

Part II Experimental and Theoretical Physics

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THEORETICAL PHYSICS 1

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Answers to Problems

(with thanks to Adam Thorn, Jo Gaunt & Bryan Webber)

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Dynamics question 1

Using the co-ordinate system described in the question, the kinetic energy of the system is

$$\begin{aligned} T &= \frac{1}{2}I_{disc}\dot{\theta}^2 + \frac{1}{2}ma^2\dot{\theta}^2 + \frac{1}{4}m(\dot{x} + a\dot{\theta})^2 \\ &= \frac{5}{4}ma^2\dot{\theta}^2 + \frac{1}{4}m\dot{x}^2 + \frac{1}{2}ma\dot{x}\dot{\theta} \end{aligned}$$

and the potential energy is

$$V = -mga \cos \theta - \frac{1}{2}mg(x + a\theta) + \frac{1}{2}kx^2$$

so the Lagrangian, $L = T - V$, is

$$L = \frac{5}{4}ma^2\dot{\theta}^2 + \frac{1}{4}m\dot{x}^2 + \frac{1}{2}ma\dot{x}\dot{\theta} + mga \cos \theta + \frac{1}{2}mg(x + a\theta) - \frac{1}{2}kx^2$$

This arises from kinetic energy terms arising from the rotational energy of the disc, the kinetic energy of the mass attached to the disk, and the kinetic energy of the mass on the string moving at speed $\dot{x} + a\dot{\theta}$. The potential energy term is straightforward to obtain. Inserting this Lagrangian into the Euler-Lagrange equations, we arrive at the equations of motion:

$$\begin{aligned} \frac{1}{2}m\ddot{x} + \frac{1}{2}ma\ddot{\theta} &= \frac{1}{2}mg - kx \\ \frac{5}{2}ma^2\ddot{\theta} + \frac{1}{2}ma\ddot{x} &= -mga \sin \theta + \frac{1}{2}mga \end{aligned}$$

In equilibrium, $\ddot{\theta} = \ddot{x} = 0$, so the equilibrium position is $x_0 = mg/2k$ and $\sin \theta_0 = 1/2$ so $\theta_0 = \pi/6$. We will now consider a small perturbation from this equilibrium position, and write $\theta = \theta_0 + \delta\theta$, $x = x_0 + \delta x$. Taylor expanding $\sin \theta$ about θ_0 , $\sin \theta \simeq 1/2 + \delta\theta\sqrt{3}/2$. If we then assume that $\delta\theta$ and δx vary with time as $e^{i\omega t}$, $\ddot{x} = -\omega^2\delta x$ and $\ddot{\theta} = -\omega^2\delta\theta$. We can then write the equations of motion in a matrix form:

$$\begin{pmatrix} -\frac{1}{2}m\omega^2 + k & -\frac{1}{2}ma\omega^2 \\ -\frac{1}{2}ma\omega^2 & -\frac{5}{2}ma^2\omega^2 + \frac{\sqrt{3}mga}{2} \end{pmatrix} \begin{pmatrix} \delta x \\ \delta\theta \end{pmatrix} = 0$$

We thus require the determinant of the matrix in the left hand side of this expression to be zero:

$$\begin{aligned} \left(k - \frac{1}{2}m\omega^2\right) \left(\frac{\sqrt{3}}{2}mga - \frac{5}{2}ma^2\omega^2\right) - \frac{1}{4}m^2a^2\omega^4 &= 0 \\ m^2\omega^4 - m\omega^2 \left(\frac{5k}{2} + \frac{\sqrt{3}mg}{4a}\right) + \frac{\sqrt{3}mgk}{2a} &= 0 \end{aligned}$$

Now, we can write a general quadratic equation as $(x-x_1)(x-x_2) = x^2 + x_1x_2 - x(x_1+x_2) = 0$ where $x_{1(2)} = m\omega_{1(2)}^2$. So, $x_1 + x_2 = 5k/2 + \sqrt{3}mg/4a$, $x_1x_2 = \sqrt{3}mgk/2a$. In the limit of

k being either very large or very small, we expect the frequencies of the two modes to be greatly different. So:

$$\begin{aligned}
 k \gg mg/a &\Rightarrow m(\omega_2)^2 \simeq 5k/2, \quad m(\omega_1)^2 \simeq \frac{\sqrt{3}mgk}{2a} \frac{2}{5k} = \frac{\sqrt{3}mg}{5a} \\
 k \ll mg/a &\Rightarrow m(\omega_2)^2 \simeq \frac{\sqrt{3}mg}{4a}, \quad m(\omega_1)^2 \simeq \frac{\sqrt{3}mgk}{2a} \frac{4a}{\sqrt{3}mg} = 2k
 \end{aligned}$$

Dynamics question 2

The Lagrangian is most easily obtained by first writing down the position and velocity of the mass:

$$\begin{aligned} x &= l \sin \theta & y &= l \cos \theta + a \cos \omega t \\ \dot{x} &= \dot{\theta} l \cos \theta & \dot{y} &= -\dot{\theta} l \sin \theta - a\omega \sin \omega t \end{aligned}$$

The Lagrangian is therefore

$$L = \frac{1}{2}m(\dot{\theta}^2 l^2 + a^2 \omega^2 \sin^2 \omega t + 2a\omega l \dot{\theta} \sin \theta \sin \omega t) - mg(l \cos \theta + a \cos \omega t)$$

Inserting this into the Euler-Lagrange equation, the equation of motion is therefore

$$l^2 \ddot{\theta} + a\omega^2 l \sin \theta \cos \omega t - gl \sin \theta = 0$$

As suggested in the question, we now write $\theta = \theta_1 + C \cos \omega t + S \sin \omega t$ where θ_1 , C and S vary slowly with time. Differentiating,

$$\begin{aligned} \dot{\theta} &= \dot{\theta}_1 + \dot{C} \cos \omega t - C\omega \sin \omega t + \dot{S} \sin \omega t + S\omega \cos \omega t \\ \ddot{\theta} &= \ddot{\theta}_1 + \ddot{C} \cos \omega t - 2\dot{C}\omega \sin \omega t - C\omega^2 \cos \omega t \\ &\quad + \ddot{S} \sin \omega t + 2\dot{S}\omega \cos \omega t - S\omega^2 \sin \omega t \end{aligned}$$

We will next expand $\sin \theta$ using a double angle formula:

$$\begin{aligned} \sin \theta &= \sin \theta_1 \cos(C \cos \omega t + S \sin \omega t) + \cos \theta_1 \sin(C \cos \omega t + S \sin \omega t) \\ &\simeq \sin \theta_1 + \cos \theta_1 (C \cos \omega t + S \sin \omega t) \end{aligned}$$

where the approximation holds for small C, S . We are only interested in the parts of the motion that are slowly varying with time, so we will keep only terms which are either constant or have frequency ω . Therefore, $\cos \omega t \sin \theta \simeq \cos \omega t \sin \theta_1 + \frac{C}{2} \cos \theta_1$ where we have kept the constant part of $\cos^2 \omega t = \frac{1}{2}(1 + \cos 2\omega t)$ and ignored the term proportional to $\cos \omega t \sin \omega t$. Considering first the constant terms in the equation of motion (i.e. the non-sinusoidal terms):

$$l^2 \ddot{\theta}_1 - gl \sin \theta_1 + \frac{1}{2}a\omega^2 l C \cos \theta_1 = 0$$

Next we consider the coefficients of the $\cos \omega t$ and $\sin \omega t$ terms in the equation of motion:

$$\begin{aligned} l^2(\ddot{C} + 2\dot{S}\omega - C\omega^2) + a\omega^2 l \sin \theta_1 - gl C \cos \theta_1 &= 0 \\ l^2(\ddot{S} - 2\dot{C}\omega - S\omega^2) - gl S \cos \theta_1 &= 0 \end{aligned}$$

Because C and S vary slowly with time we will set their time derivatives equal to zero, and the above pair of equations become

$$\begin{aligned} -Cl^2\omega^2 - gl C \cos \theta_1 &= -a\omega^2 l \sin \theta_1 \\ -Sl^2\omega^2 - gl S \cos \theta_1 &= 0 \end{aligned}$$

These equations can be solved to find $S = 0$ and

$$C = \frac{a\omega^2 \sin \theta_1}{\omega^2 l + g \cos \theta_1}$$

At this point, we make use of $\omega^2 \gg g/l$, to infer that $C \simeq a \sin \theta_1/l$. Finally, we substitute these expressions for C and S into the equation arising from considering the coefficients of the constant terms in the equation of motion:

$$\ddot{\theta}_1 + \sin \theta_1 \left(-\frac{g}{l} + \frac{a\omega^2}{2l} \frac{a \cos \theta_1}{l} \right) = 0$$

When the inverted pendulum is upright, $\theta = 0$ and $\cos \theta_1 \simeq 1$, $\sin \theta_1 \simeq \theta_1$. The above equation then becomes that for a simple harmonic oscillator:

$$\ddot{\theta}_1 + \theta_1 \left(\frac{a^2\omega^2}{2l^2} - \frac{g}{l} \right) = 0$$

from which the period of oscillation is easily found. The upright position is stable if the term in brackets is positive (compare this to a standard SHM equation $\ddot{\theta} + \omega^2\theta = 0$ which comes about due to a restoring force like $-kx$ for a mass on a spring, say. If the position $\theta = 0$ is stable, the force acting when we move away from this position must be a restoring force). Consequently,

$$\frac{a^2\omega^2}{2l^2} > \frac{g}{l} \Rightarrow \omega^2 > \frac{2gl}{a^2}$$

Dynamics question 3

The Lagrangian is

$$L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - \frac{1}{2}kr^2$$

The conjugate momenta are thus

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r} \qquad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta} \quad (\ddagger)$$

The Hamiltonian, written in terms of these canonical momenta, is then

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\theta^2}{r^2} \right) + \frac{1}{2}kr^2$$

At this point, we re-express the Hamiltonian in terms of the generalised coordinates $q_1 = r$ and $q_2 = mr^2\dot{\theta}$ - that is, we relabel the terms as follows:

$$r \rightarrow q_1 \qquad p_r \rightarrow p_1 \quad (*)$$

$$\theta \rightarrow -p_2 \qquad p_\theta \rightarrow q_2 \quad (\dagger)$$

This gives:

$$H = \frac{1}{2m} \left(p_1^2 + \frac{q_2^2}{q_1^2} \right) + \frac{1}{2}kq_1^2$$

The equations of motion derived from this Hamiltonian are:

$$\begin{aligned} \dot{p}_1 &= \frac{q_2^2}{mq_1^3} - kq_1 & \dot{q}_1 &= \frac{p_1}{m} \\ \dot{p}_2 &= -\frac{q_2}{mq_1^2} & \dot{q}_2 &= 0 \end{aligned}$$

Do these equations correspond to the expected motion? We can find out by appropriately using (\ddagger) , $(*)$ and (\dagger) with the above equations:

$$\begin{aligned} p_1 \text{ equation :} \qquad \dot{p}_1 &= m\ddot{r} & (\text{using } (*)) \\ &= \frac{q_2^2}{mq_1^3} - kq_1 \\ &= \frac{p_\theta^2}{mr^3} - kr & (\text{using } (*) \text{ and } (\dagger)) \\ \implies m\ddot{r} &= mr\dot{\theta}^2 - kr & (\text{using } (\ddagger)) \end{aligned}$$

This is the correct radial equation of motion - the rate of change of radial momentum is given by a centrifugal force term ($mr\dot{\theta}^2$) plus the contribution from the central potential ($-kr$). ✓

$$\begin{aligned} q_2 \text{ equation :} \qquad \dot{q}_2 &= \dot{p}_\theta & (\text{using } (\dagger)) \\ &= 0 \end{aligned}$$

This is the correct angular equation. It corresponds to the statement that angular momentum is conserved, which is true for the given central potential. ✓

The other two equations simply give back the definitions of q_2 and p_1 in terms of $q_1 (= r)$ and $p_2 (= -\theta)$.

Dynamics question 4

Advantages of the Hamiltonian formulation over the Lagrangian formulation include:

- The Lagrangian formulation leads to N second order differential equations while the Hamiltonian formulation leads to $2N$ first order differential equations, which may be easier to solve.
- The q_i in the Lagrangian formulation must be position co-ordinates, whereas in the Hamiltonian formulation the q_i and p_i are on an equal footing and the q_i need not be position co-ordinates. This also means that canonical transformations with mixed momenta and position can be used to greatly simplify Hamilton's equations. (This will be illustrated later in this question).
- The Hamiltonian formulation can lead to easily identifiable constants of motion (for example, if H is independent of t then energy is conserved). The presence of a conserved quantity immediately simplifies Hamilton's equations, whereas no immediate simplification would occur in the Lagrangian formulation.
- There is a simple relationship between the (classical) Hamiltonian formulation and quantum mechanics.

Starting from the Hamiltonian

$$H(q, p, t) = p\dot{q} - L(q, \dot{q}, t)$$

we find the differential dH and substitute using the Euler-Lagrange equation:

$$\begin{aligned} dH &= \frac{\partial H}{\partial p} dp + \frac{\partial H}{\partial q} dq + \frac{\partial H}{\partial t} dt \\ &= p d\dot{q} + \dot{q} dp - \frac{\partial L}{\partial q} dq - \frac{\partial L}{\partial \dot{q}} d\dot{q} - \frac{\partial L}{\partial t} dt \\ &= \dot{q} dp - p dq - \frac{\partial L}{\partial t} dt. \end{aligned}$$

Comparing the first and third lines therefore gives Hamilton's equations,

$$\dot{q} = \frac{\partial H}{\partial p}, \quad -\dot{p} = \frac{\partial H}{\partial q}, \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}.$$

We then write the first two of Hamilton's equations in matrix form,

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{pmatrix}$$

and note that our co-ordinate transformation means that

$$\begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix} = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix}, \quad \begin{pmatrix} \frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{pmatrix} = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial P} \end{pmatrix}$$

and so

$$\begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix} = \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial P} \end{pmatrix}.$$

Performing one of the matrix multiplications, we then note that for Hamilton's equations to be obeyed in the Q, P co-ordinates we require

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} -\frac{\partial Q}{\partial p} & \frac{\partial Q}{\partial q} \\ -\frac{\partial P}{\partial p} & \frac{\partial P}{\partial q} \end{pmatrix} \begin{pmatrix} \frac{\partial Q}{\partial q} & \frac{\partial P}{\partial q} \\ \frac{\partial Q}{\partial p} & \frac{\partial P}{\partial p} \end{pmatrix}.$$

The 2,1 element of this matrix equation then tells us that

$$-1 = -\frac{\partial P}{\partial p} \frac{\partial Q}{\partial q} + \frac{\partial P}{\partial q} \frac{\partial Q}{\partial p} = -\{Q, P\}_{q,p}$$

as required.

For the co-ordinate transformation given in the question,

$$\frac{\partial Q}{\partial q} = \frac{m\omega p}{p^2 + (m\omega q)^2}, \quad \frac{\partial Q}{\partial p} = \frac{-m\omega q}{p^2 + (m\omega q)^2}, \quad \frac{\partial P}{\partial q} = m\omega q, \quad \frac{\partial P}{\partial p} = \frac{p}{m\omega}$$

from which it follows that the above Poisson bracket holds. Now, the inverse co-ordinate transform is

$$\begin{aligned} p &= \sqrt{2m\omega P} \cos Q \\ q &= \frac{\sqrt{2m\omega P}}{m\omega} \sin Q \end{aligned}$$

so in the Q, P co-ordinate system the Hamiltonian for the simple harmonic oscillator is $H = \omega P$. Hamilton's equations are then

$$\dot{Q} = \frac{\partial H}{\partial P} = \omega, \quad -\dot{P} = \frac{\partial H}{\partial Q} = 0$$

the solutions to which are

$$Q = \omega t + \alpha, \quad P = \beta$$

for some constants α, β . Finally, we rewrite this solution in the q, p co-ordinate system:

$$q = \frac{\sqrt{2m\omega\beta}}{m\omega} \sin(\omega t + \alpha), \quad p = \sqrt{2m\omega\beta} \cos(\omega t + \alpha)$$

which is the familiar solution for a simple harmonic oscillator.

Dynamics question 5

Given the definition of the Lagrangian $L = T - V$ we immediately obtain the conjugate momenta

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

given that $V = V_1(\mathbf{q}) + a_i \dot{q}_i$. Then,

$$\dot{q}_i p_i = -a_i \dot{q}_i + \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = 2T - a_i \dot{q}_i \quad (\text{summation over } i \text{ is implied})$$

where we have assumed that the kinetic energy T depends quadratically on the \dot{q}_i : if $T = k_i \dot{q}_i^2$ for some coefficients k_i , then $\frac{\partial T}{\partial \dot{q}_i} = 2k_i \dot{q}_i$ so $\dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = 2k_i \dot{q}_i^2 = 2T$. The Hamiltonian is then

$$H = \dot{q}_i p_i - L = 2T - a_i \dot{q}_i - T + V = T + V_1$$

If we understand H as the total energy of the Lagrangian system, hence as a function of \mathbf{q} and $\dot{\mathbf{q}}$, we realise that the velocity-dependent part of the potential does not appear explicitly. The total energy of the system can be obtained by simply measuring the kinetic energy and the position-dependent part of the potential, $V_1(\mathbf{q})$.

However, this does not mean that Hamilton's equations of motion are independent of the velocity-dependent part of the potential! Before we are allowed to use H in Hamilton's equations, we *must* complete the Legendre transformation from the Lagrangian formalism (L as a function of \mathbf{q} and $\dot{\mathbf{q}}$) to the Hamiltonian formalism (H as a function of \mathbf{q} and \mathbf{p}). In order to do so, we ought to invert the expression for the conjugate momenta above

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i} - a_i = 2k_i \dot{q}_i - a_i \quad \rightarrow \quad \dot{q}_i = \frac{p_i + a_i}{2k_i}$$

and obtain \dot{q}_i as a function of p_i . We then substitute the new expression wherever \dot{q}_i appears in H . This completes the Legendre transform and we arrive at an expression for H in terms of \mathbf{q} , \mathbf{p} and other constants, but without any \dot{q}_i . Ipso facto, we are finally allowed to describe the dynamics of the system using Hamilton's equations:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i},$$

and we clearly see that velocity-dependent part of the potential explicitly appears in the Hamiltonian formulation through the change of variable from $\dot{\mathbf{q}}$ to the conjugate momenta \mathbf{p} .

Dynamics question 6

Consider translating the co-ordinate such that $x \rightarrow x + \delta x$. This will change the Hamiltonian by δH , so for invariance under this translation we require $\delta H = 0$. Thus:

$$\begin{aligned}\delta H &= \sum \delta x \frac{\partial H}{\partial x} \\ &= - \sum \dot{p} \delta x\end{aligned}$$

where we have used one of Hamilton's equations to obtain the \dot{p}_i term, and the summation is over all of the particles in the system. Because the perturbation $\delta x \neq 0$, $\sum \dot{p} = 0$ and so $\sum p$ is constant.

Dynamics question 7

Using the magnetic vector potential suggested in the question, $\mathbf{A} = (-By, 0, 0)$, the Lagrangian is

$$\begin{aligned} L &= \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - e(\phi - v_i A_i) \\ &= \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - eBy\dot{x} \end{aligned}$$

The conjugate momenta are

$$p_x = m\dot{x} - eBy, \quad p_y = m\dot{y}, \quad p_z = m\dot{z}$$

and so the Hamiltonian is

$$\begin{aligned} H &= p_i \dot{q}_i - L = m\dot{x}^2 - eBy\dot{x} + m\dot{y}^2 + m\dot{z}^2 - L \\ &= \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \\ &= \frac{(p_x + eBy)^2 + p_y^2 + p_z^2}{2m} \end{aligned}$$

We then use Hamilton's equations to find

$$\dot{p}_y = -\frac{eB}{m}(p_x + eBy), \quad \dot{x} = \frac{p_x + eBy}{m}, \quad \dot{y} = \frac{p_y}{m}, \quad \dot{p}_x = 0$$

The solution to the equation for p_x is of course $p_x = \text{constant}$. We can write this as $p_x = -eBy_0$, where y_0 is a constant with dimensions of length. Inserting this solution into the equation of motion for p_y , which we in turn insert into the equation of motion for y differentiated with respect to time, we obtain:

$$\ddot{y} + \frac{e^2 B^2}{m^2}(y - y_0) = 0$$

which is SHM about y_0 at a frequency of $\omega_L = eB/m$. Consequently, $y = y_0 + a \sin(\omega_L t + \varphi_0)$. We next consider the behaviour of x :

$$\dot{x} = \frac{eB}{m} \left(\frac{p_x}{eB} + y \right) = eB \left(\frac{y - y_0}{m} \right) = eB \left(\frac{a \sin \omega_L t}{m} \right)$$

so $x = x_0 - a \cos(\omega_L t + \varphi_0)$. We are told that the ion is projected into the xy plane, so $z = 0$. Putting together the x, y and z components of the motion, we see that the complete solution for the motion of the system is circular motion in the xy plane, with angular velocity $\omega = eB/m$.

The Hamiltonian of this question is not invariant under a displacement in the y direction (a dependence on y is introduced via B). Consequently the momentum conservation law derived in the previous question does not apply in the y direction - $p_y \equiv m\dot{y}$ is not conserved. The Hamiltonian is invariant under x translations, so p_x is invariant - however, it should be

emphasised that this quantity is the *canonical* x momentum, not the mechanical x momentum $m\dot{x}$. In general the two are not the same, and in the present context we see that $p_x = m\dot{x} - eBy$ - so it is this that is conserved. As we intuitively expected, neither $m\dot{x}$ nor $m\dot{y}$ are conserved (except in the special case $\dot{x} = 0, \dot{y} = 0$).

It should be noted, however, that the total momentum is conserved, if we include the momentum density of the electromagnetic field.

Dynamics question 8

Given a scalar function $f = f(q_i, p_i, t)$,

$$\frac{df}{dt} = \frac{\partial f}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial f}{\partial p_i} \frac{dp_i}{dt} + \frac{\partial f}{\partial t}$$

Using Hamilton's equations,

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) = \frac{\partial f}{\partial t} + \{f, H\}$$

For a vector function $A(\mathbf{x})$,

$$\{p_j, A_k\} = \frac{\partial p_j}{\partial q_i} \frac{\partial A_k}{\partial p_i} - \frac{\partial p_j}{\partial p_i} \frac{\partial A_k}{\partial q_i} = -\delta_{ij} \frac{\partial A_k}{\partial q_i} = -\frac{\partial A_k}{\partial x_j}$$

The analogy between the classical Poisson bracket and quantum mechanical commutators is that $\{f, g\} \rightarrow [\hat{f}, \hat{g}]/i\hbar$, so $[\hat{p}_j, \hat{A}_k] = -i\hbar \frac{\partial A_k}{\partial x_j}$.

The Lagrangian for an electron in a magnetic field is $L = \frac{1}{2}m\dot{x}^2 + e(\phi - v_i A_i)$ (n.b. charge $q = -e$), so the classical Hamiltonian is

$$H = \frac{(\mathbf{p} + e\mathbf{A})^2}{2m} - e\phi$$

and the quantum mechanical Hamiltonian is

$$H = \frac{1}{2m} \left(\hat{p}^2 + e^2 \hat{A}^2 + e\hat{A}_i \hat{p}_i + e\hat{p}_i \hat{A}_i \right) - e\hat{\phi}$$

It is important to note that the \hat{p}_i in the final term in the brackets above acts on both \hat{A}_i AND the wavefunction.

Consider the action of this term on the wavefunction ψ :

$$e\hat{p}_i(\hat{A}_i\psi) = e\hat{A}_i(p_i\psi) + e[\hat{p}_i, \hat{A}_i]\psi$$

Now:

$$\begin{aligned} [\hat{p}_i, \hat{A}_i] &= -i\hbar \frac{\partial A_i}{\partial x_i} && \text{using equation for commutator derived earlier} \\ &= -i\hbar \nabla \cdot \mathbf{A} = 0 && \text{using } \nabla \cdot \mathbf{A} = 0 \end{aligned}$$

Therefore $e\hat{p}_i(\hat{A}_i\psi) = e\hat{A}_i(p_i\psi)$, and the final QM Hamiltonian is:

$$H = -\frac{\hbar^2 \nabla^2}{2m} + \frac{e^2 A^2}{2m} - \frac{i\hbar e}{m} \mathbf{A} \cdot \nabla - e\phi$$

The Schrödinger equation is simply $H\psi = i\hbar \dot{\psi}$.

Dynamics question 9

The Lagrangian is just the potential energy U subtracted from the kinetic energy of the mass M and the sum of the kinetic energies of the n particles with mass m :

$$L = \frac{M\dot{\mathbf{R}}^2}{2} + \frac{m}{2} \sum_{i=1}^n \dot{\mathbf{R}}_i^2 - U$$

The fact that the centre of mass of the system is fixed gives us the holonomic constraint $M\mathbf{R} + \sum_{i=1}^n m\mathbf{R}_i = 0$ (taking the centre of mass of the system to be at the origin). If we switch to the relative co-ordinate system $\mathbf{r}_\alpha = \mathbf{R}_\alpha - \mathbf{R}$ the constraint can be written:

$$(M + nm)\mathbf{R} + m \sum_i \mathbf{r}_i = 0$$

$$\mathbf{R} = \frac{-m}{M + nm} \sum_i \mathbf{r}_i$$

Given the form of the Lagrangian, we want to find expressions for $\dot{\mathbf{R}}^2$ and $\sum \dot{\mathbf{R}}_i^2$:

$$\dot{\mathbf{R}}^2 = \frac{m^2}{(M + nm)^2} \left(\sum \dot{\mathbf{r}}_i \right)^2$$

$$\sum \dot{\mathbf{R}}_i^2 = \sum \left(\dot{\mathbf{R}} + \dot{\mathbf{r}}_i \right)^2 = \sum \left(\dot{\mathbf{R}}^2 + \dot{\mathbf{r}}_i^2 + 2\dot{\mathbf{R}} \cdot \dot{\mathbf{r}}_i \right)$$

The Lagrangian is now

$$L = \frac{M\dot{\mathbf{R}}^2}{2} + \frac{m}{2} \sum \dot{\mathbf{R}}^2 + \frac{m}{2} \sum \dot{\mathbf{r}}_i^2 + m \sum \dot{\mathbf{r}}_i \cdot \dot{\mathbf{R}} - U$$

We can move the $\dot{\mathbf{R}}^2$ terms outside of the sums, and arrive at

$$L = \frac{\dot{\mathbf{R}}^2}{2} (M + nm) + \frac{m}{2} \sum \dot{\mathbf{r}}_i^2 - \frac{m^2}{M + nm} \left(\sum \dot{\mathbf{r}}_i \right)^2 - U$$

$$= -\frac{1}{2} \frac{m^2}{M + nm} \left(\sum \dot{\mathbf{r}}_i \right)^2 + \frac{m}{2} \sum \dot{\mathbf{r}}_i^2 - U$$

The conjugate momenta are

$$\mathbf{p}_\alpha = m\dot{\mathbf{r}}_\alpha - \frac{m^2}{M + nm} \sum_\beta \dot{\mathbf{r}}_\beta$$

Summing the expression for the conjugate momenta over α ,

$$\begin{aligned} \sum \mathbf{p}_\alpha &= m \sum \mathbf{v}_\alpha - \frac{nm^2}{M + nm} \sum \mathbf{v}_\alpha \\ &= \frac{(Mm + nm^2) \sum \mathbf{v}_\alpha - nm^2 \sum \mathbf{v}_\alpha}{M + nm} \\ &= \frac{mM}{M + nm} \sum \mathbf{v}_\alpha \end{aligned}$$

where $\mathbf{v}_\alpha = \dot{\mathbf{r}}_\alpha$. Thus,

$$\mathbf{v}_\alpha = \frac{\mathbf{p}_\alpha}{m} + \frac{m^2}{M + nm} \frac{M + nm}{Mm} \sum \mathbf{p}_\beta = \frac{\mathbf{p}_\alpha}{m} + \frac{\sum \mathbf{p}_\beta}{M}$$

The Hamiltonian is then

$$H = \frac{\sum p_i^2}{m} + \frac{(\sum \mathbf{p}_i)^2}{M} - \frac{m}{2} \sum v_i^2 + \frac{m^2}{2} \frac{(\sum \mathbf{v}_i)^2}{M + nm} + U$$

but

$$\left(\sum \mathbf{v}_\alpha \right)^2 = \left(\frac{M + nm}{Mm} \right)^2 \left(\sum \mathbf{p}_\alpha \right)^2$$

so

$$\frac{m^2}{2} \frac{(\sum \mathbf{v}_i)^2}{M + nm} = \frac{(\sum \mathbf{p}_\alpha)^2}{2} \frac{M + nm}{M^2}$$

We next want to evaluate $\sum v_\alpha^2$:

$$\begin{aligned} v_\alpha^2 &= \frac{\mathbf{p}_\alpha^2}{m^2} + \frac{(\sum \mathbf{p}_\beta)^2}{M^2} + \frac{2\mathbf{p}_\alpha \cdot \sum \mathbf{p}_\beta}{mM} \\ \sum v_\alpha^2 &= \frac{\sum \mathbf{p}_\alpha^2}{m^2} + \frac{n(\sum \mathbf{p}_\alpha)^2}{M^2} + \frac{2(\sum \mathbf{p}_\alpha)^2}{mM} \end{aligned}$$

Inserting all of these terms into the earlier expression for the Hamiltonian, a little algebra leads us to conclude that

$$H = \frac{\sum \mathbf{p}_\alpha^2}{2m} + \frac{(\sum \mathbf{p}_\alpha)^2}{2M} + U$$

Dynamics question 10

The Lagrangian is

$$L = \frac{1}{2}mv^2 - q(\phi - v_i A_i)$$

so the conjugate momenta are

$$p_i = mv_i + qA_i$$

and the Hamiltonian is

$$\begin{aligned} H = p_i \dot{q}_i - L &= (mv_i + qA_i)v_i - \frac{1}{2}mv^2 + q(\phi - v_i A_i) \\ &= \frac{1}{2}mv^2 + q\phi \\ &= \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + q\phi \end{aligned}$$

We will use $\phi = -Ex$ and $\mathbf{A} = (0, Bx, 0)$ which gives $\mathbf{E} = -\nabla\phi = (E, 0, 0)$ and $\mathbf{B} = \nabla \times \mathbf{A} = (0, 0, B)$. For this choice of potentials, the Hamiltonian becomes

$$H = \frac{1}{2m} (p_x^2 + (p_y - qBx)^2 + p_z^2) - qEx$$

Using Hamilton's equations,

$$\begin{aligned} \dot{p}_x &= \frac{qB}{m}(p_y - qBx) + qE \\ \dot{p}_y &= \dot{p}_z = 0 \\ \dot{x} &= \frac{p_x}{m} \\ \dot{z} &= \frac{p_z}{m} \\ \dot{y} &= \frac{p_y - qBx}{m} \end{aligned}$$

from which we see

$$\begin{aligned} \ddot{x} = \frac{\dot{p}_x}{m} &= \frac{qBp_y}{m^2} - \frac{q^2 B^2 x}{m^2} + \frac{qE}{m} \\ \ddot{x} + \omega_0^2 x &= \frac{qBp_y}{m^2} + \frac{qE}{m} \end{aligned}$$

where $\omega_0 = qB/m$. If we assume a solution of the form $x = A \sin(\omega_0 t) + c$, $\ddot{x} = -\omega_0^2(x - c)$ so

$$-\omega_0^2(x - c) + \omega_0^2 x = \omega_0^2 c = \frac{qBp_y}{m^2} + \frac{qE}{m} = \frac{\omega_0 p_y}{m} + \frac{\omega_0 E}{B}$$

and thus $c = \frac{p_y}{m\omega_0} + \frac{E}{B\omega_0}$. We can then substitute this solution for x into the \dot{y} equation:

$$\begin{aligned} \dot{y} &= \frac{p_y}{m} - \frac{qB}{m} A \sin(\omega_0 t) - \left(\frac{p_y}{m\omega_0} + \frac{E}{B\omega_0} \right) \frac{qB}{m} \\ &= -\omega_0 A \sin(\omega_0 t) - \frac{E}{B} \end{aligned}$$

which integrates to give

$$y = A \cos(\omega_0 t) - \frac{Et}{B} + C$$

The particle therefore undergoes helical motion, but with an added drift in the $-y$ direction at speed E/B .

Dynamics question 11

In relativistic dynamics, the Lagrangian for a particle moving in 1D is

$$L = \frac{-m_0 c^2}{\gamma} - V$$

so the conjugate momentum is

$$\begin{aligned} p &= \frac{\partial L}{\partial v} = -m_0 c^2 \frac{\partial}{\partial v} \left(\sqrt{1 - v^2/c^2} \right) \\ &= (-m_0 c^2) \left(-\frac{2v}{c^2} \right) \left(\frac{1}{2} \right) \gamma \\ &= m_0 v \gamma \end{aligned}$$

The Hamiltonian is then

$$\begin{aligned} H &= p\dot{q} - L = m_0 \gamma v^2 + \frac{m_0 c^2}{\gamma} + V \\ &= m_0 \left(\frac{v^2}{\sqrt{1 - v^2/c^2}} + \frac{c^2(1 - v^2/c^2)}{\sqrt{1 - v^2/c^2}} \right) + V \\ &= \gamma m_0 c^2 + V \end{aligned}$$

Dynamics question 12

The Lagrangian for a charged relativistic particle in a magnetic field is

$$L = \frac{-m_0 c^2}{\gamma} - e(\phi - v_i A_i) = -m_0 c^2 \left(1 - \frac{v_x^2 + v_y^2 + v_z^2}{c^2} \right)^{1/2} - e(\phi - v_i A_i)$$

The conjugate momenta are

$$\begin{aligned} p_i &= -m_0 c^2 \cdot \frac{1}{2} \cdot -\frac{2v_i}{c^2} \cdot \gamma + eA_i \\ &= m_0 v_i \gamma + eA_i \end{aligned}$$

The Hamiltonian is therefore

$$\begin{aligned} H = p_i \dot{q}_i - L &= m_0 v^2 \gamma + e v_i A_i + \frac{m_0 c^2}{\gamma} + e(\phi - v_i A_i) \\ &= \gamma m_0 c^2 + e\phi \end{aligned}$$

where we have made use of the fact that $\gamma c^2 = v^2 \gamma + c^2/\gamma$. One can then easily rewrite the Hamiltonian in terms of the conjugate momenta

$$H = m_0 c^2 \sqrt{1 + \frac{(\mathbf{p} - e\mathbf{A})^2}{m_0^2 c^2}} + e\phi$$

This shows us that the vector potential \mathbf{A} is still explicitly present in the Hamiltonian.

Dynamics question 13

The question tells us that

$$L = \int \left(-\frac{dm_0 c^2}{\gamma} \right), \quad dm_0 = \rho_0 r \, dr \, d\theta$$

The θ integral is trivial to perform, and remembering that $v = r\omega$,

$$\begin{aligned} L &= 2\pi c^2 \rho_0 \int_0^a -r \left(1 - \frac{\omega^2 r^2}{c^2} \right)^{1/2} dr \\ &= 2\pi \rho_0 c^2 \left[\frac{1}{3} \left(1 - \frac{\omega^2 r^2}{c^2} \right)^{3/2} \frac{c^2}{\omega^2} \right]_0^a \\ &= \frac{2\pi \rho_0 c^4}{3\omega^2} \left[\left(1 - \frac{\omega^2 a^2}{c^2} \right)^{3/2} - 1 \right] \end{aligned}$$

We then find the angular momentum via $J = \frac{\partial L}{\partial \omega}$. Let us define $\alpha = 2\pi \rho_0 c^4/3$ and $\beta^2 = a^2/c^2$. Then

$$\begin{aligned} J &= \frac{\partial}{\partial \omega} \left(\frac{\alpha}{\omega^2} \left[(1 - \beta^2 \omega^2)^{3/2} - 1 \right] \right) \\ &= -\frac{2\alpha}{\omega^3} \left[(1 - \beta^2 \omega^2)^{3/2} - 1 \right] + \frac{\alpha \omega}{\omega^3} \left[-2\omega \beta^2 \frac{3}{2} (1 - \beta^2 \omega^2)^{1/2} \right] \\ &= \frac{2\alpha}{\omega^3} \left[1 - \left(1 + \frac{\beta^2 \omega^2}{2} \right) (1 - \beta^2 \omega^2)^{1/2} \right] \end{aligned}$$

But the mass of the disk is $M_0 = \rho_0 \pi a^2$, so remembering the original definitions of α and β :

$$J = \frac{4M_0 c^4}{3a^2 \omega^3} \left[1 - \sqrt{1 - \frac{a^2 \omega^2}{c^2}} \left(1 + \frac{a^2 \omega^2}{2c^2} \right) \right]$$

(You should check that this gives the expected result $\frac{1}{2} M_0 a^2 \omega$ in the non-relativistic limit.)

Field Theory question 1

We will use a Lagrange multiplier field $\lambda \equiv \lambda(x, y)$ to extremise $S = \int dx dy |Q|^\alpha$, where \mathbf{Q} is a 2D vector field, subject to the constraint $\nabla \cdot \mathbf{Q} = R(x, y)$. We will thus consider extremising

$$S' = \int dx dy \mathcal{L} = \int dx dy \left[(Q_x^2 + Q_y^2)^{\alpha/2} + \lambda(\nabla \cdot \mathbf{Q} - R) \right]$$

The generalised form of the Euler-Lagrange equations appropriate here is

$$\frac{\partial \mathcal{L}}{\partial Q_i} - \frac{\partial}{\partial x} \left(\frac{\partial \mathcal{L}}{\partial (\partial_x Q_i)} \right) - \frac{\partial}{\partial y} \left(\frac{\partial \mathcal{L}}{\partial (\partial_y Q_i)} \right) = 0$$

Remembering that $\nabla \cdot \mathbf{Q} = \partial_x Q_x + \partial_y Q_y$, the equation for Q_x is

$$\alpha Q_x (Q_x^2 + Q_y^2)^{\alpha/2-1} - \frac{\partial \lambda}{\partial x} = 0$$

with an entirely equivalent equation for Q_y . Using the relation $Q^{\alpha-2} = (Q^{\alpha/2-1})^2$, this is

$$\frac{\partial \lambda}{\partial x} = \alpha Q_x Q^{\alpha-2}$$

with an equivalent formula for y .

Field Theory question 2

The Klein-Gordon Lagrangian density is

$$\mathcal{L} = \frac{1}{2} \left[\hbar^2 \left(\frac{\partial \varphi}{\partial t} \right)^2 - \hbar^2 c^2 (\nabla \varphi)^2 - m_0^2 c^4 \varphi^2 \right]$$

The conjugate momentum density is then

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} = \hbar^2 \dot{\varphi}$$

The generalised Euler-Lagrange equation is

$$\frac{\partial \mathcal{L}}{\partial \varphi} - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\varphi}} \right) - \frac{\partial}{\partial x_i} \left(\frac{\partial \mathcal{L}}{\partial (\partial_{x_i} \varphi)} \right) = 0$$

so using the above Lagrangian density,

$$-m_0^2 c^4 \varphi - \hbar^2 \ddot{\varphi} + \hbar^2 c^2 \nabla^2 \varphi = 0$$

and the Hamiltonian density is

$$\begin{aligned} \mathcal{H} &= \pi \dot{\varphi} - \mathcal{L} = \hbar^2 \dot{\varphi}^2 - \frac{1}{2} [\hbar^2 \dot{\varphi}^2 - \hbar^2 c^2 (\nabla \varphi)^2 - m_0^2 c^4 \varphi^2] \\ &= \frac{1}{2} \left[\frac{\pi^2}{\hbar^2} + \hbar^2 c^2 (\nabla \varphi)^2 + m_0^2 c^4 \varphi^2 \right] \end{aligned}$$

Field Theory question 3

$$\mathcal{L} = \frac{\hbar}{2i} \left(\Psi \frac{\partial \Psi^*}{\partial t} - \Psi^* \frac{\partial \Psi}{\partial t} \right) - \frac{\hbar^2}{2m} \nabla \Psi \cdot \nabla \Psi^* - V(\mathbf{r}) \Psi^* \Psi$$

The Euler-Lagrange equation for Ψ is

$$\frac{\partial \mathcal{L}}{\partial \Psi} - \nabla \left(\frac{\partial \mathcal{L}}{\partial (\nabla \Psi)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial (\partial \Psi / \partial t)} \right) = 0$$

which gives

$$\frac{\hbar}{2i} \frac{\partial \Psi^*}{\partial t} - V \Psi^* + \frac{\hbar^2}{2m} \nabla^2 \Psi^* - \frac{\partial}{\partial t} \left(-\frac{\hbar}{2i} \Psi^* \right) = 0$$

and hence

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V \Psi^*$$

which is the complex conjugate of the Schrödinger equation. Similarly the Euler-Lagrange equation for Ψ^* is

$$\frac{\partial \mathcal{L}}{\partial \Psi^*} - \nabla \left(\frac{\partial \mathcal{L}}{\partial (\nabla \Psi^*)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial (\partial \Psi^* / \partial t)} \right) = 0$$

which gives

$$-\frac{\hbar}{2i} \frac{\partial \Psi}{\partial t} - V \Psi + \frac{\hbar^2}{2m} \nabla^2 \Psi - \frac{\partial}{\partial t} \left(\frac{\hbar}{2i} \Psi \right) = 0$$

and hence the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi .$$

The momentum density conjugate to Ψ is

$$\Pi = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} = \frac{1}{2} i\hbar \Psi^*$$

while that conjugate to Ψ^* is

$$\Pi^* = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}^*} = -\frac{1}{2} i\hbar \Psi .$$

Thus the Hamiltonian density is

$$\mathcal{H} = \Pi \dot{\Psi} + \Pi^* \dot{\Psi}^* - \mathcal{L} = \frac{\hbar^2}{2m} \nabla \Psi \cdot \nabla \Psi^* + V \Psi^* \Psi .$$

The integral of this over all space is

$$H = \int d^3\mathbf{r} \mathcal{H} = \int d^3\mathbf{r} \left(\frac{\hbar^2}{2m} \nabla \Psi \cdot \nabla \Psi^* + V \Psi^* \Psi \right) .$$

Integrating the first term by parts, the integrated piece is zero since the field must vanish at infinity, so

$$\begin{aligned} H &= \int d^3\mathbf{r} \left(-\frac{\hbar^2}{2m} (\nabla^2 \Psi) \Psi^* + V(\mathbf{r}) \Psi^* \Psi \right) \\ &= \int d^3\mathbf{r} \Psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi , \end{aligned}$$

which is the usual expression for the expectation value of the energy.

Field Theory question 4

$$\mathcal{L} = \frac{\partial \varphi^*}{\partial t} \frac{\partial \varphi}{\partial t} - \nabla \varphi^* \nabla \varphi - m^2 \varphi^* \varphi .$$

(a) The momentum density conjugate to φ is

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} = \frac{\partial \varphi^*}{\partial t}$$

Similarly the momentum density conjugate to φ^* is

$$\pi^* = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}^*} = \frac{\partial \varphi}{\partial t}$$

We must treat φ and φ^* as independent fields, so

$$\mathcal{H} = \pi \dot{\varphi} + \pi^* \dot{\varphi}^* - \mathcal{L} = \pi^* \pi + \nabla \varphi^* \nabla \varphi + m^2 \varphi^* \varphi .$$

(b) We have

$$\begin{aligned} \varphi(\mathbf{r}, t) &= \int \frac{d^3 \mathbf{k}}{2(2\pi)^3 \omega} \left[a(\mathbf{k}) e^{-ik \cdot x} + b^*(\mathbf{k}) e^{ik \cdot x} \right] \\ \varphi^*(\mathbf{r}, t) &= \int \frac{d^3 \mathbf{k}'}{2(2\pi)^3 \omega'} \left[a^*(\mathbf{k}') e^{ik' \cdot x} + b(\mathbf{k}') e^{-ik' \cdot x} \right] \end{aligned}$$

where (natural units) $k \cdot x = \omega t - \mathbf{k} \cdot \mathbf{r}$ etc. Therefore

$$\begin{aligned} \varphi^* \varphi &= \int \frac{d^3 \mathbf{k} d^3 \mathbf{k}'}{4(2\pi)^6 \omega \omega'} \left[a(\mathbf{k}) a^*(\mathbf{k}') e^{-i(k-k') \cdot x} + b^*(\mathbf{k}) a^*(\mathbf{k}') e^{+i(k+k') \cdot x} \right. \\ &\quad \left. + a(\mathbf{k}) b(\mathbf{k}') e^{-i(k+k') \cdot x} + b^*(\mathbf{k}) b(\mathbf{k}') e^{+i(k-k') \cdot x} \right] , \end{aligned}$$

where for example

$$\begin{aligned} \int d^3 \mathbf{r} a(\mathbf{k}) a^*(\mathbf{k}') e^{-i(k-k') \cdot x} &= \int d^3 \mathbf{r} a(\mathbf{k}) a^*(\mathbf{k}') e^{-i[(\omega-\omega')t - (\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}]} \\ &= (2\pi)^3 a(\mathbf{k}) a^*(\mathbf{k}') e^{-i(\omega-\omega')t} \delta^3(\mathbf{k}-\mathbf{k}') \end{aligned}$$

and therefore

$$\int d^3 \mathbf{r} \frac{d^3 \mathbf{k} d^3 \mathbf{k}'}{4(2\pi)^6 \omega \omega'} a(\mathbf{k}) a^*(\mathbf{k}') e^{-i(k-k') \cdot x} = \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega^2} a(\mathbf{k}) a^*(\mathbf{k})$$

where we have used the fact that $\omega = \omega'$ when $\mathbf{k} = \pm \mathbf{k}'$. Proceeding similarly with the other terms, we have

$$\int d^3 \mathbf{r} \varphi^* \varphi = \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega^2} \left[|a(\mathbf{k})|^2 + |b(\mathbf{k})|^2 + a(\mathbf{k}) b(-\mathbf{k}) e^{-2i\omega t} + b^*(\mathbf{k}) a^*(-\mathbf{k}) e^{+2i\omega t} \right] .$$

For the other terms in \mathcal{H} , we need

$$\begin{aligned}\frac{\partial \varphi}{\partial t} &= \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \left[-ia(\mathbf{k})e^{-ik \cdot x} + ib^*(\mathbf{k})e^{+ik \cdot x} \right] \\ \nabla \varphi &= \int \frac{d^3 \mathbf{k}}{(2\pi)^3 \omega} \mathbf{k} \left[ia(\mathbf{k})e^{-ik \cdot x} - ib^*(\mathbf{k})e^{ik \cdot x} \right]\end{aligned}$$

Proceeding as above, we find

$$\begin{aligned}\int d^3 \mathbf{r} \pi^* \pi &= \int \frac{d^3 \mathbf{k}}{4(2\pi)^3} [|a(\mathbf{k})|^2 + |b(\mathbf{k})|^2 - a(\mathbf{k})b(-\mathbf{k})e^{-2i\omega t} - b^*(\mathbf{k})a^*(-\mathbf{k})e^{+2i\omega t}] \\ \int d^3 \mathbf{r} \nabla \varphi^* \cdot \nabla \varphi &= \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega^2} \mathbf{k}^2 [|a(\mathbf{k})|^2 + |b(\mathbf{k})|^2 + a(\mathbf{k})b(-\mathbf{k})e^{-2i\omega t} + b^*(\mathbf{k})a^*(-\mathbf{k})e^{+2i\omega t}] .\end{aligned}$$

Adding all the terms in H together and using $\mathbf{k}^2 = \omega^2 - m^2$, the time-independent terms add while the time-dependent terms cancel, giving

$$H = \int d^3 \mathbf{r} \mathcal{H} = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} [|a(\mathbf{k})|^2 + |b(\mathbf{k})|^2] .$$

(c) The Lagrangian density has a symmetry under global phase changes of φ : $\varphi \rightarrow e^{-i\varepsilon} \varphi$. For ε small, $\varphi \rightarrow \varphi - i\varepsilon \varphi$ and $\varphi^* \rightarrow \varphi^* + i\varepsilon \varphi^*$. Writing \mathcal{L} in covariant form,

$$\mathcal{L} = (\partial_\mu \varphi^*)(\partial^\mu \varphi) - m^2 \varphi^* \varphi ,$$

the Noether current is

$$\begin{aligned}J_\mu &\propto \frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} \delta \varphi + \frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi^*)} \delta \varphi^* \\ &= -i\varepsilon(\partial_\mu \varphi^*) \varphi + i\varepsilon(\partial_\mu \varphi) \varphi^* .\end{aligned}$$

In terms of components we have $J_\mu = (J_0, -\mathbf{J})$ and $\partial^\mu J_\mu = 0$ means that

$$\frac{\partial J_0}{\partial t} = -\nabla \cdot \mathbf{J} .$$

Therefore

$$\int_V d^3 \mathbf{r} \frac{\partial J_0}{\partial t} = - \int_V d^3 \mathbf{r} \nabla \cdot \mathbf{J} = - \int d^2 \mathbf{S} \cdot \mathbf{J}$$

where the last integral is over the surface of V . Extending V to the whole of space, this surface integral must be zero since the field has to vanish at infinity. Therefore the charge Q defined by

$$Q = \int_{\text{all space}} d^3 \mathbf{r} J_0$$

has the property

$$\frac{dQ}{dt} = \int_{\text{all space}} d^3 \mathbf{r} \frac{\partial J_0}{\partial t} = 0$$

i.e. $Q = \text{constant}$.

In this case, dividing out the constant ε , we have

$$J_0 = -i \frac{\partial \varphi^*}{\partial t} \varphi + i \frac{\partial \varphi}{\partial t} \varphi^*$$

and so

$$Q = -i \int_{\text{all space}} d^3 \mathbf{r} \left(\frac{\partial \varphi^*}{\partial t} \varphi - \frac{\partial \varphi}{\partial t} \varphi^* \right) = \text{const.}$$

We use the Fourier representations of φ and φ^* in part (b) to obtain

$$\begin{aligned} \int d^3 \mathbf{r} \frac{\partial \varphi^*}{\partial t} \varphi &= \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega} [i|a(\mathbf{k})|^2 - i|b(\mathbf{k})|^2 - ia(\mathbf{k})b(-\mathbf{k})e^{-2i\omega t} + ib^*(\mathbf{k})a^*(-\mathbf{k})e^{+2i\omega t}] \\ \int d^3 \mathbf{r} \frac{\partial \varphi}{\partial t} \varphi^* &= \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega} [-i|a(\mathbf{k})|^2 + i|b(\mathbf{k})|^2 - ia(\mathbf{k})b(-\mathbf{k})e^{-2i\omega t} + ib^*(\mathbf{k})a^*(-\mathbf{k})e^{+2i\omega t}] . \end{aligned}$$

When we subtract these expressions, the time-independent terms add while the time-dependent terms cancel, giving

$$Q = \int \frac{d^3 \mathbf{k}}{2(2\pi)^3 \omega} [|a(\mathbf{k})|^2 - |b(\mathbf{k})|^2] .$$

The interpretation of these results is that the positive and negative frequency Fourier components of the field contribute to the energy with the same sign, in proportion to their amplitudes squared, but they contribute to the charge with the opposite sign. After second quantization, the quanta of the field are particles and antiparticles, associated with the positive and negative frequency Fourier components respectively. Both particles and antiparticles have positive energy, but they have opposite charges, which is consistent with the above results.

Field Theory question 5

$$\mathcal{L} = \frac{1}{2}\sigma \left[\left(\frac{\partial \varphi_x}{\partial t} \right)^2 + \left(\frac{\partial \varphi_y}{\partial t} \right)^2 \right] - \frac{1}{2}F \left[\left(\frac{\partial \varphi_x}{\partial z} \right)^2 + \left(\frac{\partial \varphi_y}{\partial z} \right)^2 \right].$$

Under the transformation

$$\begin{aligned}\varphi_x &\rightarrow \varphi_x \cos \theta - \varphi_y \sin \theta \\ \varphi_y &\rightarrow \varphi_x \sin \theta + \varphi_y \cos \theta\end{aligned}$$

(which is a rotation about the z -axis) we have

$$\begin{aligned}\dot{\varphi}_x^2 &\rightarrow \dot{\varphi}_x^2 \cos^2 \theta + \dot{\varphi}_y^2 \sin^2 \theta - 2\dot{\varphi}_x \dot{\varphi}_y \cos \theta \sin \theta \\ \dot{\varphi}_y^2 &\rightarrow \dot{\varphi}_x^2 \sin^2 \theta + \dot{\varphi}_y^2 \cos^2 \theta + 2\dot{\varphi}_x \dot{\varphi}_y \sin \theta \cos \theta\end{aligned}$$

so that

$$\dot{\varphi}_x^2 + \dot{\varphi}_y^2 \rightarrow \dot{\varphi}_x^2 + \dot{\varphi}_y^2$$

and similarly for the second term in \mathcal{L} . Therefore \mathcal{L} is invariant under rotation about the z -axis.

For $\theta = \varepsilon$ small, we have

$$\varphi_x \rightarrow \varphi_x - \varepsilon \varphi_y, \quad \varphi_y \rightarrow \varepsilon \varphi_x + \varphi_y$$

i.e. $\delta \varphi_x = -\varepsilon \varphi_y$ and $\delta \varphi_y = +\varepsilon \varphi_x$.

The corresponding Noether current is

$$J_\mu \propto \frac{\partial \mathcal{L}}{\partial (\partial^\mu \varphi_x)} \delta \varphi_x + \frac{\partial \mathcal{L}}{\partial (\partial^\mu \varphi_y)} \delta \varphi_y$$

i.e. $J_\mu = (\rho, J_x, J_y, J_z)$ where (dividing out ε)

$$\begin{aligned}\rho &= -\sigma \frac{\partial \varphi_x}{\partial t} \varphi_y + \sigma \frac{\partial \varphi_y}{\partial t} \varphi_x \\ J_z &= F \frac{\partial \varphi_x}{\partial z} \varphi_y - F \frac{\partial \varphi_y}{\partial z} \varphi_x\end{aligned}$$

and $J_x = J_y = 0$. The conservation equation $\partial^\mu J_\mu = 0$ gives

$$\frac{\partial \rho}{\partial t} = \frac{\partial J_z}{\partial z}$$

so, defining the charge

$$Q = \int_a^b dz \rho$$

where a and b are the ends of the string, we see that

$$\dot{Q} = \int_a^b dz \frac{\partial \rho}{\partial t} = J_z(b) - J_z(a) = 0$$

assuming the displacements (or the transverse velocities) vanish at the ends. Therefore Q is a conserved charge.

The transverse momentum densities are

$$\pi_x = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}_x} = \sigma \dot{\varphi}_x, \quad \pi_y = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}_y} = \sigma \dot{\varphi}_y,$$

and so

$$\rho = \varphi_x \pi_y - \varphi_y \pi_x$$

which we recognise as the z -component of angular momentum per unit length of the string. Thus Q is the total z -component of angular momentum, which is conserved because the dynamics of the system are invariant with respect to rotations about the z -axis.

Field Theory question 6

Recall from lectures that the angular momentum vector \mathbf{J} has components

$$J_i = \frac{1}{2} \varepsilon_{ijk} J^{jk}$$

where

$$\begin{aligned} J^{\mu\nu} &= \int d^3\mathbf{r} M^{0\mu\nu}, \\ M^{\lambda\mu\nu} &= x^\mu T^{\lambda\nu} - x^\nu T^{\lambda\mu}, \end{aligned}$$

$T^{\mu\nu}$ being the stress-energy tensor. Thus

$$\begin{aligned} J_i &= -\frac{1}{2} \varepsilon_{ijk} \int d^3\mathbf{r} (r^j T^{0k} - r^k T^{0j}) \\ &= -\varepsilon_{ijk} \int d^3\mathbf{r} r^j T^{0k}. \end{aligned}$$

For a real scalar Klein-Gordon field we have

$$T^{\mu\nu} = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} \partial^\nu \varphi - g^{\mu\nu} \mathcal{L}$$

with Lagrangian density

$$\mathcal{L} = \frac{1}{2} (\partial^\mu \varphi)(\partial_\mu \varphi) - \frac{1}{2} m^2 \varphi^2,$$

and therefore

$$T^{\mu\nu} = (\partial^\mu \varphi)(\partial^\nu \varphi) - g^{\mu\nu} \mathcal{L}.$$

Thus

$$T^{0k} = T^{k0} = -\dot{\varphi} \nabla_k \varphi$$

and

$$J_i = -\varepsilon_{ijk} \int d^3\mathbf{r} \dot{\varphi} r_j \nabla_k \varphi$$

i.e.

$$\mathbf{J} = - \int d^3\mathbf{r} \dot{\varphi} \mathbf{r} \times \nabla \varphi.$$

The Fourier representation of a real scalar field is

$$\varphi(\mathbf{r}, t) = \int \frac{d^3\mathbf{k}}{2(2\pi)^3 \omega} \left[a(\mathbf{k}) e^{-ik \cdot x} + a^*(\mathbf{k}) e^{+ik \cdot x} \right]$$

We can obtain \mathbf{r} from the Fourier representation by operating with $\mp i \nabla^{(k)}$ on the \pm ve frequency parts, respectively, where $\nabla^{(k)} = (\partial/\partial k_x, \partial/\partial k_y, \partial/\partial k_z)$ is the gradient operator in \mathbf{k} -space. Then we have

$$\begin{aligned} \dot{\varphi} &= \int \frac{d^3\mathbf{k}}{2(2\pi)^3} \left[-ia(\mathbf{k}) e^{-ik \cdot x} + ia^*(\mathbf{k}) e^{+ik \cdot x} \right] \\ \dot{\varphi} \mathbf{r} &= \int \frac{d^3\mathbf{k}}{2(2\pi)^3} \left\{ \left[\nabla^{(k)} a(\mathbf{k}) \right] e^{-ik \cdot x} + \left[\nabla^{(k)} a^*(\mathbf{k}) \right] e^{+ik \cdot x} \right\} \\ \nabla \varphi &= \int \frac{d^3\mathbf{k}'}{2(2\pi)^3 \omega'} \mathbf{k}' \left[ia(\mathbf{k}') e^{-ik' \cdot x} - ia^*(\mathbf{k}') e^{+ik' \cdot x} \right], \end{aligned}$$

where we have integrated by parts in the expression for $\dot{\phi} \mathbf{r}$.

Proceeding as in qu. 4, we find

$$\begin{aligned} \mathbf{J} = & -i \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega} \mathbf{k} \times \left[a^*(\mathbf{k}) \nabla^{(k)} a(\mathbf{k}) - a(\mathbf{k}) \nabla^{(k)} a^*(\mathbf{k}) \right. \\ & \left. + a(-\mathbf{k}) \nabla^{(k)} a(\mathbf{k}) e^{-2i\omega t} - a^*(-\mathbf{k}) \nabla^{(k)} a^*(\mathbf{k}) e^{+2i\omega t} \right] . \end{aligned}$$

The time-independent terms are equal by integration by parts. The two time-dependent terms cannot contribute since \mathbf{J} is a conserved quantity. To see this in detail, integrate the first term by parts (noting that $\mathbf{k} \times \nabla^{(k)} \omega = 0$ and $\nabla^{(k)} \times \mathbf{k} = 0$) to obtain

$$\int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega} a(-\mathbf{k}) (\mathbf{k} \times \nabla^{(k)}) a(\mathbf{k}) e^{-2i\omega t} = - \int \frac{d^3 \mathbf{k}}{4(2\pi)^3 \omega} a(\mathbf{k}) (\mathbf{k} \times \nabla^{(k)}) a(-\mathbf{k}) e^{-2i\omega t}$$

Changing the variable of integration to $-\mathbf{k}$ (noting that $\mathbf{k} \times \nabla^{(k)}$ is invariant under this operation) we get minus the original integral, so it must be zero. Similarly for the other time-dependent term, which is just the complex conjugate of this one. Therefore

$$\mathbf{J} = -i \int \frac{d^3 \mathbf{k}}{2(2\pi)^3 \omega} a^*(\mathbf{k}) (\mathbf{k} \times \nabla^{(k)}) a(\mathbf{k}) .$$

Field Theory question 7

$$\begin{aligned}\mathcal{L} = & \frac{1}{2}(\partial_\mu\varphi_1)(\partial^\mu\varphi_1) + \frac{1}{2}(\partial_\mu\varphi_2)(\partial^\mu\varphi_2) - \frac{1}{2}M_{11}\varphi_1^2 - M_{12}\varphi_1\varphi_2 - \frac{1}{2}M_{22}\varphi_2^2 \\ & - \frac{1}{4}\Lambda_{11}\varphi_1^4 - \frac{1}{2}\Lambda_{12}\varphi_1^2\varphi_2^2 - \frac{1}{4}\Lambda_{22}\varphi_2^4.\end{aligned}$$

(a) Recall that the dimensions of \mathcal{L} in natural units are $[M]^4$ and those of a scalar field are $[M]$. Thus M_{ij} must have dimensions $[M]^2$ and Λ_{ij} must be dimensionless.

(b) The energy of the system is given by the Hamiltonian

$$H = \int d^3\mathbf{r} \mathcal{H}$$

where

$$\mathcal{H} = \pi_1\dot{\varphi}_1 + \pi_2\dot{\varphi}_2 - \mathcal{L},$$

and $\pi_i = \dot{\varphi}_i$, so that

$$\mathcal{H} = \frac{1}{2}(\pi_1^2 + \pi_2^2 + \nabla\varphi_1 \cdot \nabla\varphi_1 + \nabla\varphi_2 \cdot \nabla\varphi_2) + V(\varphi_1, \varphi_2)$$

where the ‘potential’ V is

$$\begin{aligned}V(\varphi_1, \varphi_2) = & \frac{1}{2}M_{11}\varphi_1^2 + M_{12}\varphi_1\varphi_2 + \frac{1}{2}M_{22}\varphi_2^2 \\ & + \frac{1}{4}\Lambda_{11}\varphi_1^4 + \frac{1}{2}\Lambda_{12}\varphi_1^2\varphi_2^2 + \frac{1}{4}\Lambda_{22}\varphi_2^4.\end{aligned}$$

Clearly \mathcal{H} will be bounded from below as long as V does not diverge to $-\infty$ at large values of φ_1 and/or φ_2 .

As long as the Λ_{ij} ’s do not satisfy special conditions (which we shall determine), there will be no constraints on the M_{ij} ’s, since the quartic terms in V will always dominate at large φ_i . Assuming this to be the case, write $\varphi_2^2 = \alpha\varphi_1^2$. Then we require

$$\Lambda_{11} + 2\Lambda_{12}\alpha + \Lambda_{22}\alpha^2 \geq 0$$

for all $\alpha \geq 0$. Hence $\Lambda_{11} \geq 0$, $\Lambda_{22} \geq 0$, and the roots

$$\alpha_{\pm} = \left(-\Lambda_{12} \pm \sqrt{\Lambda_{12}^2 - \Lambda_{11}\Lambda_{22}} \right) / \Lambda_{22}$$

are either complex or both negative. Hence we require $\Lambda_{12} \geq \sqrt{\Lambda_{11}\Lambda_{22}}$ or $\sqrt{\Lambda_{11}\Lambda_{22}} \geq \Lambda_{12} \geq -\sqrt{\Lambda_{11}\Lambda_{22}}$. So in summary the conditions are

$$\Lambda_{11} \geq 0, \quad \Lambda_{22} \geq 0 \quad \Lambda_{12} \geq -\sqrt{\Lambda_{11}\Lambda_{22}}.$$

There are two special cases where we get conditions on the M_{ij} ’s, as follows. First, if $\Lambda_{12} = -\sqrt{\Lambda_{11}\Lambda_{22}}$, $\Lambda_{11} = 0$ or $\Lambda_{22} = 0$ there is a ‘flat direction’ along which the quartic term vanishes. This direction corresponds to $\alpha = \sqrt{\Lambda_{11}/\Lambda_{22}}$ in the first case, $\alpha = 0$ in the second,

and $\alpha = \infty$ in the third. The quadratic term must be non-negative along the flat direction, which means that in this case (only) we require

$$\begin{aligned} M_{11}\sqrt{\Lambda_{22}} + M_{22}\sqrt{\Lambda_{11}} \pm 2M_{12}(\Lambda_{11}\Lambda_{22})^{1/4} &\geq 0 && \text{if } \Lambda_{12} = -\sqrt{\Lambda_{11}\Lambda_{22}} \\ M_{11} &\geq 0 && \text{if } \Lambda_{11} = 0 \\ M_{22} &\geq 0 && \text{if } \Lambda_{22} = 0 \end{aligned}$$

Notice that if both Λ_{11} and Λ_{22} are zero then we have two flat directions and we require both $M_{11} \geq 0$ and $M_{22} \geq 0$ if the potential is to be bounded from below.

A second special case is when all the Λ_{ij} 's are zero: then we require that the quadratic term should not go to $-\infty$ in any direction. Setting $\varphi_2 = \beta\varphi_1$, we require

$$M_{11} + 2M_{12}\beta + M_{22}\beta^2 \geq 0$$

for all β . Hence $M_{11} \geq 0$, $M_{22} \geq 0$, and the roots

$$\beta_{\pm} = \left(-M_{12} \pm \sqrt{M_{12}^2 - M_{11}M_{22}} \right) / M_{22}$$

are complex or coincident, which means $M_{12}^2 \leq M_{11}M_{22}$.

(c) For the symmetry to be spontaneously broken, we require the origin $(\varphi_1, \varphi_2) = (0, 0)$ to be a point of unstable equilibrium. Assuming that the Λ_{ij} 's are non-zero and satisfy the conditions in part (b), there will then be a pair of points of stable equilibrium elsewhere, say at (v_1, v_2) and $(-v_1, -v_2)$. In the state of minimum energy the field must choose one of these, breaking the symmetry.

Near the origin, the quartic terms in V will be negligible, so the conditions that the origin be a point of stable equilibrium will be just those discussed in part (b) when the Λ_{ij} 's are all zero. To break the symmetry requires the converse conditions, i.e.

$$M_{11} < 0 \quad \text{or} \quad M_{22} < 0 \quad \text{or} \quad M_{12}^2 > M_{11}M_{22} .$$

Field Theory question 8

We have

$$S[\varphi] = \int d^4x \left[\frac{1}{2} (\partial_\mu \varphi) (\partial^\mu \varphi) - \frac{1}{4} \lambda \varphi^4 \right] .$$

Making the transformation $\varphi(x) \rightarrow \varphi'(x) = \alpha \varphi(\alpha x)$, we have

$$\partial_\mu \varphi' = \alpha \frac{\partial \varphi(\alpha x)}{\partial x^\mu} = \alpha^2 \frac{\partial \varphi(\alpha x)}{\partial (\alpha x^\mu)}$$

and so

$$\begin{aligned} S[\varphi'] &= \int d^4x \left[\frac{1}{2} (\partial_\mu \varphi') (\partial^\mu \varphi') - \frac{1}{4} \lambda (\varphi')^4 \right] \\ &= \int d^4x \alpha^4 \left[\frac{1}{2} \frac{\partial \varphi(\alpha x)}{\partial (\alpha x^\mu)} \frac{\partial \varphi(\alpha x)}{\partial (\alpha x_\mu)} - \frac{1}{4} \lambda [\varphi(\alpha x)]^4 \right] \\ &= \int d^4x' \left[\frac{1}{2} \frac{\partial \varphi(x')}{\partial (x'^\mu)} \frac{\partial \varphi(x')}{\partial (x'_\mu)} - \frac{1}{4} \lambda [\varphi(x')]^4 \right] , \end{aligned}$$

where in the last line we have defined $x' = \alpha x$. But since x' is just a variable of integration, we can replace it by x to see that this is identical to $S[\varphi]$.

Under a small change in the field $\delta\varphi$, we have

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\varphi} \delta\varphi + \frac{\partial\mathcal{L}}{\partial(\partial^\mu\varphi)} \delta(\partial^\mu\varphi) .$$

As in the derivation of the Noether current, we may use the Euler-Lagrange equation of motion

$$\frac{\partial\mathcal{L}}{\partial\varphi} = \partial^\mu \left(\frac{\partial\mathcal{L}}{\partial(\partial^\mu\varphi)} \right)$$

and $\delta(\partial^\mu\varphi) = \partial^\mu(\delta\varphi)$ to write this as

$$\delta\mathcal{L} = \partial^\mu \left(\frac{\partial\mathcal{L}}{\partial(\partial^\mu\varphi)} \right) \delta\varphi + \frac{\partial\mathcal{L}}{\partial(\partial^\mu\varphi)} \partial^\mu(\delta\varphi) = \partial^\mu \left(\frac{\partial\mathcal{L}}{\partial(\partial^\mu\varphi)} \delta\varphi \right) .$$

In the case of a symmetry of \mathcal{L} , the l.h.s. would be zero and this would already define a conserved current. However, a dilatation of this system leaves the action but not \mathcal{L} itself invariant, so we need to evaluate the l.h.s. explicitly and express it as a 4-divergence.

In the case of a small dilatation $\alpha = 1 + \varepsilon$ we have

$$\delta\varphi = (1 + \varepsilon)\varphi(x + \varepsilon x) - \varphi(x) = \varepsilon\varphi + \varepsilon x^\nu \partial_\nu \varphi + \mathcal{O}(\varepsilon^2)$$

so to first order $\delta\varphi = \varepsilon(\varphi + x^\nu \partial_\nu \varphi)$. Thus

$$\frac{\partial\mathcal{L}}{\partial\varphi} \delta\varphi = -\varepsilon \lambda \varphi^3 (\varphi + x^\nu \partial_\nu \varphi) = -\varepsilon (4 + x^\nu \partial_\nu) \frac{1}{4} \lambda \varphi^4 .$$

Also

$$\delta(\partial^\mu\varphi) = \partial^\mu(\delta\varphi) = \varepsilon \partial^\mu \varphi + \varepsilon \partial^\mu (x^\nu \partial_\nu \varphi) + \mathcal{O}(\varepsilon^2)$$

and

$$\partial^\mu(x^\nu \partial_\nu \varphi) = \partial^\mu(x_\nu \partial^\nu \varphi) = \partial^\mu \varphi + x^\nu \partial_\nu \partial^\mu \varphi ,$$

so that, again to first order,

$$\delta(\partial^\mu \varphi) = \varepsilon(2 + x^\nu \partial_\nu) \partial^\mu \varphi .$$

Thus

$$\frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} \delta(\partial^\mu \varphi) = \varepsilon(\partial_\mu \varphi)(2 + x^\nu \partial_\nu) \partial^\mu \varphi = \frac{1}{2} \varepsilon(4 + x^\nu \partial_\nu)(\partial_\mu \varphi)(\partial^\mu \varphi)$$

and therefore

$$\delta \mathcal{L} = \varepsilon(4 + x^\nu \partial_\nu) \mathcal{L} = \varepsilon(4 + x_\mu \partial^\mu) \mathcal{L} = \varepsilon \partial^\mu (x_\mu \mathcal{L}) .$$

[Remark: Notice that in general any quantity Q with mass dimension (in natural units) p changes by $\delta Q = \varepsilon(p + x^\nu \partial_\nu)Q$ under a small dilatation.]

Putting everything together, we see that

$$\varepsilon \partial^\mu (x_\mu \mathcal{L}) = \partial^\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} \delta \varphi \right) = \varepsilon \partial^\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} [\varphi + x^\nu \partial_\nu \varphi] \right)$$

and therefore a conserved current, J_μ such that $\partial^\mu J_\mu = 0$, may be defined by

$$\begin{aligned} J_\mu &= \frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} (\varphi + x^\nu \partial_\nu \varphi) - x_\mu \mathcal{L} \\ &= (\partial_\mu \varphi) (\varphi + x^\nu \partial_\nu \varphi) - x_\mu \mathcal{L} . \end{aligned}$$

Recalling that the stress-energy tensor is

$$T_{\mu\nu} = \frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} \partial_\nu \varphi - g_{\mu\nu} \mathcal{L}$$

we may write this *dilatation current* in the alternative form

$$J_\mu = x^\nu T_{\mu\nu} + \varphi \partial_\mu \varphi .$$

Field Theory question 9

We want to determine the energy levels of an electron in a uniform constant magnetic field along the z axis. It is convenient to use the second order form of the Dirac equation, which for the case in question reduces to

$$\left[\left(\frac{i\hbar}{c} \partial_t \right)^2 - (i\hbar \nabla + e\mathbf{A})^2 - m^2 c^2 + e\hbar \boldsymbol{\Sigma} \cdot \mathbf{B} \right] \varphi = 0.$$

Given that the magnetic field is along the z axis, we can choose ϕ to be an eigenstate of the corresponding component of the spin, namely $\Sigma_z \varphi = \sigma \varphi$, with $\sigma = \pm 1$. Moreover, with the choice of vector potential $\mathbf{A} = (0, Bx, 0)$, we can further choose φ to be an eigenstate of definite momentum in the y and z directions, p_y, p_z . If the electron has total energy E , the equation above reduces to

$$\left[\left(\frac{E}{c} \right)^2 - p_z^2 - m^2 c^2 + e\hbar \sigma B \right] \varphi = \left[-\hbar^2 \partial_x^2 + (eBx - p_y)^2 \right] \varphi.$$

The term in square brackets on the l.h.s. is a constant and the equation can be recognised to be equivalent to the time-independent Schrödinger equation for a simple harmonic oscillator in one dimension (w.r.t. the x coordinate), with energy $\hbar|e|B(2n+1)$, with $n = 0, 1, 2, \dots$

One can similarly use the known form of the wave function of the oscillator to construct the wave function of the Dirac equation, $\psi = [\gamma(p - eA) + m] \varphi$ (left as an exercise). We note here that, contrary to φ , the solution ψ is no longer an eigenstate of Σ_z . This is expected: we have seen in the lecture notes that the spin is not a conserved quantity for a relativistic particle in motion.

Field Theory question 10

In this question we derive Pauli's phenomenological equation for a particle with spin 1/2 as the low energy, non-relativistic limit of the Dirac equation. Consider the Dirac equation minimally coupled to an EM field:

$$\gamma^\mu (i\hbar\partial_\mu - eA_\mu) \psi - mc\psi = 0,$$

where $A^\mu = (\phi/c, \mathbf{A})$. It is convenient to write it as

$$\gamma^0 \left(i\frac{\hbar}{c}\partial_t - \frac{e\phi}{c} \right) \psi + \boldsymbol{\gamma} \cdot (i\hbar\boldsymbol{\nabla} + e\mathbf{A}) \psi - mc\psi = 0$$

and introduce the simplified notation $E = i\hbar\partial_t$ and $\mathbf{p} = -i\hbar\boldsymbol{\nabla}$:

$$\gamma^0 (E - e\phi) \psi - c\boldsymbol{\gamma} \cdot (\mathbf{p} - e\mathbf{A}) \psi - mc^2\psi = 0,$$

where we have also multiplied by an overall factor c .

Using the standard representation of the γ matrices,

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix},$$

where I is the 2×2 identity matrix and σ_i are Pauli matrices, and representing the 4-spinor ψ as a 2-component vector

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

where each component ψ_\pm is a 2-spinor, we can expand the Dirac equation in matrix form

$$\begin{pmatrix} E - e\phi - mc^2 & -c\boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A}) \\ c\boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A}) & -E + e\phi - mc^2 \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = 0,$$

which is equivalent to the desired result

$$\begin{cases} (E - e\phi)\psi_+ - c\boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A})\psi_- = mc^2\psi_+ \\ -(E - e\phi)\psi_- + c\boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A})\psi_+ = mc^2\psi_- \end{cases}.$$

If we apply the low energy and non-relativistic approximation $E - e\phi \simeq mc^2$ to the second equation, we obtain

$$\psi_- \simeq \frac{1}{2mc} \boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A}) \psi_+.$$

Notice that at low energies (hence small EM fields) and in the non-relativistic limit $\mathbf{p} \simeq m\mathbf{v}$, ψ_- is suppressed with respect to ψ_+ (by a factor of the order of v/c).

Substituting this result into the first equation and rearranging the terms, we arrive at Pauli's phenomenological equation:

$$(E - mc^2)\psi_+ = \frac{1}{2m} [\boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A})]^2 \psi_+ + e\phi\psi_+,$$

where $E - mc^2$ is the classical energy of the particle, namely its total minus rest energy.

In order to evaluate the second term on the r.h.s. of Pauli's equation, let us introduce for convenience the shorthand notation $\mathbf{O} = \mathbf{p} - e\mathbf{A}$. Using the form of the Pauli matrices

$$\sigma^1 \equiv \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 \equiv \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 \equiv \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

we observe that

$$\boldsymbol{\sigma} \cdot \mathbf{O} = \begin{pmatrix} O_z & O_x - iO_y \\ O_x + iO_y & -O_z \end{pmatrix}$$

and

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \mathbf{O})^2 &= \begin{pmatrix} O_x^2 + O_y^2 + O_z^2 + i[O_x, O_y] & [O_z, O_x] + i[O_y, O_z] \\ -[O_z, O_x] + i[O_y, O_z] & O_x^2 + O_y^2 + O_z^2 - i[O_x, O_y] \end{pmatrix} \\ &= \mathbf{O}^2 I + i \begin{pmatrix} [O_x, O_y] & -i[O_z, O_x] + [O_y, O_z] \\ i[O_z, O_x] + [O_y, O_z] & -[O_x, O_y] \end{pmatrix}, \end{aligned}$$

where $[,]$ denotes the commutator of two operators and I is once again the 2×2 identity matrix (which will be omitted for simplicity in the following). We then evaluate

$$[O_i, O_j] = [p_i, p_j] + e^2[A_i, A_j] - e[p_i, A_j] - e[A_i, p_j],$$

for $i \neq j$. The first two terms vanish trivially but the last two need to be evaluated with care, e.g.

$$(p_x A_y - A_y p_x) \psi = -i\hbar[\partial_x(A_y \psi) - A_y \partial_x \psi] = -i\hbar[(\partial_x A_y) \psi + A_y \partial_x \psi - A_y \partial_x \psi] = -i\hbar(\partial_x A_y) \psi.$$

After a few lines of similar algebra, one obtains:

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \mathbf{O})^2 &= \mathbf{O}^2 - e\hbar \begin{pmatrix} \partial_x A_y - \partial_y A_x & -i(\partial_z A_x - \partial_x A_z) + (\partial_y A_z - \partial_z A_y) \\ i(\partial_z A_x - \partial_x A_z) + (\partial_y A_z - \partial_z A_y) & -(\partial_x A_y - \partial_y A_x) \end{pmatrix} \\ &= \mathbf{O}^2 - e\hbar \begin{pmatrix} B_z & -iB_y + B_x \\ iB_y + B_x & -B_z \end{pmatrix} \\ &= \mathbf{O}^2 - e\hbar \boldsymbol{\sigma} \cdot \mathbf{B}. \end{aligned}$$

Substituting finally into the r.h.s. of Pauli's equation, we arrive at the result

$$\frac{1}{2m} (\mathbf{p} - e\mathbf{A})^2 \psi_+ - \frac{e\hbar}{2m} (\boldsymbol{\sigma} \cdot \mathbf{B}) \psi_+ + e\phi \psi_+.$$

This is one of the several successes of Dirac's equation: the ability to derive the gyromagnetic ratio from first principles based on relativistic invariance, therefore demonstrating the need for half-integer particles, formerly introduced by Pauli on purely phenomenological grounds.

Phase transitions and critical phenomena question 1

The scope of this question is to obtain the phase diagram of a fully-connected uniform Ising model and study its phase transition. In order to do so, several tasks have been set up to guide you through the calculation of the energy and partition function, and to study their dependence on temperature and applied magnetic field.

(a) The Hamiltonian of the model is

$$H = -\frac{J}{N} \sum_{i,j} s_i s_j, \quad s_i = \pm 1, \quad s_i^2 = 1. \quad (1)$$

The energy of the system is the ensemble average of H , and therefore the sum over i, j of the ensemble average of $s_i s_j$. The system clearly has translation invariance and thus the latter can only depend on the distance $|i - j|$, as customary. Moreover, this system is rather special in that every spin is equally connected to every other, and thus the system is *scale free* in that no meaningful notion of distance between two spins can be introduced (alternatively: all the spins are nearest neighbours to one another). Therefore, the ensemble average of $s_i s_j$ does not even depend on the difference $|i - j|$, but rather takes on a constant value ε independent of i or j . As a result, the energy of the system can be written as $-JN\varepsilon$, indeed proportional to N as anticipated (here we used the fact that $\sum_{i,j} 1 = N^2$).

(b) As the sum over i, j in Eq. (1) runs over all indices $i, j = 1, \dots, N$, it is proportional to the sum of the double product terms in the square of the sum of all the spins $(\sum_i s_i)^2$. All terms that are not double products add up to a trivial constant that will be neglected in the remainder of the exercise:

$$H = -\frac{J}{2N} \left[\left(\sum_i s_i \right)^2 - N \right] \equiv -\frac{J}{2N} \left(\sum_i s_i \right)^2. \quad (2)$$

(c) Using the definition $m = N^{-1} \sum_i s_i$ in Eq. (2), we see that the Hamiltonian depends on a spin configuration $\{s_i\}$ only via its magnetisation $m(\{s_i\})$, $H = -JNm^2/2$ [Note: since $m \in (-1, 1)$ by definition, this is an alternative way to show that the energy of the system is proportional to N]. Therefore, all configurations $\{s_i\}$ that have the same magnetisation m are in fact energetically degenerate. In order for a configuration to have magnetisation m , it must have N^+ positive spins such that $N^+ - (N - N^+) = mN$, i.e., $N^+ = N(1 + m)/2$. The total number of such configurations is nothing but the combinatorial factor of choosing N^+ positive spins out of an ensemble of N total spins, that is:

$$W(m) = \binom{N}{N^+} = \frac{N!}{N^+!(N - N^+)!} = \frac{N!}{[N(1 + m)/2]![N(1 - m)/2]!}. \quad (3)$$

(d) Since the Hamiltonian of the system depends on the spin configuration only through the value of the magnetisation, $H = H(m)$, and using Eq. (3), we can write the partition function of the system as:

$$Z = \sum_{\{s_i\}_{i=1}^N} e^{-H/k_B T} = \sum_m e^{-H(m)/k_B T} \left(\sum_{\{s_i\}_m} 1 \right) = \sum_m W(m) e^{-H(m)/k_B T}, \quad (4)$$

where $\{s_i\}_m$ indicates the ensemble of configurations that have the same value m of the magnetisation.

In the thermodynamic limit ($N \gg 1$) and assuming that the fully polarised configurations $m \simeq \pm 1$ do not play a significant role (hence $N(1 \pm m)/2$ is also a large number), we can use Stirling's approximation $n! \sim n^n e^{-n}$ to obtain a more transparent expression for $W(m)$:

$$\begin{aligned} W(m) &\simeq \frac{N^N e^{-N}}{[N(1+m)/2]^{N(1+m)/2} [N(1-m)/2]^{N(1-m)/2} e^{-N(1+m)/2 - N(1-m)/2}} \\ &= \left[\left(\frac{1+m}{2} \right)^{\frac{1+m}{2}} \left(\frac{1-m}{2} \right)^{\frac{1-m}{2}} \right]^{-N} \\ &= \exp \left[-N \left(\frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2} \right) \right]. \end{aligned}$$

The exponent in the final expression above takes the well-known form of the entropy of mixing, $\rho \ln \rho + (1-\rho) \ln(1-\rho)$, where $\rho = (1+m)/2$ is the density of up spins (and $1-\rho$ is the density of down spins).

In general, in order to obtain the partition function of a system one ought to find a way to compute explicitly the summation in Eq. (4). This task rarely comes easy. However, this fully connected model where each spin interacts with every other spin is one of the few cases that are amenable to an explicit calculation that is exact in the thermodynamic limit. Let us start from the partition function written as a sum over m after substituting the expanded version of $W(m)$ and $H = -JNm^2/2$,

$$\begin{aligned} Z &= \sum_m \exp \left\{ \frac{N}{2k_B T} \left[Jm^2 - k_B T [(1+m) \ln(1+m) + (1-m) \ln(1-m)] \right] \right\} \\ &\equiv \sum_m e^{-NF(m)/2k_B T}, \end{aligned}$$

where an irrelevant overall constant factor $e^{N \ln 2}$ was left out for simplicity. The partition function is a summation of positive real numbers and therefore can be bounded from below by the value of any of the elements in the summation; here we choose the largest one and rename it $e^{-NF_{\min}/2k_B T}$ for convenience (clearly the maximum of the exponential coincides with the minimum of the function $F(m)$). Conversely, the summation can be bounded from above by replacing each element by their maximum one. The total number of elements in the summation is the number of values that m can take on; since the spins are discrete, the total magnetisation of the system can only take the values $-N, -N+2, \dots, N-2, N$, which is a number of the order of N for large N . Therefore, we can write the following lower and upper bounds for Z :

$$e^{-NF_{\min}/2k_B T} \leq Z \leq N e^{-NF_{\min}/2k_B T}. \quad (5)$$

These bounds can be equivalently re-written as

$$-F_{\min}/2k_B T \leq \frac{\ln Z}{N} \leq \frac{\ln N}{N} - F_{\min}/2k_B T. \quad (6)$$

In the thermodynamic limit, $\ln N/N \rightarrow 0$ and $\ln Z/N \rightarrow -F_{\min}/2k_B T$. Therefore, the partition function of this fully connected system is controlled asymptotically by the largest value

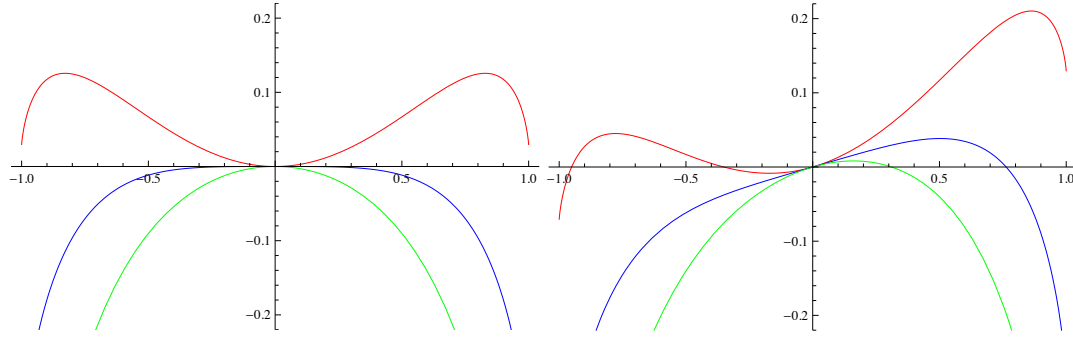


Figure 1: Left panel: Dependence of the function $-F(m)$ on $m \in (-1, 1)$ for $J = 1$ and different values of $k_B T = 0.7, 1.0, 1.3$ (red, blue, green). Right panel: same function and parameter values with the addition of a magnetic field of strength $B = 0.05$.

of the elements in the summation over m . It is important to notice that this is *not* a general property of partition functions, and indeed it would not apply to this very same system if we had instead considered the expression for Z as a summation over spin configurations $\{s + i\}$: in that case, it would have been *wrong* to approximate Z by the largest value of $e^{-H/k_B T}$. [Recall that in a proper thermodynamic system Z is exponential in the volume and thus $\ln Z \sim N$, and the ratio $\ln Z/N$ does not vanish in the thermodynamic limit in Eq. (6).]

In conclusion, the partition function of this system and therefore all of its thermodynamic properties are determined by the minimum of $F(m)$, or equivalently the maximum of

$$-F(m) = Jm^2 - k_B T [(1+m) \ln(1+m) + (1-m) \ln(1-m)]. \quad (7)$$

The dependence of this function on $m \in (-1, 1)$ for $J = 1$ and different values of $k_B T$ is illustrated in Fig. 1.

(e) The maximum of the function $-F(m)$ can be found by studying its stationary point(s),

$$-\frac{dF(m)}{dm} = 2Jm - k_B T \ln \frac{1+m}{1-m} = 0. \quad (8)$$

Using the suggestion given in the problem set, $2 \tanh^{-1}(x) \equiv \ln[(1+x)/(1-x)]$, this equation can be re-expressed in a form that should be immediately familiar from the lecture notes on mean-field theory for the Ising model:

$$\tanh\left(\frac{Jm}{k_B T}\right) = m. \quad (9)$$

[It is noteworthy to remark that the above equation is *exact* in the thermodynamic limit for this fully connected model, whereas mean field equations are generally only an approximation to finite range models (in dimensions less than or equal to 3, at least).]

A solution at $m = 0$ always exists. If the slope of the hyperbolic tangent at $m = 0$ is smaller than unity, i.e., $J/k_B < T$, then there are no further solutions and one can show that $m = 0$ is indeed a maximum (see for instance Fig. 1 or the second derivative hereafter). If the slope is larger than unity, i.e., $J/k_B > T$, then two more solutions appear which are

equal maxima of $-F(m)$ at $m = \pm m_0 \neq 0$ whereas $m = 0$ becomes a minimum. This is the characteristic signature of *spontaneous symmetry breaking* that takes place in the system as the temperature is lowered below the *critical temperature* $T_c = J/k_B$.

The second derivative of $-F(m)$ yields

$$-\frac{d^2 F(m)}{dm^2} = 2J - \frac{2k_B T}{1 - m^2}. \quad (10)$$

Given that the denominator $1 - m^2$ is bounded between 0 and 1, for $J < k_B T$ the second derivative is negative for all values of m . At $J = k_B T$, the second derivative vanishes at $m = 0$ (typical of a second order phase transition) and it is negative elsewhere. For $J > k_B T$ the second derivative is positive for values of m close to 0 and negative close to $m = \pm 1$. This is consistent with the behaviour illustrated in Fig. 1.

(f) Expanding the (negative of) Eq. (7), recalling that $\ln(1+x) \simeq x - x^2/2 + x^3/3 - x^4/4 + \mathcal{O}(x^5)$, one obtains

$$F(m) \simeq -Jm^2 + k_B T \left[m^2 + \frac{m^4}{6} \right] + \mathcal{O}(m^5). \quad (11)$$

Comparing to the expression from Landau theory $F(T) = F_0 + \alpha(T)m^2 + \beta(T)m^4/2$, one obtains

$$\alpha(T) = k_B T - J \quad \beta(T) = k_B T/3. \quad (12)$$

As in the lectures, one finds that $\alpha(T_c) = 0$, and α takes positive values above the transition ($m = 0$) and negative values below ($m = \pm m_0$).

(g) Generalising the model by adding a uniform magnetic field B changes the Hamiltonian to $H = -JNm^2/2 - BNm$. The dependence on the spin configurations remains a dependence solely on their magnetisation m and therefore many of the discussions above carry through with minimal changes.

The place where a magnetic field plays a key role is in the determination of the maximum of $-F(m)$ (i.e., the determination of the equilibrium value of m that in turn determines the value of the partition function of the system). In the presence of a field, Eq. (8) and Eq. (9) need to be replaced by,

$$-\frac{dF(m)}{dm} = 2Jm + B - k_B T \ln \frac{1+m}{1-m} = 0$$

$$\tanh \left(\frac{Jm+B/2}{k_B T} \right) = m \quad .$$

In the new form, the place where the hyperbolic tangent vanishes is shifted to a negative value of $m = -B/2J$. For large temperatures $T > J/k_B$, using a graphic solution of the second equation above, one can readily observe that the shift results in the intersection with m moving from $m = 0$ to a finite positive value of m . As the temperature is lowered, eventually two further solutions of the equation appear. However, the former one – which in the mean time kept moving to larger and larger values of m – remains the maximum of the function at all temperatures. The two new solutions are a secondary maximum and a minimum, respectively (see the right panel of Fig. 1). Therefore, nothing special happens in the system at the temperature where the two new solutions appear. As expected, the applied uniform magnetic field explicitly breaks the symmetry of the system and removes any trace of the thermodynamic transition. [Albeit of no consequences for thermodynamic properties

of the system, the appearance of a secondary maximum in $-F(m)$ means that a special value of m exists that the system favours over “nearby” values. This feature can have important consequences in the dynamical properties of the system, as it can for instance give rise to long-lived metastable states: if we prepare the system near the secondary maximum, it may take a long time for thermal fluctuations to allow the system to relax to the absolute thermodynamic maximum. However, discussing these phenomena is beyond the scope of this lecture course.]

Phase transitions and critical phenomena question 2

The Landau free energy expansion for a uniaxial ferromagnet in a magnetic field can be written as

$$F = F_0 - hm + \frac{a}{2}m^2 + \frac{b}{4}m^4.$$

(a) Phase transitions occur when a new state (ordered) state develops from the disordered (high temperature) phase. The appearance of the new state is typically described using an order parameter, say the magnetisation in an Ising model. Ginzburg-Landau theory provides a phenomenological description of critical phenomena based on an appropriately coarse grained order parameter m . It is constructed on the basis of symmetries rather than precise knowledge of the microscopic properties of the system.

Near the transition temperature, where the order parameter vanishes, one can expand the Ginzburg-Landau free energy in powers of m and its derivatives. The latter often penalise spatial variations of the parameter m and thus one can further simplify the free energy expansion by considering the case of uniform m , as in this example.

In an expansion of the form

$$F = F_0 - hm + \frac{a}{2}m^2 + \frac{b}{4}m^4$$

we require that $b > 0$ for the free energy to be bounded from below ($b = 0$ is acceptable if $a > 0$); we also recognise the second term on the right hand side as an externally applied magnetic field; finally, we also know that a transition in this free energy occurs when a changes sign (and therefore $a(T_c) = 0$).

(b) The magnetisation of the system scales like a power law of the applied field along the critical isotherm (for small fields), and the exponent is $1/\delta$.

Along the critical isotherm $T = T_c$, $a(T_c) = 0$ and

$$F(T_c) = F_0 - hm + \frac{b}{4}m^4.$$

The equilibrium value of m can be obtained from the equation $\partial F/\partial m = 0$,

$$\frac{\partial F(T_c)}{\partial m} = -h + bm^3 = 0 \quad \Rightarrow \quad m = \sqrt[3]{\frac{h}{b}}$$

and therefore $\delta = 1/3$.

(c) The dependence of the magnetisation on the applied field and temperature can be obtained as above,

$$\frac{\partial F(T)}{\partial m} = -h + a(T)m + b(T)m^3 = 0.$$

However, rather than solving for m , it is convenient to take a further derivative with respect to h :

$$\frac{\partial^2 F(T)}{\partial h \partial m} = -1 + a(T)\chi + 3b(T)m^2\chi = 0 \quad \Rightarrow \quad \chi = \frac{1}{a(T) + 3b(T)m^2}.$$

For $t > 0$ ($T > T_c$), we know that $m = 0$ and therefore $\chi = a(T)^{-1}$.

For $t < 0$, $m \neq 0$ and we can re-write the first equation as

$$b(T)m^2 = \frac{h - a(T)m}{m}.$$

Substituting into the expression for χ , one obtains

$$\chi = \frac{1}{a(T) + 3(h/m - a(T))} \Big|_{h=0} = \frac{1}{-2a(T)} = \frac{1}{2|a(T)|},$$

where we used the fact that $a(T)$ is negative for $T < T_c$.

Finally, it is straightforward to combine these results and show that

$$\lim_{t \rightarrow 0^+} \frac{\chi(t)}{\chi(-t)} = \frac{2|a(-t)|}{a(t)} = 2,$$

where we used knowledge of the fact that $a(T) \propto (T - T_c)/T_c$ for T close to T_c .

(d) Once we add $dm^3/3$ to the free energy F and set $h = 0$,

$$F = F_0 + \frac{a}{2}m^2 + \frac{d}{3}m^3 + \frac{b}{4}m^4,$$

the equilibrium value of the magnetisation is given by

$$\frac{\partial F}{\partial m} = 0 = am + dm^2 + bm^3,$$

which admits solutions of the form

$$m = 0 \quad \text{and} \quad m = \frac{-d \pm \sqrt{d^2 - 4ab}}{2b}.$$

The latter of course are acceptable only if $d^2 > 4ab$.

By looking at the form of the second derivative with respect to m ,

$$\frac{\partial^2 F}{\partial m^2} = a + 2dm + 3bm^2,$$

we see immediately that the sign at $m = 0$ is controlled solely by the parameter a : if $a > 0$ then $m = 0$ is a minimum; if $a < 0$, it is a maximum.

If $a < 0$, the other two solutions of $\partial F/\partial m = 0$ are acceptable ($d^2 > 4ab$) and therefore they both have to be minima (observe that in this case the two solutions lie on opposite sides of $m = 0$, and that $F(m) \rightarrow +\infty$ for $m \rightarrow \pm\infty$).

If $a > 0$, then the other two solutions (if they exist) are either both positive or both negative. They are therefore a maximum and a minimum, respectively. So long as d is sufficiently small however, the global minimum remains at $m = 0$ (one can check that this is indeed the case for $d < 9ab/2$). The case of larger values of d can well be studied using this very same approach but it is more involved and beyond the scope of the question (an interesting exercise nonetheless!).

Similarly to the case $d = 0$ considered in the lectures, it is the sign of a that drives a transition from a state with $m = 0$ to a state with $m \neq 0$. However, the cubic term introduces two major changes: (i) the symmetry in the ordered phase is broken explicitly, since $m = (-d - \sqrt{d^2 - 4ab})/(2b)$ has a lower free energy than $m = (-d + \sqrt{d^2 - 4ab})/(2b)$; (ii) the change in the order parameter across the critical point $a = 0$ is discontinuous, hence the transition has become *first order*.

Phase transitions and critical phenomena question 3

Consider the Landau free energy expansion of a system with complex order parameter $\phi(x)$ in 1D:

$$\beta H = \int f dx = \int \left[a\phi^*\phi + \frac{1}{2}(\phi^*\phi)^2 + c(\partial_x\phi^*)(\partial_x\phi) + (\partial_x^2\phi^*)(\partial_x^2\phi) \right] dx$$

with the coefficients a, c real.

(a) The physical state of the system is obtained by minimizing the free energy. When $c > 0$, this is equivalent to the free energy expected for an Ising ferromagnet discussed in the lecture notes, which is minimized by a uniformly constant order parameter $\phi(x) = \bar{\phi}$, except that the order parameter is now complex. We thus need to minimize the function

$$f|_{\phi(x)=\bar{\phi}} = a\bar{\phi}^*\bar{\phi} + \frac{1}{2}(\bar{\phi}^*\bar{\phi})^2 = a|\bar{\phi}|^2 + \frac{1}{2}|\bar{\phi}|^4$$

This is the mexican hat potential encountered when studying spontaneous symmetry breaking in the context of the relativistic scalar complex ϕ^4 field theory. For $a > 0$, the solution is $\bar{\phi} = 0$, whereas for $a < 0$ a continuous line of solutions equally minimize the free energy, $|\bar{\phi}| = \sqrt{-a}$.

The order parameter develops continuously across the transition at $a = 0$, with a discontinuity in its first derivative. This is therefore a second order phase transition, which spontaneously breaks a global phase change symmetry.

(b) Let us consider a uniform magnetic field B coupled to the order parameter $\phi(x)$, where B points along the real axis in the complex ϕ plane. The free energy should then include a further term $-B(\phi + \phi^*)/2$.

As suggested in the question, the response of the system to such field will be in the real component of ϕ , and we can therefore simplify the expression for the free energy by considering ϕ to be a real scalar field. Once again, for $c > 0$ the free energy is minimised by a uniform constant field $\phi(x) = m$, with m real in this case:

$$f|_{\phi(x)=m} = am^2 + \frac{1}{2}m^4 - Bm, \quad \frac{\partial f}{\partial m} = 0 = 2am + 2m^3 - B$$

This is equivalent to the case of the Ising ferromagnet considered in the lecture notes. The zero-field susceptibility is obtained by taking the derivative with respect to B of the equation that determines the physical value of m (above, right hand side),

$$2a\chi + 6m^2\chi = 1$$

where $\chi = \partial m / \partial B|_{B=0}$. Above the transition ($a > 0$), $m(B=0) = 0$ and $\chi = 1/2a$. Below the transition ($a < 0$), $m(B=0) = \pm\sqrt{-a}$ and $\chi = -1/4a$.

(c) We then consider the general case where both a and c are allowed to take on negative values and assume, as suggested in the question, an order parameter of the form $\phi(x) = \phi_0 e^{i(kx+\delta)}$, where $\phi_0 > 0$, k and δ are real constants. A straightforward substitution into the free energy of the system gives:

$$f|_{\phi(x)=\phi_0 e^{i(kx+\delta)}} = a\phi_0^2 + \frac{1}{2}\phi_0^4 + ck^2\phi_0^2 + k^4\phi_0^2 = (a + ck^2 + k^4)\phi_0^2 + \frac{1}{2}\phi_0^4$$

In order to minimize the free energy, we need to solve the system of differential equations

$$\begin{cases} \frac{\partial f}{\partial \phi_0} = 2(a + ck^2 + k^4)\phi_0 + 2\phi_0^3 = 0 \\ \frac{\partial f}{\partial k} = 2k(c + 2k^2)\phi_0^2 = 0 \end{cases}$$

- If $a > 0$ and $c > 0$, then the only solution is $\phi_0 = 0$ for any k . This corresponds to the disordered “paramagnetic” phase where the order parameter vanishes.
- If $a < 0$ and $c > 0$, then an additional solution appears, for $k = 0$ and $\phi_0^2 = -a$. In order to see which of the two solutions is the global minimum (and thus corresponds to the physical state), we need to compare the free energies: (i) $f|_{\phi_0=0} = 0$; and (ii) $f|_{k=0, \phi_0^2=-a} = -a^2/2$. Clearly the free energy (ii) is lowest, and this region of parameter space corresponds to an ordered phase with uniform ($k = 0$) order parameter $\phi_0^2 = -a$.
- If $c < 0$, a new solution to the second differential equation appears for $k^2 = -c/2$. With this choice for k , the first differential equation gives $\phi_0^2 = c^2/4 - a$ (in addition to $\phi_0 = 0$, which is always a solution). Notice that this new finite value of the order parameter for finite k is allowed only if $a < c^2/4$. The free energy of this new solution

$$f|_{k^2=-c/2, \phi_0^2=c^2/4-a} = -\frac{1}{2} \left(\frac{c^2}{4} - a \right)^2,$$

is always negative, thus lower than that for $\phi_0 = 0$, $f = 0$.

In the region of parameter space where $a < 0$ and $c < 0$, this new solution should also be compared to the other one: $k = 0$, $\phi_0^2 = -a$, $f = -a^2/2$:

$$-\frac{1}{2} \left(\frac{c^2}{4} - a \right)^2 < -\frac{a^2}{2} \quad \rightarrow \quad \frac{c^2}{2} \left(\frac{c^2}{8} - a \right) > 0$$

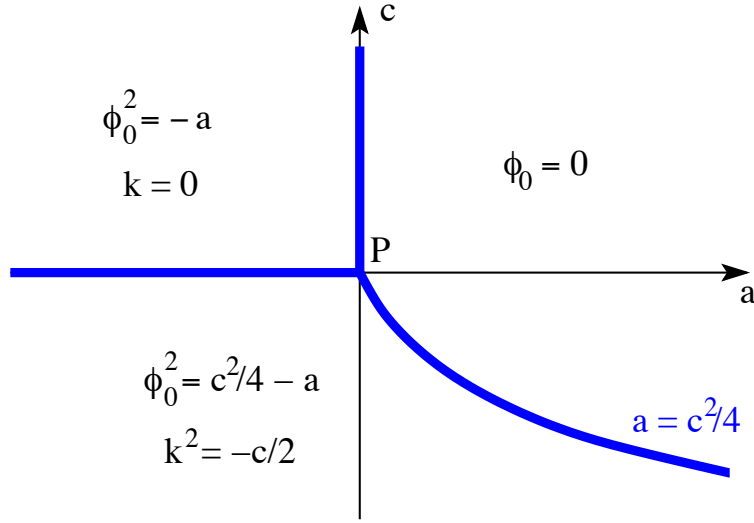
which is always satisfied for $a < 0$. Therefore, whenever the new finite- k solution is allowed, it is indeed the global minimum of the free energy and thus the physical state of the system. Notice that $k^2 = -c/2$, $\phi_0^2 = c^2/4 - a$ corresponds to a modulated rather than uniform order parameter, with wave vector $k = \pm\sqrt{-c/2}$.

There is no dependence on δ in the free energy. This term represents a global phase in the order parameter, and the free energy is symmetric upon changes in the global phase; therefore it cannot depend on δ .

As discussed in part (b), the system undergoes a spontaneous breaking of the global phase symmetry. In the ordered phase, the system will spontaneously choose a value for δ , but this choice is arbitrary rather than being dictated by a free energy minimisation principle.

(d) Using the information obtained in part (c), it is straightforward to draw the phase transi-

tion lines (or phase boundaries) in the ac plane:



The point P where three transition lines meet is called a tricritical point (indeed characteristic of a Lifshitz free energy).

Let us consider the cases $a = c$ and $a = 0, c < 0$ and study the behaviour of the order parameter when it approaches the tricritical point ($a = 0, c = 0$) from the ordered phase. In both cases, the latter phase corresponds to $k^2 = -c/2, \phi_0^2 = c^2/4 - a$, and therefore:

$$\begin{cases} \phi_0^2 = c^2/4 - c \simeq -c & (a = c, c < 0) \\ \phi_0^2 = c^2/4 & (a = 0, c < 0) \end{cases}$$

where we used the fact that, close to the phase transition, $|c|$ is small and thus $c^2 \ll |c|$. The critical exponent of the order parameter changes from $\beta = 1/2$ to $\beta = 1$, depending on the direction of approach to the critical point.

Phase transitions and critical phenomena question 4

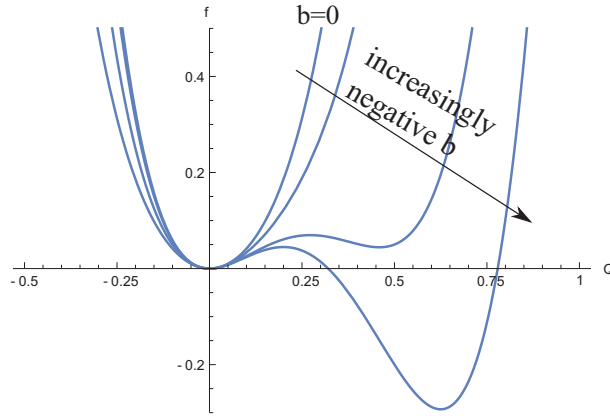
(a) The nematic energy, $E \propto -(\mathbf{s}_i \cdot \mathbf{s}_j)^2$, equally favors alignment or anti-alignment. Thus the ferro-magnet aligned state has the spins all pointing in the same direction, giving a finite $\langle \mathbf{s} \rangle$, whereas the nematic ground state can contain equal numbers of aligned and anti-aligned spins giving $\langle \mathbf{s} \rangle = 0$. The nematic energy does not actually distinguish between alignment and anti-alignment, so the fully aligned state is also a ground state. However, on combinatorial grounds there are many more ground states with $\langle \mathbf{s} \rangle = 0$, hence this is what is observed.

(b) $S_{\alpha\alpha} = \frac{1}{N} \sum_{i=1}^N (3s_{i\alpha}s_{i\alpha} - \delta_{\alpha\alpha}) = \frac{1}{N} \sum_{i=1}^N (3(1) - 3) = 0$

(c) Substituting $S_{\alpha\beta} = Q(3n_\alpha n_\beta - \delta_{\alpha\beta})$ into the provided energy (easy if you remember it is symmetric, and hence diagonal in its principal frame) yields

$$f = 6aQ^2 + 6bQ^3 + 18cQ^4.$$

This is graphed for various values of $b < 0$ below:



If $b = 0$ this is a simple symmetric energy with a single minimum. As b is reduced below 0 the energy loses symmetry, and eventually a second minimum appears at positive Q . At some value of b it becomes the global minimum. The transition is thus discontinuous.

(d) f always has one minimum with $f = 0$ at $Q = 0$. The second minimum will become the global minimum when it passes $f = 0$, so we examine

$$\begin{aligned} f &= 6aQ^2 + 6bQ^3 + 18cQ^4 = 0 \\ \implies &= aQ^2 + bQ^3 + 3cQ^4 = 0 \end{aligned}$$

which has three solutions, $Q = 0$ (as expected) and

$$Q = \frac{-b \pm \sqrt{b^2 - 12ca}}{6c}.$$

The point where we go from one to three solutions is the point when the second minimum cuts the x axis, which occurs when $b^2 = 12ca$.

So the transition happens when $b = -\sqrt{12ac}$, and the system jumps from $Q = 0$ to

$$Q = \frac{-b}{6c} = \sqrt{\frac{a}{3c}}.$$

Propagators and Causality question 1

We wish to find

$$I = \int_0^{2\pi} \frac{d\theta}{a + b \sin \theta}$$

We will assume a and b to be real, and that $a > b$. We will make the substitution $z = e^{i\theta}$ and integrate around the unit circle.

$$\begin{aligned} I &= \int \frac{dz/iz}{a + b(z - z^{-1})/2i} \\ &= \int \frac{2dz/b}{z^2 + \frac{2aiz}{b} - 1} \end{aligned}$$

The integrand has poles at

$$\begin{aligned} z_{\pm} &= -\frac{2ai}{2b} \pm \frac{\sqrt{-\frac{4a^2}{b^2} + 4}}{2} \\ &= -i \left(\frac{a}{b} \pm \sqrt{\frac{a^2}{b^2} - 1} \right) \end{aligned}$$

Given $a > b$, only z_- lies within the unit circle. It is a simple pole, so the residue there is

$$\lim_{z \rightarrow z_-} \frac{2/b}{z - z_+} = \frac{2/b}{2i\sqrt{\frac{a^2}{b^2} - 1}}$$

The integral is $2\pi i$ times this, so

$$I = \frac{2\pi}{\sqrt{a^2 - b^2}}$$

Next, we wish to evaluate

$$I = \int_0^{\infty} \frac{dx}{1 + x^6}$$

It is possible to evaluate this integral (or rather, twice the integral), using a semi-circular contour closed either in the upper or the lower half plane. However, this method requires the computation of three residues. A much more efficient way to tackle this problem is to use a wedge shaped contour which is composed from the following three parts:

C_1 : A line running from $z = 0$ to $z = \infty$ along the real axis.

C_2 : A curve running between $\theta = 0$ and $\theta = \pi/3$ at infinity.

C_3 : A line returning to $z = 0$ from infinity along the line $z = te^{\pi i/3}$ ($t \in \mathbb{R}, 0 < t < \infty$).

The complete contour $C \equiv C_1 + C_2 + C_3$ only encloses one of the poles of the integrand - i.e. the pole at $z = e^{\pi i/6}$. The integral of $f(z) \equiv (1 + z^6)^{-1}$ over C is therefore given by:

$$\begin{aligned}
\oint_C \frac{dz}{1+z^6} &= 2\pi i \times \text{residue of pole at } z = e^{\pi i/6} \\
&= 2\pi i \times \lim_{z \rightarrow e^{\pi i/6}} \left(\frac{z - e^{\pi i/6}}{1+z^6} \right) \\
&= 2\pi i \times \lim_{z \rightarrow e^{\pi i/6}} \left(\frac{1}{6z^5} \right) \\
&= \frac{\pi}{3} \frac{1}{e^{\pi i/3}}
\end{aligned}$$

In the third line of the above, we have made use of l'Hôpital's rule. We now consider the integral of $f(z)$ over each of the individual sections $C_1 - C_3$. The integral along C_1 is of course I , whilst that along C_2 vanishes. The integral of $f(z)$ along C_3 is given by:

$$\begin{aligned}
\int_{C_3} \frac{dz}{1+z^6} &= \int_{\infty}^0 \frac{e^{\pi i/3} dt}{1+t^6} \\
&= -e^{\pi i/3} I
\end{aligned}$$

So the integral of $f(z)$ along the contour C_3 is just the integral we want multiplied by a phase factor. Finally, using $\oint_C = \int_{C_1} + \int_{C_2} + \int_{C_3}$ we obtain:

$$\begin{aligned}
\frac{\pi}{3} \frac{1}{e^{\pi i/3}} &= \left(1 - e^{\pi i/3} \right) I \\
\Rightarrow I &= \frac{\pi}{3}
\end{aligned}$$

Propagators and Causality question 2

We want to find the response V of the circuit for a given input I , which in the Fourier domain will be just $V(\omega) = Z(\omega)I(\omega)$ for the complex impedance Z . We will write the impedance of a capacitor as $Z_C = 1/i\omega C$ and the impedance of an inductor as $Z_L = i\omega L$. In doing this, we have made the important assumption that all currents and voltages in the system behave like $e^{i\omega t}$. When we perform a Fourier integral to find $Z(t)$ from $Z(\omega)$ we must therefore be aware that we are using a different sign convention to the usual Fourier integral which has $e^{-i\omega t}$. Furthermore, the fact that we are assuming sinusoidal behaviour requires the system to be lightly damped. Damping in an LCR circuit comes from the resistance R , so we will later require R to be in some sense small. This will correspond to ensuring that the poles of our complex function are in sensible places. The first step is to find the impedance of the circuit:

$$\begin{aligned}\frac{1}{Z} &= \frac{1}{Z_C} + \frac{1}{Z_L + Z_R} \\ &= \frac{i\omega RC - \omega^2 LC + 1}{R + i\omega L}\end{aligned}$$

We can take the inverse Fourier transform to find $Z(t)$:

$$\begin{aligned}Z(t) &= \int Z(\omega) e^{i\omega t} \frac{d\omega}{2\pi} \\ &= - \int \frac{d\omega}{2\pi} e^{i\omega t} \frac{R + i\omega L}{LC(\omega^2 - i\omega R/L - 1/LC)}\end{aligned}$$

where we remember the earlier discussion on the sign conventions used. The integrand has poles at

$$\omega_{1,2} = \frac{iR}{2L} \pm \sqrt{\frac{1}{LC} - \frac{R^2}{4L^2}}$$

Following the earlier remark about light damping, we will take $R^2 < 4L/C$ so the square root is of a positive number, and both poles lie in the upper half plane. For causal behaviour of the system, we require that there is only a response when $t > 0$. We will use a standard semi-circular contour, and consider what happens if we close in the upper and lower half planes for $t < 0$ and $t > 0$. For $t < 0$, the contribution from the semi-circular arc will diverge if we close in the upper half plane and be zero if we close in the lower half plane. We must therefore close in the lower half plane for $t < 0$, where we find there is no response because the contour encloses no poles. For $t > 0$, we must close in the upper half plane, where we will enclose the two poles and so there will be some response of the system as expected. Both of the poles are of order one so their residues are straightforward to obtain:

$$Z(t) = -\frac{i}{LC} \left[\frac{R + i\omega_1 L}{\omega_1 - \omega_2} e^{i\omega_1 t} + \frac{R + i\omega_2 L}{\omega_2 - \omega_1} e^{i\omega_2 t} \right]$$

The difference in frequencies is

$$\omega_1 - \omega_2 = \Delta\omega = 2\sqrt{\frac{1}{LC} - \frac{R^2}{4L^2}} = \frac{2}{L}\sqrt{\frac{L}{C} - \frac{R^2}{4}} = 2\omega_0$$

We wish to find the voltage $V(t)$ set up as a result of the following input current $I(t)$:

$$I(t) = \begin{cases} 0 & t < 0 \\ I_0 \cos(\Omega t) & t > 0 \end{cases}$$

To do this, we use the inverse Fourier transformed version of $V(\omega) = Z(\omega)I(\omega)$:

$$V(t) = \int dt' Z(t') I(t - t')$$

We insert the explicit forms for $Z(t)$ and $I(t)$ into this expression. We then use the fact that $\cos(\Omega t) = \Re e^{i\Omega t}$ and the fact that $Z(t)$ must be real to write:

$$\begin{aligned} V(t) &= -\frac{iI_0}{2LC\omega_0} \Re \left(e^{i\Omega t} \int_0^t dt' (R + i\omega_1 L) e^{i(\omega_1 - \Omega)t'} - (R + i\omega_2 L) e^{i(\omega_2 - \Omega)t'} \right) \\ &= -\frac{I_0}{2LC\omega_0} \Re \left(e^{i\Omega t} \left[\frac{(R + i\omega_1 L) e^{i(\omega_1 - \Omega)t'}}{(\omega_1 - \Omega)} - \frac{(R + i\omega_2 L) e^{i(\omega_2 - \Omega)t'}}{(\omega_2 - \Omega)} \right]_0^t \right) \\ &= \frac{I_0}{2\omega_0} \Re \left(\frac{e^{i\Omega t}}{(1 + i\Omega RC - \Omega^2 LC)} \left[(\omega_2 - \Omega)(R + i\omega_1 L) e^{i(\omega_1 - \Omega)t'} - (\omega_1 - \Omega)(R + i\omega_2 L) e^{i(\omega_2 - \Omega)t'} \right]_0^t \right) \end{aligned}$$

The “ $t' = 0$ ” terms from the above expression correspond to the steady state response, which is:

$$V(t)_S = I_0 \Re (Z(\Omega) e^{i\Omega t})$$

exactly as one would expect. The “ $t' = t$ ” terms give the following transient:

$$V(t)_T = \frac{I_0}{2\omega_0} e^{-Rt/(2L)} \frac{(2L/C - R^2 - 2L^2\Omega^2) \sin(\omega_0 t) - 2L\omega_0 R \cos(\omega_0 t)}{L((1 - \Omega^2 LC)^2 + (\Omega RC)^2)}$$

The full solution for $V(t)$ is of course $V(t)_S + V(t)_T$ (for $t > 0$).

Propagators and Causality question 3

The Green's function (by definition) satisfies the equation

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 \right) G(\mathbf{r}, \mathbf{r}'; t, t') = \delta^3(\mathbf{r} - \mathbf{r}') \delta(t - t')$$

The Fourier transform of the right hand side is 1. To Fourier transform the left hand side, we will change variables to $\tau = t - t'$, so

$$i\hbar \int d\tau e^{iz\tau/\hbar} \frac{\partial G(\tau)}{\partial t} = -i\hbar \int \frac{iz}{\hbar} e^{iz\tau/\hbar} G(\tau) d\tau = zG(\mathbf{r}, \mathbf{r}'; z)$$

where we have integrated by parts, noting that the boundary term is zero. Thus,

$$\left(z + \frac{\hbar^2}{2m} \nabla^2 \right) G(\mathbf{r}, \mathbf{r}'; z) = \delta^3(\mathbf{r} - \mathbf{r}')$$

Next, we note that $\nabla^2 \leftrightarrow -k^2$ under Fourier transformation and let $\mathbf{p} = \mathbf{r} - \mathbf{r}'$ so that

$$\begin{aligned} G(\mathbf{r}, \mathbf{r}'; z) &= \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')}}{z - \hbar^2 k^2 / 2m} \\ &= \frac{1}{(2\pi)^3} \int k^2 dk \sin \theta d\theta d\phi \frac{e^{i\mathbf{k} \cdot \mathbf{p}}}{z - \hbar^2 k^2 / 2m} \\ &= \frac{1}{(2\pi)^2} \int_0^\infty \frac{k^2 dk}{z - \hbar^2 k^2 / 2m} \int_0^\pi d\theta \sin \theta e^{ikp \cos \theta} \\ &= \frac{1}{(2\pi)^2} \int_0^\infty \frac{k^2 dk}{z - \hbar^2 k^2 / 2m} \frac{e^{ikp} - e^{-ikp}}{ikp} \\ &= \frac{2m}{i(2\pi)^2 p \hbar^2} \int_{-\infty}^\infty \frac{k e^{ikp}}{2mz/\hbar^2 - k^2} dk \end{aligned}$$

where the symmetry properties of the k integrand were used to change the range of k integration. The integrand has poles at $k = \pm \sqrt{2mz/\hbar}$. We first consider the case $z = E + i\epsilon$, which has poles at $k_{1,2} = \pm(\sqrt{2m/\hbar})E^{1/2}e^{i\epsilon/2}$ (because $(E^{1/2}e^{i\epsilon/2})^2 = Ee^{i\epsilon} \simeq E + i\epsilon$ when ϵ is small). We will close the contour of integration with a semi-circle in the upper half plane; the contribution from the semi-circular arc vanishes due to Jordan's lemma. Only the pole at k_1 is enclosed which has residue $-e^{ik_1 p}/2$, using l'Hôpital's rule. When $z = E - i\epsilon$ the poles move to $k_{1,2} = \pm(\sqrt{2m/\hbar})E^{1/2}e^{-i\epsilon/2}$ and the pole enclosed by the contour is the one at $k_2 = -(\sqrt{2m/\hbar})E^{1/2}e^{-i\epsilon/2}$ with residue $-e^{ik_2 p}/2$. (For the $E < 0$ cases, we just need to replace \sqrt{E} by $i\sqrt{E}$). We multiply the residues by $2\pi i$ to arrive at the required integrals, and then use the definition of ΔG given in the question along with the integrals for the $E > 0$ cases to arrive at

$$\Delta G = -2\pi i \frac{2m}{\hbar^2} \frac{\sin\left(\sqrt{2mE}|\mathbf{r} - \mathbf{r}'|/\hbar\right)}{4\pi^2|\mathbf{r} - \mathbf{r}'|} \Theta(E)$$

For a particle in free space, $E = \hbar^2 k^2 / 2m$ so $dk/dE = \sqrt{2m}/2\hbar\sqrt{E}$. Each state in k -space occupies a volume $(2\pi)^3$, so the number in a sphere of radius k is $n = 4\pi k^3 / 3(2\pi)^3$.

Therefore, the density of states is

$$\begin{aligned}\frac{dn}{dE} &= \frac{4\pi k^2}{(2\pi)^3} \frac{dk}{dE} \\ &= \frac{m}{2\pi^2 \hbar^3} \sqrt{2mE}.\end{aligned}$$

Noting that the limit of $\sin(x)/x$ as x tends to zero is 1, comparing this to the earlier equation for ΔG shows that in this case

$$\rho(E) = \lim_{\mathbf{r} \rightarrow \mathbf{r}'} \frac{\Delta G(\mathbf{r}, \mathbf{r}'; E)}{-2\pi i}.$$

For the last part we again use $G = 1/(z - H)$, so

$$G = \sum_n \frac{|n\rangle\langle n|}{z - E_n}$$

because the eigenstates $|n\rangle$ form a complete set, and

$$\begin{aligned}G(\mathbf{r}, \mathbf{r}'; z) \equiv \langle \mathbf{r} | G | \mathbf{r}' \rangle &= \sum_n \frac{\langle \mathbf{r} | n \rangle \langle n | \mathbf{r}' \rangle}{z - E_n} \\ &= \sum_n \frac{\phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}')}{z - E_n}\end{aligned}$$

Writing $z = E \pm is$,

$$G^\pm(\mathbf{r}, \mathbf{r}'; z) = \sum_n \frac{\phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}')}{(E - E_n) \pm is}.$$

Using the identity given in the question,

$$\Delta G(\mathbf{r}, \mathbf{r}; E) = -2\pi i \sum_n \phi_n(\mathbf{r}) \phi_n^*(\mathbf{r}') \delta(E - E_n)$$

and so

$$\rho(\mathbf{r}, E) = \lim_{\mathbf{r} \rightarrow \mathbf{r}'} \frac{\Delta G(\mathbf{r}, \mathbf{r}'; E)}{-2\pi i}$$

as required.

Propagators and Causality question 4

The derivation of the Kramers-Kronig relations is given in the lecture notes.

The relationship between x , G and f can be found in the following way. Define the operator

$$L_t = \frac{d^2}{dt^2} + \gamma \frac{d}{dt} + \omega_0^2$$

so that the equation of motion has the form

$$L_t x(t) = f(t)$$

Insert a delta function into the right hand side:

$$L_t x(t) = \int dt' \delta(t - t') f(t')$$

and substitute for it using the definition of the Green's function

$$L_t G(t - t') = \delta(t - t')$$

Therefore,

$$L_t x(t) = \int dt' L_t G(t - t') f(t') = L_t \int dt' G(t - t') f(t')$$

which implies

$$x(t) = \int dt' G(t - t') f(t')$$

Note that from this we can deduce that $G(t - t')$ is a generalized susceptibility and therefore, its Fourier transform $G(\omega)$ will obey the Kramers-Kronig relations.

By definition

$$\left(\frac{d^2}{dt^2} + \gamma \frac{d}{dt} + \omega_0^2 \right) G(t - t') = \delta(t - t')$$

Taking the Fourier transform of this equation, we see that

$$(-\omega^2 - i\gamma\omega + \omega_0^2) G(\omega) = 1$$

and hence

$$G(\omega) = \frac{1}{-\omega^2 - i\gamma\omega + \omega_0^2}$$

To simplify the algebra we rewrite $G(\omega)$ in the form

$$G(\omega) = \frac{-1}{(\omega + b + ia)(\omega - b + ia)}$$

where $a = \gamma/2 > 0$ and $b = \sqrt{\omega_0^2 - \gamma^2/4} > 0$. This corresponds to damped oscillation. Splitting $G(\omega)$ into its real and imaginary parts we have

$$G(\omega) = \frac{(\omega^2 - b^2 - a^2) - 2ia\omega}{(\omega + b + ia)(\omega - b + ia)(\omega + b - ia)(\omega - b - ia)}$$

In order to show that $G(\omega)$ satisfies the first Kramers-Kronig relation we need to prove:

$$P \int_{-\infty}^{\infty} \Im G(\omega) \cdot \frac{1}{\omega - \zeta} \frac{d\omega}{\pi} = \Re G(\zeta)$$

In the complex plane, the integrand is

$$f(z) = \Im G(z) \frac{1}{z - \zeta} = \frac{-2az}{(z + b + ia)(z - b + ia)(z + b - ia)(z - b - ia)(z - \zeta)}$$

The easiest way to integrate this function is to rewrite as the sum of two functions

$$f_1(z) = \frac{-2a}{(z + b + ia)(z - b + ia)(z + b - ia)(z - b - ia)}$$

$$f_2(z) = \frac{-2a\zeta}{(z + b + ia)(z - b + ia)(z + b - ia)(z - b - ia)(z - \zeta)}$$

so that

$$f(z) = f_1 + f_2$$

The poles of these functions (all of which are simple) are at $z_1 = b + ia$, $z_2 = -b + ia$, $z_3 = \zeta$, $z_4 = b - ia$, $z_5 = -b - ia$. The pole at $z = \zeta$ on the real axis is not present in $f_1(z)$. As usual, we consider a semi-circular contour which we close in the upper half plane. For both functions the integral along the semi-circular arc vanishes as $R \rightarrow \infty$. Therefore for f_1 :

$$\begin{aligned} \oint f_1(z) dz &= P \int_{-\infty}^{\infty} f_1(z) dz = 2\pi i (\text{Res.}(z_1) + \text{Res.}(z_2)) \\ &= -2a \cdot 2\pi i \cdot \left[\frac{1}{(2ia)(-2b + 2ia)(-2b)} + \frac{1}{(2b + 2ia)(2ia)(2b)} \right] \\ &= -\frac{\pi}{b^2 + a^2} \end{aligned}$$

For f_2 we note that the pole on the real axis at $z = \zeta$ contributes half the usual value, i.e. $\pi i \text{Res.}(z)$. We therefore have:

$$\begin{aligned} \oint f_2(z) dz &= P \int_{-\infty}^{\infty} f_2(z) dz = 2\pi i \left(\text{Res.}(z_1) + \text{Res.}(z_2) + \frac{\text{Res.}(z_3)}{2} \right) \\ &= -2a\zeta \cdot 2\pi i \left[\frac{1}{(2ia)(-2b + 2ia)(-2b)(ia - b - \zeta)} + \frac{1}{(2b + 2ia)(2ia)(2b)(ia + b - \zeta)} \right. \\ &\quad \left. + \frac{1}{2} \frac{1}{(\zeta + b + ia)(\zeta - b + ia)(\zeta + b - ia)(\zeta - b - ia)} \right] \\ &= -\frac{\zeta^2 \pi (-b^2 + 3a^2 + \zeta^2)}{(\zeta + b + ia)(\zeta - b + ia)(\zeta + b - ia)(\zeta - b - ia)(b^2 + a^2)} \end{aligned}$$

We therefore have

$$\begin{aligned} P \int_{-\infty}^{\infty} \Im G(\omega) \cdot \frac{1}{\omega - \zeta} d\omega &= P \int_{-\infty}^{\infty} f_1(\omega) d\omega + P \int_{-\infty}^{\infty} f_2(\omega) d\omega \\ &= -\frac{\pi}{b^2 + a^2} - \frac{\zeta^2 \pi (-b^2 + 3a^2 + \zeta^2)}{(\zeta + b + ia)(\zeta - b + ia)(\zeta + b - ia)(\zeta - b - ia)(b^2 + a^2)} \end{aligned}$$

Rearranging this, we find as required

$$P \int_{-\infty}^{\infty} \Im G(\omega) \cdot \frac{1}{\omega - \zeta} \frac{d\omega}{\pi} = \frac{\zeta^2 - a^2 - b^2}{(\zeta + b + ia)(\zeta - b + ia)(\zeta + b - ia)(\zeta - b - ia)} = \Re G(\zeta)$$