

3 Lagrangian and Hamiltonian Framework

3.1 Particle Mechanics

Lagrange's equations are derived from the Principle of Least Action, which is a fundamental theorem of Classical Mechanics (and also can be interpreted in terms of Quantum Mechanics). In this we begin by defining a quantity called the Lagrangian by

$$L = T - V, \quad (3.1)$$

where T is the total kinetic energy of a system and V the total potential energy. We then consider the motion of the particle between the fixed positions $q_i(t_1)$ and $q_i(t_2)$ for times t_1 and t_2 . The Action is defined by

$$S = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t) dt, \quad (3.2)$$

and the degrees of freedom are the coordinates q_i and the velocities \dot{q}_i . The Principle of Least Action states that S is at an extremum, either a maximum or a minimum, for the actual paths between the fixed positions at fixed times. This then provides equations for the paths of the particles. Suppose $q_i^0(t)$ represents the true path, and we make infinitesimal variations about this.

$$q_i(t) = q_i^0(t) + \epsilon_i(t). \quad (3.3)$$

By definition $\epsilon_i(t_1) = \epsilon_i(t_2) = 0$. Expanding to 1st order about the $q_i^0(t)$ we obtain

$$\begin{aligned} S &= \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t) dt \equiv S^0 + \delta S = \int_{t_1}^{t_2} L(q_i^0 + \epsilon_i, \dot{q}_i^0 + \dot{\epsilon}_i, t) dt \\ &= S^0(q_i^0, \dot{q}_i^0) + \int_{t_1}^{t_2} \sum_i \left[\left(\frac{\partial L}{\partial \dot{q}_i} \right) \dot{\epsilon}_i + \left(\frac{\partial L}{\partial q_i} \right) \epsilon_i \right] dt \\ &= S^0(q_i^0, \dot{q}_i^0) + \sum_i \left[\epsilon_i(t) \left(\frac{\partial L}{\partial \dot{q}_i} \right) \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \sum_i \left[-\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) + \left(\frac{\partial L}{\partial q_i} \right) \right] \epsilon_i dt, \end{aligned} \quad (3.4)$$

where to obtain the second term we have integrated by parts with respect to t . This second term is identically zero from the boundary conditions, so we have

$$\delta S = \int_{t_1}^{t_2} \sum_i \left[-\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) + \left(\frac{\partial L}{\partial q_i} \right) \right] \epsilon_i dt. \quad (3.5)$$

This must be true for arbitrary small variations $\epsilon_i(t)$, so we obtain the Euler-Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) = \frac{\partial L}{\partial q_j}. \quad (3.6)$$

Note that in this derivation we have made no reference at any point to what any set of coordinates is, or the constraints – Lagrange's equations are true for any set q_i which describe the independent degrees of freedom of the system.

Let us check that these new equations look plausible. Consider the simplest general case of a single particle of mass m moving in one dimension with coordinate x in potential $V(x)$. In this case the Lagrangian takes the simple form

$$L = \frac{1}{2}m\dot{x}^2 - V(x). \quad (3.7)$$

$\frac{\partial L}{\partial x} = m\dot{x}$ and $\frac{\partial L}{\partial \dot{x}} = -\frac{\partial V}{\partial x}$ so Lagrange's equation becomes

$$\frac{d}{dt}m\dot{x} \equiv m\ddot{x} = -\frac{\partial V}{\partial x}. \quad (3.8)$$

So for this simple case we recover Newton's equation that mass \times acceleration is equal to the applied force.

However, in quantum mechanics we are not familiar with the Lagrangian. The quantity which appears in the Schrödinger equation and which determines the time evolution of quantities is the Hamiltonian, which is closely related to the Lagrangian. Defining the generalised momentum $p_i = \frac{\partial L}{\partial \dot{q}_i}$ we can choose to use the p_i as the complementary degrees of freedom to the q_i rather than the generalised velocities \dot{q}_i . Using these we can define a new function, the Hamiltonian

$$H(p_i, q_i, t) = \sum_i p_i \dot{q}_i(p_i, q_i) - L(\dot{q}_i(p_i, q_i), q_i, t). \quad (3.9)$$

This is known as a Legendre transformation (also used in thermodynamics) and the independent degrees of freedom are now defined to be the p_i and the q_i . If we consider the case of the particle moving in a central potential $V(r)$ then

$$p_r = m\dot{r}, \quad p_\theta = mr^2\dot{\theta}, \quad (3.10)$$

and

$$\begin{aligned} H(p, q) &= p_r \dot{r} + p_\theta \dot{\theta} - \frac{1}{2}m\dot{r}^2 - \frac{1}{2}mr^2\dot{\theta}^2 + V(r) \\ &= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + V(r) \quad \left[= \frac{1}{2}m\dot{r}^2 + \frac{1}{2}mr^2\dot{\theta}^2 + V(r) \right] \\ &= T + V. \end{aligned} \quad (3.11)$$

Thus, in this case the Hamiltonian has the physical interpretation of the energy. This is not always true, but will be as far as we are concerned in this course.

However, have we lost a simple set of equations of motion by making this change in definition? We can see by deriving Hamilton's equations.

$$\frac{\partial H}{\partial q_i} = \sum_j \left(\frac{\partial \dot{q}_j}{\partial q_i} p_j - \frac{\partial L}{\partial q_i} - \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i} \right), \quad (3.12)$$

where the derivative with respect to q_i is for fixed generalised momenta. $\frac{\partial L}{\partial \dot{q}_j} \equiv p_j$ and the first and third terms cancel, leaving

$$\frac{\partial H}{\partial q_i} = -\frac{\partial L}{\partial q_i} = -\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = -\dot{p}_i. \quad (3.13)$$

Also we can differentiate with respect to p_i (for fixed coordinates),

$$\frac{\partial H}{\partial p_i} = \sum_j \left(\dot{q}_j \delta_{ij} + p_j \frac{\partial \dot{q}_j}{\partial p_i} - \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial p_i} \right). \quad (3.14)$$

But $\frac{\partial L}{\partial \dot{q}_j} \equiv p_j$ and so the second and third terms cancel. Hence, we obtain the full set of Hamilton's equations

$$\frac{\partial H}{\partial q_i} = -\dot{p}_i, \quad \frac{\partial H}{\partial p_i} = \dot{q}_i. \quad (3.15)$$

These are just as simple as for the Lagrangian case, i.e. if we can write down the kinetic and potential energy it is a straightforward progression to the equations of motion. In our example of the particle in a central potential the \dot{q}_i equations give

$$\dot{r} = \frac{p_r}{m}, \quad \dot{\theta} = \frac{p_\theta}{mr^2}, \quad (3.16)$$

i.e. the expected relation between velocities and generalised momenta, and the \dot{p}_i equations give

$$\dot{p}_r = -\frac{\partial V}{\partial r} + \frac{p_\theta^2}{mr^3}, \quad \dot{p}_\theta = 0. \quad (3.17)$$

The conservation laws are immediately apparent. If $H(p_i, q_i)$ is independent of one of the q_i the conjugate momentum p_i is conserved. In this case the independence on θ leads to conservation of angular momentum p_θ . Also, we see that the equation for \dot{p}_r has two terms on the right-hand side. The first, $-\frac{\partial V}{\partial r}$, is the conventional radial force, which may be attractive towards the origin or repulsive away from it. The second, $\frac{p_\theta^2}{mr^3}$ is guaranteed to be positive and is the fictitious “centrifugal force”. It simply reflects that a particle with conserved angular momentum cannot get too close to $r = 0$ else its orbital kinetic energy get very large.

The Hamiltonian and Lagrangian formulations are completely equivalent. However, certain physical aspects are more clear in the Hamiltonian framework. Consider the time dependence of the Hamiltonian

$$\begin{aligned} \frac{dH}{dt} &= \sum_i \left(\frac{\partial H}{\partial q_i} \dot{q}_i + \frac{\partial H}{\partial p_i} \dot{p}_i \right) + \frac{\partial H}{\partial t} \\ &\equiv \sum_i (-\dot{p}_i \dot{q}_i + \dot{q}_i \dot{p}_i) + \frac{\partial H}{\partial t} \\ &= \frac{\partial H}{\partial t} \equiv -\frac{\partial L}{\partial t}. \end{aligned} \quad (3.18)$$

Hence, if H (or L) have no explicit time dependence, which will be the case throughout this course, then H is a conserved quantity. Hence, we will consider H to be equivalent to the energy, which is a conserved quantity.

Since the Hamiltonian is directly related to the time-dependence of the system we can illustrate one more property. Consider any function of the coordinates and conjugate momenta $f(q_i, p_i, t)$. The time-dependence of f is given by

$$\frac{df}{dt} = \sum_i \left(\frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial p_i} \dot{p}_i \right) + \frac{\partial f}{\partial t}. \quad (3.19)$$

Using the Hamiltonian equations of motion this can be re-expressed as

$$\frac{df}{dt} = \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) + \frac{\partial f}{\partial t}. \quad (3.20)$$

Thus, up to the explicit time dependence the evolution of f is driven by the Hamiltonian. In fact the quantity

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) \quad (3.21)$$

is a form which appears frequently in Hamiltonian physics and is called the Poisson bracket of f and g . This actually provides the direct link between the classical and the quantum theory. This may be seen if we consider the following Poisson brackets:

$$\begin{aligned} \{x, x\} &= \{p, p\} = 0, \\ \{x, p\} &= 1. \end{aligned} \quad (3.22)$$

The non-zero element can be compared to the quantum commutation relation

$$[x, p] = i\hbar. \quad (3.23)$$

Additionally, using the Poisson brackets we can write eq. (3.20) as

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t}. \quad (3.24)$$

This has clear parallels to quantum mechanics where the time evolution of the expectation value of an operator f is

$$\left\langle \frac{df}{dt} \right\rangle = \frac{1}{i\hbar} \langle [f, H] \rangle + \left\langle \frac{\partial f}{\partial t} \right\rangle. \quad (3.25)$$

Indeed the Hamiltonian framework is central to the quantization of a classical system, and Poisson brackets and commutators relate the two regimes. We can define the quantum version of a classical theory by replacing the Poisson brackets in the classical theory with the commutation relations for the operators defining the quantum theory.

As an explicit example of the time evolution being governed by the Hamiltonian we consider the example of the angular momentum component L_x when a particle is moving in a spherically symmetric potential $V(r)$ where $r = \sqrt{x^2 + y^2 + z^2}$. Using the definition $\mathbf{L} = \mathbf{r} \wedge \mathbf{p}$ we have $L_x = yp_z - zp_y$. We consider the Poisson bracket $\{L_x, H\}$. This is given by

$$\{L_x, H\} = \frac{\partial L_x}{\partial x} \frac{\partial H}{\partial p_x} - \frac{\partial L_x}{\partial p_x} \frac{\partial H}{\partial x} + \frac{\partial L_x}{\partial y} \frac{\partial H}{\partial p_y} - \frac{\partial L_x}{\partial p_y} \frac{\partial H}{\partial y} + \frac{\partial L_x}{\partial z} \frac{\partial H}{\partial p_z} - \frac{\partial L_x}{\partial p_z} \frac{\partial H}{\partial z}. \quad (3.26)$$

Since L_x has no x or p_x dependence and $H = \mathbf{p}^2/2m + V(r)$ we obtain

$$\{L_x, H\} = p_z \frac{p_y}{m} + z \frac{\partial V}{\partial y} - p_y \frac{p_z}{m} - y \frac{\partial V}{\partial z}. \quad (3.27)$$

The first and third terms obviously cancel. Also

$$\frac{\partial V}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial V}{\partial r} = \frac{y}{r} \frac{\partial V}{\partial r} \quad \text{and} \quad \frac{\partial V}{\partial z} = \frac{z}{r} \frac{\partial V}{\partial r}, \quad (3.28)$$

so the second and fourth terms cancel and

$$\{L_x, H\} = 0. \quad (3.29)$$

Since L_x has no explicit time dependence this also means that

$$\frac{dL_x}{dt} = 0 \quad (3.30)$$

for the system, and the vanishing Poisson bracket of L_x and H results in the well-known conclusion that angular momentum components are conserved if there is a spherically symmetric potential. This is a general rule. Any quantity (if not explicitly time dependent) will be conserved if its Poisson bracket with the Hamiltonian is zero. Similarly any quantum operator which commutes with the Hamiltonian represents a conserved quantity

3.2 Lagrangian Field Theory.

So far we have considered the description of a system of discrete particles. However, the formalism can be extended to cover continuous systems. For example, electromagnetism cannot be described as above, in terms of an object at point x at time t , but exists as a field strength as a function of position and time, i.e. $\mathbf{E}(\mathbf{x}, t)$ and $\mathbf{B}(\mathbf{x}, t)$. Hence, fields are functions of four parameters (in three space dimensions), rather than one.

In order to extend our discussion we avoid the complications involved with the vector like nature of the electromagnetic field, and introduce a scalar field $\phi(\mathbf{x}, t)$. In order to generalise particle mechanics to fields we first imagine splitting space up into a lattice of points labelled by i , where each of the points has a separation $\Delta x = a$, and similarly for the y and z coordinates. The Lagrangian for the field at each lattice point is then relatively easy to construct. The kinetic energy of each discrete part of the lattice is given by

$$t_i = \frac{1}{2} \left(\frac{\partial \phi_i}{\partial t} \right)^2, \quad (3.31)$$

and for a simple harmonic type potential for the field

$$v_i = \frac{1}{2} \omega^2 \phi_i^2. \quad (3.32)$$

Hence, the total Lagrangian is

$$L_0 = a^3 \sum_i \left(\frac{1}{2} \left(\frac{\partial \phi(\mathbf{x}_i, t)}{\partial t} \right)^2 - \frac{1}{2} \omega^2 \phi_i^2(\mathbf{x}_i, t) \right). \quad (3.33)$$

where a is the lattice spacing and the factor a^3 , the volume per lattice site, has been inserted to obtain the correct dimension for the Lagrangian. We can also introduce an interaction potential

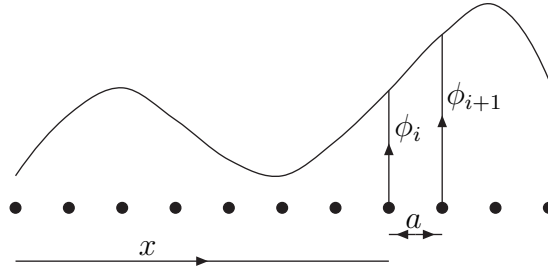


Figure 2: The representation of a wave on a string as a series of discrete points.

between neighbouring points on the lattice. A model for this would be to consider the motion of a wave on a string in terms of discrete points on the string, as shown in the figure below. The amplitude of transverse motion of the string at point i is defined by ϕ_i .

If the transverse displacement of two adjacent points is different then they will be separated by a distance equal to $\sqrt{a^2 + (\phi_{i+1} - \phi_i)^2}$. Hence, the increase in length of the string between the two points, if the transverse displacements are small compared to the equilibrium separation a , is

$$(a^2 + (\phi_{i+1} - \phi_i)^2)^{\frac{1}{2}} - a \approx \frac{(\phi_{i+1} - \phi_i)^2}{2a}. \quad (3.34)$$

Therefore, if the tension in the string is T , the potential energy V is the sum of the tension multiplied by the extension summed over all segments, i.e.

$$V = \sum_i \frac{T(\phi_{i+1} - \phi_i)^2}{2a}. \quad (3.35)$$

Extending this to all three dimensions and introducing an unknown coupling constant κ instead of T we get

$$V_{int} = a^3 \kappa \sum_{i, \mu_k} (\phi(\mathbf{x}_i + \mu_k, t) - \phi(\mathbf{x}_i, t))^2, \quad (3.36)$$

where the μ_k are the lattice vectors in each direction to the nearest neighbour. We can now add this to the previous Lagrangian. However, in order for this to become a field theory we must let $a \rightarrow 0$ and $i \rightarrow \infty$ in such a way that we obtain a finite result with ϕ being a continuous function of space as well as time. In the interaction potential we see that in this limit

$$\left(\phi(\mathbf{x}_i + \mu_k, t) - \phi(\mathbf{x}_i, t) \right) = \phi(\mathbf{x}_i, t) + a \left(\frac{d\phi}{dx_k} \right) - \phi(\mathbf{x}_i, t) + \mathcal{O}(a^2) \quad (3.37)$$

$$\rightarrow a \left(\frac{d\phi}{dx_k} \right). \quad (3.38)$$

So in the continuum limit

$$a^3 \sum_i \rightarrow \int d^3 \mathbf{x}, \quad (3.39)$$

and in order to obtain a Lorentz invariant result we must have $\kappa = 1/(2a^2)$. This then results in the Lagrangian

$$L = \int d^3\mathbf{x} \left(\frac{1}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} (\nabla \phi)^2 - \frac{1}{2} \omega^2 \phi^2 \right). \quad (3.40)$$

But using the previous definition of the Action S in terms of the Lagrangian we obtain

$$S[\phi] = \int dt \int d^3\mathbf{x} \mathcal{L}(\partial_\mu \phi, \phi), \quad (3.41)$$

where $\mathcal{L}(\partial_\mu \phi, \phi)$ is a Lorentz covariant Lagrangian density.

The equations of motion are derived in the same way as for the case of particle mechanics, i.e. the true behaviour of the system is determined to be that at which the Action is an extremum for fixed boundary conditions. Hence, we consider making a small change in ϕ away from the true value ϕ^0 , i.e.

$$\phi(\mathbf{x}, t) = \phi^0(\mathbf{x}, t) + \epsilon(\mathbf{x}, t) \quad \text{and} \quad \partial_\mu \phi(\mathbf{x}, t) = \partial_\mu \phi^0(\mathbf{x}, t) + \partial_\mu \epsilon(\mathbf{x}, t), \quad (3.42)$$

where $\epsilon(\mathbf{x}, t)$ are small variations which vanish on some three-dimensional space-time boundary, often taken to be at infinity. We may then derive the equations of motion as before.

$$S[\phi] = \int dt \int d^3\mathbf{x} \mathcal{L}(\partial_\mu(\phi^0 + \epsilon), \phi^0 + \epsilon) \quad (3.43)$$

$$= S[\phi^0] + \int dt \int d^3\mathbf{x} \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \partial_\mu \epsilon + \frac{\partial \mathcal{L}}{\partial \phi} \epsilon \right) \quad (3.44)$$

$$= S[\phi^0] + \int dt \int d^3\mathbf{x} \left(-\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} + \frac{\partial \mathcal{L}}{\partial \phi} \right) \epsilon, \quad (3.45)$$

where in the final step we have used the 4-d divergence theorem. Again for the Action to be at an extremum for arbitrary small variations of the field on the second term on the right hand side must vanish, and we obtain the classical field equations

$$\left(\frac{\partial \mathcal{L}}{\partial \phi} \right) = \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right). \quad (3.46)$$

For our particular example

$$\frac{\partial \mathcal{L}}{\partial \phi} = -\omega^2 \phi; \quad \frac{\partial \mathcal{L}}{\partial(\partial \phi / \partial t)} = \frac{\partial \phi}{\partial t}; \quad \frac{\partial \mathcal{L}}{\partial(\partial \phi / \partial x_k)} = -\frac{\partial \phi}{\partial x_k}, \quad (3.47)$$

and the field equation is

$$\frac{\partial}{\partial t} \frac{\partial \phi}{\partial t} + \nabla \cdot (-\nabla \phi) + \omega^2 \phi^2 = 0, \quad (3.48)$$

i.e.

$$\frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi + \omega^2 \phi = 0. \quad (3.49)$$

So this is exactly the same as the Klein Gordon equation for a relativistic scalar particle in zero potential, and has solutions which are simply plane waves in four dimensions, i.e. $\phi \sim \exp(ip_\mu x^\mu)$ where $p^\mu p_\mu = p^2 = \omega^2$, so ω plays the same role as the mass m .

Hence, we have constructed a relativistically invariant scalar field theory with recognisable and easily interpretable solutions. In order to consider quantisation, as well as to investigate potential symmetries it would be useful to have a corresponding Hamiltonian formulation of classical field theory. Here we have to be careful - the Hamiltonian density corresponds to the energy density, which unlike the Lagrangian density is therefore not Lorentz invariant. In order to have a sensible Hamiltonian density it must be defined as one component of a Lorentz structure which has well-defined transformation rules under Lorentz transformations, and which also satisfies conservation laws.

If we consider small variations of the space-time coordinates $x^\mu \rightarrow x^\mu + \alpha^\mu$ where α^μ vanishes on some space-time boundary, then the invariance of the Action under such a change of coordinates (which is after all just a change in the definition of integration variables in the Action) can be shown to lead to the conservation equation

$$\partial^\lambda \Theta_{\lambda\rho} = 0, \quad (3.50)$$

where

$$\Theta_{\lambda\rho} = \frac{\partial \mathcal{L}}{\partial(\partial^\lambda \phi)} \partial_\rho \phi - g_{\lambda\rho} \mathcal{L}, \quad (3.51)$$

and where $g_{\lambda\rho}$ is the space-time metric. The quantity $\Theta_{\lambda\rho}$ is known as the energy momentum tensor, and we notice that its definition in terms of the Lagrangian density has some similarity to the definition of the Hamiltonian in terms of the Lagrangian. We can make this analogy more precise by considering the single component

$$\Theta_{00} = \frac{\partial \mathcal{L}}{\partial(\partial^0 \phi)} \partial_0 \phi - \mathcal{L}. \quad (3.52)$$

If we can identify this as an energy density then we require $\int d^3\mathbf{x} \Theta_{00} = E$ to be conserved. In fact

$$\frac{\partial E}{\partial t} = \int d^3\mathbf{x} \frac{\partial \Theta_{00}}{\partial t}, \quad (3.53)$$

and from our conservation rule $\partial^0 \Theta_{00} - \nabla \cdot \Theta_0 = 0$, and therefore

$$\frac{\partial E}{\partial t} = \int d^3\mathbf{x} \nabla \cdot \Theta_0 = \int d^2\mathbf{S} \cdot \Theta_0. \quad (3.54)$$

This is the continuity equation relating the change of energy with time in a volume to the flow of energy across the surface of the volume considered, and is zero if the flow is zero.

Hence, the component of the four-tensor $\Theta_{\lambda\rho}$

$$\Theta_{00} = \frac{\partial \mathcal{L}}{\partial(\partial^0 \phi)} \partial_0 \phi - \mathcal{L}, \quad (3.55)$$

is the suitable generalisation of the Hamiltonian to classical field theory. By comparison to particle mechanics where $H = p\dot{x} - L$, if we have a conjugate momentum field $\pi(\mathbf{x}, t)$ defined by

$$\pi = \frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial t)}. \quad (3.56)$$

the Hamiltonian density is then defined by

$$\Theta_{00} = \mathcal{H}(\pi, \phi, \partial\phi/\partial x, \dots) = \pi \frac{\partial\phi}{\partial t} - \mathcal{L}, \quad (3.57)$$

and in the above example would be

$$\mathcal{H} = \frac{1}{2} \left(\pi^2 + (\nabla\phi)^2 + m^2\phi^2 \right). \quad (3.58)$$

Quantum field theory is then associated with imposing the same type of commutation relations between the field and its conjugate momentum as between x and p in quantum mechanics. this is the topic of the next section.