Comprehensive Examination

Department of Physics and Astronomy

Stony Brook University

Fall 2021 (in 4 separate parts: CM, EM, QM, SM)

General Instructions:

Three problems are given. If you take this exam as a placement exam, you must work on all three problems. If you take the exam as a qualifying exam, you must work on two problems (if you work on all three problems, only the two problems with the highest scores will be counted).

Each problem counts for 20 points, and the solution should typically take approximately one hour.

Use one exam book for each problem, and label it carefully with the problem topic and number and your ID number.

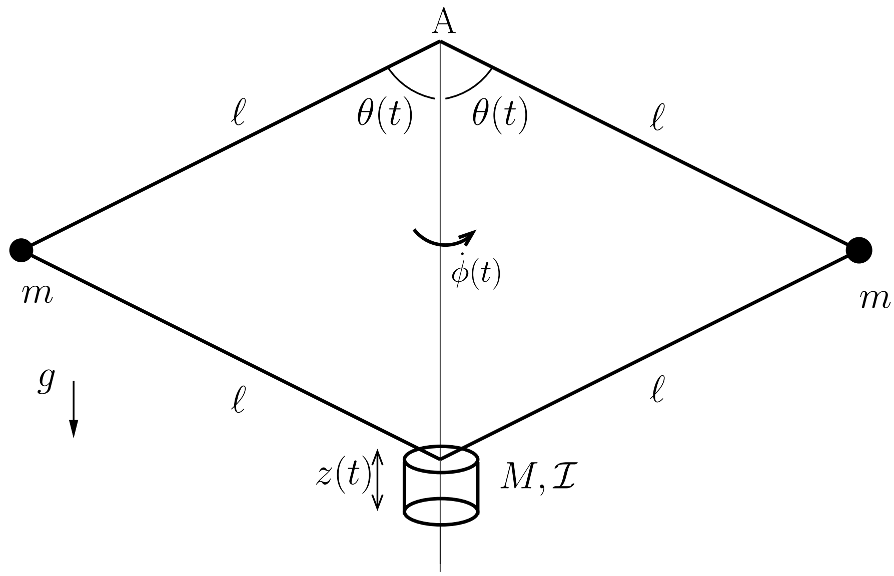
Write your ID number (not your name!) on each exam booklet.

You may use, one sheet (front and back side) of handwritten notes and, with the proctor's approval, a foreign-language dictionary. **No other materials may be used**.

Classical Mechanics 1

Oscillations of a rotating system

Consider two point masses of mass m and a cylinder with moment of inertia $\mathcal{I}$ and mass M connected with four massless hinges and massless connecting rods of fixed length ℓ lying in a plane. The system is suspended in the earth's gravitational field from a fixed point, point A shown below. The cylinder is constrained to slide along the z-axis, and as it slides its position $z(t)$, and the corresponding angle $\theta(t)$, change in time. The whole system rotates around the z-axis with angular velocity $\dot{\phi}(t)$.



(a) (8 points) Introduce suitable generalized coordinates and determine the Lagrangian of the system.

(b) (5 points) Determine all integrals (or constants) of the motion. Interpret these constants physically.

(c) (Not graded – see below) Consider the stable configurations with $\dot{\phi} = \omega = \text{const}$ and $\theta = 0$, i.e. maximally extended. At time t=0 the cylinder is given an upward impulsive upward kick performing work W over an infinitessimal displacement of the system. Find an equation that determines the maximum deflection angle $\theta_{\rm max}$

(d) (7 points) Consider the configurations with $\theta = 0$ and $\dot{\phi} \equiv \omega = \text{const}$. Show that the configuration becomes unstable for $\omega > \omega_c$ and determine ω_c.

Solution:

(a) The kinetic energy has a translational and a rotational component, $T = T_{\text{translational}} + T_{\text{rotational}}$. Taking $I_m = 2m\ell^2 \sin^2\theta$ for the moment of inertia of the point masses, we may write

$$\begin{aligned} T_{\text{rot}} = & \quad \tfrac{1}{2}\mathcal{I}\dot{\phi}^2 + \tfrac{1}{2}I_m\dot{\phi}^2 \\ = & \quad \tfrac{1}{2}\mathcal{I}\dot{\phi}^2 + m\ell^2\sin^2\theta\dot{\phi}^2 \end{aligned}$$

Taking the $+x$-direction as to the right and the $+y$-direction as up and taking x and y as the positions of the point masses and Y as the position of the cylinder, we may write the translational kinetic energy as

$$T_{\text{trans}} = \quad 2\cdot\tfrac{1}{2}m\dot{y}^2 + 2\cdot\tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}M\dot{Y}$$

With

$$\begin{aligned} y = \ell\cos\theta \quad & x = \ell\sin\theta \\ \dot{y} = -\ell\sin\theta\dot{\theta} \quad & \dot{x} = \ell\cos\theta\dot{\theta} \end{aligned}$$

Looking at the cylinder, we have

$$\begin{aligned} Y = & \quad 2\ell\cos\theta \\ \dot{Y} = & \quad -2\ell\sin\theta\dot{\theta} \end{aligned}$$

and the translational kinetic energy is then

$$\begin{aligned} T_{\text{trans}} = & \quad m\left(\ell^2\cos^2\theta\dot{\theta}^2 + \ell^2\sin^2\theta\dot{\theta}^2\right) + \tfrac{1}{2}4M\ell^2\sin^2\theta\dot{\theta} \\ = & \quad m\ell^2\dot{\theta}^2\left(\sin\theta^2 + \cos\theta^2\right) + 2M\ell^2\sin^2\theta\dot{\theta} \\ = & \quad m\ell^2\dot{\theta}^2 + 2M\ell^2\sin^2\theta\dot{\theta} \end{aligned}$$

Then

$$T = m\ell^2\dot{\theta}^2 + 2M\ell^2\sin^2\theta\dot{\theta}^2 + m\ell^2\sin^2\theta\dot{\phi}^2 + \frac{1}{2}\mathcal{I}\dot{\phi}^2$$

Taking $V = 0$ at the suspension point A we get the potential energy

$$\begin{aligned} V = & \quad V_{\text{cylinder}} + V_{\text{pointmasses}} \\ = & \quad -Mg\left(2\ell\cos\theta\right) - 2mg\left(\ell\cos\theta\right) \\ = & \quad -2\left(M+m\right)g\ell\cos\theta \end{aligned}$$

And the Lagrangian is

$$L = \left(m\ell^2 + 2M\ell^2\sin^2\theta\right)\dot{\theta}^2 + m\ell^2\sin^2\theta\dot{\phi}^2 + \frac{1}{2}\mathcal{I}\dot{\phi}^2 + 2\left(M+m\right)g\ell\cos\theta \tag{1}$$

(b) A cyclic coordinate q_i is one for which $\frac{\partial L}{\partial q_i} = 0$. The momentum associated with coordinate q_i is

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

and with this the Euler-Lagrange equation becomes

$$\frac{\partial L}{\partial q_i} = \frac{dp_i}{dt}$$

For a cyclic coordinate, $\frac{\partial L}{\partial q_i} = 0$ so $\frac{dp_i}{dt} = 0$, which says that p_i is constant in time. This is a case of Noether's theorem. For this system,

$$\frac{\partial L}{\partial \phi} = 0 \longrightarrow \left(\mathcal{I} + 2m\ell^2 \sin\theta^2\right)\dot{\phi} = L_z$$

which we recognize is conservation of angular momentum about the z axis.

The other conserved quantity is the energy

$$E = T + V = \left(m\ell^2 + 2M\ell^2\sin^2\theta\right)\dot{\theta}^2 + m\ell^2\sin^2\theta\dot{\phi}^2 + \frac{1}{2}\mathcal{I}\dot{\phi}^2 - 2\left(M+m\right)g\ell\cos\theta \qquad (2)$$

It is useful to replace $\dot{\phi}$ with L_z and to write

$$E = \frac{1}{2}m_{\text{eff}}(\theta)\ell^2\dot{\theta}^2 + V_{\text{eff}}(\theta) \qquad (3)$$

where

$$V_{\text{eff}}(\theta) = \frac{1}{2}\frac{L_z^2}{\mathcal{I} + 2m\ell^2\sin^2(\theta)} - 2(M+m)g\ell\cos\theta \qquad (4)$$

and

$$m_{\text{eff}}(\theta) = 2m + 4M\sin^2\theta \qquad (5)$$

(c) The problem was misstated. It was stated:

Consider the stable configurations with $\dot{\phi} = \omega =$ const and $\theta = 0$, i.e. maximally extended. At time t=0 the cylinder is given an upward impulsive upward kick imparting momentum p_0. Find an equation that determines the maximum deflection angle $\theta_{\max}$ (This equation could be solved numerically for $\theta_{\max}$.)

The problem with this is that if the cylinder gets momentum p_0 in a short time, then the velocity of the side masses infinite, i.e. we have done an infinite amount of work.

It should have been stated:

Consider the stable configurations with $\dot{\phi} = \omega =$ const and $\theta = 0$, i.e. maximally extended. At time t=0 the cylinder is given an upward impulsive upward kick performing work W over a short period of time and infinitessimal displacement of the system. Find an equation that determines the maximum deflection angle $\theta_{\max}$ (This equation could be solved numerically for $\theta_{\max}$.)

We can use energy conservation to write down the required equation. The initial energy just after the work is the kinetic energy the cylinder plus potential energy of the cylinder and the two masses

$$E = W + \frac{1}{2}\mathcal{I}\omega^2 - 2(M+m)g\ell\,. \tag{6}$$

The work that is done goes into increasing the kinetic energy of the two side masses, i.e. just after impulse the angle θ has scarcely changed, but the two side masses are moving with constant velocity

$$W = \frac{1}{2}m_{\text{eff}}(\theta)\ell\dot{\theta}^2\Big|_{\theta=0} \tag{7}$$

The bottom mass initially has no vertical motion.

Comparing this initial energy in Eq. 6 with the final energy at angle $\theta_{\max}$, Eq. 3, and noting that at the maximum height we have $\dot{\theta}_{\max} = 0$, leads to an equation which must be solved numerically

$$E = \frac{1}{2}\mathcal{I}\omega^2\left(\frac{1}{1 + (2m\ell^2/\mathcal{I})\sin^2\theta_{\max}}\right) - 2(M+m)g\ell\cos\theta_{\max}\,. \tag{8}$$

(d) To study the dynamics at small θ we expand the Langrangian in Eq. 1 to quadratic order in θ

$$L \simeq m\ell^2\dot{\theta}^2 + m\ell^2\theta^2\dot{\phi}^2 + \frac{1}{2}\mathcal{I}\dot{\phi}^2 - (M+m)\,g\theta^2 + \text{const}\,, \tag{9}$$

We have neglected terms of order $\theta^2\dot{\theta}^2$ which are quartic order in θ. The Euler-Lagrange equations of motion to linear order in θ are

$$\partial_t(\mathcal{I}\dot{\phi}) = 0\,, \tag{10}$$

$$\partial_t(m\ell^2\dot{\theta}) = 2m\ell^2\theta\dot{\phi}^2 - 2(M+m)g\theta\,. \tag{11}$$

Recognizing that $\mathcal{I}\omega \equiv L_z$ is constant, the equation of motion for θ reads

$$\partial_t(m\ell^2\dot{\theta}) = -\left[2(M+m)g\ell - \frac{2m\ell^2}{\mathcal{I}^2}L_z^2\right]\theta\,. \tag{12}$$

Thus, $\theta = 0$ is unstable whenever

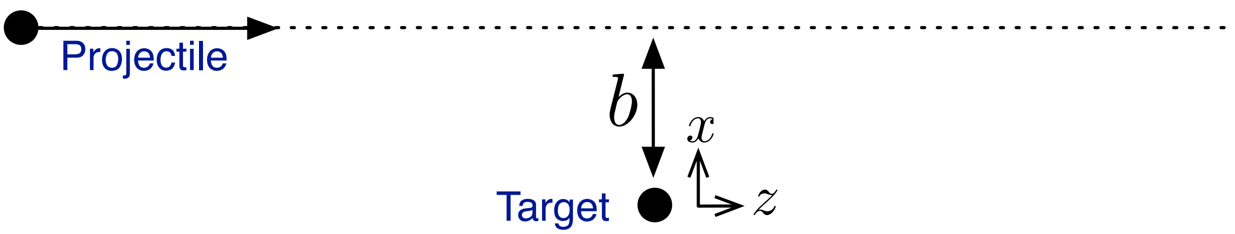
$$L_z > \left(\frac{(M+m)g\ell\mathcal{I}^2}{m\ell^2}\right)^{1/2}\,. \tag{13}$$

Classical Mechanics 2

Energy loss in a classical collision

A particle at position $\boldsymbol{r}(t) = (x, y, 0)$ (the target) is constrained to move in the x, y plane (transverse to the beam), and is bound to the origin in a harmonic potential, $U = \frac{1}{2}m\omega_0^2\boldsymbol{r}^2$. The target is initially at rest at the origin.

A second particle at position $\boldsymbol{r}_p(t)$ (the projectile) has high energy E, and scatters off the first particle at an impact parameter b relative to the origin. The two particles interact via the potential, $V(|\boldsymbol{r} - \boldsymbol{r}_p|) = U_0 e^{-\kappa|\boldsymbol{r}-\boldsymbol{r}_p|^2}$, during the projectile's passage. Since the projectile has high energy, you should assume that it moves with constant velocity throughout the collision. You should also assume that the displacement of the target $\boldsymbol{r}(t)$ is always small compared to b, $|\boldsymbol{r}| \ll b$.



(a) (2 points) Compute the force $\boldsymbol{F}(t)$ on the target by the projectile as a function of time.

Within the *approximations* given above, you should find that the x component of the force takes the form

$$F_x(t) = f\, e^{-\kappa(v_0 t)^2}\,, \tag{1}$$

where f and v_0 are constant in time, and the projectile is at $(b, 0, 0)$ at $t = 0$.

(b) (6 points) Determine the displacement and velocity of the target as a function of time throughout the duration of the collision. You may leave any explicit integrals unevaluated.

(c) (7 points) Determine the total energy absorbed by the oscillator after a collision at impact parameter b. Some integrals are given below.

(d) (5 points) Now consider a dilute infinite medium consisting of n targets per volume, randomly distributed in space. As above, the targets move in the x and y directions only and are harmonically bound. What is the energy lost per length by the projectile? Some integrals are given below.

Hint: First find the number of collisions per length with impact parameter between b and $b + db$.

Possibly Useful Integrals:

Here $n = 0, 1, 2, 3, \ldots$ is a non-negative integer:

$$\int_{-\infty}^{\infty} dx\, e^{ikx} e^{-ax^2} = \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \tag{2}$$

$$\int_{0}^{\infty} dx\, e^{-x} x^n = n! \tag{3}$$

Solution

(a) The trajectory of the projectile is is

$$\boldsymbol{r}_b = b\hat{\boldsymbol{x}} + v_0 t\hat{\boldsymbol{z}} \tag{4}$$

where $v_0 = \sqrt{2mE}$. Then

$$F_x = -\frac{\partial V}{\partial x} \tag{5}$$

The force is clearly in the xz plane. Since

$$(\boldsymbol{r} - \boldsymbol{r}_b)^2 = (x-b)^2 + (v_0 t)^2 + y^2\,, \tag{6}$$

we find

$$F_x = U_0 e^{-\kappa(x-b)^2 - \kappa(z - v_0 t)^2} 2\kappa(x-b)\,, \tag{7}$$

Since the displacement is small $x, z \ll b$ we find

$$F_x = -\,U_0 e^{-\kappa b^2 - \kappa(v_0 t)^2} 2\kappa b. \tag{8}$$

So the final result for the force is

$$F_x(t) = -\,f e^{-\kappa(v_0 t)^2} \tag{9}$$

where $f = (2U_0\kappa b)\, e^{-\kappa b^2}$.

(b) The displacement is the convolution of the retarded Green function of the harmonic oscillator

$$G_R(t,t') = \theta(t,t')\frac{\sin(\omega_0(t-t'))}{m\omega_0}\,, \tag{10}$$

and the force $F_x(t')$

$$x(t) = \int_{-\infty}^{\infty} G_R(t,t')\, F_x(t')\, dt'\,. \tag{11}$$

Computing the displacement of the oscillator we have

$$x(t) = -\int_{-\infty}^{t} \frac{f}{m\omega_0} \sin(\omega_0(t-t')) e^{-\kappa(v_0 t')^2}\,. \tag{12}$$

The velocity is given by differentiation and is displayed in Eq. 15

(c) The energy of the oscillator is best computed using by evaluating

$$a_x(t) = v_x(t) + i\omega_0\, x(t) \tag{13}$$

The energy in the oscillator is

$$\epsilon(b) = \frac{1}{2} m |a_x|^2 \tag{14}$$

At intermediate times

$$v_x(t) = -\int_{-\infty}^{t} \frac{f}{m}\cos(\omega_0(t-t'))e^{-\kappa(v_0 t')^2} \tag{15}$$

$$i\omega_0 x(t) = -\int_{-\infty}^{t} \frac{f}{m} i\sin(\omega_0(t-t'))e^{-\kappa(v_0 t')^2} \tag{16}$$

So

$$a_x = -\frac{f}{m}\int_{-\infty}^{t} e^{i\omega(t-t')}e^{-\kappa(v_0 t')^2} \tag{17}$$

At large times we define $\Omega^2 = \kappa v_0^2$

$$a_x(t\to\infty) = e^{i\omega t}\int_{-\infty}^{\infty} dt' \frac{f}{m} e^{-i\omega_0 t'} e^{-\kappa(v_0 t')^2} \tag{18}$$

$$= \sqrt{\pi} e^{i\omega t}\, \frac{f}{m\Omega} e^{-\omega_0^2/4\Omega^2} \tag{19}$$

The point to remember is that the amplitude of the oscillator after being acted upon by a force $F(t)$ is the Fourier transform of the force.

Evaluating the energy we find

$$\epsilon(b) = \frac{\pi f^2}{2m\Omega^2} e^{-\omega_0^2/2\Omega^2} \tag{20}$$

Restoring what is $f = (2U_0\kappa)be^{-\kappa b^2}$ we find

$$\epsilon(b) = \frac{2\pi U_0^2}{m v_0^2}\left[\kappa b^2 e^{-\kappa b^2 - \omega_0^2/2\Omega^2}\right]\,. \tag{21}$$

(d) From geometry the number of collisions between b and and $b+db$ per length $d\mathcal{N}$, is

$$d\mathcal{N} = n(2\pi b)db\,. \tag{22}$$

were $n = N/V$ is the number of targets per volume. The energy absorbed per length by collisions between b and $b+db$ is

$$d\mathcal{E} = n(2\pi b)\epsilon(b)db \tag{23}$$

Substituting $\epsilon(b)$ and integrating over b we find the total energy lost per length

$$\mathcal{E} = \int_0^\infty n(2\pi b)\frac{2\pi U_0^2}{m v_0^2}\left[\kappa b^2 e^{-\kappa b^2 - \omega_0^2/2\Omega^2}\right] db\,. \tag{24}$$

The last integral is elementary. Switching to the dimensionless variable $u \equiv \kappa b^2$, and $du = 2\kappa b db$, we find

$$\mathcal{E} = (2\pi)^2 \frac{U_0^2}{m v_0^2}\left(\frac{n}{2\kappa}\right) e^{-\omega_0^2/2\Omega^2}\int_0^\infty u e^{-u} du\,. \tag{25}$$

The last integral is $\Gamma(2) = 1!$, and so

$$\mathcal{E} = (2\pi)^2 \frac{U_0^2}{m v_0^2}\left(\frac{n}{2\kappa}\right) e^{-\omega_0^2/2\Omega^2}\,. \tag{26}$$

Classical Mechanics 3

Phase shifts and time delays from classical mechanics

(**A**) (5 points) Consider a free particle of mass m in one spatial dimension, and a straight-line path in spacetime connecting (t_0, x_0) to (t, x).

(i) Evaluate the action, $S[x(t')] = \int_{t_0}^{t} dt' \, \frac{1}{2} m\dot{x}^2$, for this path. The result is called $S_{\text{free}}(t, x, t_0, x_0)$ below.

(ii) Compute $-\partial S_{\text{free}}(t, x, t_0, x_0)/\partial t$ and $\partial S_{\text{free}}(t, x, t_0, x_0)/\partial x$ and interpret them physically.

(iii) Determine $S_{\text{free}}(t, x, t_0, x_0)$ for $t_0 \to -\infty$ with $v_0 \equiv x_0/t_0$ held fixed. You should find that the limiting action takes the form

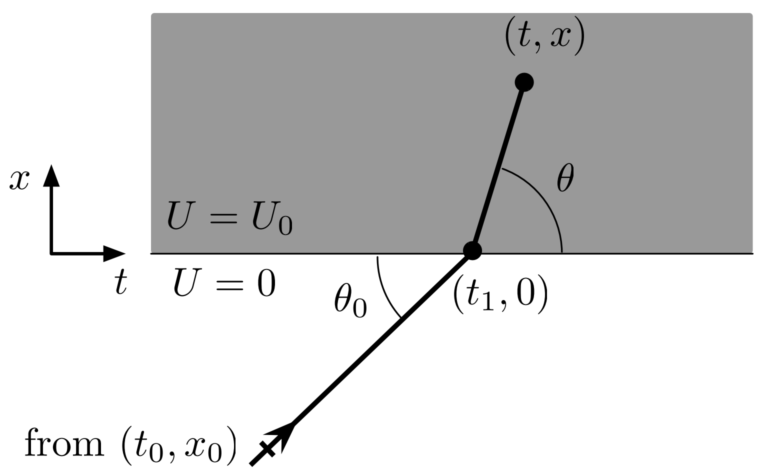
$$S_{\text{free}}(t, x, t_0, x_0) \to S_{\text{free}}(t, x, E_0, t_0) = \Delta S_{\text{free}}(t, x, E_0) - E_0 t_0 \, ,$$

where $E_0 \equiv = \frac{1}{2} m v_0^2$. Sketch lines of constant $\Delta S_{\text{free}}(t, x, E_0)$ in the (t, x) plane for a given $v_0 > 0$.

(**B**) (9 points) Now consider the same particle in a step potential

$$U(x) = \begin{cases} U_0 & x > 0, \\ 0 & x < 0. \end{cases}$$

Consider the spacetime path, shown below, that connects (t_0, x_0) to (t, x) via an arbitrary intermediate point $(t_1, 0)$ on the interface. Take t_0 to negative infinity as in part (A), and assume that $E_0 > U_0$ in what follows.



(i) Evaluate the action for the illustrated path to find $S(t, x, E_0, t_0; t_1)$. Extremize this action to find the relation between the velocities before and after the step, v_0 and v, and the relation between the angles, θ_0 and θ (see figure).

(ii) For the classical trajectory, evaluate the action $S(t, x, E_0, t_0)$ for x both above and below the interface.

(iii) For the classical trajectory, compute and interpret the differences:

$$\left.\frac{\partial S}{\partial t}\right|_{x=0^+} - \left.\frac{\partial S}{\partial t}\right|_{x=0^-}, \qquad \text{and} \qquad \left.\frac{\partial S}{\partial x}\right|_{x=0^+} - \left.\frac{\partial S}{\partial x}\right|_{x=0^-},$$

where $x{=}0^+$ and $x{=}0^-$ are infinitesimally above and below the interface respectively.

(**C**) (6 points) Now replace the step function of part (B) by the localized potential barrier $U(x)$:

$$U(x) = \begin{cases} 0 & x < 0\,, \\ U_0 & 0 < x < a\,, \\ 0 & x > a\,. \end{cases}$$

Assume that $E_0 > U_0$ in what follows

(i) For the classical path and $x > a$, determine the extremized action $S(t, x, E_0, t_0)$ as defined in the previous parts. Compute the difference in action relative to the free case:

$$\delta \equiv S(t, x, E_0, t_0) - S_{\text{free}}(t, x, E_0, t_0)\,.$$

(ii) Compute $\partial\delta/\partial E_0$ and interpret the result.

Solution

Throughout this problem it is useful to recognize that the action S is the phase of the quantum mechanical wave function $\psi \sim Ae^{iS/\hbar}$.

A. The free particle:

(i) The action is

$$S(t, x, t_0, x_0) = \frac{1}{2}mv^2(t - t_0) = \frac{1}{2}m\frac{(x - x_0)^2}{(t - t_0)} \,. \tag{1}$$

Lines of constant S and the associated straight-line trajectories are shown in Fig. **??**(a).

(ii) We have

$$\partial S/\partial x = m\frac{(x - x_0)}{t - t_0} \,, \tag{2}$$

and

$$\partial S/\partial t = -\frac{1}{2}m\frac{(x - x_0)^2}{(t - t_0)^2} \,. \tag{3}$$

These are clearly interpreted as the momentum and (minus) the energy of the particle. The momentum depends on the position and time

(iii) Expanding for large t_0 and $x_0 = v_0 t_0$ to first order in (t, x) we have

$$S(t, x, t_0, x_0) \simeq mv_0 x - \frac{1}{2}mv_0^2 t + \frac{1}{2}mv_0^2 t_0 \,. \tag{4}$$

So

$$S(t, x, t_0, x_0) \to S(t, x, E_0, t_0) = (p_0 x - E_0 t) + E_0 t_0 \tag{5}$$

or

$$\Delta S(t, x, E_0) = p_0 x - E_0 t \tag{6}$$

where $E_0 = \frac{1}{2}mv_0^2$ and $p_0 = \sqrt{2mE_0}$. The constant $E_0 t_0$ will be retained but is unimportant in practice. Lines of constant $p_0 x - E_0 t$ are plane waves.

B. The step potential:

(i) The action takes the form

$$S(t, x, E_0, t_1) = S_{\text{free}}(t_1, x, E_0, t_0)|_{x=0} + \int_{t_1}^{t} dt' \left[\frac{1}{2}m(\dot{x}(t'))^2 - U_0\right] \,. \tag{7}$$

The first term represents the action from negative infinity to t_1 and is evaluated on the interface $x = 0$. The second term represents the propagation for $t > t_1$ and is a straight line path (the second leg). Evaluating the integral for the straight line path we find the result

$$S(t, x, E_0, t_0; t_1) = -E_0 t_1 + \frac{1}{2}m\frac{x^2}{t - t_1} - U_0(t - t_1) + E_0 t_0 \,. \tag{8}$$

Differentiating with respect to t_1 and setting the result to zero to extremize the action we have

$$\frac{\partial S}{\partial t_1} = -E_0 + \frac{1}{2} m \frac{x^2}{(t-t_1)^2} + U_0 = 0\,. \tag{9}$$

The extremization condition fixes the slope or velocity for $x > 0$

$$v = \tan\theta = \frac{x}{(t-t_1)} = \sqrt{\frac{2}{m}(E_0 - U_0)}\,. \tag{10}$$

For $x < 0$ the slope is

$$v_0 = \tan\theta_0 = \frac{x_0}{t_0} = \sqrt{\frac{2}{m} E_0}\,, \tag{11}$$

and so the relationship between the angles is

$$\tan\theta = \sqrt{\tan^2\theta_0 - (2U_0/m)}\,. \tag{12}$$

(ii) First we will find the action for $x > 0$. From the extremization condition in Eq. 9 we have

$$v \equiv x/(t-t_1) \qquad \frac{1}{2} m v^2 = (E_0 - U_0). \tag{13}$$

Thus the value of the action at the extremal point is

$$S(t, x, E_0, t_0) = \underset{t_1}{\text{extrm}} \left\{ S(t, x, E_0, t_0; t_1) \right\}\,, \tag{14}$$

$$= -\,E_0 t_1 + \frac{1}{2} m \frac{x^2}{(t-t_1)^2}(t-t_1) + E_0 t_0 \tag{15}$$

Then, using the identities in Eq. 13 we find after minor rearrangements

$$S(t, x, E_0, t_0) = px - E_0 t + E_0 t_0 \tag{16}$$

where $p = mv = \sqrt{2m(E_0 - U_0)}$. For $x < 0$ the action is the free one. Thus the extremized action (minus the constant $E_0 t_0$) is

$$\Delta S(t, x, E_0) = \begin{cases} p_0 x - E_0 t & x < 0\,, \\ px - E_0 t & x > 0 \end{cases} \tag{17}$$

Lines of constant S are shown in Fig. 1(a) and (b). The classical trajectories comes from differences in S shown in Fig. 1(c), and can found by setting $\partial S(t, x, E_0)/\partial E_0) = \text{const.}$

(iii) The time derivatives is clearly continuous across the interface

$$\left.\frac{\partial S}{\partial t}\right|_{x=0^+} - \left.\frac{\partial S}{\partial t}\right|_{x=0^-} = -E_0 + E_0 = 0 \tag{18}$$

reflecting energy conservation. The spatial derivative is discontinuous

$$\left.\frac{\partial S}{\partial x}\right|_{x=0^+} - \left.\frac{\partial S}{\partial x}\right|_{x=0^-} = p - p_0 \tag{19}$$

Which records the jump in momentum (impulse) that is expected as the particle crosses $x = 0$.

The lines of constant action are shown in Fig. 1(a) and (b) for $E = 1$ and $E = 1.1$. The classical trajectores are when $\partial S/\partial E_0$ is constant as shown in Fig. 1(c). This is explored graphically in the figure.

C. The barrier potential

(i) To evaluate the action for the classical path with energy E_0 we switch to the Hamiltonian formalism. The action associated with a path γ (or $x'(t')$) is

$$S_\gamma = \int_\gamma p dx' - H dt' \tag{20}$$

The energy of the path is $H(x, p) = E_0$ is constant. If particle arrives at the barrier $x = 0$ at time t_1, the subsequent change in action, ΔS_γ, is found by integrating from $(t_1, 0)$ up to (t, x) is

$$\Delta S_\gamma = - E_0(t - t_1) + \int_0^a p dx' + \int_a^x p_0 dx' \tag{21}$$

$$= - E_0(t - t_1) + pa + p_0(x - a) \tag{22}$$

where $p = \sqrt{2m(E_0 - U_0)}$ and $p_0 = \sqrt{2mE_0}$. In the last step we have separated the integral into a regions with $0 < x' < a$ and $a < x' < x$. So, adding the free contribution (from $t' = t_0$ to t_1), the extremized action from negative infinity to the point (t, x) is

$$S(t, x, E_0) = S_{\rm free}(t_1, x, E_0)|_{x=0} + \Delta S_\gamma \, . \tag{23}$$

Using $S_{\rm free}(t_1, x, E_0)|_{x=0} = -E_0(t_1 - t_0)$ we find

$$S(t, x, E_0, t_0) = -E_0(t - t_0) + p_0(x - a) + pa \, . \tag{24}$$

The action difference relative to the free case is simply

$$\delta = -p_0 a + pa \, . \tag{25}$$

(ii) Differentiating δ with respect to E_0, and using that the velocity is quite generally $v = \partial E/\partial p$:

$$\frac{\partial p_0}{\partial E_0} = \frac{1}{v_0} = \sqrt{\frac{m}{2E_0}} \, , \tag{26}$$

$$\frac{\partial p'}{\partial E_0} = \frac{1}{v} = \sqrt{\frac{m}{2(E_0 - U_0)}} \, , \tag{27}$$

we see that

$$\frac{d\delta}{dE_0} = \frac{a}{v} - \frac{a}{v_0} \, . \tag{28}$$

This is the amount of time that the particle was delayed relative to the free propagation by crossing the potential barrier.

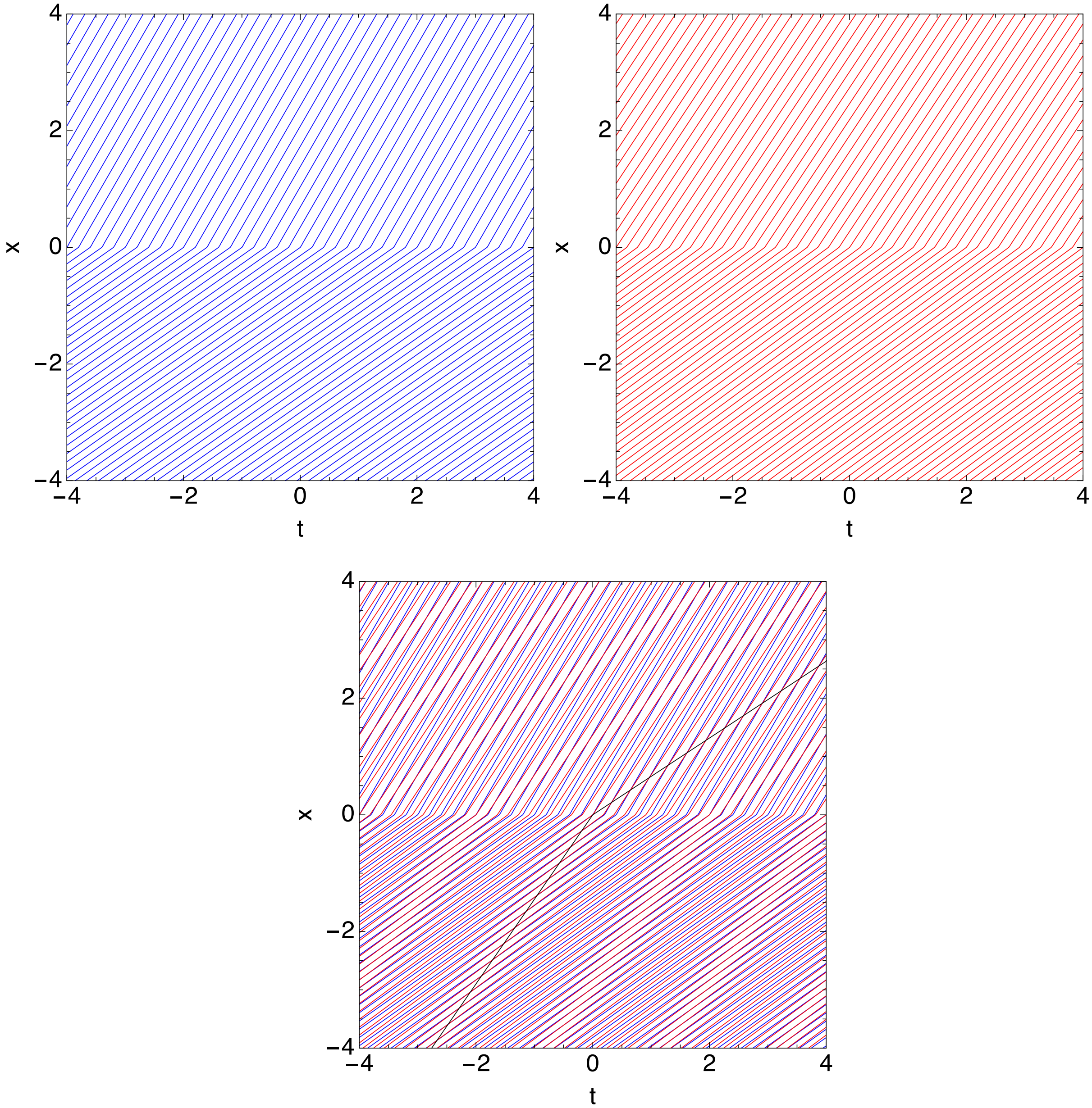


Figure 1: The classical trajectory are places where the phase *difference* is constant. The first figure (a) shows contour lines of constant $S(t,x,E_0)$ for $m=1$, $E_0=1$ and $U_0=5/6$. The second figure shows lines of constant S for $E_0=1.1$ (i.e. almost 1). The third figure overlays the first two figures and illustrates a visual interference pattern. The patterns which emerges from the interference are the lines of constant difference $S(E_0)-S(E+\Delta E_0)\simeq \Delta E_0 \partial S/\partial E_0 = C$ are constant. This condition determine the classical trajectories. The thin black line shows one such classical trajectory, where $\partial S/\partial E_0 = 0$.

Electromagnetism 1

Capacitor with a hemisphere

Consider a large parallel plate capacitor with a hemispherical bulge of radius a on one of plates as shown in Fig. A. The plate with the hemisphere is grounded and the other is at a constant potential V_0. The plates are separated by a distance b with $b \gg a$ (Fig. A is not to scale).

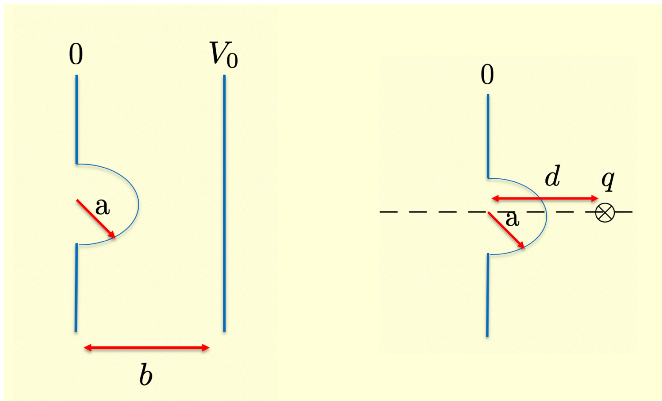


Fig.A Fig.B

(a) (6 points) Find the potential everywhere inside the capacitor.

(b) (4 points) Calculate the surface charge density on the flat portion of the grounded plate. Sketch the result.

(c) (4 points) What is the total charge on the hemisphere?

(d) (6 points) Consider now Fig. B, where the second plate is removed and replaced by a charge q located at distance d (see figure). Find the force on the charge q. Is it attractive or repulsive?

Solution

a. Let (r, θ) be the polar coordinate of an arbitrary point within the capacitor, with θ measured with respect to the perpendicular to the plate. Using the image method, the potential within the capacitor shown in Fig. A reads

$$V(r, \theta) = -E_0 \left(r - \frac{a^3}{r^2} \right) \cos\theta \tag{1}$$

with $E_0 = V_0/b$.

b. The surface density on the grounded plate is

$$\sigma_P(r) = -\frac{1}{4\pi r} \left(\frac{\partial V}{\partial \theta} \right)_{r=a} = \frac{E_0}{4\pi} \left(1 - \frac{a^3}{r^3} \right) \tag{2}$$

Thus the density approaches zero as $r \to a$.

c. The surface charge density on the hemisphere is

$$\sigma_H(\theta) = -\frac{1}{4\pi} \left(\frac{\partial V}{\partial r} \right)_{r=a} = \frac{3E_0}{4\pi} \cos\theta \tag{3}$$

The total charge on the hemisphere is

$$Q_H = \int_0^{\pi/2} 2\pi a^2 \sin\theta \, d\theta \, \sigma_H(\theta) = \frac{3}{4} E_0 a^2 \tag{4}$$

d. Using the image methods (plane + sphere) we place three image charges on the x axis, to compensate the charge q at $x = d$. Two image charge are of strength $\mp aq/d$ and placed at positions $x = \pm a^2/d$, and one of strength $-q$ is placed at position $x = -d$. The force on the charge q is attractive

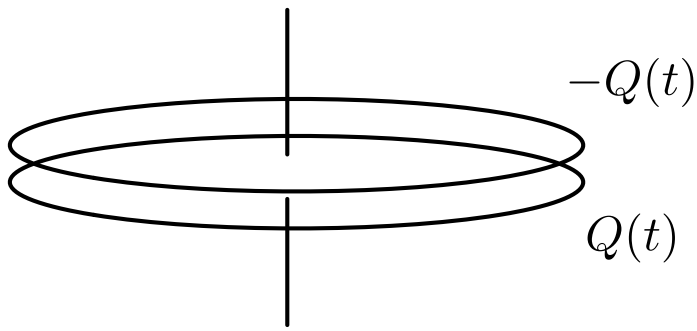
$$F = -\frac{aq^2/d}{(d - a^2/d)^2} + \frac{aq^2/d}{(d + a^2/d)^2} - \frac{q^2}{(2d)^2} \tag{5}$$

The negative sign indicates an attractive force.

Electromagnetism 2

A circular capacitor

A circular capacitor of radius R and separation a, with $a \ll R$, is charged with a *slowly varying* sinusoidal current, *i.e.* the charge on the plates is $Q(t) = Q_o \sin(\omega t)$ as illustrated below. Neglect any fringing of the fields.



(a) (4 points) Determine the electric and magnetic fields in between the plates. Draw a picture to indicate the directions of the fields while the charge on the bottom plate is negative and increasing, i.e. becoming less negative.

(b) (3 points) Using the fields from part (a), compute the energy stored in the capacitor in the electric fields, U_E, and the magnetic fields, U_B. The total is $U = U_E + U_B$.

(c) (8 points)

(i) Using the fields from part (a), determine the energy flowing into the capacitor as a function of time, by computing Poynting vector and evaluating Poynting flux.

(ii) The Poynting flux in (i) does not equal the change in energy per time dU/dt for the energy computed in (b). Explain why clearly and precisely.

Hint: What is the relative size of U_B/U_E and what approximations were made in part (a)?

(d) (5 points) (i) Determine the gauge potentials $(\phi, \mathbf{A})$ in the Coulomb gauge for the fields of part (a). (ii) Write down the *exact* Maxwell equations in the capacitor for $(\phi, \mathbf{A})$ in the Coulomb gauge. Show that the $(\phi, \mathbf{A})$ of (i) satisfy these equations to the required accuracy.

Possibly useful formulae:

The curl of vector a field $\mathbf{V}$ in cylindrical coordinates ($\rho = \sqrt{x^2 + y^2}$ and $\phi = \tan^{-1}(y/x)$) is

$$\nabla \times \mathbf{V} = \left(\frac{1}{\rho} \frac{\partial V_z}{\partial \phi} - \frac{\partial V_\phi}{\partial z} \right) \hat{\boldsymbol{\rho}} + \left(\frac{\partial V_\rho}{\partial z} - \frac{\partial V_z}{\partial \rho} \right) \hat{\boldsymbol{\phi}} + \frac{1}{\rho} \left(\frac{\partial (\rho V_\phi)}{\partial \rho} - \frac{\partial V_\rho}{\partial \phi} \right) \hat{\boldsymbol{z}}\,.$$

The Laplacian of a scalar field u is

$$\Delta^2 u = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial u}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 u}{\partial \phi^2} + \frac{\partial^2 u}{\partial z^2}\,.$$

Solution

(a) The electric field is

$$E^z = \frac{Q(t)}{A}\hat{\mathbf{z}} = \sigma_0 \sin(\omega t)\,\hat{\mathbf{z}}, , \tag{1}$$

with $\sigma_0 = Q_0/A$ and $A = \pi R^2$. The magnetic field is determined from Amperes law with the displacement current

$$\boldsymbol{j}_D = \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t} . \tag{2}$$

So we find

$$B^\phi(2\pi\rho) = \frac{1}{c}\pi\rho^2 \partial_t E^z , \tag{3}$$

or finally

$$B^\phi = \frac{\rho\omega}{2c}\sigma_0 \cos(\omega t) . \tag{4}$$

(b) The electric energy is

$$U_E = \frac{1}{2}\int_V E^2 = \tfrac{1}{2} A a \sigma_0^2 \sin^2(\omega t) . \tag{5}$$

The magnetic energy is

$$U_B = \frac{1}{2} a \int 2\pi\rho d\rho (B^\phi)^2 = \frac{1}{16} A a \sigma_0^2 \left(\frac{\omega R}{c}\right)^2 \cos^2(\omega t) . \tag{6}$$

(c) The Poynting vector is

$$\boldsymbol{S} = c\,\boldsymbol{E}\times\boldsymbol{B} \tag{7}$$

$$= -\frac{1}{2}\left[\omega\rho\sigma_0^2 \cos(\omega t)\sin(\omega t)\right]\hat{\boldsymbol{\rho}} \tag{8}$$

To find the energy flowing into the capacitor we evaluate the Poynting flux on the area of rim, where the normal $d\boldsymbol{a} = -\hat{\rho}$ to points into the capacitor

$$\frac{dU}{dt} = \int_A \boldsymbol{S}\cdot d\boldsymbol{a} = A a \sigma_0^2 \cos(\omega t)\sin(\omega t). \tag{9}$$

We see that this gives only the change in the change in the electric contribution per time $\dot{U}_E$.

The “issue" is that we are computing the fields in an approximation scheme where the frequency is small, $\omega R/c \ll 1$

$$E = E^{(0)} + E^{(2)} + \ldots \tag{10}$$

and worked in a zeroth order approximation, i.e. the electric field in (a) is $E^{(0)}$. Note that the magnetic field energy is smaller by a factor of $(\omega R/c)^2$, i.e.

$$U_B \sim \left(\frac{\omega R}{c}\right)^2 U_E \tag{11}$$

In order capture the change in U_B per time we would need to compute $\boldsymbol{E}$ and $\boldsymbol{S}$ to quadratic order. $E^{(2)}$ comes from the time-dependent B field and is of order

$$E^{(2)} \sim \frac{R}{c}\partial_t B \tag{12}$$

(d) The two Maxwell equations with the charges and currents are

$$\nabla \cdot \boldsymbol{E} = \rho \tag{13}$$

$$\nabla \times \boldsymbol{B} = \frac{\boldsymbol{j}}{c} + \frac{1}{c}\partial_t \boldsymbol{E} \tag{14}$$

The remaining two Maxwell equations (the Bianchi identities) guarantee that $\boldsymbol{E}$ and $\boldsymbol{B}$ can be expressed in terms of $(\phi, \boldsymbol{A})$

$$\boldsymbol{E} = -\frac{1}{c}\partial_t \boldsymbol{A} - \nabla\phi \tag{15}$$

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \tag{16}$$

The charges and currents are zero inside the capacitor. Using the identity and the Coulomb gauge condition $\nabla \cdot \boldsymbol{A} = 0$

$$\nabla \times \nabla \times \boldsymbol{A} = \nabla(\nabla \cdot \boldsymbol{A}) - \nabla^2 \boldsymbol{A} = -\nabla^2 \boldsymbol{A} \tag{17}$$

We have for the Maxwell equations to be solved

$$-\nabla^2 \phi = 0 \tag{18}$$

$$\frac{1}{c^2}\partial_t^2 \boldsymbol{A} - \nabla^2 \boldsymbol{A} = -\frac{1}{c}\partial_t(\nabla \cdot \phi) \tag{19}$$

Solving Laplace equation for the scalar potential gives

$$\phi = -E^z(t) z \tag{20}$$

For $\boldsymbol{A}$ we have only a z component. We may drop $\partial_t^2 A^z$ in a quasi-static approximation as discussed in part (c)

$$\underbrace{\frac{1}{c^2}\partial_t^2 A^z}_{\text{discard}} - \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\frac{\partial A^z}{\partial\rho}\right) = -\frac{1}{c}\partial_t \partial^z \phi \tag{21}$$

$$-\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial A^z}{\partial\rho}\right) = \frac{\omega}{c}\sigma_0 \cos(\omega t) \tag{22}$$

Integrating this equation we find

$$A^z = -\frac{\sigma_0 \omega}{4c}\cos(\omega t)\rho^2 + C_1 \log\rho + C_2 \tag{23}$$

Demanding regularity at the origin we set $C_1 = 0$, and C_2 is of no physical relevance, yielding finally

$$A^z = -\frac{\sigma_0 \omega}{4c}\cos(\omega t)\rho^2 \,. \tag{24}$$

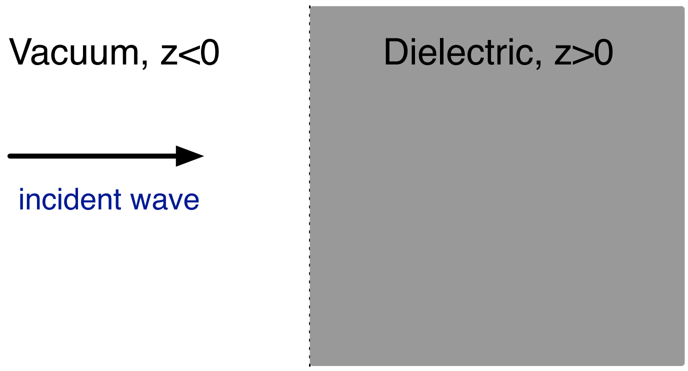
A straight forward sanity check gives $\mathbf{B} = \nabla \times \boldsymbol{A}$

$$B^\phi = -\frac{\partial}{\partial\rho}A^z = \sigma_0 \frac{\rho\omega}{2c}\cos\omega t \tag{25}$$

Electromagnetism 3

Reflection from an imperfect dielectric

A linearly polarized plane wave in vacuum $\boldsymbol{E}_I(t,z) = \mathrm{Re}[Ae^{-i\omega t + ik_0 z}]\,\hat{\boldsymbol{x}}$ is normally incident upon a semi-infinite slab of dielectric with real permittivity $\epsilon \equiv 1 + \chi$. The dielectric is imperfect, and conducts current with a small conductivity σ. The dielectric fills the region $z > 0$ shown below. Take $\mu = 1$ everywhere[1].



(a) (5 points) Show that dielectric supports plane wave solutions of the form $e^{ik(\omega)z - i\omega t}$ with $\boldsymbol{E}$ and $\boldsymbol{B}$ transverse. Determine the dispersion relation $k(\omega)$ and the relation between $\boldsymbol{E}$ and $\boldsymbol{B}$. You should find that $k(\omega)$ is complex valued.

(b) (8 points) Determine the electric and magnetic fields, $\boldsymbol{E}(t,z)$ and $\boldsymbol{B}(t,z)$, both for $z < 0$ and $z > 0$.

(c) (3 points) What is the ratio of the reflected and incident power per unit area? Show that the result is independent of σ to first order in σ when σ is small.

Note: for X small (with X any real number), $|1 + iX|^2 \simeq 1$ up to corrections of order X^2.

(d) (4 points) Assume that σ is small but non-zero. Compute the time averaged energy density in the dielectric at a distance z from the interface. Over what distance does the energy density decrease to 50% of its initial value?

[1] In SI units take $\mu = \mu_0$ everywhere.

Solution

(a) We take solutions of the plane wave form

$$\boldsymbol{E}(t,z) = Ae^{ik(\omega)z - i\omega t}\,\hat{\boldsymbol{x}}\,, \tag{1}$$

with an analogous equations for $\boldsymbol{B}$ and $\boldsymbol{J}$. These vectors are transverse to $\hat{\boldsymbol{z}}$. Ampere's Law reads

$$\nabla \times \boldsymbol{B} = (4\pi/c)\boldsymbol{J} + \frac{1}{c}\partial_t \boldsymbol{E}\,,$$

and the constitutive relation is

$$\boldsymbol{J} = \sigma \boldsymbol{E} + \chi \partial_t \boldsymbol{E} \tag{2}$$

$$= \sigma \boldsymbol{E} - i\omega\chi \boldsymbol{E} \tag{3}$$

We find

$$i\boldsymbol{k} \times \boldsymbol{B} = \frac{4\pi}{c}\boldsymbol{J} - \frac{i\omega \boldsymbol{E}}{c}\,, \tag{4}$$

$$= -\frac{i\omega}{c}\left(+i\frac{4\pi\sigma}{\omega} + \epsilon\right)\boldsymbol{E}\,, \tag{5}$$

$$\equiv -\frac{i\omega}{c}\varepsilon(\omega)\boldsymbol{E}\,. \tag{6}$$

In passing to the second equation, we used the constitutive relation and defined $\epsilon = 1 + \chi$.

From Eq. (4), the effective dielectric constant is given by is $\varepsilon(\omega) = \epsilon + i4\pi\sigma/\omega$, leading us to take

$$k^2(\omega) = \frac{\omega^2}{c^2}\varepsilon(\omega)\,. \tag{7}$$

This reasoning is corroborated by crossing Eq. (4) with $i\boldsymbol{k}$, using the Faraday relation $i\boldsymbol{k} \times \boldsymbol{E} = i\omega/c\boldsymbol{B}$ and the transversity of $\boldsymbol{B}$

$$i\boldsymbol{k} \times i\boldsymbol{k} \times \boldsymbol{B} = -\boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{B}) + k^2\boldsymbol{B} = k^2\boldsymbol{B}\,, \tag{8}$$

to find

$$\left[k^2(\omega) - \frac{\omega^2}{c^2}\varepsilon(\omega)\right]\boldsymbol{B} = 0\,. \tag{9}$$

In vacuum $k_0 = \omega/c$ and thus the dispersion curve is finally

$$k^2 = k_0^2\varepsilon(\omega)\,. \tag{10}$$

(b) The electric field of the incoming wave, reflected wave and transmitted wave are given by

$$\boldsymbol{E}_I = Ae^{ik_0z - i\omega t}\hat{\boldsymbol{x}}, \qquad \boldsymbol{E}_R = A_Re^{-ik_0z - i\omega t}\hat{\boldsymbol{x}}, \qquad \boldsymbol{E}_T = A_Te^{ik_Tz - i\omega t}\hat{\boldsymbol{x}}. \tag{11}$$

The corresponding magnetic fields are $\boldsymbol{B} = \boldsymbol{k} \times \boldsymbol{E}$. At the interface the transverse components $\boldsymbol{E}_T$ and $\boldsymbol{B}_T = \boldsymbol{k} \times \boldsymbol{E}$ are continuous. This gives the matching conditions

$$A + A_R = A_T, \qquad A - A_R = \sqrt{\varepsilon(\omega)}A_T. \tag{12}$$

We used that $k_T = \sqrt{\varepsilon(\omega)}k_0$. They are solved by

$$A_T = \frac{2A}{1+\sqrt{\varepsilon(\omega)}}, \qquad A_R = \frac{1-\sqrt{\varepsilon(\omega)}}{1+\sqrt{\varepsilon(\omega}}A. \tag{13}$$

This gives the electric and magnetic fields everywhere.

(c) The power flow per unit area is given by $c/(8\pi)\mathrm{Re}\boldsymbol{E}_\omega \times \boldsymbol{B}^*_\omega$. Since everything is perpendicular, we obtain for the energy flow of the reflected wave in units of the incoming wave

$$\mathcal{R} = \left|\frac{1-\sqrt{\varepsilon(\omega)}}{1+\sqrt{\varepsilon(\omega)}}\right|^2. \tag{14}$$

For small σ we have

$$\sqrt{\varepsilon(\omega)} = \sqrt{\epsilon}\left(1 + i\,\frac{4\pi\sigma/\epsilon}{2\omega}\right) \equiv n + in_\sigma \tag{15}$$

where we have defined n and n_σ as the real and imaginary parts of the index of refraction. We expand $\mathcal{R}$ for small n_σ and find

$$\frac{A_R}{A} = \left(\frac{1-n}{1+n}\right)\cdot\frac{1-in_\sigma/(1-n)}{1+in_\sigma/(1+n)}. \tag{16}$$

Since for small X (with X anything)

$$|1+iX|^2 \simeq 1 + O(X^2)\,, \tag{17}$$

we see that the reflection coefficient is independent of σ to first order and reads

$$\mathcal{R} = \left|\frac{A_R}{A}\right|^2 = \left(\frac{1-n}{1+n}\right)^2 \tag{18}$$

(d) The energy density stored in the wave

$$u(z) = \frac{1}{8\pi}\mathrm{Re}(\varepsilon(\omega))|E(z)|^2 = \frac{\epsilon}{8\pi}|A_T e^{ik_T z}|^2\,. \tag{19}$$

The transmitted wave number is complex

$$k_T = \sqrt{\varepsilon(\omega)}k_0 = k_0(n + in_\sigma)\,. \tag{20}$$

As in the previous part, the square of the transmission amplitude is independent of the σ to first order

$$|A_T|^2 = |A|^2\frac{4n^2}{(1+n)^2}\,, \tag{21}$$

and the energy density is

$$u(z) = \frac{|A|^2}{8\pi}\,\frac{4n^2}{(1+n)^2}e^{-2n_\sigma k_0 z}\,. \tag{22}$$

Unpacking the definitions of k_0 and n_σ, we find finally

$$u(z) = \frac{|A|^2}{8\pi} \frac{4n^2}{(1+n)^2} e^{-n(4\pi\sigma/\epsilon)/cz} \,. \tag{23}$$

From the form of this equation the decay length, L, is given by

$$\frac{1}{2} = e^{-n(4\pi\sigma/\epsilon)/cL} \,. \tag{24}$$

Thus

$$L = 0.7 \frac{c/n}{4\pi\sigma/\epsilon} \,, \tag{25}$$

and is independent of frequency in this limit.

Quantum Mechanics 1

Two particles and a potential

Consider two particles, both of mass m in a plane, but with one allowed to move only on the full x axis (from $-\infty$ to $+\infty$), and the other constrained to the full y axis, (from $-\infty$ to $+\infty$). With x labeling the position of the first particle, and y the position of the second, the potential energy of the system is taken as

$$V(x,y) \;=\; \frac{k}{2}\,(x+y)^2\;. \tag{1}$$

(Please note, this is not $x^2 + y^2$.) Also note that $V = 0$ at the origin, which is available to both particles. Assume first that the particles are distinguishable, and can pass each other without a collision.

(a) *(2 pts)* Write down the Hamiltonian, and the Schrödinger equation for stationary states of this system.

(b) *(6 pts)* Find the eigenfunctions $\psi_n(x,y)$ and corresponding energy eigenvalues E_n in terms of those for one-dimensional harmonic oscillator and plane-wave systems. Normalize the plane-wave assuming that the particles are confined to an interval of length L, with periodic boundary conditions at the ends.

(c) *(4 pts)* Suppose the system is in one of its eigenfunctions, $\psi_n(x,y)$, corresponding to a state of energy E_n. Give an expression for the probability density for finding a particle at point x, regardless of where the other particle is, $-\infty < y < \infty$, and if possible evaluate it.

(d) *(4 pts)* From now on, assume that the two particles are indistinguishable and have spin $1/2$ each. Construct the wavefunctions of the stationary states with definite spin symmetry in this case, using the wavefunctions from part (b).

(e) *(4 pts)* As the final step, assume now that in addition to the potential used above, there is a contact potential $U(x,y) = \lambda\delta(x-y)$. Describe as quantitatively as you can how the wavefunctions in part (d) are modified by this potential.

Solution

a) The stationary Schrödinger equation has the usual form:

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \; + \; \frac{k}{2} (x+y)^2 \right] \psi_n(x,y) \; = \; E_n \psi_n(x,y) \,. \tag{2}$$

b) The point for the solution is to change variables to

$$\begin{aligned} u &= \frac{1}{\sqrt{2}} (x+y) \\ v &= \frac{1}{\sqrt{2}} (x-y) \end{aligned} \tag{3}$$

and to use the fact that in these variables the Schrödinger equation separates in two, leading to a harmonic oscillator equation for u and a free particle equation for v. The solutions are then

$$\psi_{I,q}(u,v) \; \propto \; \phi_I(u) \, e^{\pm iqv} \,, \tag{4}$$

where ϕ_I are the wave functions of the harmonic oscillator stationary states. The total energies are

$$E_{I,q} \; = \; \left(I + \frac{1}{2} \right) \hbar\omega \; + \; \frac{(\hbar q)^2}{2m} \,, \tag{5}$$

where $\omega = \sqrt{\frac{k}{m}}$ and q is a wave number. Imposing the periodic boundary condition on the plane wave, we can write $\psi_{I,q}(u,v)$ as

$$\psi_{I,q}(u,v) \; = \; \phi_I(u) \frac{1}{\sqrt{L}} \, e^{\pm iqv} \,, \quad q = \frac{2\pi}{L} N \,, \tag{6}$$

with integer N.

c) The probability density for x is given by the probability density in x and y, i.e., $|\psi_{I,q}|^2$, integrated over y:

$$\begin{aligned} p(x) &= \int_{-\infty}^{\infty} dy \; |\psi_{I,q}(u,v)|^2 \\ &= \frac{1}{L} \int_{-\infty}^{\infty} dy \; |\phi_I(x+y)|^2 \\ &= \frac{1}{L} \int_{-\infty}^{\infty} dz \; |\phi_I(z)|^2 = \frac{1}{L} \,. \end{aligned} \tag{7}$$

This is for any x or I, when the ϕ_Is are normalized to unity as necessary.

d) Identical particles with spin 1/2 are fermions, implying that the total wavefunction of the two-particle state should be antisymmetric with respect to permutation of the particle coordinates. This means that in the case of antisymmetric spin part of the wavefunction, the singlet state

$$\chi_s = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\,,$$

the coordinate part should be symmetric with respect to the interchange of x and y. This condition is satisfied if the wavefunctions (6) with the same energy (5) are combined to form the function even in v. Therefore, the total wavefunction of the spin 1/2 fermions in the singlet state with energy $E_{I,q}$ is:

$$\psi^{(s)}_{I,q}(u,v,\sigma_1,\sigma_2) \;=\; \chi_s \cdot \phi_I(u)\frac{\sqrt{2}}{\sqrt{L}}\,\cos qv\,. \qquad (8)$$

If the spin part of the wavefunction is symmetric, i.e., the particles are in the triplet state χ_t, which is an arbitrary superposition of the states

$$|\uparrow\uparrow\rangle\,,\quad |\downarrow\downarrow\rangle\;,\quad \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\,,$$

the coordinate part of the wavefunction should be antisymmetric with respect to the interchange of x and y, and the total wavefunction then is:

$$\psi^{(t)}_{I,q}(u,v,\sigma_1,\sigma_2) \;=\; \chi_t \cdot \phi_I(u)\frac{\sqrt{2}}{\sqrt{L}}\,\sin qv\,. \qquad (9)$$

e) Since the wavefunctions of the triplet states as obtained in part (d) vanish at $x = y$, the delta-functional potential $U(x,y) = \lambda\delta(x-y)$ does not have any effect on them. To find the wavefunctions of the singlet states in the presence of this potential, we need to solve the v-part of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial v^2} + \;\lambda\delta(\sqrt{2}v)\right]\,\psi_q(v) \;=\; \frac{(\hbar q)^2}{2m}\psi_q(v)\,, \qquad (10)$$

for the wavefunction $\psi_q(v)$ even in v. This means that one can look for a solution in the form

$$\psi_q(v) = \frac{\sqrt{2}}{\sqrt{L}}\cos(q|v| + \phi)\,. \qquad (11)$$

The discontinuity

$$\frac{\partial}{\partial v}\,|v| \;=\; \theta(v) \,-\, \theta(-v) \qquad (12)$$

in the derivative of $|v|$ at $v = 0$ and the relation

$$\frac{\partial}{\partial v}\,\theta(v) \;=\; \delta(v) \qquad (13)$$

lead to the standard condition on the wavefunction imposed by the delta-functional potential,

$$\psi_q'(+0) - \psi_q'(-0) = \frac{\sqrt{2}\lambda m}{\hbar^2}\psi_q(0)\,. \tag{14}$$

This relation can be used to determine the phase ϕ directly, and we find,

$$\phi = \arctan\left(\frac{\lambda m}{\sqrt{2}q\hbar^2}\right)\,. \tag{15}$$

As one can see from this expression, the phase ϕ vanishes, as it should, with the magnitude λ of the potential, and tends to $\pi/2$, for large λ.

Quantum Mechanics 2

Entanglement in quantum mechanics

This problem discusses the concept of entanglement in quantum mechanics: correlated states of distinct quantum system. In the most basic setup, entanglement is defined quantitatively through the reduced density matrix. If two quantum systems have a pure-state density matrix $\rho_{1+2} = |\psi\rangle\langle\psi|$, entanglement E is defined as the entropy of the reduced density matrix $E = -\mathrm{Tr}\{\rho_1 \ln \rho_1\}$, where $\rho_1 = \mathrm{Tr}_2\{\rho_{1+2}\}$.

(a) *(3 pts)* Consider an arbitrary state of a quantum system composed of two distinct two-state systems:

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle \,.$$

Here α, β, γ, δ are the arbitrary complex coefficients that satisfy the appropriate normalization condition, and in the state $|ij\rangle$, i denotes the state of the first, and j – the second two-state system. Find the reduced density matrix ρ_1.

(b) *(5 pts)* From ρ_1, calculate the entanglement E in terms of the coefficients α, β, γ, δ. [*Hint:* A convenient way to do this is to find directly the eigenvalues of the 2×2 matrix ρ_1.] Repeat this calculation by reversing the roles of the two subsystems, i.e.:

$$E = -\mathrm{Tr}\{\rho_2 \ln \rho_2\}\,, \qquad \rho_2 = \mathrm{Tr}_1\{\rho_{1+2}\}\,,$$

and show that the definition of entanglement used above satisfies the natural requirement that E does not depend on which subsystem is taken to be the "first" and the "second".

(c) *(4 pts)* For the states ψ for which only *two* out of four coefficients α, β, γ, δ are nonvanishing, find all the states that have maximum entanglement $E = ln2$.

(d) *(4 pts)* Consider the states ψ for which all *four* coefficients α, β, γ, δ are nonvanishing. For these states, characterize all the states that have vanishing entanglement $E = 0$. Write these states explicitly as the product of the normalized states of the two subsystems.

(e) *(4 pts)* Entanglement can manifest itself as the correlations in the results of the measurements done on the subsystems. Consider the two states, which are examples of the states in parts (c) and (d):

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}[|00\rangle + i|11\rangle]\,, \qquad |\psi_2\rangle = \frac{1}{2}[|00\rangle + i|01\rangle - i|10\rangle + |11\rangle]\,.$$

Assume that the projective measurement of the observable σ_x (σ_x is a Pauli matrix) is done on the first two-state system. What are the outcomes of such a measurement, if the system is in the state $|\psi_1\rangle$ or $|\psi_2\rangle$, and what will be the state of the second two-state system system after the measurement depending on it outcome?

Solution

(a) To find ρ_1, one needs to sum the terms in the outer product $|\psi\rangle\langle\psi|$ that have the second two-state system in the same state 0 and the same state 1. Doing this for the state $|\psi\rangle$ in the problem, we get

$$\rho_1 = \begin{pmatrix} |\alpha|^2 + |\beta|^2 & \alpha\gamma^* + \beta\delta^* \\ \alpha^*\gamma + \beta^*\delta & |\gamma|^2 + |\delta|^2 \end{pmatrix} .$$

(b) To find the two eigenvalues p_1 and p_2 of ρ_1, it is convenient to use the fact that their sum is the trace, while the product is the determinant of ρ_1:

$$p_1 + p_2 = |\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1 , \qquad p_1 p_2 = (|\alpha|^2 + |\beta|^2)(|\gamma|^2 + |\delta|^2) - |\alpha\gamma^* + \beta\delta^*|^2$$

$$= |\alpha|^2|\delta|^2 + |\beta|^2|\gamma|^2 - 2\mathrm{Re}[\alpha^*\delta^*\beta\gamma] \equiv D .$$

Solving the quadratic equation that follows from these two relations, we get

$$p_1 = \frac{1}{2} + \sqrt{\frac{1}{4} - D} , \qquad p_2 = \frac{1}{2} - \sqrt{\frac{1}{4} - D} .$$

In terms of these eigenvalues, the entanglement is:

$$E = -(p_1 \ln p_1 + p_2 \ln p_2) .$$

Finding ρ_2 in the same way as ρ_1, we get:

$$\rho_2 = \begin{pmatrix} |\alpha|^2 + |\gamma|^2 & \alpha\beta^* + \gamma\delta^* \\ \alpha^*\beta + \gamma^*\delta & |\beta|^2 + |\delta|^2 \end{pmatrix} .$$

This expression shows that while this matrix is different from ρ_1, its trace and determinant, and therefore the eigenvalues, are the same. Thus, it gives the same magnitude of the entanglement, the condition that is essential for the entanglement to be the characteristics of the correlations between the two subsystems, not the property of the subsystems themselves.

(c) From the expression for E obtained in part (b), we see that entaglement has the maximum value of $\ln 2$ if $D = 1/4$. Expression for D shows directly that if only two coefficients are nonvanishing, condition $D = 1/4$ can be satisfied only if either

$$|\alpha| = |\delta| = \frac{1}{\sqrt{2}} , \quad \text{or} \quad |\beta| = |\gamma| = \frac{1}{\sqrt{2}} .$$

This means that all possible maximally-entangled states with the two non-vanishing coefficients are

$$\frac{1}{\sqrt{2}}[|00\rangle + e^{i\phi}|11\rangle] , \quad \text{and} \quad \frac{1}{\sqrt{2}}[|01\rangle + e^{i\chi}|10\rangle] ,$$

where ϕ and χ are possible arbitrary phases.

(d) Entanglement vanishes, if one of the eigenvalues of ρ_1 is zero, i.e., if $D = 0$. If all four coefficients are non-vanishing, this happens if

$$|\alpha|^2|\delta|^2 + |\beta|^2|\gamma|^2 = 2\mathrm{Re}[\alpha\beta\gamma^*\delta^*] \quad \Rightarrow \quad \frac{|\alpha||\delta|}{|\beta||\gamma|} + \frac{|\beta||\gamma|}{|\alpha||\delta|} = \cos\eta\,,$$

where $\eta = \arg[\alpha^*\delta^*\beta\gamma]$. This equation is satisfied only if

$$\frac{|\alpha||\delta|}{|\beta||\gamma|} = 1\,, \quad \eta = 0\,.$$

These two condition which can be summarized as one relation for the coefficients

$$\alpha\delta = \beta\gamma\,. \tag{1}$$

This means that $\delta = \beta\gamma/\alpha$, and one can express the state $|\psi\rangle$ as the product state:

$$|\psi\rangle = (\alpha|0\rangle + \gamma|1\rangle)_1(|0\rangle + (\beta/\alpha)|1\rangle)_2\,.$$

As the last step, the subsystem states are transformed into the properly normalized states:

$$|\psi\rangle = \frac{|\alpha|}{\alpha}\frac{1}{\sqrt{|\alpha|^2+|\gamma|^2}}(\alpha|0\rangle + \gamma|1\rangle)_1\frac{1}{\sqrt{|\alpha|^2+|\beta|^2}}(\alpha|0\rangle + \beta|1\rangle)_2\,,$$

making use of the fact that the relation (1) between the coefficients implies that the normalization condition for the total state $|\psi\rangle$ can be written as

$$(|\alpha|^2 + |\beta|^2)(|\alpha|^2 + |\gamma|^2) = |\alpha|^2\,.$$

The overall phase factor $|\alpha|/\alpha$ can be omitted if necessary.

(e) The eigenstates of the σ_x observable with eigenvalues ±1 are

$$\frac{1}{\sqrt{2}}[|0\rangle \pm |1\rangle]\,.$$

Calculating the overlap of these states with the state $|\psi_1\rangle$ we see that the outcomes ±1 of the measurements of σ_x on the first subsystem are obtained with equal probabilities 1/2 and the second subsystem is left in the state that depends on the outcome of the measurement on the first subsystem:

$$\frac{1}{\sqrt{2}}[|0\rangle + i|1\rangle]_2 \quad \text{for } +1\,, \qquad \frac{1}{\sqrt{2}}[|0\rangle - i|1\rangle]_2 \quad \text{for } -1\,.$$

The state $|\psi_2\rangle$ can be written as the product state:

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)_1\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)_2\,.$$

This means that the state of the second subsystem will remain the same,

$$\frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)_2\,,$$

regardless of the measurement, which will again produce the outcomes ±1 with probabilities 1/2, when done on the state $|\psi_2\rangle$.

Quantum Mechanics 3

Aharonov-Bohm effect with 1D scattering

A free quantum particle with coordinate x, mass m, and charge q moves along a ring with circumference L: $x \in [-L/2, L/2]$ threaded by a magnetic flux Φ. The effect of the flux on the particle can be described by imposing on the wavefunction $\psi(x)$ the quasipaeriodic boundary conditions with the phase $\phi = q\Phi/\hbar$ at the ends of the interval. The particle undergoes potential scattering at $x \simeq 0$ characterized by the scattering matrix S that relates the amplitudes A, B, C, D of the wavefunction components propagating in two different directions along the ring (see Figure):

$$\begin{pmatrix} C \\ D \end{pmatrix} = S \begin{pmatrix} A \\ B \end{pmatrix} , \qquad S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} .$$

The particle is transmitted through/reflected from the $x \simeq 0$ region with probabilities T and R, respectively, $T + R = 1$, and propagates freely, i.e., has the Hamiltonian $H = p^2/2m$ (in the standard notations) everywhere else.

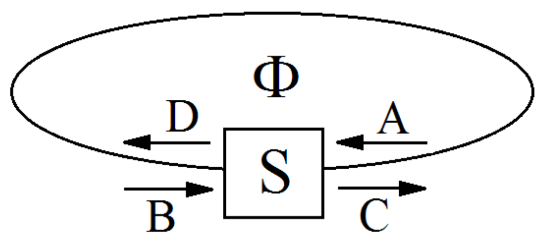


Figure 1: Diagram of a ring threaded by a magnetic flux Φ with potential scattering described by the scattering matrix S.

(a) *(4 pts)* Write down all (different) relations among the scattering coefficients r, t, r', t' that follow from the scattering matrix S being unitary.

(b) *(3 pts)* Write down the relations between the amplitudes A and D, and B and C, that follow from the free propagation of the particle along the ring at energy E. Parameterize the energy through the wavevector k: $E = \hbar^2 k^2/2m$.

(c) *(5 pts)* Combine the relations from (b), the scattering conditions described by the scattering matrix, and the relations among the scattering amplitudes from part (a), to derive the equation that determines the wavevectors k (and thus the energies E) of the particle stationary states:

$$\cos\left(kL + \frac{\eta + \eta'}{2}\right) = \sqrt{T} \cos\left(\phi - \frac{\eta - \eta'}{2}\right) .$$

Here η and η' are the phases of the transmission amplitudes t and t'.

(d) *(5 pts)* Solve this equation in the limit of small transmission probability, $T \ll 1$ (keeping only the leading non-vanishing terms in T in all relevant expressions) to obtain the energies E_n of the stationary states as functions of the flux Φ. Calculate the current I_n carried by the particles in the the state $|n\rangle$.

(e) *(3 pts)* Derive the condition the scattering matrix S satisfies if the scattering has the time-reversal symmetry. How this affects the result in part (d) for the currents I_n?

Solution

(a) As for any unitary matrix, the fact that the scattering matrix is unitary means that the matrix elements satisfy the following relations:

$$|r|^2+|t|^2=|t'|^2+|r'|^2=|r|^2+|t'|^2=|t|^2+|r'|^2=1\,, \qquad r^*t'+t^*r'=0\,.$$

The first set of the relations means that the magnitudes of the scattering amplitudes in the two directions are the same:

$$|r|=|r'|=\sqrt{R}\,, \qquad |t|=|t'|=\sqrt{T}\,,$$

while the second defines the phase of the reflection amplitude r':

$$r'=-r^*(t'/t^*)\,.$$

(b) Free propagation of particle in the positive or negative direction along the ring with the wavevector k implies that the wavefunction is

$$\psi(x)\propto e^{\pm ikx},$$

i.e.,the wavefunction amplitudes accumulates the phase kL in the direction of propagation, when they move through the whole ring. The magnetic flux threading the ring means that the amplitude acquires the phase ϕ when circling the ring in one direction, and the phase $-\phi$ – in the opposite direction. Combining these two phases, we get the relations between the amplitudes of the plane wave components of the wavefunction

$$A=e^{i(kL-\phi)}D\,, \qquad B=e^{i(kL+\phi)}C\,.$$

(c) The wavefunction amplitudes are also related by the potential scattering described by the scattering matrix S:

$$C=rA+t'B\,, \qquad D=tA+r'B\,.$$

These relations, combined with those from the free propagation, give the system of two equations that should be satisfied by the amplitudes A and B:

$$rA+(t'-e^{-i(kL+\phi)})B=0\,, \qquad (t-e^{i(\phi-kL)})A+r'B=0\,.$$

Condition that the determinant of this homogeneous system vanishes so that it has a non-zero solution, gives the equation for the wavevector k, and therefore, the energy of the stationary state of the particle:

$$rr'-tt'-e^{-i2kL}+e^{-ikL}(te^{-i\phi}+t'e^{i\phi})=0\,.$$

Introducing explicitly the phases of the transmission amplitudes: $t=\sqrt{T}e^{i\eta}$, and $t'=\sqrt{T}e^{i\eta'}$, and using the unitarity relation between the scattering amplitudes, $r'=-r^*e^{i(\eta+\eta')}$ we transform this equation simplifies to

$$e^{-i2kL}-\sqrt{T}e^{-ikL}(e^{i(\eta-\phi)}+e^{i(\eta'+\phi)})+e^{i(\eta+\eta')}=0\,.$$

Introducing the phase $\delta = \phi - (\eta - \eta')/2$ and variable $z = e^{-i[kL+(\eta+\eta')/2]}$, we see that this equation cab be cast as the following quadratic equation for z:

$$z^2 - 2\sqrt{T} z \cos\delta + 1 = 0\,,$$

with the solution

$$z = \sqrt{T}\cos\delta \pm i\sqrt{1 - T\cos^2\delta}\,.$$

Real and imaginary parts of this equation are consistent with each other, and therefore, only one of them is sufficient, e.g.,

$$\cos\left(kL + \frac{\eta+\eta'}{2}\right) = \sqrt{T}\cos\delta\,. \tag{1}$$

(d) For $T = 0$, Eq. (1) reduces to

$$\cos\left(kL + \frac{\eta+\eta'}{2}\right) = 0$$

and solutions for the wavevector k are

$$k_n = \frac{1}{L}\left(\pi n - \frac{\pi+\eta+\eta'}{2}\right),$$

with integer n. As should be, k_n is independent of the flux-induced phase ϕ, and corresponds to the standing wave in what effectively is a potential well.

For small but non-vanishing T, we can solve Eq. (1) by iterations to find a small correction δk_n to k_n induced by the non-vanishing right-hand-side of this equation. Using the fact that the derivative of $\cos[kL + (\eta+\eta')/2]$ at $k = k_n$ is $(-1)^n$, we get:

$$\delta k_n = \frac{(-1)^n}{L}\sqrt{T}\cos\delta\,.$$

From this, the energies E_n are:

$$E_n = \frac{\hbar^2}{2m}\big(k_n + \delta k_n\big)^2 \simeq \frac{\hbar^2 k_n^2}{2m} + \frac{\hbar^2 k_n}{m}\delta k_n\,.$$

As usual, the current in a stationary state $|n\rangle$ can be calculated from E_n:

$$I_n = -\frac{dE_n}{d\Phi} = -\hbar v_n \frac{d\delta k_n}{d\Phi} = (-1)^n \frac{q v_n}{L}\sqrt{T}\sin\delta = (-1)^n \frac{q v_n}{L}\sqrt{T}\sin\left(\phi - \frac{\eta-\eta'}{2}\right), \quad v_n = \frac{\hbar k_n}{m}\,.$$

We see that the current I_n depends periodically on the flux Φ with the period $2\pi\hbar/q = h/q$ consistent with the Aharonov-Bohm effect.

(e) Time-reversal symmetry implies that complex conjugation of a scattering solution of the Schrödinger equation produces a valid solution. Since onplex conjugation of the plane waves interchanges the incoming and the outgoing state, this means that the scattering matrix of the time-reversal scattering satisfies the condition

$$S^* = S^{-1}\,.$$

Combined with the unitarity condition, this means that the scattering matrix is symmetric, $S^T = S$, i.e.,

$$t = t' , \quad \eta = \eta' .$$

As we can see from the definition of the phase δ, in this case, $\delta = \phi$, and the current I_n vanishes for vanishing flux Φ: $\sin\delta = \sin\phi = 0$ for $\Phi = 0$. Without time-reversal symmetry, the current I_n can be non-vanishing even without the flux.

Statistical Mechanics 1

Mean-field interactions

Consider a system of N distinguishable particles. Each particle has two energy levels: the ground level has energy zero and is non-degenerate, while the excited level has energy ε and consists of g_e degenerate states.

(a) (3pt) Compute the partition function $Z_N(T)$ of the N-particle system.

(b) (2pt) Find the temperature T_x at which the numbers of particles in the ground and excited states are equal.

(c) (2pt) Derive an expression for the average particle energy, $\langle\varepsilon\rangle$, as a function of temperature T. What is the average energy $\langle\varepsilon\rangle$ at the transition temperature T_x?

(d) (3pt) Write an expression for the heat capacity $C_V(T)$ as a function of temperature. Find the maximum value of the heat capacity $C_V(T)$ and compare it to its value at temperature T_x. How is the heat capacity related to the fluctuations of the energy?

(e) (3pt) Express the entropy as a function of temperature, $S(T)$.

(f) (7pt) Now consider an attractive interaction amongst only the excited particles adding an interaction energy

$$E_{\text{int}} = -\alpha \frac{N_{\text{e}}^2}{N},$$

to the energy of the non-interacting system. Here $N_{\text{e}} \gg 1$ is the number of excited particles and $0 < \alpha < \varepsilon/2$ is the interaction strength. In a *mean-field approximation*, particle states are independent from each other, and the effect of the interaction on each individual particle can be approximated by a shift in its energy $\Delta\varepsilon$ created by all other excited particles.

(i) The excitation energy of a particle is the energy required to raise one additional partilce from the ground to the excited state for a given N_e. Find how the excitation energy $\varepsilon \to \varepsilon' = \varepsilon + \Delta\varepsilon$ is modified due to the interaction for a mean number of excited particles, $\bar{N}_e$.

(ii) Write a self-consistency equation for the average number of excitations, $n_{\text{e}} = \bar{N}_{\text{e}}/N$.

(iii) Sketch a graphical solution to the self-consistency equation. Use your sketch to describe qualitatively the high temperature limit, the low temperature limit, and possible transition points.

Solutions

(a) For N independent two-level particles, the partition function is

$$Q = q^N = \left(1 + g_e e^{-\beta\varepsilon}\right)^N = \left(1 + g_e e^{-\tau_0/T}\right)^N. \tag{1}$$

where q is the single-particle partition function and where we have made the temperature explicit by expressing $\beta\varepsilon = \varepsilon/(kT) = \tau_0/T$. k is Boltzmann's constant, T is temperature and $\tau_0 = \varepsilon/k$ is a constant that gives the liquid-state energy level in terms of a temperature τ_0.

(b) Find the point at which the population p_s^* of the solid equals the population p_ℓ^* of the liquid, where the * indicates the populations specifically at this transition temperature.

$$p_s^* = \frac{1}{q} = \frac{1}{1 + g_e x}, \qquad \text{and} \qquad p_\ell^* = \frac{g_e e^{-\beta\varepsilon}}{q} = \frac{g_e x}{1 + g_e x}. \tag{2}$$

where $x = \exp(-\tau_0/T)$ is a useful simplification for other steps below.

Now, setting $p_s^* = p_\ell^*$ means that $g_e x^* = 1$, which gives the transition temperature to be

$$T_x = \frac{\tau_o}{\ln g_e} \tag{3}$$

in terms of the known model quantities τ_0 and g_e. If $g_e = 1$, note that there is no crossover point because $T_x = \infty$. For larger g_e, there is a finite temperature of the liquid to solid transition in this model. Also, at this transition point, you find have $p_s^* = p_\ell^* = 1/2$.

(c) Sum the probability-weighted energies over the two states to get:

$$\langle\varepsilon\rangle = \sum p_j^* \varepsilon_j = 0 \cdot p_s^*(0) + \varepsilon \cdot p_\ell^* = \frac{\varepsilon g_e e^{-\tau_0/T}}{1 + g_e e^{-\tau_0/T}} = \frac{\varepsilon g_e x}{1 + g_e x}. \tag{4}$$

(or you can get this by taking the derivative $\langle\varepsilon\rangle = -q^{-1}(\partial q/\partial\beta)$). Substitute the transition point condition, $g_e x^* = 1$, into Eq 4 to get $\langle\varepsilon^*\rangle = \varepsilon/2$.

(d) To compute the heat capacity, use the definition $C_V = (\partial U/\partial T)$ from thermodynamics and sum over the particles, to get:

$$C_V = N\left(\frac{\partial\langle\varepsilon\rangle}{\partial T}\right)_{V,N} = N\left(\frac{\partial\langle\varepsilon\rangle}{\partial\beta}\right)\left(\frac{d\beta}{dT}\right) = -\frac{N}{kT^2}\left(\frac{\partial\langle\varepsilon\rangle}{\partial\beta}\right), \tag{5}$$

where the right-hand expressions convert from T to β to make the next step of the differentiation simpler. Take derivative of the form $d(u/v) = (vu' - uv')/v^2$, where $u = g_e\varepsilon e^{-\beta\varepsilon}$ and $v = 1 + g_e e^{-\beta\varepsilon}$, to get

$$\begin{aligned}\left(\frac{\partial\langle\varepsilon\rangle}{\partial\beta}\right) &= \frac{(1 + g_e e^{-\beta\varepsilon})(-\varepsilon^2 g_e e^{-\beta\varepsilon}) - \varepsilon g_e e^{-\beta\varepsilon}(-g_e\varepsilon e^{-\beta\varepsilon})}{(1 + g_e e^{-\beta\varepsilon})^2} \\ &= \frac{-\varepsilon^2 g_e e^{-\beta\varepsilon}}{(1 + g_e e^{-\beta\varepsilon})^2}.\end{aligned} \tag{6}$$

Substitute Equation (6) into the right-hand side of Equation (5) to find the heat capacity C_V in terms of the energy level spacing ε:

$$C_V = \frac{N\varepsilon^2}{kT^2}\frac{g_e e^{-\beta\varepsilon}}{(1+g_e e^{-\beta\varepsilon})^2} = \frac{Nk\tau_0^2 g_e x}{(1+g_e x)^2}. \tag{7}$$

Substitute $g_e x^* = 1$ into Eq 7 to get $C_V = Nk\tau_0^2/4$ at the liquid-solid transition temperature. And yes, the heat capacity reaches a peak at temperature T_x, as you can see by taking the derivative and finding that it is zero at that point.

$$\frac{dC_V}{dx} = \frac{d}{dx}\left[\frac{g_e x}{(1+g_e x)^2}\right]_{x^*} = 1 - (g_e x^*)^2 = 0. \tag{8}$$

(e) Entropy is defined as

$$\frac{S}{Nk} = \ln q + \frac{\langle\varepsilon\rangle}{kT} \tag{9}$$

So, for this model, we have:

$$\frac{S}{Nk} = \ln(1+g_e x) + \left(\frac{\varepsilon}{kT}\right)\left(\frac{g_e x}{1+g_e x}\right). \tag{10}$$

and $g_e x \to 0$ as $T \to 0$, so $S(0) = 0$.

(f) The mean-field approximation treats all particles independently. Therefore, the additional excitation energy is due to the change of the total energy upon excitation of (any) one particle:

$$\Delta\varepsilon = E_{\text{int}}(N_{\text{e}}+1) - E_{\text{int}}(N_{\text{e}}) \approx -2\alpha\frac{N_{\text{e}}}{N} = -2\alpha n_{\text{e}} \tag{11}$$

Since all particles are independent, the number of excited ones can still be found using the same Gibbs distribution as above but replacing $\varepsilon \to \varepsilon' = \varepsilon - 2\alpha n_{\text{e}}$, which leads to the following transcendental equation:

$$n_{\text{e}} = \frac{N_{\text{e}}}{N} = \frac{1}{1 + \frac{1}{g_e}\exp\left[(\varepsilon - 2\alpha n_{\text{e}})/kT\right]} \tag{12}$$

It is useful to resolve it for ε',

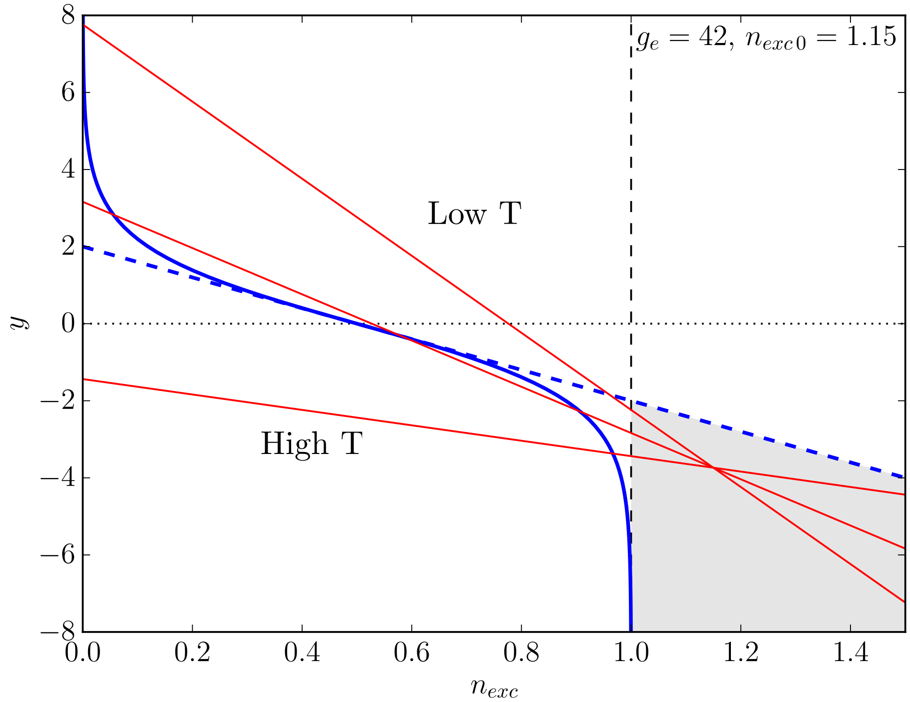
$$\frac{\varepsilon'}{kT} = \frac{\varepsilon - 2\alpha n_{\text{e}}}{kT} = \log g_e + \log(1-n_{\text{e}}) - \log n_{\text{e}} \tag{13}$$

This equation can be solved numerically. For qualitative analysis, it can be solved graphically by plotting the curve $y = \log(1-n_{\text{e}}) - \log(n_{\text{e}})$ (the blue curve) and straight lines (the red lines) passing through the point $(n_{\text{e}0}, y_0) = (\frac{\varepsilon}{2\alpha}, -\log g_e)$ with slope $-\frac{2\alpha}{kT}$. The intersections points are the solutions to eq. 13. Note that $n_{\text{e}0}$ (the x coordinate of the interesction point) is greater than unity due to the constraint $\alpha < \varepsilon/2$. Thus the intersection point could be in the gray region shown in the figure.

In the high-temperature limit, the slope of the red line, $-2\alpha/kT$, is small and the red line is nearly horizontal. The only intersection in this case is at $y = -\log g_e$ and $n_\mathrm{e} = \frac{g_e}{1+g_e}$, i.e., the system is completely random. In the zero-temperature limit the slope is a large and negative, the only intersection is at $y \to \infty$ and $n_\mathrm{e} \to 0$, so the entire system is in the ground state. Abrupt changes of the energy with temperature are possible when the line can cross the blue curve at more than one point, which is possible if the point $(n_{\mathrm{e}0}, y_0)$ is in the shaded region, or

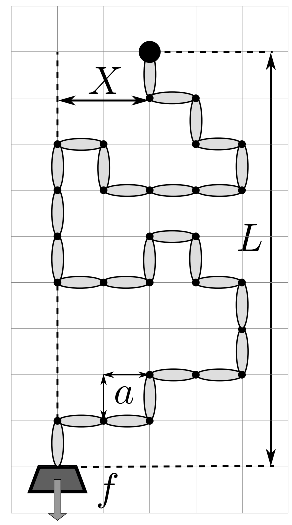
$$-4n_{\mathrm{e}0} + 2 > y_0 \quad \Longleftrightarrow \alpha > \frac{2\varepsilon}{2 + \log g_e}\,, \tag{14}$$

i.e., either at large enough interaction constant α or large enough excited-state degeneracy.



Statistical Mechanics 2

Thermodynamics of a polymer molecule

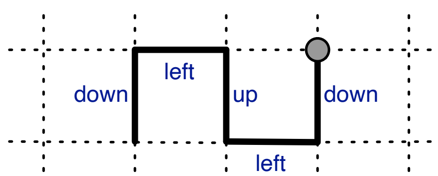


Consider a 2-dimensional polymer chain molecule consisting of $N \gg 1$ links that can be oriented only along the square lattice and that can intersect and overlap freely without any effect. Each link has length $a = 1$ and has constant intrinsic heat capacity c (i.e., due to excitations of its internal degrees of freedom). The kinetic energy of the links is negligible. One end of the molecule is fixed in space, and a vertical force f is applied to the other end, so that the energy of the entire system is equal to

$$E(L) = -fL\,,$$

where L is the length of the molecule in the vertical direction.

(a) (1pt) Each link orientation can be in four states: up (u), down (d), left (l), or right (r). Consider the chain of five links in the configuration shown below with (d, l, u, l, d). The configuration below has energy $E = -f$ since the total vertical length is $L = 1$. How many configurations are there with five links? Draw another five link configuration and find its energy.



(b) (5pt) Find the partition function $Z(T, f)$ as a function of the force f and temperature T.

Hint: it may be convenient to use coordinates (x_i, y_i) *to represent each link as a vector with* $i = 1 \ldots N$ *labelling the links, e.g.* $(1, 0)$ *is a left link.*

(c) (5pt) Compute the mean vertical length $\overline{L}$, the entropy S, and the heat capacity of the polymer chain at constant tension f as functions of f and T.

(d) (4pt) Find the fluctuation $\langle(\Delta L)^2\rangle$ and $\langle(\Delta X)^2\rangle$ of the end of the molecule stretched to mean length $\overline{L}$ in the vertical direction. (X is the transvese displacement of the end as shown in the figure above.)

(e) (3pt) If the molecule stretched approximately to half of its maximal length $\overline{L} = N/2$ in the vertical direction, how much work can be extracted from it if the temperature is maintained constant?

(f) (2pt) Compute the isothermic elasticity $\left(\frac{\partial \overline{L}}{\partial f}\right)_T$ in the vertical direction. How does the answer change if the system (e.g., a macroscopic sample of such molecules) is thermally insulated?

Solution

(a) [2pt] For a link directed up or down, its contribution to the energy is $\pm f$, respectively. For a horizontal link, the energy contribution is zero.

(b) [4pt] For each link i, let's introduce its coordinates x_i, y_i describing its orientation such that

$$x_i = \pm 1,\; y_i = 0 \quad \text{or} \quad x_i = 0,\; y_i = \pm 1\,.$$

With the static force f applied to the end of the molecule, the energy function depends on the position of the molecule's end $\sum_i y_i = L$,

$$E = -fL = -f\sum_i y_i\,. \tag{1}$$

For each link, there are four possible states : $y_i = \pm 1$ or $x_i = \pm 1$. Since the energy of the molecule is linear in $L = \sum_i y_i$, the partition function can be factorized into sums over states of individual links,

$$Z(T,f) = \sum_{\{y_i=\pm 1 \text{ or } x_i=\pm 1\}} e^{\frac{f}{T}\sum_i y_i} = \prod_i \left(e^{f/T} + 2 + e^{-f/T}\right) = \left(4\cosh^2\frac{f}{2T}\right)^N\,. \tag{2}$$

(c) [5pt] Since the partition function above is a function of temperature and external force, it is appropriate to define the Gibbs potential as

$$G(T,f) = -T\log Z(T,f) = -2NT\log\left(2\cosh\frac{f}{2T}\right) \tag{3}$$

from which one can compute the molecule's mean elongation

$$L = \frac{T}{Z}\left(\frac{\partial Z}{\partial f}\right)_T = -\left(\frac{\partial G}{\partial f}\right)_T = N\tanh\frac{f}{2T} \tag{4}$$

and the molecule's entropy

$$S = -\left(\frac{\partial G}{\partial T}\right)_f = 2N\log\left(2\cosh\frac{f}{2T}\right) - \frac{Nf}{T}\tanh\frac{f}{2T}\,. \tag{5}$$

Now, the additional heat capacity due to the entropy of the molecule is easy to determine as

$$(\Delta C)_f = T\left(\frac{\partial S}{\partial T}\right)_f = N\frac{f^2}{2T^2}\frac{1}{\cosh^2\frac{f}{2T}} = N\frac{f^2}{2T^2}\left[1 - \left(\frac{L}{N}\right)^2\right]\,, \tag{6}$$

so that the total heat capacity is $C_f = Nc + (\Delta C)_f$.

(d) [4pt] Fluctuation of the molecule's length can be found as the second derivative of the Gibbs potential,

$$(\delta L)^2 = \langle L^2\rangle - \langle L\rangle^2 = -T\left(\frac{\partial^2 G}{\partial f^2}\right)_T = T\left(\frac{\partial L}{\partial f}\right)_T \tag{7}$$

Evaluating the derivative yields

$$(\delta L)^2 = T\left(\frac{\partial}{\partial f}\right)_T \left(N\tanh\frac{f}{2T}\right) = N\frac{1}{2\cosh^2\frac{f}{2T}} = \frac{N}{2}\left[1-\left(\frac{L}{N}\right)^2\right] \tag{8}$$

Since all the links can be in $x_i = \pm 1$ state independently of each other, one can calculate the mean-square transverse displacement as

$$(\delta X)^2 = \langle X^2\rangle = N\langle x_i^2\rangle = N\frac{2}{e^{f/T}+2+e^{-f/T}} = \frac{N}{2\cosh^2\frac{f}{2T}} = (\delta L)^2\,, \tag{9}$$

i.e. the fluctuations in both directions are equal to each other independent of the applied tension. In case of maximal elongation $L = N$, the molecule has no freedom to fluctuate in either direction.

(e) [2pt] The question about the maximal possible work is equivalent to the question about free energy. The free energy of the molecule can be calculated by Legendre transformation $G(T, f) \to F(T, L)$

$$F(T, L) = G - f\left(\frac{\partial G}{\partial f}\right)_T \equiv G + fL = -TS \tag{10}$$

(the latter identity follows from the results of part **(b)**). In order to determine the change of entropy, one has to find the tension f_1/T corresponding to length $L_1 = N/2$:

$$L_1 = N\tanh\frac{f_1}{2T} = N/2 \quad\Leftrightarrow\quad \tanh\frac{f_1}{2T} = \frac{1}{2} \quad\Leftrightarrow\quad f_1 = T\log 3\,. \tag{11}$$

The maximal work is achieved when the tension is reduced to zero, i.e. $f_2 = 0$, $L_2 = 0$ and $S_2 = 2N\log 2 = \log(4^N)$, which corresponds to the maximally disordered state. The work is equal to decrease in the free energy, thus

$$W = F_1 - F_2 = T(S_2 - S_1) = NT\log 4 - NT\log\left(4\cosh^2\frac{f_1}{2T}\right) + Nf_1\tanh\frac{f_1}{2T} = NT\log\frac{3\sqrt{3}}{4}\,. \tag{12}$$

(f) [3pt] The isothermal elasticity is easily computed by taking the derivative

$$\kappa_T = \left(\frac{\partial L}{\partial f}\right)_T = \frac{N}{2\cosh^2\frac{f}{2T}} = \frac{N}{2}\left[1-\left(\frac{L}{N}\right)^2\right] \tag{13}$$

If the molecule is thermally insulated, then the elasticity is "adiabatic" with $S = const$, so

$$\kappa_S = \left(\frac{\partial L}{\partial f}\right)_S = \frac{\partial(L,S)}{\partial(f,S)} = \frac{\partial(L,T)}{\partial(f,T)}\cdot\frac{\partial(L,S)}{\partial(L,T)}\cdot\frac{\partial(f,T)}{\partial(f,S)} = \kappa_T\frac{C_L}{C_f} \tag{14}$$

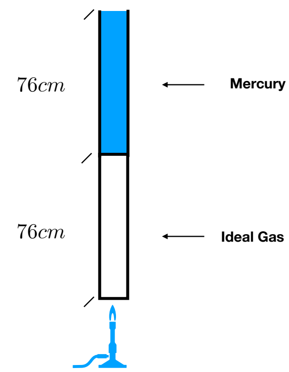
The heat capacity at constant tension $C_f = Nc + \Delta C$ was computed in part **(b)**. If the elongation of the molecule is kept constant, its heat capacity is given only by the intrinsic heat capacity of the links, therefore $C_L = Nc$. Thus, the adiabatic elasticity is

$$\kappa_S = \frac{\kappa_T}{1+\Delta C/(Nc)} = \frac{N}{2}\frac{1-L^2/N^2}{1+\frac{f^2}{2cT^2}\left(1-L^2/N^2\right)} \leq \kappa_T\,. \tag{15}$$

Statistical Mechanics 3

Unexpected explosion

A tube is separated into two equal 76-cm parts by a mobile weightless disc. The tube and the disc have negligible heat capacity. The lower part contains *diatomic* ideal gas with initial volume V_0. The upper part contains mercury and is open to air at the atmospheric pressure P_0. (Recall that the weight per area of 76cm of mercury is equivalent to atmospheric pressure P_0, so the gas is initially at pressure $2P_0$). Initially, the gas has temperature T_0 and is insulated from the environment and the mercury, and the whole system is in equilibrium. The gas is then gradually heated, so the disc rises and the mercury is *slowly* spilled out.



(A) (2 pt) If after a time period the volume of the gas increases from V_0 to $V \equiv xV_0$, determine its temperature and pressure assuming equilibrium at all times; sketch $P(V)$ and $T(V)$ versus x.

(B) (4 pt) Suppose an infinitesimal amount of heat δQ is supplied to the gas by a candle. Find the effective heat capacity

$$C(V) = \frac{dQ}{dT},$$

as a function of the volume of the gas in the tube and sketch $C(V)$ versus x.

(C) (3 pt) Determine the points $x = V/V_0$ where the heat capacity $C(V)$ becomes infinite and zero, and the range of x where $C(V)$ is negative. When $C(V)$ is negative, how does the temperature of the gas change upon heating? Give a qualitative explanation for this behavior.

(D) (4 pt) Assume that the system is slowly heated. Write down the condition for mechanical stability of the system. Show that the system becomes unstable when $C(V) = 0$.

(E) (3 pt) Compute the amount of heat required to reach the point of instability, after which all the mercury is pushed out of the tube. Compare it to the mechanical energy of lifting the disc all the way up until the mercury is pushed out and explain the difference (if any).

(F) (4 pt) Now the candle is removed, and assume that the tube conducts heat perfectly. The gas is heated by increasing the temperature of the environment (i.e. the air around the bottom of the tube), but the external pressure P_0 (at the top of the tube) remains constant. Find the fluctuation of the gas temperature as a function of $x = V/V_0$. At which point does the system become unstable under these conditions?

Solution

(A) [2pt] The external pressure is determined by the height of the mercury column, which depends linearly on the volume of the gas; thus, the pressure changes linearly between $P(V_0) = 2P_0$ and $P(2V_0) = P_0$,

$$P(V) = P_0\left(3 - \frac{V}{V_0}\right) = P_0(3 - x)\,, \tag{1}$$

where it is convenient to introduce $x = V/V_0$, V_0 is the initial gas volume, and $V_0 \le V \le 2V_0$ is the current volume of the gas (thus $1 \le x \le 2$). The ideal gas equation of state yields

$$PV = NT = \frac{2P_0V_0}{T_0}T\,, \tag{2}$$

from which the temperature is

$$T = \frac{1}{2}x(3 - x)T_0\,. \tag{3}$$

Note that the maximum temperature is achieved at $x = \frac{3}{2}$: $T(x = \frac{3}{2}) = \frac{9}{8}T_0$, and temperature is the same at the beginning and the end of the gas expansion: $T(V_0) = T(2V_0) = T_0$.

(B) [4pt] First, relate dV and dT of the gas with the pressure given by Eq. (1)

$$dP = -P_0\frac{dV}{V_0}\,, \tag{4}$$

$$NdT = PdV + VdP = P_0\left(3 - 2\frac{V}{V_0}\right)dV = P_0V_0(3 - 2x)dx\,, \tag{5}$$

$$dT = \frac{1}{2}T_0(3 - 2x)dx\,. \tag{6}$$

(Can also be obtained directly from Eq. (3)). Assuming that the $V = \text{const}$ heat capacity of the gas $C_V = Nc$,

$$dQ = Nc\,dT + P\,dV = N\left[c + \frac{3 - x}{3 - 2x}\right]dT \tag{7}$$

and the heat capacity of the gas under the mercury column is

$$C = N\left[c + \frac{3 - x}{3 - 2x}\right] \tag{8}$$

(C) [3pt] The heat capacity (8) reaches infinite value at $x = \frac{3}{2}$ and zero at

$$x_0 = 3\frac{1 + c}{1 + 2c} > \frac{3}{2} \tag{9}$$

At $\frac{3}{2} < x < x_0$, the heat capacity is negative, $C(x) < 0$. In this interval, the gas continues to expand while it is heated, and its temperature decreases, because the pressure decreases simultaneously and the gas performs work in part at the expense of its internal energy. When the heat capacity reaches zero, $C(x = x_0) = 0$, no more heat is required by the gas to continue expansion. The system becomes unstable and the gas expands spontaneously until all the mercury is pushed out of the tube ("explosion").

(D) [4pt] The previous point can be illustrated by examining mechanical stability of the gas upon adiabatic expansion or contraction. If the external pressure (mercury column) decreases faster than the internal pressure of the gas upon adiabatic expansion ($\delta Q = 0$, $dV > 0$), the system is unstable:

$$\left|\frac{dP_{ext}}{dV}\right| > \left|\left(\frac{\partial P_{gas}}{\partial V}\right)_S\right| \quad \Longleftrightarrow \quad \frac{dP_{ext}}{dV} < \left(\frac{\partial P_{gas}}{\partial V}\right)_S < 0\,. \tag{10}$$

It is crucial to use adiabatic ($S = 0$) compressibility, since the system is insulated *up to very slow heating*. We have also used the general stability requirement $\left(\frac{\partial P}{\partial V}\right)_S < 0$. To compute the left side of the inequality, one should use Eq. (1),

$$\frac{dP_{ext}}{dV} = -\frac{P_0}{V_0}\,, \tag{11}$$

and to compute the right side of the inequality, one should use the equation state of the gas directly, without the constraint (1), since the system may no longer be at the equilibrium with the mercury column,

$$0 = TdS = NcdT + pdV = (1+c)PdV + cVdP \quad \Longleftrightarrow \quad \left(\frac{\partial P}{\partial V}\right)_S = -\frac{1+c}{c}\cdot\frac{P}{V}\,. \tag{12}$$

Up to the point the equilibrium is lost, it is assumed that $P = P_{ext}$, therefore

$$\left(\frac{\partial P}{\partial V}\right)_S = -\frac{1+c}{c}\cdot\frac{3-x}{x}\cdot\frac{P_0}{V_0} \tag{13}$$

Solving inequality (10), one obtains

$$x > 3\frac{1+c}{2+c} = x_0\,, \tag{14}$$

i.e., the same as the $C(x) = 0$ condition.

(E) [3pt] One has to integrate the heat capacity from $x = 1$ to x_0, after which the expansion is self-driven. Using Eqs. (6,8),

$$\begin{aligned} Q_{\text{tot}} &= \int CdT \\ &= \int_1^{x_0} N\left[c + \frac{3-x}{3-2x}\right]\cdot\frac{1}{2}T_0(3-2x)dx \quad = P_0V_0\frac{(2+c)^2}{2(1+2c)}\,. \end{aligned} \tag{15}$$

To obtain the mechanical energy required to push all the mercury out of the tube, one can integrate the pressure between $x = 1$ and $x = 2$:

$$W = \int_{V_0}^{2V_0} P(V)dV = P_0V_0\int_1^2 (3-x)dx = \frac{3}{2}P_0V_0\,. \tag{16}$$

Note that this work is equivalent to expansion $\Delta V = 2V_0 - V_0 = V_0$ against the constant pressure P_0 plus lifting the center of mass of the mercury column to the top of the tube,

$$W_{ext} = P_0 V_0 + \frac{1}{2} P_0 V_0 = \frac{3}{2} P_0 V_0 \,. \tag{17}$$

The difference is

$$Q - W_{ext} = P_0 V_0 \frac{(c-1)^2}{2(1+2c)} \geq 0 \,. \tag{18}$$

The excess energy will be transferred to the kinetic energy of the mercury since the expansion of the gas will not be a slow, near-equilibrium process.

(F) [4pt] In a canonical ensemble, temperature fluctuation is determined by the heat capacity,

$$\langle (\Delta T)^2 \rangle = C(V) T^2 \,. \tag{19}$$

In the region where $C(V) < 0$, the fluctuation appears to have imaginary value. While this would be nonsense physics-wise, mathematically it means that there is no stable equilibrium for the temperature if it is allowed to vary.

Taking into account the temperature of the gas as a function of volume (part A), the system can no longer be in equilibrium with a heat bath at the temperature above the maximum temperature of the gas $T_{max} = T(x = \frac{3}{2}) = \frac{9}{8} T_0$. Temperature does not exceed $\frac{9}{8} T_0$ for $x < \frac{3}{2}$, and for $x > \frac{3}{2}$ the heat capacity is negative. It means that any heat transferred to the gas from the heat bath with temperature at or above T_{max} will result in expansion of the gas and *decrease* of its temperature, leading to further "runaway" heat transfer and uncontrolled expansion.