

CHM 532

Notes on Classical Mechanics

Lagrange's and Hamilton's Equations

It is not possible to understand the principles of quantum mechanics without some understanding of classical mechanics. In class, we have reviewed the basic principles of Newton's Laws of Motion. We have also recast Newton's second law into the forms developed by Lagrange and Hamilton. These notes provide some of the details about the Lagrangian and Hamiltonian formulations of classical mechanics.

1 Newton's Second Law

We consider N particles moving in three-dimensional space, and we describe the location of each particle using Cartesian coordinates. We let m_i be the mass of particle i , and we let x_i, y_i and z_i be respectively the x, y and z -coordinates of particle i . For time derivatives of the coordinates (and all other physical observables), we use the "dot" notation first introduced by Isaac Newton

$$\dot{x}_i = \frac{dx_i}{dt} \tag{1}$$

and

$$\ddot{x}_i = \frac{d^2x_i}{dt^2}. \tag{2}$$

We let F_{x_i} be the x -component of the force on particle i . Then Newton's Second Law takes the form

$$F_{x_i} = m\ddot{x}_i. \tag{3}$$

For example, if we study the motion of a single particle of mass m moving in one dimension in a harmonic potential with associated force $F_x = -kx$, Newton's second law takes the form

$$-kx = m\ddot{x}. \tag{4}$$

Solution of this differential equation for the coordinate x as a function of the time t gives a complete description of the motion of the particle; i.e. at any time t one knows the location and velocity of the particle.

2 Conservative Systems

In quantum mechanics we often restrict our attention to a class of physical systems that are called conservative. In a qualitative sense conservative systems are those for which the total energy E is the sum of the kinetic and potential energies. For any system E is conserved (i.e. $dE/dt = 0$), and for conservative systems, the sum of the potential energy and kinetic energy is conserved. Explicitly, we have the following definition:

Definition: A classical mechanical system is conservative if there exists a function $V(x_1, y_1, z_1, x_2, \dots, z_N)$ called the *potential energy* such that for any coordinate x_i (or y_i or z_i) we can write

$$F_{x_i} = -\frac{\partial V}{\partial x_i} \left(\text{or } F_{y_i} = -\frac{\partial V}{\partial y_i} \text{ or } F_{z_i} = -\frac{\partial V}{\partial z_i} \right) \quad (5)$$

where F_{x_i} (or F_{y_i} or F_{z_i}) is the x (or y or z) -component of the force on particle i .

As an example, we can consider the one-dimensional particle moving in the harmonic well with force $F = -kx$. For such a system, a potential energy exists and is given by $V(x) = 1/2 kx^2$. By differentiating the potential energy with respect to x , the force is obtained. We can then be sure that for a harmonic oscillator the total energy

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 \quad (6)$$

is conserved. We have not yet proved that the sum of the kinetic and potential energies is conserved for conservative systems. Such a proof is possible most readily after we develop Hamilton's formulation of classical mechanics.

Before leaving this section it is important to give an example of a classical system that is not conservative. Consider a block sliding on a flat surface parallel to the surface of the earth that experiences a frictional force. If the block has some initial kinetic energy, the speed of the block must slow to zero owing to the friction. The total energy includes dissipation of the kinetic energy into heat (from the frictional force). Frictional forces always depend on the velocity of an object and are not derivable from a potential energy function.

3 Notation

In the next section we recast Newton's Second Law in the form introduced by Lagrange. To proceed, we emphasize the notation used for derivatives. We need to distinguish the explicit and implicit dependence of a function on a variable. As an example, the expression for the kinetic energy T of our system of N particles in Cartesian coordinates is given by

$$T = \frac{1}{2} \sum_{i=1}^N m_i [\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2]. \quad (7)$$

Equation (7) for the kinetic energy is an explicit function of the velocities of each particle; i.e. the $\{\dot{x}_i, \dot{y}_i, \dot{z}_i\}$, but no other variables. We can write

$$\frac{\partial T}{\partial \dot{x}_j} = m_j \dot{x}_j. \quad (8)$$

However, in the expression for T , there is no explicit dependence on the time t or the coordinates $\{x_i, y_i, z_i\}$. Consequently, we write

$$\frac{\partial T}{\partial t} = 0 \quad (9)$$

and

$$\frac{\partial T}{\partial z_j} = 0. \quad (10)$$

Equations (9) and (10) do not imply that the kinetic energy is independent of the time or the z -component of the coordinate for particle j . Equations (9) and (10) only state that in the expression for T *as written*, there is no explicit dependence of T on t or z_j . If we want the actual (i.e. implicit) dependence of the kinetic energy on time, we write

$$\frac{dT}{dt}$$

which is not zero in the general case (dT/dt does equal zero for a free particle). We understand the notation ∂ to represent a derivative of the explicit dependence of a function *as written* on a variable and the notation d to represent a derivative for the actual (i.e. implicit) dependence of a function on a variable. It is important that the differences between ∂ and d are clear for the developments that follow.

4 Lagrange's Equations

We now derive Lagrange's equations for the special case of a conservative system in Cartesian coordinates. An extension to more general systems is possible. The proof of such an extension is beyond the scope of this course. However, using Lagrange's equations in more general coordinate systems is an important part of this course and must be discussed after the derivation in Cartesian coordinates.

We begin with Eq.(7) for the kinetic energy. We first differentiate the expression with respect to one of the velocities

$$\frac{\partial T}{\partial \dot{x}_j} = m_j \dot{x}_j. \quad (11)$$

We next take the implicit derivative of Eq.(11) with respect to time

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{x}_j} = m_j \ddot{x}_j. \quad (12)$$

The right hand side of Eq. (12) is the mass of the particle multiplied by the acceleration of the particle, which by Newton's second law must be the force on the particle. For a conservative system, we can express this force by $-\partial V/\partial x_j$ so that

$$\frac{d}{dt} \frac{\partial T}{\partial \dot{x}_j} = -\frac{\partial V}{\partial x_j}. \quad (13)$$

We now give a defining relation for the classical Lagrangian:

Definition: The classical Lagrangian L is given by

$$L = T - V \quad (14)$$

The classical Lagrangian is the difference between the kinetic and potential energies of the system. Using this definition in Eq.(13), we obtain

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}_j} - \frac{\partial L}{\partial x_j} = 0. \quad (15)$$

Equations (15) are Lagrange's equations in Cartesian coordinates. We use the plural (equations), because Lagrange's equations are a set of equations. We have a separate equation for each coordinate x_j . A completely analogous set of equations is obtained for the other Cartesian directions y and z .

We emphasize that Lagrange's equations are just a new notation for Newton's second law. For example, consider once again the one-dimensional harmonic oscillator. The Lagrangian for the system is

$$L = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 \quad (16)$$

and Lagrange's equation is

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = \frac{d}{dt}m\dot{x} + kx = 0 \quad (17)$$

or

$$m\ddot{x} = -kx \quad (18)$$

which is just Newton's second law. To understand the utility of the new notation, we need to introduce the notion of generalized coordinates.

4.1 Generalized Coordinates

Much of Lagrange's work was concerned with methods useful for systems subject to external constraints. You may be familiar with the method of Lagrange multipliers, a method that enables you to find extrema of functions subject to constraints. The method of Lagrange multipliers

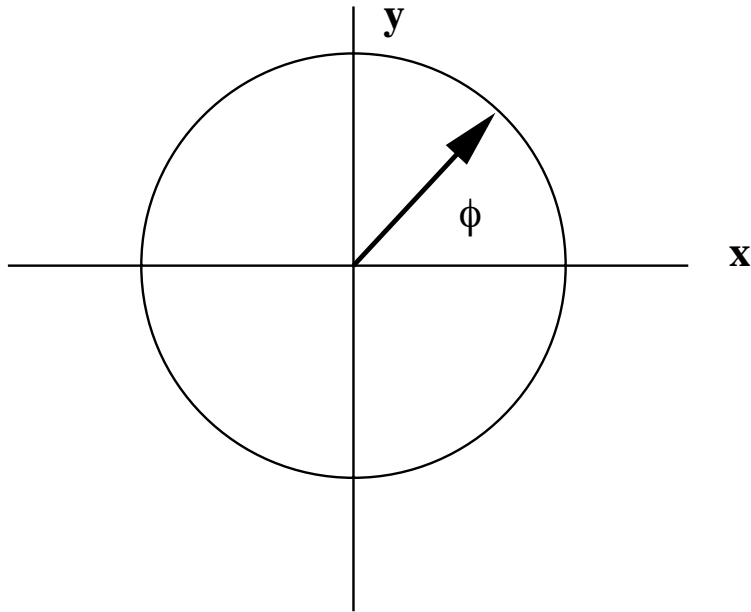


Figure 1:

is used frequently in developing the formulas in statistical mechanics. Lagrange was also interested in the effect of constraints on systems in classical mechanics.

A simple example of the kind of problem that interested Lagrange is the motion of a free particle of mass m confined to move on the perimeter of a ring of radius R depicted in Fig. 1. Constraints on a particle's motion arise from some set of unspecified forces. For the particle on a ring, it is possible to imagine some force of infinite strength that limits the motion of the particle. The exact nature of the force is not important to us. We only need to consider the confined space.

For a particle on a ring, the Cartesian coordinates x and y are not the most convenient to describe the motion of the particle. As a result of the constraint, a single coordinate ϕ is sufficient to locate the particle. The coordinate ϕ is defined to be the angle that a line connecting the current location of the particle with the origin of coordinates makes with the x -axis. The connections between ϕ and the Cartesian coordinates are given by

$$x = R \cos \phi \tag{19}$$

and

$$y = R \sin \phi. \tag{20}$$

The angle ϕ is an example of a *generalized coordinate*. Generalized coordinates are any set of coordinates that are used to describe the motion of a physical system. Cartesian coordinates and spherical polar coordinates are other examples of generalized coordinates. We may choose any convenient set of generalized coordinates for a particular problem. For the particle in a ring example, the convenient coordinate is ϕ . For systems with spherically symmetric potentials (the motion of the earth about the sun, the hydrogen atom), we can choose spherical polar coordinates. We label the i 'th generalized coordinates with the symbol q_i , and we let \dot{q}_i represent the time derivative of q_i .

4.2 Lagrange's Equations in Generalized Coordinates

Lagrange has shown that the form of Lagrange's equations is invariant to the particular set of generalized coordinates chosen. For any set of generalized coordinates, Lagrange's equations take the form

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0, \quad (21)$$

exactly the same form that we derived in Cartesian coordinates. The proof that Lagrange's equations looks the same in any coordinate system is beyond the scope of this course. We do emphasize that the invariance to coordinate system is not a property of the equations of motion when expressed in the usual form of Newton's second law.

We now illustrate how to use Lagrange's equations in generalized coordinates by applying the approach to the free motion of a particle confined to move on the perimeter of a ring as discussed previously. We use the following procedure that is general:

1. express the Lagrangian L in Cartesian coordinates;
2. transform L to generalized coordinates;
3. give Lagrange's equations in generalized coordinates.

The meaning of the expression of "free particle" is the absence of any external forces. We can arbitrarily set the potential energy V to zero. Then in Cartesian coordinates, the Lagrangian for any free particle in the xy -plane can be expressed

$$L = \frac{1}{2}m[\dot{x}^2 + \dot{y}^2]. \quad (22)$$

We next transform L to generalized coordinates using Eqs. (19) and (20). We need the time derivatives of x and y expressed in terms of the generalized coordinate system

$$\dot{x} = -R \sin \phi \dot{\phi} + \dot{R} \cos \phi \quad (23)$$

and

$$\dot{y} = R \cos \phi \dot{\phi} + \dot{R} \sin \phi. \quad (24)$$

Owing to the constraint, R is a constant and $\dot{R} = 0$. Then

$$\dot{x} = -R \sin \phi \dot{\phi} \quad (25)$$

and

$$\dot{y} = R \cos \phi \dot{\phi}, \quad (26)$$

so that L becomes

$$L = \frac{1}{2} m R^2 \dot{\phi}^2 [\cos^2 \phi + \sin^2 \phi] \quad (27)$$

$$= \frac{1}{2} m R^2 \dot{\phi}^2 \quad (28)$$

Because of the constraint, the Lagrangian is a function of a single coordinate ϕ . We finally give Lagrange's equations

$$\frac{\partial L}{\partial \dot{\phi}} = m R^2 \dot{\phi} \quad (29)$$

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}} = m R^2 \ddot{\phi} \quad (30)$$

$$\frac{\partial L}{\partial \phi} = 0 \quad (31)$$

so that

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\phi}} = \frac{d}{dt} m R^2 \dot{\phi} = m R^2 \ddot{\phi} = 0. \quad (32)$$

Equation (32) implies the acceleration of the coordinate ϕ is zero so that the particle moves with a constant generalized velocity $\dot{\phi}$.

5 Generalized Momenta

Equation (32) can be interpreted to mean that the quantity $\partial L / \partial \dot{\phi} = m R^2 \dot{\phi}$ is conserved. To fully explore the meaning of the conservation of a quantity like $\partial L / \partial \dot{\phi}$, consider the Lagrangian in Cartesian coordinates for a particle of mass m moving in one dimension

$$L = \frac{1}{2} m \dot{x}^2 - V(x). \quad (33)$$

By differentiating L with respect to the velocity \dot{x} we obtain the linear momentum

$$\frac{\partial L}{\partial \dot{x}} = m \dot{x}, \quad (34)$$

which is conserved in the case of no external forces; i.e. the linear momentum is conserved if $V(x)$ is a constant. Using these simple equations we are lead to the following definition:

Definition: The generalized momentum p_i conjugate to the coordinate q_i is defined by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}. \quad (35)$$

For the case of a Lagrangian expressed in Cartesian coordinates, the generalized momentum conjugate to each coordinate reduces to the linear momentum. In the particle in a ring example, the generalized momentum conjugate to the coordinate ϕ , $\partial L/\partial \dot{\phi} = p_\phi$, can be shown to be the angular momentum of the particle. Notice that a generalized momentum conjugate to any coordinate is conserved if the coordinate is absent in the Lagrangian. For a particle of mass m moving in one dimension in Cartesian coordinates, the linear momentum is conserved if the Lagrangian is independent of the coordinate x ; i.e. if the potential is a constant. Similarly, the particle in a ring has conserved angular momentum, because the Lagrangian is independent of ϕ .

Shortly, we shall see that it is possible to express the equations of motion using a formulation due to Hamilton where the generalized momenta appear explicitly. Before developing the formulation of Hamilton, in the next section we introduce the concept of a Legendre transform.

6 The Legendre Transform

The Legendre transform is a method of changing the dependence of a function of one set of variables to another set of variables. The Legendre transform is most often used in the study of thermodynamics. Recall from thermodynamics, there are two free energy functions called the Gibbs free energy and the Helmholtz free energy. The total differential of the Helmholtz free energy is given by

$$dA = -SdT - pdV \quad (36)$$

where S is the entropy, T is the temperature, V is the volume and p is the pressure. From the total differential, it is evident that the Helmholtz free energy is expressed as a function of the temperature and the volume; i.e. $A = A(T, V)$. Now suppose we prefer to express the state of our system in terms of temperature and pressure rather than temperature and volume. We can define a new function G by

$$G = A + pV \quad (37)$$

where we have added to A the product of the variable we want (p) and the variable we want to eliminate (V). The algebraic sign of the included pV product is chosen to be the opposite of the algebraic sign of the pdV term in Eq.(36). Taking the differential of the expression for G we obtain

$$dG = dA + pdV + Vdp = -SdT - pdV + pdV + Vdp = -SdT + Vdp. \quad (38)$$

It is evident that G is a function of T and p as desired. In thermodynamics, G is called the Gibbs free energy, and G is said to be the Legendre transform of A . As previously mentioned, in Eq.(37) the product pV is included with an algebraic sign opposite to the sign of pdV in Eq.(36), so that the cancellation of the two pdV terms is assured.

7 The Classical Hamiltonian and Hamilton's Equations

We now apply the notion of the Legendre transform to the classical Lagrangian. In our previous developments, we have taken L to be a function of all the generalized coordinates and their respective time derivatives; i.e. $L = L(\{q_i\}, \{\dot{q}_i\}, t)$. For generality, we have also included the possibility that the Lagrangian has an explicit time dependence. Such an explicit time dependence can occur when the external forces acting on a system are time dependent. The resulting time-dependent potentials can be important in quantum systems, as for example, the study of the interaction of radiation with matter. Light is composed of electric and magnetic fields that oscillate in time, and when light interacts with matter, the electrons are subjected to time-dependent potentials. The quantum treatment of spectroscopy includes time dependent potentials, and we generalize the Lagrangian to admit such time dependences. However, in CHM 532, a detailed treatment of time dependence is beyond the scope of the course, and we only see examples of Lagrangians that have no explicit time dependence.

We now use the Legendre transform to define a new function where we replace the velocity (the \dot{q}_i) dependence by a dependence on the generalized momenta. The transformed function is given by the definition that follows:

Definition: For a system of particles each having masses m_i described by a set of generalized coordinates q_i , the classical Hamiltonian is defined by

$$H = \sum_i p_i \dot{q}_i - L(\{q_i\}, \{\dot{q}_i\}, t) \quad (39)$$

As we now show, the particular choice of the relative signs of the first and second terms in Eq.(39) makes the classical Hamiltonian a natural function of the generalized coordinates and momenta rather than the generalized coordinates and the velocities. The reason that the sum is included with a positive sign and the Lagrangian is included with a negative sign (rather than the opposite) is made clear shortly when we identify the meaning of the classical Hamiltonian.

We now take the total differential of Eq.(39)

$$dH = \sum_i \left(p_i d\dot{q}_i + \dot{q}_i dp_i - \frac{\partial L}{\partial q_i} dq_i - \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i \right) - \frac{\partial L}{\partial t}. \quad (40)$$

The derivative $\partial L / \partial \dot{q}_i$ is the definition of the generalized momentum p_i . From Lagrange's

equations [Eq.(21)], we can write

$$\frac{d}{dt}p_i - \frac{\partial L}{\partial q_i} = 0 \quad (41)$$

or

$$\frac{\partial L}{\partial q_i} = \dot{p}_i. \quad (42)$$

Then the total differential of the classical Hamiltonian becomes

$$dH = \sum_i (p_i dq_i + \dot{q}_i dp_i - \dot{p}_i dq_i - p_i d\dot{q}_i) - \frac{\partial L}{\partial t} \quad (43)$$

$$= \sum_i (\dot{q}_i dp_i - \dot{p}_i dq_i) - \frac{\partial L}{\partial t}. \quad (44)$$

The classical Hamiltonian is manifestly a function of the generalized coordinates and momenta rather than the generalized coordinates and velocities. From Eq.(44) we have

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \quad (45)$$

$$\frac{\partial H}{\partial q_i} = -\dot{p}_i \quad (46)$$

and

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \quad (47)$$

Equations (45)-(47) are called *Hamilton's equations of motion*.

To understand the meaning of the classical Hamiltonian and Hamilton's equations of motion, it is useful to consider the motion of a particle of mass m in one dimension with the Lagrangian given in Eq.(33). As discussed previously, the generalized momentum for the system is given by $p_x = \partial L / \partial \dot{x} = m\dot{x}$, and from the definition of the Hamiltonian, we have

$$H = p_x \dot{x} - L = m\dot{x}^2 - \left(\frac{1}{2}m\dot{x}^2 - V(x) \right) \quad (48)$$

$$= \frac{1}{2}m\dot{x}^2 + V(x). \quad (49)$$

The Hamiltonian is seen to be the sum of the kinetic and potential energies of the system. For conservative systems, H is the total energy.

As written, Eq.(49) is not correct, because H is not written explicitly as a function of the generalized momentum. To make the expression for H correct, we must substitute $\dot{x} = p_x/m$ so that Eq.(49) becomes

$$H = \frac{p_x^2}{2m} + V(x). \quad (50)$$

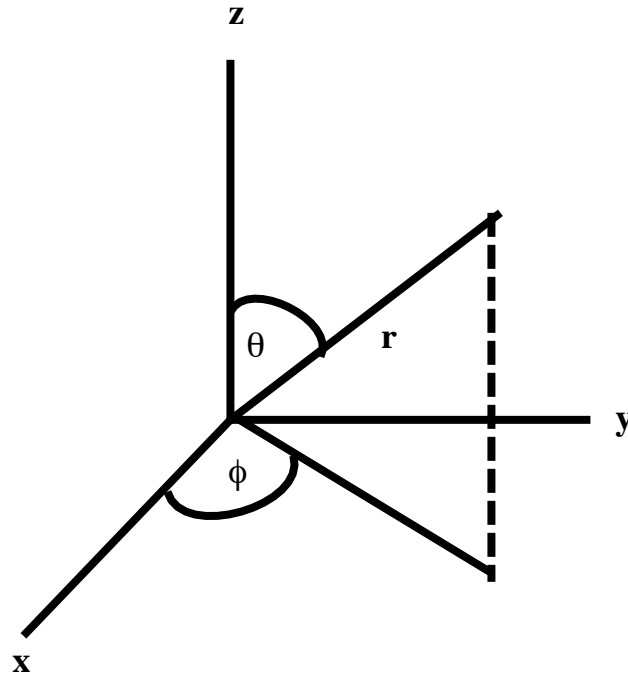


Figure 2:

The Hamiltonian is then seen to be an expression for the total energy of a conservative system in terms of the generalized coordinates and momenta. With the Hamiltonian expressed in terms of the proper variables, we can give Hamilton's equations of motion for the system

$$\frac{\partial H}{\partial p_x} = \frac{p_x}{m} = \dot{x} \quad (51)$$

and

$$\frac{\partial H}{\partial x} = \frac{dV}{dx} = -\dot{p}_x. \quad (52)$$

Equation (51) relates the generalized momentum to the velocity, and Eq.(52) is easily seen to be Newton's second law of motion for the system. Consequently, Hamilton's equations are just another formulation of Newton's second law. As an exercise, you can construct the Hamiltonian for the particle confined to move on the perimeter of a ring and give Hamilton's equations of motion. The result should be identical to Newton's second law.

8 Construction of the Hamiltonian in Spherical Polar Coordinates - Central Force Motion

For systems with spherical symmetry (e.g. the hydrogen atom), spherical polar coordinates are the most convenient set of generalized coordinates. As depicted in Fig. 2, the spherical

polar coordinates are r, θ and ϕ . The coordinate r is the distance from the origin of coordinates to the particle, θ is the angle a line connecting the origin of the coordinates to the particle position makes with the z -axis and ϕ is the angle a projection of the line defining θ onto the xy -plane makes with the x -axis. The connections between Cartesian coordinates and spherical polar coordinates can be derived readily using trigonometry. The result is

$$x = r \sin \theta \cos \phi \quad (53)$$

$$y = r \sin \theta \sin \phi \quad (54)$$

and

$$z = r \cos \theta. \quad (55)$$

Another important relation is the direct result of the Pythagorean theorem

$$r = \sqrt{x^2 + y^2 + z^2}. \quad (56)$$

We now consider a particle of mass m moving in three-dimensional space subject to a conservative central force with associated potential energy $V(r)$. The meaning of a central force is the potential energy is a function only of the r -coordinate and independent of θ and ϕ . In Cartesian coordinates, the Lagrangian for the system is

$$L = \frac{1}{2}m[\dot{x}^2 + \dot{y}^2 + \dot{z}^2] - V. \quad (57)$$

To transform L from Cartesian to spherical polar coordinates, we need expression for the time derivatives of each Cartesian coordinate in terms of spherical polar coordinates. The time derivatives are obtained using a combination of the chain and product rules from calculus. Using Eq. (53) we have

$$\dot{x} = \dot{r} \sin \theta \cos \phi + r\dot{\theta} \cos \theta \cos \phi - r\dot{\phi} \sin \theta \sin \phi. \quad (58)$$

Similarly,

$$\dot{y} = \dot{r} \sin \theta \sin \phi + r\dot{\theta} \cos \theta \sin \phi + r\dot{\phi} \sin \theta \cos \phi. \quad (59)$$

and

$$\dot{z} = \dot{r} \cos \theta - r\dot{\theta} \sin \theta. \quad (60)$$

We then substitute Eqs. (58)-(60) into Eq.(57). After some algebra (that is left as an exercise), the result is

$$L = \frac{1}{2}m[\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2 \theta \dot{\phi}^2] - V(r). \quad (61)$$

Before constructing the classical Hamiltonian, it is a useful exercise to generate Lagrange's equations using the Lagrangian given in Eq.(61). For the r -coordinate, we have

$$\frac{d}{dt}m\dot{r} - mr\dot{\theta}^2 - mr \sin^2 \theta \dot{\phi}^2 + \frac{dV}{dr} = 0, \quad (62)$$

for the θ -coordinate we have

$$\frac{d}{dt}(mr^2\dot{\theta}) - mr^2 \sin \theta \cos \theta \dot{\phi}^2 = 0, \quad (63)$$

and for the ϕ -coordinate we have

$$\frac{d}{dt}(mr^2 \sin^2 \theta \dot{\phi}) = 0. \quad (64)$$

The equation for the ϕ -coordinate is an expression of the conservation of the momentum conjugate to the coordinate ϕ (the angular momentum).

To construct the classical Hamiltonian, we need expressions for the generalized momenta conjugate to each of the spherical polar coordinates. These expressions have already been obtained when constructing Lagrange's equations. In particular

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}, \quad (65)$$

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2\dot{\theta}, \quad (66)$$

and

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2 \sin^2 \theta \dot{\phi}. \quad (67)$$

Then using the definition of the classical Hamiltonian

$$H = p_r \dot{r} + p_\theta \dot{\theta} + p_\phi \dot{\phi} - L \quad (68)$$

$$= \frac{1}{2}m[\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2 \theta \dot{\phi}^2] + V(r) \quad (69)$$

Finally, Eq. (69) must be transformed to replace the velocities with generalized momenta. Using Eqs. (65)-(67) we finally obtain

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2 \sin^2 \theta} + V(r). \quad (70)$$

If needed, the equations of motion can be obtained by applying Hamilton's equations to the constructed Hamiltonian.

9 Poisson's Equation

As a final topic, in this section we discuss an important relation usually called "Poisson's equation." Poisson's name has been given to several equations in mechanics and the study of electricity and magnetism, so we sometimes call the resulting equation "Poisson's equation of motion," to distinguish it from other equations with the name Poisson. We consider any

function of coordinates, momenta and possibly the time $f(\{q_i\}, \{p_i\}, t)$. For the function f , we can take any mechanical variable like the kinetic energy, the total energy, or one of the momenta. Using the chain rule, we now give an expression for the implicit time derivative of f

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_i \left[\frac{\partial f}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial f}{\partial p_i} \frac{dp_i}{dt} \right]. \quad (71)$$

Using Hamilton's equations of motion, the above expression becomes

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_i \left[\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right]. \quad (72)$$

We now make use of the following definition:

Definition: Let $A(\{q_i\}, \{p_i\})$ and $B(\{q_i\}, \{p_i\})$ be two functions of the generalized coordinates and momenta of a system. Then the Poisson bracket of A and B is defined by

$$\{A, B\}_{pb} = \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right). \quad (73)$$

Substituting the definition of the Poisson bracket into Eq.(72), we obtain the Poisson equation

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{f, H\}_{pb}. \quad (74)$$

The Poisson equation shows that the time evolution of any dynamical variable is governed by the classical Hamiltonian through the Poisson bracket of the variable with the Hamiltonian.

An important application of the Poisson equation is the proof that the Hamiltonian is conserved for conservative classical systems. The demonstration involves taking the implicit time derivative of the Hamiltonian

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \{H, H\}_{pb}. \quad (75)$$

It is easy to show that for any variable $\{A, A\}_{pb} = 0$. Then if H is not an explicit function of time, $dH/dt = 0$ and H is conserved.

For the purposes of CHM 532, an important reason to study the Poisson bracket is to be made clear later in the course, when we study quantum commutators.