problem could also explain that mysterious scene in Gravity where some force is pulling George Clooney away from Sandra Bullock and she ends up releasing him.

Statistical Mechanics 2: Atom-Molecule Equilibrium in a Harmonic Trap

In this problem we are analyzing the equilibrium between atoms and molecules trapped in three-dimensional, spherically symmetric harmonic potentials. There are two species of atoms A, B with masses m_A, m_B . Atoms A and B can form a molecule M in a reaction $A + B \leftrightarrow M$, where the molecular binding energy is $-E$ with $E > 0$, i.e., a molecule at rest has less energy than a pair of atoms A, B at rest. We assume that two atoms of the same species do not form molecules, and that there is only one relevant state of the molecule (rotational and vibrational modes are frozen out). The numbers of particles of each species are denoted by N_A, N_B , and N_M . The system is assumed to be in thermal equilibrium at sufficiently high temperature T , such that the fermionic or bosonic character of the particles is irrelevant.

- (a) (1 pt) For each particle, the eigenenergies are given by $E_j = (j + 3/2)\hbar\omega$, with degeneracy g_j , where the same value of ω applies independently of whether the particles are atoms A or B , or molecule M . What is the degeneracy g_j for the energy E_j ? If you do not know how to compute g_j , you may simply leave it in symbolic form and go on to do the rest of the problem.
- (b) (2 pts) Determine the single-particle partition functions Z_α , where $\alpha = A, B, M$. Given particle numbers N_α , what is the condition on Z_α and N_α that allows one to ignore the fermionic or bosonic character of the particles?
- (c) (2 pts) Find the partition function for the complete system of atoms and molecules at fixed particle numbers N_A, N_B , and N_M expressed in terms of the single-particle atomic partition function Z_A .
- (d) (5 pts) Assume that initially there are N_{A_0} and N_{B_0} atoms A, B and no molecules. The system then reaches atom-molecule equilibrium at temperature T with particle number N_α , with $\alpha = A, B, M$. Determine the equilibrium molecule number N_M in terms of N_A, N_B , the single-particle partition functions, and the other quantities given in the problem. Explain why the conversion efficiency of atom pairs into molecules remains small for $E \sim kT$ even though the molecules have less energy. Use Stirling's approximation: $\ln N! \approx N \ln N - N$ to simplify the calculations.

- Solutions by Markus Klute (December 2015) An earlier version of this problem also appeared on the Spring 2007 exam.

- (a) The potential V can be written in cartesian coordinates as $V(x, y, z) = \frac{1}{2}m_\alpha\omega^2(x^2 + y^2 + z^2)$, $\alpha = A, B, M$. For a level with energy $E_j = (j + 3/2)\hbar\omega$, if $n_z = j$, there is one possible way to redistribute the remaining energy between x and y , $(n_x, n_y) = (0, 0)$, if $n_z = j - 1$, there are two ways, $(n_x, n_y) = (1, 0), (0, 1)$, etc. The degeneracy of the level with eigenenergy E_j is thus $g_j = 1 + 2 + 3 + \dots + (j + 1) = \frac{1}{2}(j + 1)(j + 2)$.
- (b) Since the atoms A, B have the same trapped potential energies, the single-particle partition function is the same, and given by

$$Z_A = Z_B = \sum g_j e^{-\beta E_j} = e^{-\frac{3}{2}\beta\hbar\omega} \frac{1}{2} \sum (j + 1)(j + 2) e^{-j\beta\hbar\omega} \equiv e^{-\frac{3}{2}\beta\hbar\omega} Z_1, \quad (1)$$

where $\beta \equiv (k_B T)^{-1}$. In order to simplify the following formulas, we have defined the partition function Z_1 that is obtained if one ignores the zero-point energy $\frac{3}{2}\hbar\omega \ll kT$. The molecule is trapped in a harmonic potential with the same frequency ω , but its energy is lower, $E_{M_j} = E_j - E$. Consequently

$$Z_M = \sum g_j e^{-\beta(E_j - E)} = e^{\beta E} Z_A. \quad (2)$$

Quantum statistical effects can be ignored if the population of the ground state, n_0 , and hence any trap state remains much smaller than unity. Since the ground state for $A, B, (M)$ has energy $E_0 = \frac{3}{2}\hbar\omega$ ($E_0 = \frac{3}{2}\hbar\omega - E$), its population in thermal equilibrium is

$$n_0 = \frac{N_{A,B} e^{-\frac{3}{2}\beta\hbar\omega}}{Z_{A,B}} = \frac{N_{A,B}}{Z_1} \text{ for the atoms,} \quad (3)$$

$$n_0 = \frac{N_M e^{-\beta(\frac{3}{2}\hbar\omega - E)}}{Z_M} = \frac{N_M}{Z_1} \text{ for the molecules.} \quad (4)$$

The system behaves like a classical gas as long as $N_{A,B,M}/Z_1 \ll 1$.

- (c) We either know that for subsystems of different atoms the partition functions simply multiply, while for N subsystems of identical particles the product of partition functions has to be divided by $N!$ to avoid multiple counting of the same many-particle states.

$$Z = \frac{e^{N_M \beta E} (Z_A)^{N_A + N_B + N_M}}{N_A! N_B! N_M!}. \quad (5)$$

Or we can proceed as follows: If the N_A of A atoms have the same set of single-particle energies $\{E_j\}$, with the set of indices denoted by $\{j\} = \{j_1, \dots, j_{N_A}\}$, and similarly for the B atoms, $\{E_k\}$, with $\{k\} = \{k_1, \dots, k_{N_B}\}$, and the molecules, $\{E_l - E\}$, with $\{l\} = \{l_1, \dots, l_{N_M}\}$, then the total energy is

$$E_{\{j\}\{k\}\{l\}} = \sum_{i=1}^{N_A} E_{j_i} + \sum_{i=1}^{N_B} E_{k_i} + \sum_{i=1}^{N_M} (E_{l_i} - E). \quad (6)$$

The degeneracy of the many-particle state is

$$g_{\{j\}\{k\}\{l\}} = \Pi_{i=1}^{N_A} g_{j_i} \Pi_{i=1}^{N_B} g_{k_i} \Pi_{i=1}^{N_M} g_{l_i}. \quad (7)$$

For each of the subsystems $\alpha = A, B, M$ there are $N_\alpha!$ permutations of the indices that represent the same N_α particle state. (Strictly, this is only true if all indices $\{j\}$ are different, but this represents the dominant contribution.) For different particles, there are no such considerations. Consequently, we have

$$Z = \frac{1}{N_A! N_B! N_M!} \sum_{\{j\}} \sum_{\{k\}} \sum_{\{l\}} g_{\{j\}\{k\}\{l\}} e^{-\beta E_{\{j\}\{k\}\{l\}}} \quad (8)$$

$$= \frac{1}{N_A!} \left(\sum_{j=0}^{\infty} g_j e^{-\beta E_j} \right)^{N_A} \frac{1}{N_B!} \left(\sum_{k=0}^{\infty} g_k e^{-\beta E_k} \right)^{N_B} \frac{1}{N_M!} \left(\sum_{l=0}^{\infty} g_l e^{-\beta E_l - E} \right)^{N_M} \quad (9)$$

$$= \frac{(Z_A)^{N_A} (Z_B)^{N_B} (Z_M)^{N_M}}{N_A! N_B! N_M!} \quad (10)$$

$$= \frac{e^{N_M \beta E} (Z_A)^{N_A + N_B + N_M}}{N_A! N_B! N_M!}. \quad (11)$$

- (d) The system can lower its energy by creating more molecules. However, two atoms have more degrees of freedom (their relative motion) than a molecule in a single state. Therefore, the entropy is increased by dissociating molecules. The equilibrium is determined by the minimum of the free energy $F = W - TS$ that can also be written as $F = -kT \ln Z$. Thus it is sufficient to find the maximum of the partition function as the molecule number is varied.

If N_A, N_B, N_M denote the particle numbers in equilibrium, particle conservation requires that $N_A = N_{A_0} - N_M$ and $N_B = N_{B_0} - N_M$. Using the results from part (c),

$$\ln Z = \beta N_M E + (N_{A_0} + N_{B_0} + N_M) \ln Z_A - \ln(N_{A_0} - N_M)! - \ln(N_{B_0} - N_M)! - \ln N_M!, \quad (12)$$

the Stirling approximation yields

$$\frac{\partial \ln N_M!}{\partial N_M} = \ln N_M + N_M / N_M - 1 = \ln N_M, \quad (13)$$

$$\frac{\partial \ln(N_{A_0} - N_M)!}{\partial N_M} = -\ln(N_{A_0} - N_M), \quad (14)$$

and thus

$$\frac{\partial \ln Z}{\partial N_M} = \beta E - \ln Z_A + \ln(N_{A_0} - N_M) + \ln(N_{B_0} - N_M) - \ln N_M = \beta E + \ln \frac{N_A N_B}{Z_A N_M} \quad (15)$$

The condition $\frac{\partial Z}{\partial N_M} = 0$ requires

$$e^{-\beta E} = \frac{N_A N_B}{Z_A N_M}. \quad (16)$$

Consequently the molecule number is given by

$$N_M = e^{\beta E} \frac{N_A N_B}{Z_A}. \quad (17)$$

Since $N_A/Z_A, N_B/Z_B \ll 1$, for $E \sim kT$ the molecule number $N_M \simeq (N_A/Z_A)/N_B = (N_B/Z_B)/N_A \ll N_A, N_B$ remains small. This is because there are more degrees of freedom for two atoms than for one molecule. Therefore, unless the molecule is strongly energetically favored ($E \gg kT$), the number of molecules remains small because there are many more two-atom states than molecule states.