

§8. HAMILTONIAN MECHANICS

In order to proceed from the classical formulation of Maxwell's electrodynamics to the quantum mechanical description a new mathematical language will be needed. In the previous sections the electromagnetic field was described using partial differential equations — Maxwell's equations — for the field components and their vector and scalar potentials. These equations provided the basis for the development of the equations of motion of charged particles embedded in the electromagnetic field. However these equations of motion were simplified descriptions of the actual motions of large numbers of charges in a conducting material. In this previous formulation, the electromagnetic field was an abstract mathematical entity. This approach was a consequence of the classical nature of electromagnetism since the field is treated as an ethereal entity that serves as the medium to carry electromagnetic waves, their energy and momentum.

Special methods have been developed by Lagrange in order to deal with the large — possibly infinite — number of particles. By formulating Newton's 2nd Law in terms of the kinetic and potential energy as functions of the coordinate system in which the particles are moving, Lagrange succeeded in *generalizing* the use of the coordinates. This approach allows the equations of motion to be isolated from a specific coordinate system, which in turn allows the *variational principle* to be applied to a variety of problems including the description of the electromagnetic field and its quantum mechanical formulation.

The formulation of the electromagnetic field can be restated in terms of Hamilton's theory of mechanics using the electromagnetic field's vector potential as a starting point [Heil81]. This method provides a classically consistent transition to the quantum mechanical description of the effect of the electromagnetic field on charged particles. In order to proceed with this formulation several new concepts must be presented. The quantum nature of matter will be briefly described followed by the description of Hamiltonian mechanics. The formulation of the equations of motion was first used in classical mechanics [Gold55], but now serves as the *introductory* method to quantizing the electromagnetic field.

§8.1. NEWTON'S EQUATIONS IN LAGRANGIAN FORM

Special methods have been developed by Lagrange in order to deal with the large — and possibly infinite — number of particles to be described by the equations of motion. By formulating Newton's 2nd Law in terms of

the kinetic and potential energy as functions of the coordinate system in which the particles are moving. Lagrange succeed in *generalizing* the use of coordinates.

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Isaac Newton formulated the laws of motion using a calculus of his own invention. Using the Cartesian coordinate system, Newton's equations for the i^{th} particle with mass m_i are:

$$\left. \begin{aligned} m_i \frac{d^2 x_i}{dt^2} &= X_i \\ m_i \frac{d^2 y_i}{dt^2} &= Y_i \\ m_i \frac{d^2 z_i}{dt^2} &= Z_i \end{aligned} \right\} \quad i = 1, 2, \dots, n \quad (8.1)$$

where, X_i , Y_i and Z_i are the three components of the force acting on the i^{th} particle.

The transformation of the equations from Newtonian form to the Lagrangian form will be make use of both the kinetic and potential energy definition in the Cartesian coordinate system. The kinetic energy, T , is defined as:

$$\begin{aligned} T &= \frac{1}{2m} (\dot{x}_1^2 + \dot{y}_1^2 + \dot{z}_1^2) + \dots + \frac{m_n}{2} (\dot{x}_n^2 + \dot{y}_n^2 + \dot{z}_n^2), \\ &= \frac{1}{2} \sum_{i=1}^n m_n (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2). \end{aligned} \quad (8.2)$$

If only conservative systems of particles are considered, then the potential energy, V , can be defined as a function of the coordinates $x_1, y_1, z_1, \dots, x_n, y_n, z_n$ of all the particles. In this approach the force experienced by each particle is equal to the partial derivative of the potential energy, such that,

$$\left. \begin{aligned} X_i &= -\frac{\partial V}{\partial x_i} \\ Y_i &= -\frac{\partial V}{\partial y_i} \\ Z_i &= -\frac{\partial V}{\partial z_i} \end{aligned} \right\} i = 1, 2, \dots, n. \quad (8.3)$$

These equations can now be used to restate Newton's equation of motion. By removing the references to the individual coordinates, the notation for the equations of motion can be simplified. Assuming that the force applied to the particle can be found from a potential, which is a function of both position and time, $V(\mathbf{r}, t)$, according to the relationship $F(\mathbf{r}, t) = -\partial V(\mathbf{r}, t)/\partial \mathbf{r}$. Substituting this expression into Newton's equation of motion gives,

$$m\ddot{\mathbf{r}} + \underbrace{\frac{\partial V(\mathbf{r}, t)}{\partial \mathbf{r}}}_{-F} = 0. \quad (8.4)$$

Since the momentum of the particle is $p = m\dot{\mathbf{r}}$, Newton's equation can be rewritten as,

$$\underbrace{\dot{p}}_{m\ddot{x}} + \underbrace{\frac{\partial V(\mathbf{r}, t)}{\partial \mathbf{r}}}_{-F} = 0. \quad (8.5)$$

Since the mass of the particle, m , is a constant, the momentum can be rewritten in terms of the particle's kinetic energy,

$$\dot{p} = \frac{d}{dt}(m\dot{\mathbf{r}}) = \frac{d}{dt} \underbrace{\frac{\partial}{\partial \mathbf{r}} \left(\frac{m\dot{\mathbf{r}}^2}{2} \right)}_{m\dot{\mathbf{r}}} = \frac{d}{dt} \underbrace{\frac{\partial (m\dot{\mathbf{r}}^2/2)}{\partial \mathbf{r}}}_p \quad (8.6)$$

By defining the kinetic energy as, $T = m\dot{\mathbf{r}}^2/2$, and using this expression to eliminate the momentum p from Newton's Law gives,

$$\underbrace{\frac{d}{dt} \frac{\partial T}{\partial \dot{\mathbf{r}}}}_p + \underbrace{\frac{\partial V}{\partial \mathbf{r}}}_{-F} = 0. \quad (8.7)$$

The kinetic energy is now a function of $\dot{\mathbf{r}}$ but not \mathbf{r} . The potential energy V as a function of \mathbf{r} but not $\dot{\mathbf{r}}$. This allows the Lagrangian to be defined again as using the relations $\partial L/\partial \dot{\mathbf{r}} = \partial T/\partial \dot{\mathbf{r}}$ and $\partial L/\partial \mathbf{r} = -\partial V/\partial \mathbf{r}$ as,

$$L(\dot{\mathbf{r}}, \mathbf{r}) = T(\dot{\mathbf{r}}) - V(\mathbf{r}). \quad (8.8)$$

This now allows Newton's Law to be stated as the *Euler-lagrange* equation (in Cartesian coordinates),

$$\underbrace{\frac{d}{dt} \frac{\partial L(\mathbf{r}, \dot{\mathbf{r}})}{\partial \dot{\mathbf{r}}}}_{m\dot{\mathbf{r}}} - \underbrace{\frac{\partial L(\mathbf{r}, \dot{\mathbf{r}})}{\partial \mathbf{r}}}_F = 0. \quad (8.9)$$

So far the changes from the description of Newton's Law as the simple equations of motion, to the Lagrangian description has not simplified anything. In the next sections, the Lagrangian description of the motion of a particle will be used to remove the dependence on the Cartesian coordinate system. In addition the Hamiltonian description of the particles motion will be developed. This description will be used as the basis for the quantum mechanical description of the electromagnetic field interacting with charged matter.

§8.2. VARIATIONAL DESCRIPTION OF THE EQUATIONS OF MOTION

The equations of motion of an object moving in a Cartesian coordinate system was first described by Isaac Newton. In Newton's mechanics the motion of a particle is uniquely determined by the *vectorial* force acting on the particle at every instance of time [Lanc70], [Byro70], [Byro69], [Chan95]. In Newton's mechanics the action of a force is described by the momentum produced by that force. There are other descriptions of the action of a force. One such description was provided by Gottfried Wilhelm Leibniz (1646–1716), who was a contemporary of Newton's. Leibniz' formulation included a quantity known as *vis viva* (Latin for *living force*) which in modern terms is called the kinetic energy [Asim66]. Leibniz replaced Newton's momentum by the kinetic energy and replaced Newton's *force* by the *work of the force*. This *work of the force* was later replaced by the *work function*. Leibniz is now credited with founding a second branch of mechanics — analytical mechanics, which is based on the maintenance of the equilibrium between the kinetic energy and the *work function*. In modern terms the *force function* is replaced by the potential energy. This approach laid the foundation for the *Principle of Least Action*.

It is convenient to divide the development of classical mechanics into three periods, the first based on Newton's *Philosophiae Naturalis Principia Mathematica* published in 1687 [Cajo62], the second based on Lagrange's *Mécanique Analytique (Analytical Mechanics)* published in 1788 [Lagr88] and the third based on Hamilton's *General Method of Dynamics* published in 1834 and 1835 [Hami34] and well as Carl Gustav Jacob Jacobi's (1804–

1851) *Vorlesungen über Dynamics* published by Clebsh in 1866. These works established mechanics as a mathematical science complete with *theoretical* explanation of the behavior of objects and like the previous descriptions of Fourier's mathematical physics works, formed a paradigm for the methods used by Maxwell and the description of electromagnetic phenomenon.

On New Year's Day 1697, Johann Bernoulli (1667–1748) of the University of Basal posed the question to the *sharpest mathematicians in the whole world* — given two points A and B in a vertical plane, find the path $A-M-B$ which the movable particle M will traverse in the shortest time, assuming the acceleration on M is due solely to gravity. Using Bernoulli's description [Stru86], the curve $ACEDB$ shown in Figure 8.1, has a path of least time from A to B . Letting C and D be two points on the curve, Bernoulli said CED must have the same path of least time.

This is the essential point of Bernoulli's argument and the power of this development in modern physics. Any curve which has a minimum property globally (in the large) must also have this property locally (in the small). If it were not the least time path than there would be some other path CFD which would be faster. If that were the case, the new path $ACFDB$ would be faster than the path $ACEDB$, which would be contrary to the original hypothesis.

The result is Bernoulli's contribution to modern physics..

...the path quickest overall must be the quickest in between any intermediate points, and the property which holds globally most also hold locally.

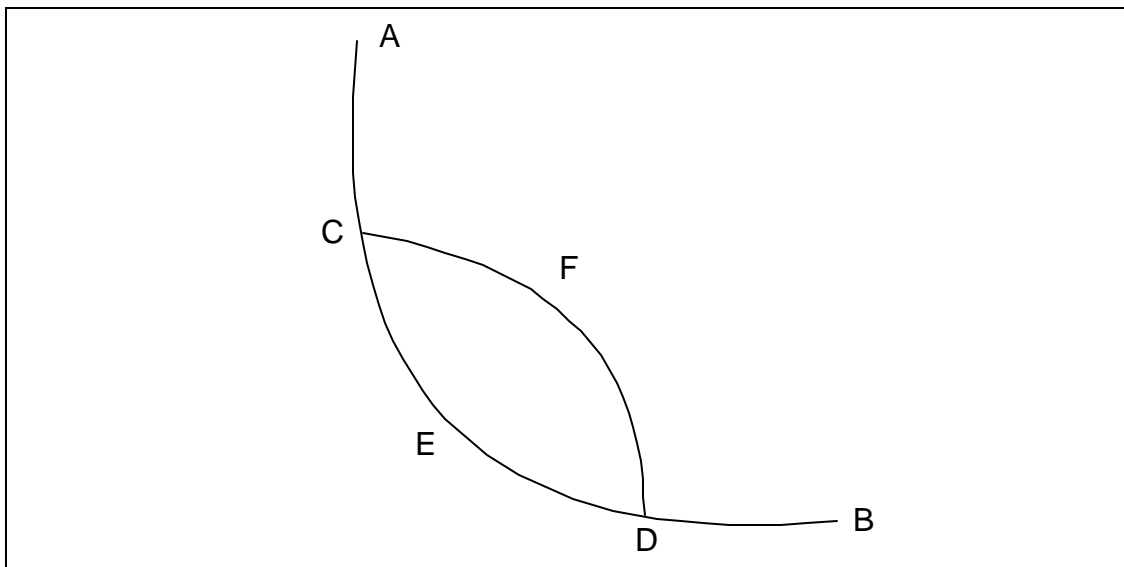


Figure §8.1 — Bernoulli's curve which describes the *least time path* between to points A and B. The mathematical problem was posed to the world's mathematicians as a challenge. Although the solution was already known to Bernoulli, a simple solution was also known to Newton, who did not respond to Bernoulli's challenge.

This problem is known as the *brachistochrone* problem — *brachistos* = shortest and *chronos* = time — and it marks the beginning of the general interest in the calculus of variations [Byro69], [Chan95], [Stru86], [Reid69].^[1] Using Bernoulli's approach the *local principal* allows the integral equations of motion to be transformed into differential equations of motion. The result is a greatly simplified method of analyzing the motion of the particle *M* along the path of least time.

In any change which occurs in nature, the sum of the product of each body multiplied by the space it traverses and by its speed (referred to as "the action") is always the least possible.

— Pierre Louis de Maupertuis [Maup46], [Doug90].

The development of analytical mechanics is associated with Leonhard Euler (1707–1783), Joseph Louis Lagrange (1736–1813), Simeon Poisson (1781–1840) and William Rowan Hamilton (1805–65). It is essentially a reformulation of Newton's mechanics which allows many problems to be solved more simply.

¹ When Bernoulli first issued the challenge there were no responses. He forwarded the problem to Charles Montagu (-), who was the president of the Royal Society. Isaac Newton responded to the question with an anonymous solution in a letter dated Jan 30, 1697. The results were published in *Philosophical Transactions*, for January 1696/7. Although Bernoulli is given credit for the solution to his problem, Newton's solution was recognized by Bernoulli in a letter to Basange de Beauval...

...although it's author, in excessive modesty, does not reveal his name, we can be certain beyond any doubt that the author is the celebrated Mr. Newton... [Chan95]

When Bernoulli solved the brachistochrone problem he boasted of having discovered a wonderful solution, but did not publish it immediately. Instead he proceeded to challenge other mathematicians, especially his elder brother, Jacob (1654–1705). Bernoulli carried on a bitter feud in which he publicly characterized his brother as incompetent. He finally published his solution in 1697 which described the motion of a *bob* traveling on a cycloid path. Before Bernoulli published his work Huygens had discovered that a mass point oscillating without friction under the influence of gravity on a vertical cycloid has a period independent of amplitude. This cycloid was called a *tautochrone* with Bernoulli's discovery, this curve was renamed the *brachistochrone* [Cour56].

Newtonian mechanics was founded on the concept of point masses, that is objects with no dimensional form. Newton's equations of motion are stated in terms of the Cartesian coordinates of the particle in motion. While the problems of dynamics can theoretically be solved by such means, in systems containing large numbers of particles, the integration of the equations of motion is generally too complex. Special methods were developed to deal with this complexity.

Lagrange's approach makes use of an integral equation containing the potential and kinetic energies. The kinetic energy (T) depends on the object's velocity $v = dx/dt$, while the potential energy (V), depends only on the object's position x . The form of Lagrange's solution is the difference between the kinetic and potential energies.

Lagrange formulated the solution to the equations of motion by means of *generalized coordinates*, i.e. any set of variables sufficient in number to define unambiguously the configuration of the system. The generalized coordinates in the Lagrange and Hamilton descriptions of motion utilizing the expressions for kinetic and potential energy as functions of these coordinates.

In the classical description of motion, two measurable quantities of a particle in motion are its spatial position and momentum. If these values are known for any point in space and time, the particle's motion or path can be calculated from Newton's second law of motion and knowledge of the external force law acting on the particle. If the particle's motion is observed over a small portion of its path its momentum is nearly constant. The product of the particle's momentum and small distance is called the *increase in the particle's action*. This action is a scalar quantity that the particle *carries* with it and increases as the particle moves along its path.^[2]

§8.3. CALCULUS OF VARIATIONS

The principal of *stationary action* appeared in Hero of Alexandria's (62 A. D.) *Cataptrica (Optics)* which described the reflection of light from a plane mirror as the shortest path taken. Pierre de Fermat (1601–1665)

² This description of action differs from the original concept developed by P. Maupertuis who proposed that *brachistochrone* problem could be better solved by not considering the transit time of the movable particle, but rather by a quantity called *action*. Maupertuis incorrectly defined this action as the product of the distance the particle travels and its speed [Motz89]

reformulated this concept as the *principal of Least Time* in 1657. Fermat stated that a light ray required the least time even if deviated from the shortest physical path,

... nature operates by the simplest and most expeditious way and means.

Fermat's principal was capable of producing the correct law of reflection and lead to the law relating the angle of incidence and reflection at an interface to the ratio of the refractive indices of the media. The relationship was confirmed experimentally by Willebrord Snell van Royen (1591–1626) in 1621 and is known as Snell's law.

The calculus of variations and the *principle of least action* combine to form a powerful method of investigating problems in dynamics. Pierre-Louis Moreaude Maupertuis (1698–1759), the author of the *Principle of Least Action* in 1774, declared it to be a metaphysical principle on which all canons of motion are based.^[3] The Newtonian equations of motion can be written in a form which makes the transition to quantum mechanics appear natural [Byro69].

The concept and principle of least action were generalized by Hamilton to include the propagation of light as well as the motion of particles. By placing a restriction on the definition of action Newtonian mechanics can be transformed into quantum mechanics. Newtonian mechanics assumes that a particles motion can be followed in infinite detail and infinite precision. If this were possible than the motion of a

³ Eighteenth century *philosopher scientists* learned to compute the paths taken by planets and objects using Newton's equations of motion. A French geometer and *philosophe*, Pierre-Louis Moreau de Maupertuis [Maup46] along with Joseph Louis Lagrange showed that the paths taken by these objects are always the most economical when the kinetic and potential energy are computed as a single quantity. In the way the moving object minimizes its *action* — a quantity based on the objects velocity, mass and the space through which it travels. No matter what forces were applied to the object, it somehow *choose* the cheapest of all possible paths. Unlike the total energy of an object — its kinetic and potential energy — which are always conserved, the quantity of *action* is constantly changing. No matter what value the *action* may assume during the objects *flight*, at the destination the *action* will a minimum of all the possible *actions* that could have occurred. In this view of mechanics, the object seems to *choose* its path, with the knowledge of all possible paths — at the beginning of the motion. Maupertuis wrote...

It is not in the little details ... that we must look for the supreme Being, but in phenomena whose universality suffers no exception and whose simplicity lay them quite open to our sight. [Glei92], [Feyn64], [Your68].

particle could be described by the particles position and momentum at a single point in space and time.

This process would be observable if all physical entities were infinitely divisible. However if nature is somehow limited in its divisibility than the *action* during a process can change only by a finite amount \hbar , than the precise determination of a particle's motion can never be determined. In order to determine the particles motion precisely, the momentum and position must be known at the same point in space and time.

Since the action is the product of momentum and a measured spatial interval that must be taken as infinitesimal, the action becomes infinitesimal and thus smaller than some limit \hbar . The result is that the momentum becomes infinite, losing all knowledge of the particles action. The result is that the particle's action becomes *quantized* so that its position and momentum can not be simultaneously known. The full impact of this result will be developed in later sections.

§8.4. ORDINARY MAXIMUM AND MINIMUM THEORY

The calculus of variations has been an important branch of mathematical physics for nearly three centuries. The task of finding points at which a functions possesses a maximum or minimum is common in the analysis physical problems. In the calculus of variations, functional forms are found in which integrals assume maximum or minimum values. These forms may contain several variables and describe multidimensional processes. Before considering maxima and minima of an integral function, the theory of the calculus of functions of a single variable will be examined.

Let $f(x)$ be a continuous function of a single variable, x , having a maximum or minimum value at $x = a$. The for a sufficiently small ϵ , there is a maximum at,

$$f(a + \epsilon) - f(a) < 0, \tag{8.10}$$

and a minimum at,

$$f(a + \epsilon) - f(a) > 0. \tag{8.11}$$

Taking the maximum case and assuming $f(a + \epsilon)$ can be expanded in positive integral powers of ϵ , by Taylor's theorem, gives,

$$f(a + \epsilon) - f(a) = \epsilon \dot{f}(a) + \frac{1}{2} \epsilon^2 \ddot{f}(a) + O(\epsilon^3). \tag{8.12}$$

The Landau symbol, O , has the meaning: $O(\epsilon^3)$ possesses the property that as $\epsilon \rightarrow 0$, the quantity $1/\epsilon^3 O(\epsilon^3)$ is bounded. From Eq. (8.10) and Eq. (8.12) at a maximum or a minimum the sign of $f(a+\epsilon) - f(a)$ is independent of the sign of ϵ , and so from Eq. (8.12) $\dot{f}(a) = 0$.

From Eq. (8.10) and Eq. (8.12) it follows that at a maximum $\ddot{f}(a)$ is negative and from Eq. (8.11) and Eq. (8.12) that at a minimum $\ddot{f}(a)$ is positive. Alternatively at a maximum $\dot{f}(a)$ is a decreasing function of a and at a minimum it is an increasing function of a .

It is possible that $\dot{f}(a) = 0$ and that $f(a)$ is neither a maximum or minimum of $f(x)$. Such a condition occurs when $\dot{f}(a) = 0$ and $\ddot{f}(a) = 0$, and $\dddot{f}(a) \neq 0$. It is then customary to say that $f(a)$ is a stationary value of $f(x)$. In general all roots of $\dot{f}(x) = 0$ are said to give rise to stationary values of $f(x)$. With this *brief* background the Lagrangian formalism will be developed in the next section.

§8.4.1. Lagrangian Formalism and the Calculus of Variations

The Lagrange formalism will be developed through a simple example — the motion of a particle with mass m in a harmonic oscillator potential given by $V(x) = kx^2/2$. According to Newton's second law of motion, the acceleration of the particle is determined by,

$$m\ddot{x} = -kx, \quad (8.13)$$

which has the well known solution,

$$x = x_0 \cos(\omega t + \phi), \quad (8.14)$$

where $\omega = \sqrt{k/m}$, is the angular frequency, the constants x_0 and ϕ are determined by the initial conditions.

Consider two times t_1 when the particle is at position x_1 and t_2 when the particle is at position x_2 . The path the particle follows between times t_1 and t_2 can be described by the quantity,

$$S = \int_{t_1}^{t_2} L\left(x, \frac{dx}{dt}\right) dt, \quad (8.15)$$

where the difference between the kinetic energy T and the potential energy V , $L = T - V$ is called Lagrangian. The quantity S , which in the past was called *Hamilton's Principal Function*, but is now called the *action function*. Dimensionally, the action is an energy times a time and has similar dimensions as Planck's constant.

The action, S , is a functional of x , that is it is a function of the function $x(t)$, which describes the path satisfying the two constraints that $x(t)$ at time $t = t_1$ assumes the value x_1 , while $x(t)$ at time $t = t_2$ assumes the value x_2 . Apart from these constraints the path may be arbitrary.

The action S is then a function of the different paths satisfying the two constraints. In order to formulate the extremum on S , a family of functions is considered, given by,

$$x(t, \alpha) = x(t, 0) + \alpha \eta(t), \quad (8.16)$$

where the function $x(t, 0)$ is the one corresponding to the extremum. The function $\eta(t)$ is arbitrary, except that it satisfies the constraints $\eta(t_1) = \eta(t_2) = 0$.

The action S is then a function $S(\alpha)$ of the parameter α ,

$$S(\alpha) = \int_{t_1}^{t_2} dt L(x(t, \alpha), \dot{x}(t, \alpha), t). \quad (8.17)$$

This expression allows for the possibility that the extremum may depend explicitly on time with the force constant of the harmonic oscillator being a function of time, $k = k(t)$.

The extremum condition is given by,

$$\left. \frac{\partial S}{\partial \alpha} \right|_{\alpha=0} = 0, \quad (8.18)$$

By differentiating Eq. (8.18) with respect to the parameter α gives,

$$\frac{\partial S}{\partial \alpha} = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right) \eta(t) dt \quad (8.19)$$

Integrating by parts ^[4] in order to replace η by $\dot{\eta}$, results in,

$$\frac{\partial S}{\partial \alpha} = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial x} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right) \eta(t) dt, \quad (8.20)$$

since,

$$\begin{aligned} \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial \dot{x}} \dot{\eta} \right) dt &= \left[\eta \frac{\partial L}{\partial \dot{x}} \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \eta(t) \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) dt, \\ &= 0 - \int_{t_1}^{t_2} \eta(t) \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) dt. \end{aligned} \quad (8.21)$$

The extremum condition Eq. (8.21) then becomes,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0, \quad (8.22)$$

since $\eta(t)$ is arbitrary except for the condition $\eta(t_1) = \eta(t_2) = 0$.

Eq. (8.22) is named the Lagrange equation. The derivative of Lagrange's equation started from a consideration of the instantaneous state of the system and small virtual displacements about the instantaneous state, i.e. from a *differential principle* such as D'Alembert's principle. ^[5] It is also possible to obtain Lagrange's equations from a

⁴ The method of integration by parts employs the identity $f(dg/dt) = d(fg)/dt - g(df/dt)$, where f and g both are functions of t . When both sides of this equation are integrated with respect to t over the interval from t_1 to t_2 the result is

$$\int_{t_1}^{t_2} \{ f(dg/dt) \} dt = [fg]_{t_1}^{t_2} - \int_{t_1}^{t_2} \{ (df/dt)g \} dt.$$

⁵ It is surprising that there can be several formulations of the principals of mechanics. Once it is understood that mechanics is a *description* of motion, then different methods of describing this motion can serve different purposes. Although Newton's method of describing the motion of particles has long been the most useful *simple* approach other formulations have been created which attempt to simplify the solutions of various types of problems. These alternative formulations differ considerably in their concepts of mass and force.

Some are restatements of Newton's laws, while others introduce new concepts. D'Alembert's principal is a restatement of Newton's Laws which seeks to reduce dynamics to statics using Newton's concept of mass and force. D'Alembert formulated his principal in 1743 in the work *Traité de Dynamique*, which was revised in 1758 as *A general principal for finding the motions of several bodies which react on each other in any fashion*. In

principle which considers the entire motion of the system between times t_1 and t_2 and small virtual variations of the entire motion from the actual motion.

§8.5. GENERALIZED COORDINATES

It is not always convenient to use Cartesian coordinates when solving problems in Newtonian mechanics. Alternative coordinate systems result in simpler solutions. The analysis of the motion of a pendulum is an example. The Lagrangian formulation of the equations of motion is well suited for these non-Euclidean or *constrained dynamical* variables. The generalized coordinates presented in this section are not alternatives to Euclidean coordinate systems, but are descriptions of the *configuration* of the mechanical system with z_i degrees of freedom. An example of such a

D'Alembert's formulation the concept of *virtual displacements* is used to describe the motions of particles in the presence of external forces. This principal can be stated in a general form as:

... if there are n particles 1, 2, 3, ..., n acted on by forces F_1, F_2, F_3, \dots , respectively, and if these are given arbitrary (virtual) displacements dr_1, dr_2, dr_3, \dots , where \mathbf{r} is the position vector of the particle, the condition of equilibrium under the action of the forces is $F_1 \cdot dr_1 + F_2 \cdot dr_2 + F_3 \cdot dr_3 + \dots + F_n \cdot dr_n = 0$ [Lind56]

The second type of formulation employs the concept of energy, Hamilton's principal being the one utilized here. In 1894 Heinrich Hertz published *Principals of Mechanics* in which he re-established the principals of mechanics with logical consistency not found in the usual Newtonian presentations of the day. Such late 19th century works usually contained metaphysical uncertainties and vagueness. Hertz attempted to reduce dynamics to kinematics, avoiding concepts like force, mass and energy. The fundamental principal of Hertzian mechanics is:

Every free system remains either in a state of rest or in uniform motions along a straightest path [Lind56].

Since most systems encountered in practical situations are non-free Hertz assumes that every part of a non-free system is part of a free system. Every motion of a free system or its non-free parts obeys the fundamental principal called *natural* motion, and Hertzian mechanics is only concerned with natural motion. There were serious problems with the description of motion, since in order to make the principal work it was necessary to invoke the existence of other particles, which may not be immediately discernible. The words *concealed* became associated with Hertz's principals.

Even though Hertz's concept did not lead to a particle method of computing the motions of particles it did lay the foundation for Hamilton's principal, in which the *concealed* aspects of the motion become the energy of the system which is minimized during the particles motion.

system is n particles each with mass m_i and coordinates z_i , where $i=1, 2, \dots, n$. By choosing any independent functions of the original $3n$ dynamical coordinates z_i , $q = q(t) = q_i(t) = q_j(z_i(t))$, where $j=1, 2, \dots, 3n$, the new dynamical variables can be defined. These new variables are the *generalized coordinates*, $q = q_i(t)$ and the *generalized velocities*, $\dot{q} = dq_i(t)/dt$ [Doug90].

It is straightforward to generalize the Lagrange formalism to systems with more degrees of freedom than are found in classical mechanics. This may be done by considering a system described by the set of generalized coordinates q_r , where r assumes the values $1, 2, \dots, s$. As before, the Lagrangian is the difference between the kinetic and potential energies is given by $L = T - V$.

The Lagrange equations are derived by requiring the action,

$$S = \int_{t_2}^{t_1} L(q_1, q_2, \dots, q_r, \dots; \dot{q}_1, \dot{q}_2, \dots, \dot{q}_r, \dots; t) dt, \quad (8.23)$$

to have an extremum. The equations of motion or Lagrange's equations, then become,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_r} \right) - \frac{\partial L}{\partial q_r} = 0, \quad (8.24)$$

where the time derivative of the generalized coordinate is now given by, $\dot{q} = \frac{dq}{dt}$ [Whit37].^[6] This formulation of Lagrange's equations is most powerful for theoretical purposes and will be used in the development of the electromagnetic field Hamiltonian. The most significant property of Eq. (8.24) is its invariance with respect to arbitrary coordinate transformations. Proof of this important attribute is given in [Your68], pp. 37–39.

The Lagrangian of a system is not unique. The total time derivative of an arbitrary function can be added to the Lagrangian L to give a new Lagrangian L' , such that,

⁶ For a particle moving in a time independent potential, the Lagrangian does not depend explicitly on time. If the system is isolated in such a manner so that time transformation invariance is preserved, the Lagrange equations can be shown without an explicit time dependence and written as, $L(q_i, \dot{q}_i)$.

$$L'(q_r, \dot{q}_r, t) = L(q_r, \dot{q}_r, t) + \dot{f}(q_r, t), \quad (8.25)$$

which has the same properties as the initial Lagrangian L with respect to the principle of least action. The action function S' relative to the Lagrangian L' is given as,

$$S' = \int_{t_1}^{t_2} L' dt = S + f(q_r(t_2), t_2) - f(q_r(t_1), t_1). \quad (8.26)$$

Since the initial and final positions are fixed S and S' have the same extremum and differ only by a constant.

§8.6. HAMILTONIAN FORMALISM

If the only use of the Lagrangian action principle is to regenerate the equations of motion it would be considered interesting but redundant. However, the Lagrangian action principle provides a description of the dynamics of a system which contains more information than supplied by Newton's equations of motion. First the action function, S , is a *global* statement about the system, from which a *local* differential equation can be derived by imposing the extremum condition. The action is global in the sense that it receives contributions from the entire trajectory of the particle in motion. As such the action *records* the *history* of the particle's motion. Second, although the action is extremized by the set of classical trajectories that are the solution to Eq. (8.24), the action can be evaluated for any trajectory. Third, the action approach allows the definition of the canonical coordinates of position and momentum to be generalized by describing the energy of the system through the Hamiltonian.

The solution of a dynamical problem by Lagrange's method requires the integration of n second-order differential equations in the n unknowns q_1, \dots, q_n . An alternative system proposed by Hamilton consists of $2n$ first-order differential equations in $2n$ unknowns, and has the advantage that it is simple and concise in its formulation [Hami35]^[7]. In

⁷ Hamilton was an astronomer and mathematician in Dublin, Ireland. As a child prodigy he was able to translate from Latin and Greek at age 5 and had mastered 13 languages by age 13. He studied at Trinity College, Cambridge and was appointed professor of astronomy at age 22. Hamilton's works include mechanics and optics as well as the discovery of *quaternions*, which generalize complex numbers to a non-commutative algebra. Although Hamilton died 35 years before Planck published his theory of quantum mechanics, Hamilton has been immortalized through his association with the energy operator in Schrödinger's wave equation.

Hamilton's equations, the *canonical equations* constitute the basis for the quantum mechanical formulation of electrodynamics. An original concept introduced by Hamilton is the *generalized momentum*, which is defined as,

$$p_r(t) \equiv \frac{\delta S}{\delta \dot{q}_r(t)} = \frac{\partial L}{\partial \dot{q}_r(t)}. \quad (8.27)$$

Defining the generalized momenta as $p = m\dot{x}$ allows the introduction of the Hamiltonian by the transformation,

$$\mathbb{H}(p, q) = p_r \dot{q}_r(p, q) - L(q, \dot{q}(p, q)). \quad (8.28)$$

The differential $\frac{d\mathbb{H}}{dt}$ is,

$$\frac{d\mathbb{H}}{dt} = p d\dot{q} + \dot{q} dp - dL = -\dot{p} dq + \dot{q} dp = -\frac{\partial L}{\partial t}, \quad (8.29)$$

since,

$$\dot{p} = \frac{\partial L}{\partial q}. \quad (8.30)$$

It follows from Eq. (8.29) that the equations of motion for the system may be written as,

$$\begin{aligned} \frac{\partial \mathbb{H}}{\partial q_r} &\equiv \left(\frac{\partial \mathbb{H}}{\partial q_r} \right)_p, \\ &= \sum_s p_s \left(\frac{\partial \dot{q}_s}{\partial q_r} \right)_p - \left(\frac{\partial L}{\partial q_r} \right)_p, \\ &= \sum_s p_s \left(\frac{\partial \dot{q}_s}{\partial q_s} \right) - \left(\frac{\partial L}{\partial q_r} \right)_q - \sum_s \left(\frac{\partial L}{\partial \dot{q}_s} \right) \left(\frac{\partial \dot{q}_s}{\partial q_r} \right)_p, \quad [8] \quad (8.31) \\ &= \sum_s p_s \left(\frac{\partial \dot{q}_s}{\partial q_s} \right) - \frac{d}{dt} \left(\frac{\partial L}{\partial q_r} \right)_q - \sum_s \left(\frac{\partial L}{\partial \dot{q}_s} \right) \left(\frac{\partial \dot{q}_s}{\partial q_r} \right)_p, \\ &= -\dot{p}_r. \end{aligned}$$

⁸ In this derivation of the Lagrange equations the index subscript r or s is used to indicate the r th or s th coordinate, in order to distinguish between each generalized coordinate in a multidimensional coordinate space. The suffix to the bracketed derivative indicates that the q 's are kept constant while the index is summed over the s 's.

$$\begin{aligned}
 \frac{\partial \mathbf{H}}{\partial p_r} &\equiv \left(\frac{\partial \mathbf{H}}{\partial p_r} \right)_q, \\
 &= \dot{q}_r + \sum_s p_s \left(\frac{\partial \dot{q}_s}{\partial p_r} \right)_q - \left(\frac{\partial \mathbf{L}}{\partial p_r} \right)_q, \\
 &= \dot{q}_r + \sum_s p_s \left(\frac{\partial \mathbf{L}}{\partial q_s} \right)_q \left(\frac{\partial \dot{q}_s}{\partial p_r} \right)_q - \sum_s \left(\frac{\partial \mathbf{L}}{\partial \dot{q}_s} \right)_q \left(\frac{\partial \dot{q}_s}{\partial p_r} \right)_q, \\
 &= \dot{q}_r.
 \end{aligned} \tag{8.32}$$

which constitute Hamilton's equations. The change of variables from (q, \dot{q}) to (q, p) results from the transformation in Eq. (8.31) which is known as a Legendre transformation.^[9]

Restating the equations of motion in terms of the coordinates and the momenta results in the *Hamiltonian* of the system,

$$\mathbf{H}(p_r, q_r, t) = \sum p_r \dot{q}_r - \mathbf{L}(q, \dot{q}, t), \tag{8.33}$$

which describes the dynamics of the system in terms of the sum of the kinetic energy and the potential energy. Hamilton's principle requires that the path taken by any physical system between two states at specified times and with fixed values of the variables must be such that the value of the function $\delta \int_{t_0}^{t_1} (T - V) dt$ must be an extremum. In this form Hamilton's principle is sufficient to generate both the equations of motion of the system and the boundary conditions for any continuous field with localized forms of energy.^[10]

For the actual solution of problems, the equations of Lagrange are more convenient than those of Hamilton, since the first step in integrating

⁹ The change in basis from (x, \dot{x}, t) to (x, p, t) is accomplished through the Legendre transformation. Consider a function of the variables $f(x, y)$ so that a differential of f has the form $df = udx + vdy$, where $u = \partial f / \partial x$ and $v = \partial f / \partial y$. To change the basis of the description from x, y to the independent variables u, y , so that differential quantities are expressed in terms of the differentials du and dy . Let g be a function of u and y defined by the equation $g = f - ux$. A differential of g is then given as $dg = df - udx - xdu$ which has the desired form. The quantities x and v are now functions of the variables u and y by the relations $x = -(\partial g / \partial u)$, $v = -(\partial g / \partial y)$, which are the converse of the above relations for u and v .

¹⁰ For physical applications, $\mathbf{L}(x_i, \dot{x}_i, t)$ must be chosen so that the Euler-Lagrange equations represent the correct equations of motion.

Hamilton's equations is to reduce their number by half, an operation which leads back to the original Lagrange equations.

The dominate position of the equations of Lagrange in the history of dynamics can best be cited in Hamilton's own words.

The theoretical development of the laws of motion of bodies is of such interest and importance, that it has engaged the attention of all the most eminent mathematicians, since the invention of dynamics as a mathematical science by Galileo... Among the successors of those illustrious men, Lagrange has perhaps done more than any other analyst, to give extent and harmony to such deductive researches, by showing the motions of systems of bodies may be derived from one radical formula; the beauty of the method so suiting the dignity of the results, as to make his great work a kind of scientific poem. [Hami34].

§8.6.1. Canonical Coordinates and Poisson Brackets

The Hamiltonian and the Lagrangian are related as,

$$\left(\frac{\partial H}{\partial \lambda}\right)_{p, q} = -\left(\frac{\partial L}{\partial \lambda}\right)_{\dot{p}, \dot{q}}. \quad (8.34)$$

The Hamiltonian equations of motion are also known as the *canonical equations*, resulting in,

$$\dot{q}_r = \frac{\partial H}{\partial p_r}; \quad \dot{p}_r = -\frac{\partial H}{\partial q_r}; \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \quad (8.35)$$

The Hamiltonian formulation provides an elegant description of mechanics in which the position and momentum of each particle is treated as though they were independent quantities. The coordinates q_r and the momentum p_r are actually allowed to be more general than just Cartesian coordinates. In particular Hamilton's equations form the basis of the quantum formulation of Maxwell's equations, since the field potential becomes an integral part of the canonical momentum and is treated as if it were a generalized coordinate in the Lagrange equations. ^[11]

¹¹ Equations Eq. (8.31) and Eq. (8.32) are also valid for a system of N particles with coordinates $(x_1, x_2, \dots, x_{3N})$. The forces between the particles can be represented by the potential energy $V(x_1, x_2, \dots, x_{3N})$. The Newtonian equations of motion in Eq. (8.33) may be

Hamilton's equations can be restated using the Poisson bracket notation. For a system of s generalized coordinates and s generalized momenta, the Poisson bracket can be defined for any two functions $u(p, q)$ and $v(p, q)$ is an antisymmetric operation given as,

$$\{u, v\} = \sum_{i=1}^s \frac{\partial u}{\partial q_i} \frac{\partial v}{\partial p_i} - \frac{\partial v}{\partial q_i} \frac{\partial u}{\partial p_i} \quad (8.36)$$

This form can be rewritten as,

$$\dot{u} = \sum_{i=1}^s \left(\frac{\partial u}{\partial q_i} \dot{q}_i + \frac{\partial u}{\partial p_i} \dot{p}_i \right) \quad (8.37)$$

for the variation of any physical quantity u . Using Hamilton's equations,

$$\dot{u} = [\mathbf{H}, u]. \quad (8.38)$$

Substituting the generalized coordinates of position and momentum gives,

$$\dot{q}_i = \{q_i, \mathbf{H}\}, \quad (8.39)$$

and

$$\dot{p}_i = \{p_i, \mathbf{H}\}. \quad (8.40)$$

Several identities result from the Poisson bracket notation that will be useful in the formulation of quantum mechanics,

First,

$$\{q_i, p_j\} = \delta_{i,j}. \quad (8.41)$$

The Poisson brackets involving only p or q vanish as,

considered as Euler equations corresponding to the requirement that the function S should be an extremum. This alternative concept is important because it enables the equations of motion to be expressed in a form that is invariant with respect to the coordinates. The extremum requirement (Hamilton's Principle) contains only physical quantities such as kinetic and potential energy, which are independent of the coordinate system. For any arbitrary coordinate system, the *momenta* $p_j = \partial L / \partial \dot{x}_j$ do not in general have dimensions of true momentum, with the coordinate x_j being a dimensionless angular quantity. The product of any momentum p_j with its associated coordinate x_j always has the dimensions of action (energy \times time). The momentum p_j and the coordinate x_j are said to be *canonically conjugate*.

$$\{p_i, p_i\} = \{q_i, q_i\} = 0. \quad (8.42)$$

Quantities whose Poisson brackets are zero, commute, and those whose Poisson brackets are equal to 1 are canonically conjugate. From Eq. (8.39), it can be seen that any quantity that commutes with the Hamiltonian does not vary with time.

Using Eq. (8.36), if the Poisson bracket of a function u with a constant c gives,

$$\{u, c\} = 0, \quad (8.43)$$

and,

$$\{u, v\} = -\{v, u\}. \quad (8.44)$$

Using the rules of differentiation,

$$\{u + v, w\} = \{u, w\} + \{v, w\}, \quad (8.45)$$

and,

$$\{u, vw\} = \{u, v\}w + v\{u, w\}. \quad (8.46)$$

Using the Poisson brackets and Hamilton's equations of motion,

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \{u, H\}_{p,q} \quad (8.47)$$

and

$$\{q_i, q_j\}_{p,q} = \delta_{i,j} \quad (8.48)$$

It is the Poisson bracket formalism that will serve as the basis of the quantum mechanical commutator algebra developed in the subsequent sections.

§8.7. STANDARD LAGRANGIAN OF CLASSICAL ELECTRODYNAMICS

To this point in the monograph the radiation field density has been treated in form described by Eq. (4.33). As such the details behind this equation have not been developed. Before proceeding with the *operator* approach to the quantum field equations, the Hamiltonian form of the field equations will be addressed.

The field energy described in Eq. (4.33) can be derived through the expansion of Maxwell's equations using Hamilton's equations of motion

with equations (VI) and (VII) representing the electric and magnetic energy densities of the field proper. These energies are considered to reside *in the field* and to be localized by (VI) and (VII) in every volume element, such that a volume dv contains field energy in the amount $\frac{1}{2} \int_V (\mathbf{E}^2 + \mathbf{B}^2) dv$. The development of the Hamiltonian form of the field energy, starting from Maxwell's equations is one approach.^[12] Another approach is to construct the field equations and their associated Hamiltonian, by searching for the Lagrangian that results in the proper field equations. That is the approach taken here and by [Your68].^[13]

The Lagrange and Hamilton equations of motion developed in the previous section will be used to derive the Hamiltonian for the radiation field, which in turn will be used to derive the operator formulation of the electromagnetic radiation field. This approach will be worked out in detail starting with the equations of motion for a charged particle in an electromagnetic field and concluding with the Hamiltonian for the same field.

In this case the forces on the particle are not derived from the field potential, but rather arise from the velocity of the particle as it travels through the field. The acceleration (change in momentum) of the charged particle is given by the Lorentz equation,

$$F \equiv \dot{p} = e\{\mathbf{E} + (\mathbf{v} \times \mathbf{B})\} \quad (8.49)$$

where v of the velocity of the particle, e is the particle's charge and \mathbf{E} and \mathbf{B} are the electric and magnetic fields. The \mathbf{E} and \mathbf{B} fields are derived from the vector potentials in the usual manner,

$$\left. \begin{aligned} \mathbf{E} &= -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t}, \\ \mathbf{B} &= \nabla \times \mathbf{A}. \end{aligned} \right\} \quad (8.50)$$

The acceleration equation, Eq. (8.49), becomes,

¹² For a more rigorous development of the radiation field energy and the associated conservation laws derived from Maxwell's equations rather than the Lagrangian, see §11 of [Eyge72].

¹³ This approach depends on developing the detailed Lagrangian for the radiation field equations in both vacuum and source forms. This section and the reference [Your68] provides the lowest details of the Lagrangian approach to quantum field problems. As such it gives insight to the current research activities in particle physics and quantum field theory.

$$\begin{aligned} \dot{p} &= e \left\{ -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + (\dot{q} \times \nabla \times \mathbf{A}) \right\}, \\ &= e \left[-\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + \{ \nabla(\dot{q} \cdot \mathbf{A}) - (\dot{q} \cdot \nabla) \mathbf{A} \} \right]. \end{aligned} \quad (8.51)$$

In order to express the equations in the Lagrangian form, Eq. (8.28), the following Lagrangian function is used,

$$L = T - e\phi + e \sum_r A_r \dot{q}_r \quad (8.52)$$

The generalized momenta, using Eq. (8.32), as,

$$\begin{aligned} p_r &= \frac{\partial L}{\partial \dot{q}_r}, \\ &= p'_r + e \mathbf{A}_r. \end{aligned} \quad (8.53)$$

The form of Eq. (8.53) is similar to the Gauge transformations given in Eq. (4.7) and Eq. (4.8) and developed further .

Finally the Hamiltonian is still equal to the total energy, using Eq. (8.52),

$$H = \sum_r p_r \dot{q}_r - L. \quad (8.54)$$

Moving to the Lagrangian for a *charged body* rather than a singular point, the Lagrangian is given by,

$$L = T + \int \rho \left(\sum_r \mathbf{A}_r v_r - \phi \right) dV. \quad (8.55)$$

where v is the velocity of the charge at any point, ρ is the charge density and dV is an element of volume. To obtain Eq. (8.55) the charged body is considered as a system of mutually attracting particles. The v 's and ρ are treated as functions of the generalized coordinates used to define the system. According to Eq. (8.55), the generalized momenta will be determined by,

$$p_r = p'_r + \int \sum_s \rho \frac{\partial v_s}{\partial \dot{q}_r} \mathbf{A}_s dV, \quad (8.56)$$

and the Hamiltonian, using the notation of Eq. (8.33) is given as,

$$\mathbb{H} = \mathbb{H} \left(q_r, p_r - \int \sum_s \rho \frac{\partial v_s}{\partial \dot{q}_r} \mathbf{A}_s dV \right) + \int \rho \phi dV. \quad (8.57)$$

§8.7.1. Time Independent Lagrangian

The development of the actual electromagnetic field equations depends on a fundamental difference between the pervious equations. Up to this point the field equations contained one independent variable, t , and several dependent variables, q_r . In the electromagnetic field equations both the q_r 's and t are independent variables, and the quantities specifying the field are the dependent variables.

This situation can be described by considering a field defined by the quantities $f_r(q_r, t)$. A Lagrangian, L , can be found which is a function of the f_r 's, the $\frac{\partial f_r}{\partial q_r}$'s and the \dot{f}_r 's, so chosen that Lagrange's differential equations,

$$\left. \begin{aligned} \frac{\partial}{\partial s} \left(\frac{\partial f}{\partial \left(\frac{\partial q_1}{\partial s} \right)} \right) + \frac{\partial}{\partial t} \left(\frac{\partial f}{\partial \left(\frac{\partial q_1}{\partial t} \right)} \right) + \dots - \frac{\partial f}{\partial q_1} &= 0 \\ \frac{\partial}{\partial s} \left(\frac{\partial f}{\partial \left(\frac{\partial q_2}{\partial s} \right)} \right) + \frac{\partial}{\partial t} \left(\frac{\partial f}{\partial \left(\frac{\partial q_2}{\partial t} \right)} \right) + \dots - \frac{\partial f}{\partial q_2} &= 0 \\ \frac{\partial}{\partial s} \left(\frac{\partial f}{\partial \left(\frac{\partial q_r}{\partial s} \right)} \right) + \frac{\partial}{\partial t} \left(\frac{\partial f}{\partial \left(\frac{\partial q_r}{\partial t} \right)} \right) + \dots - \frac{\partial f}{\partial q_r} &= 0 \end{aligned} \right\} \quad (8.58)$$

for the integral $\int L dq_r dt$ to be stationary resulting in the equations of the field. Rewriting Eq. (8.58) by considering f_r 's to be functions of the generalized coordinates *evaluated* at a specific point in space, results in the ordinary Lagrange equations for L and Eq. (8.58) for L ,

$$\frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{f}_r} \right) + \sum_s \frac{\partial}{\partial q_s} \left(\frac{\partial L}{\partial \left(\frac{\partial f_r}{\partial q_r} \right)} \right) - \frac{\partial L}{\partial f_r} = 0, \quad (8.59)$$

are now equivalent, that is Lagrange's equations are valid for both point charges and distributed charges moving in the electromagnetic field. The Lagrangian L , which is a function of the dynamical variables can be rewritten as,

$$L = \int L d^3 q_r , \quad (8.60)$$

where L is now called the *Lagrangian density*.^[14]

§8.7.2. Lagrangian Density

In order to develop the underlying mathematics necessary for the quantum field description of electromagnetism, the standard Lagrangian will be extended. What is needed is a formalism that describes the observed phenomena of the radiation interaction with charged matter. This description must define the total Lagrangian L and maintain internal consistency, when the number of degrees of freedom becomes infinite.

The Lagrangian formalism for systems of point particles and the derivation of the Hamiltonian provides an easy transition to quantum mechanics. The systems presented so far consist of a finite number of variables. Although there are many physical systems with a finite number of degrees of freedom, the electromagnetic field is not one of them. There are other cases such as gases or liquids all of which have one or more

¹⁴ In the development of electrodynamics, the Lagrangian density is a function of the dynamical variables $A_i(\mathbf{r})$ and $dA_i(\mathbf{r})/dt$ where i describes all the individual points in the discrete space and \mathbf{r} describes all the possible coordinate values. The Lagrangian density function of the coordinates $A_i(\mathbf{r})$ and the velocities $dA_i(\mathbf{r})/dt$ and the spatial derivatives, denoted by $\partial_j A_i$, whose presence shows that the motion of the coordinate $A_i(\mathbf{r})$ is coupled to the motion of a neighboring point in the same manner the discrete variable q_i depends on q_{i-1} and q_{i+1} [Cohe89].

These spatial derivatives are not new independent variables but are linear combinations of generalized coordinates. In the study of electromagnetic theory the Lagrangian density takes on the form $L(A_i, dA_i/dt, \partial_j A_i)$.

The Lagrangian density that is used in electrodynamics contains generalized coordinate derivatives. Such a structure allows Maxwell's equations to be describe the motions of fields coupled from point to point in space. The absence of these spatial derivatives in the Lagrangian density would lead to a theory where the electromagnetic field evolves independently at each point in space. Since Maxwell's equations involve the spatial derivative of the field, the Lagrangian density also depends on spatial derivatives.

variables which are functions of continuous variables. There are various methods of transforming a discrete system to a continuous one. One method is to consider a continuous linear elastic structure as the limit of a system of point particles and then to generalize the results. A second method is to construct a generalized variational principle and the third method is to employ the Fourier transform to construct a generalized set of variables in Fourier space. There are several advantages to the third approach. First the continuous system which was a function of the continuous variable x is transformed to a discrete system of variables with an index of k , as long as the system is enclosed in a finite volume.

By combining the first and third approach — using the Fourier spatial description of a linear elastic medium — a transition to the quantum field description can be made. The starting point for this new Lagrangian will be the same as the transition from classical to quantum mechanics — Classical Hamiltonian dynamics. A generalized approach can be formulated by letting $\phi(\mathbf{r})$ represent the displacement amplitude of the field at a point \mathbf{r} . This results in the field having an infinite number of degrees of freedom which must be specified at each point where \mathbf{r}_i where $i \rightarrow \infty$.

For a continuous space the summation in Eq. (8.59) becomes infinite and must be replaced by the integral in Eq. (8.60). In this way $L(\mathbf{r})$ depends on the amplitude of the field at or near the point \mathbf{r} . This amplitude might be a function of $\phi(\mathbf{r})$ itself and must contain the time derivatives of ϕ , just as the Lagrangian of a particle contains the kinetic energy, which is a function of velocity. The Lagrangian density L must also depend on the spatial derivatives of $\phi(\mathbf{r})$, otherwise there would be no connection between the field amplitudes at neighboring points in space.

The system is more easily quantized as a discrete formulation, since the Fourier coefficients can be directly introduced as *creation* and *annihilation* operators. There are some difficulties with this approach, but they will be dealt with in the section on gauge theory. Because of the *difficulty* a simplified mechanical example will be used in which a *longitudinal* wave in one dimension is used to illustrate the idea.

Starting with the one dimension longitudinal wave described by the wave equation,

$$\rho \frac{\partial^2 \phi}{\partial t^2} - \mu \frac{\partial^2 \phi}{\partial x^2} = 0, \quad (8.61)$$

where $\phi(x, t)$ is the displacement of point x at time t . The density of the elastic medium is ρ and the restoring force of the media is μ . The length of the one dimensional media is L which requires $\partial\phi/\partial x$ vanishes at the boundaries. Given these conditions, the displacement function can be expanded in a Fourier series as,

$$\phi(x, t) = \sum \phi'_k(t) \sin kx, \quad (8.62)$$

where k has the periodic values $n\pi/L, n = 0, 1, 2, \dots$. The periodic boundary condition $\partial\phi/\partial x = 0$ can now be replaced by,

$$\phi(x + L, t) = \phi(x, t). \quad (8.63)$$

Another simplification is to expand the Fourier series is an exponential such that,

$$\phi(x, t) = \frac{1}{\sqrt{L}} \sum_k \phi_k(t) e^{ikx}, \quad (8.64)$$

where k is now the wave number which can be positive as well as negative. Since the Fourier expansion given in Eq. (8.64) involves complex numbers and $\phi(x, t)$ is a real quantity in terms of ϕ_k and ϕ_{-k} are related to each other through this complex conjugate $\phi_k = \phi_{-k}^*$ resulting in k independent variables.

The k^{th} instance of ϕ can be obtained from the continuous function through Fourier transform,

$$\phi_k = \frac{1}{\sqrt{L}} \int \phi(x) e^{ikx} dx. \quad (8.65)$$

By letting the extent of the medium tend to infinity $L \rightarrow \infty$ and using the following limits,

$$\sum_k \rightarrow \frac{L}{2\pi} \int dk, \quad (8.66)$$

and,

$$\phi_k \rightarrow \sqrt{\frac{2\pi}{L}} \phi(k). \quad (8.67)$$

The Fourier transform pairs can be given as,

$$\phi(x, t) = \frac{1}{\sqrt{2\pi}} \int \phi(k, t) e^{ikx} dx, \quad (8.68)$$

$$\phi(k, t) = \frac{1}{\sqrt{2\pi}} \int \phi(x, t) e^{-ikx} dx. \quad (8.69)$$

The Fourier transform of the wave equation now becomes,

$$\rho \frac{\partial \phi_k}{\partial t^2} + k^2 \phi_k = 0 \quad (8.70)$$

which is now the equations of motion of the system, but containing an infinite number of degrees of freedom. These equations can be derived from the Lagrangian,

$$\mathcal{L}(\phi_k, \dot{\phi}_k) = \frac{1}{2} \rho \sum_k \dot{\phi}_k \dot{\phi}_{-k} - \frac{1}{2} \mu \sum_k k^2 \phi_k \phi_{-k}. \quad (8.71)$$

Using the relations given in Eq. (281) and Eq. (280) these transitions from the discrete formulation using ϕ_k to the continuous formulation using $\phi(x)$ can be made.

Considering the first term of the Lagrangian,

$$\begin{aligned} \frac{1}{2} \rho \sum_k \dot{\phi}_k \dot{\phi}_{-k} &= \frac{1}{2} \rho \int \dot{\phi}(k) \dot{\phi}(-k) dk, \\ &= \frac{1}{2} \rho \sqrt{2\pi} \int \dot{\phi}(x) dx \int e^{-ikx} \dot{\phi}(-k) dk, \\ &= \frac{1}{2} \rho \int \dot{\phi}(x) \dot{\phi}(x) dx, \\ &= \int \mathcal{T}(x) dx = \frac{1}{2} \int \dot{\phi}(x) \dot{\phi}(x). \end{aligned} \quad (8.72)$$

which is the kinetic energy *density*. The second term,

$$\begin{aligned}
 \frac{1}{2}\mu \sum_k k^2 \phi_k \phi_{-k} &= \frac{1}{2}\mu \int k^2 \phi(k) \phi(-k) dk, \\
 &= \frac{1}{2}\mu \sqrt{2\pi} \iint \phi(x) k^2 e^{-ikx} \phi(-k) dx dk, \\
 &= \frac{1}{2}\mu \sqrt{2\pi} \iint \phi(x) \left(-\frac{\partial^2}{\partial x^2} e^{-ikx} \right) \phi(-k) dx dk, \\
 &= \frac{1}{2}\mu \sqrt{2\pi} \int \left(-\frac{\partial^2}{\partial x^2} \phi(x) \right) dx \int e^{-ikx} \phi(k) dk, \quad (8.73) \\
 &= \frac{1}{2}\mu \int \left(-\frac{\partial^2}{\partial x^2} \phi(x) \right) dx \phi(x), \\
 &= \frac{1}{2}\mu \int \left(\frac{\partial^2 \phi}{\partial x^2} \right) dx, \\
 &= \int V(x) dx.
 \end{aligned}$$

which is the potential energy *density*.

Frustra fit per plura, quod feiri potest per pauciora

OR

Essentia non sunt multiplicanda praeter necessitatem

(It is vain to do with more what one can do with less)

OR

(Entities are not to be multiplied beyond necessity)^[15]

— Occam's Razor

¹⁵ Attributed to William of Occam, or Ockham, or probably Oakham in Surrey (1300–1349), Oxford scholar in the Order of Franciscan Friars. Occam's razor is widely used in scientific analysis with an interpretation akin to: *One should always choose the simpler of two otherwise competing descriptions of physical phenomena.* [Doug90].