Hamilton-Jacobi Theory in Classical Mechanics

Patrick Van Esch

August 28, 2003

1 Lagrangian and Hamiltonian formulation.

1.1 Configuration space.

It is assumed that the momentary, well, eh, configuration of a dynamical system can be described by a finite number n of real parameters, the **generalized coordinates**:

$$q \leftrightarrow \{q_1, q_2, ..., q_n\} \tag{1}$$

For a featureless point particle in 3-dimensional Euclidean space on which a reference frame has been defined, there are 3 such generalized coordinates, namely the 3 cartesian coordinates of the point in space that is occupied by the point particle at the instant in time we're considering:

$$q_1 = x, q_2 = y, q_3 = z \tag{2}$$

We do not need to have cartesian coordinates, of course. For example, spherical coordinates do just as well:

$$q_1 = r, q_2 = \theta, q_3 = \phi \tag{3}$$

For Nfeatureless point particles, we can in an evident way describe the system by $3N$ such coordinates. But of course, 'mixed' coordinates are also possible, such as the relative positions of certain particles with respect to others etc...

For a rigid body, 6 coordinates are needed, for example, the 3 cartesian coordinates of the center of gravity and 3 Euler angles. For ensembles of rigid bodies with constraints, called mechanisms, the choice of generalized coordinates has to take into account the constraints.

So there is a (part of) R^n that is called "configuration space" and corresponds to the possible values of the n-tuple $\{q_1, ..., q_n\}$ that makes sense. In fact, we should be more general and allow for a differentiable manifold, and not just a chunk of R^n to be the configuration space, but we won't go into that here.

1.2 Hamilton's Principle

The basic idea is that the time evolution of our dynamical system is determined by a path, followed by a "point in configuration space", that is parameterized in

time. This simply comes down to say that the dynamical behavior of our system is described by letting the generalized coordinates be functions of time t. There are supposed to be laws of nature that determine these paths, so not just all lines in configuration space correspond to time evolutions of our dynamical system. In fact, it is taken to be a fundamental principle of nature that there is only one single path that describes the dynamics of the system when the system has configuration $\{q_i^{(1)}\}$ at moment $t = t^{(1)}$, and configuration $\{q_i^{(2)}\}$ at moment $t = t^{(2)}$. This fundamental principle is called **Hamilton's Principle**. It says two things. First, it says that there exists a function, the **Lagrangian**, of the generalized coordinates, their time derivatives, and time:

$$L\left(q_1, ..., q_n, \dot{q}_1, ..., \dot{q}_n, t\right) \tag{4}$$

Second, it says that for a true path in configuration space, as it is actually followed by the dynamical system, which is in configuration $q^{(1)}$ at time $t^{(1)}$ and in configuration $q^{(2)}$ at time $t^{(2)}$ satisfies:

$$\delta\left(\int_{t=t^{(1)}}^{t^{(2)}} L\left(q_1(t), ..., q_n(t), \dot{q}_1(t), ..., \dot{q}_n(t), t\right) dt\right) = 0 \tag{5}$$

Here, δ stands for a variation amongst paths. Let us look closer at what is precisely stated: For each potential path $q(t)$, that satisfies the two boundary conditions: $q^{(1)}$ at time $t^{(1)}$ and $q^{(2)}$ at time $t^{(2)}$, the integral has a value. If the potential paths change a little, then this value changes a little too. But for the true path the integral has a certain value, and slightly changed potential paths from the true path give us *the same value* in first order of the change. Meaning the true path has an extremum (usually a minimum) of the integral. We say that the integral is stationary for this path. In fact, the condition imposed by Hamilton's Principle puts a severe constraint on what are possible true paths, and in most cases only one path survives. That is then the true path followed by the dynamics of the system. In fact, Hamilton's Principle can be reduced to a set of differential equations which the true path has to satisfy:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \tag{6}$$

These are called **Euler-Lagrange's equations** and are mathematically equivalent to Hamilton's principle. They are second-order differential equations for $q_i(t)$.

A remark is maybe due on derivatives. When we have a function, like a Lagrangian, and we take a partial derivative to, say, $\dot{q}_i$, it might be a bit disturbing, because there is also q_i somewhere. The partial derivative has to be understood as with respect to a slot in the functional prescription: simply write $L(a, b, c)$, derive with respect to b, and after that, place back q_i and $\dot{q}_i$. A total derivative with respect to time however, means that we consider q to be a function of time, that $\dot{q}$ is the derivative of this function of time and that we have to apply the chain rule. Both kinds of derivatives appear in the way the Euler-Lagrange equations have been written down.

1.3 Hamilton's formulation

Lagrangian dynamics, the prescription of true paths in configuration space through Hamilton's Principle, or equivalently, solving the Euler-Lagrange equations in configuration space, gives a priori a full description of the dynamics, once we know the Lagrangian. There is, however, something which is unsatisfactory, and that is this configuration space. Knowing the point in configuration space which is occupied at a certain moment in time does not completely fix the time evolution, so this point in configuration space does not contain all the information of the dynamical state of the system. In fact, that's obvious, because the Euler-Lagrange equations are second-order equations, so in order to fix a solution one needs a value of q_i and of their derivatives.

Hamilton introduces 'phase space', in order to remedy this. The idea is that a point in phase space contains all the dynamical information of the system, and that from there on, only one possible evolution in time is possible. So we could simply define phase space as the direct sum of configuration space, and a copy of it, representing the derivatives, but Hamilton does something more subtle. Starting from the Lagrangian, he defines the following variables, called **conjugate momenta**:

$$p_i = \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}} \tag{7}$$

He proposes to invert these equations, so that we can write the derivatives of q_i as functions of only the q and the p (and t):

$$\dot{q}_i = r_i(q, p, t) \tag{8}$$

He then introduces the function: $H = \dot{q}_i p_i - L(q, \dot{q}, t)$ but written as a function of q and p:

$$H(q, p, t) = r_i(q, p, t) p_i - L(q, r(q, p, t), t) \tag{9}$$

This function $H(q, p, t)$ is called the **Hamiltonian**. The space spanned by the variables q_i and p_i (so a $2n$ dimensional space) is called **phase space**. We want to stress here that equation 7 is only needed to define a variable transformation between the Lagrangian formalism and the phase space formalism. Once this has been done (once the Hamiltonian has been found using equation 9), we should forget about this relationship, and consider p and q as independent variables. Again, a path in phase space determines the dynamics of the system, where by "path" we understand a curve parameterized in time, $\{q_i(t), p_i(t)\}$. Of course not all such curves in phase space correspond to a dynamics of the system. In fact, paths are much more restricted in phase space than in configuration space, because, by construction, we want only one single true path to go through each of the points in phase space. Indeed, we wanted a point in phase space to fix completely the dynamical evolution of the system, and that comes down to saying that only one true path can go through that point. It can be shown that the equivalent dynamics is given by the set of first order differential equations which the true paths have to satisfy:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \tag{10}$$

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \tag{11}$$

They are called the **canonical equations of Hamilton**. In fact, the dynamics in phase space (the dynamically allowed paths in (p, q) space) can also be derived from a variational principle. There is indeed such a principle, called **the modified Hamilton Principle**, and it takes on the following form:

$$\delta \left(\int_{t=t^{(1)}}^{t^{(2)}} \left(p_i(t)\dot{q}_i(t) - H\left(q_1(t), ..., q_n(t), p_1(t), ...p_n(t), t\right)\right) dt \right) = 0 \tag{12}$$

We have to consider all different paths $(q(t), p(t))$ in phase space, that satisfy the requirement that $q(t^{(1)}) = q^{(1)}$ and $q(t^{(2)}) = q^{(2)}$. Note that there is no requirement on the boundary values of p. p and q have to be considered as independent variables here that can independently take on values as a function of time. Each of these paths satisfying these requirements gives rise to a certain value of the integral. The true path followed by the dynamical system has then the property that the value of the integral is the same (to first order) for this path, and other, potential paths near to it. Note that in the integral, we use of course the Hamiltonian as a function of p and q, but we explicitly use $\dot{q}$ in the front term. This must not be replaced by the function $r(q, p)$. Working out the consequences of the modified Hamilton Principle, we find back the canonical equations of Hamilton, proving the equivalence of both formulations.

A final remark: if a generalized coordinate q_j doesn't explicitly occur in the Hamiltonian, then p_j is a constant of motion (meaning, a constant, independent of time for a true dynamical motion). q_j then becomes a linear function of time. Such a coordinate q_j is called a **cyclic coordinate**.

2 Canonical Transformations

2.1 What are Canonical Transformations ?

In configuration space, any change of generalized coordinates:

$$Q_i = Q_i(q_j, t) \tag{13}$$

is a possibility (as long as the transformation is smooth and regular). We substitute, in the Lagrangian, the old q_j by the new Q_i (using the inverse transformation) and the old $\dot{q}_j$ by the new $\dot{Q}_i$ using the chain rule in the inverse transformation. We then obtain a new function L' which serves as the new Lagrangian and which gives us the same dynamical behavior of the system as a function of the new variables Q_i. Such a transformation of generalized coordinates is called **a point transformation**. But in Hamilton's formulation, we can go further. We can have transformations of phase space:

$$Q_i = Q_i(p, q, t) \tag{14}$$

$$P_i = P_i(p, q, t) \tag{15}$$

However, the point transformations of configuration space could take on any form ; there are only certain kinds of transformations allowed in phase space, in order to be able to have a new Hamiltonian formulation in the new variables. The allowed transformations in phase space are called **Canonical Transformations**. The requirement is that there exists a new Hamiltonian, $K(Q, P, t)$, such that this Hamiltonian, and the associated canonical equations, give rise to allowed dynamical paths in the phase space (Q, P), that are the transformed paths of the allowed dynamical paths in the phase space (q, p). From the variational principles explained earlier, it can be shown that the most general transformation from the old to a new Hamiltonian takes on the form:

$$K = \lambda H + \frac{dF}{dt} \tag{16}$$

A canonical transformation hence will give rise to the above transformation of the Hamiltonian. There is actually another requirement, namely that of scale. Indeed, we can always introduce a global scale factor in the transformation. So it is always possible to re-scale a transformation so that $\lambda = 1$. In fact, it is just a matter of definition: if we drop this requirement, we talk of extended canonical transformations, but when we apply the requirement, we talk about canonical transformations.

A way to generate canonical transformations is by using a generating function F_2. Just consider a general function:

$$F_2(q, P, t) \tag{17}$$

We can then build a transformation from the following equations:

$$p_i = \frac{\partial F_2}{\partial q_i} \tag{18}$$

$$Q_i = \frac{\partial F_2}{\partial P_i} \tag{19}$$

If we now introduce:

$$K = H + \frac{\partial F_2}{\partial t} \tag{20}$$

we obtain again a Hamiltonian system, with Hamiltonian function K, in the variables (Q_i, P_i). This dynamics is equivalent, through the transformation, with the original Hamiltonian dynamics, so the proposed transformations are canonical transformations. There are similar transformations possible from other generating functions. For example, we can play a similar game with a generating function $F_1(q, Q, t)$.

2.2 Poisson Brackets

If u and v are two functions defined on phase space, we can define a new function on phase space, called the **Poisson bracket** of the two functions:

$$[u, v]_{q,p} \equiv \frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial v}{\partial q_i}\frac{\partial u}{\partial p_i} \tag{21}$$

It turns out that for the variables (q, p) themselves, the Poisson bracket takes on particularly simple values:

$$[q_j, q_k]_{q,p} = 0 = [p_j, p_k]_{q,p} \quad (22)$$

$$[q_j, p_k]_{q,p} = \delta_{jk} = -[p_k, q_j]_{q,p} \quad (23)$$

These relationships are called the **fundamental Poisson brackets**. It turns out that Poisson brackets are invariant under Canonical transformations. This means that a necessary and sufficient condition for a transformation to be a Canonical transformation, is that the transformation functions satisfy the fundamental Poisson brackets.

The invariance of Poisson brackets under canonical transformations allows us to write all time evolution as follows:

$$\frac{du}{dt} = [u, H] + \frac{\partial u}{\partial t} \quad (24)$$

A special case are the canonical equations of Hamilton:

$$\dot{q}_i = [q_i, H] \quad (25)$$

$$\dot{p}_i = [p_i, H] \quad (26)$$

3 Hamilton-Jacobi theory

3.1 The Hamilton-Jacobi equation.

We saw that a point in phase space represents the full dynamical information a system has, and only one single dynamical time evolution is possible with as initial condition, a particular point in phase space. The complete solution to the dynamical problem of a system is hence given by the functions:

$$q_i = q_i(q_i^0, p_i^0, t) \quad (27)$$

$$p_i = p_i(q_i^0, p_i^0, t) \quad (28)$$

Here, (q^0, p^0) stands for the initial point in phase space at time $t = 0$. This can be any point. Now the idea is the following: if we can somehow find a canonical transformation, that inverts the above equations, meaning, the new variables are (q^0, p^0), then the dynamical problem is simple: in these variables, nothing moves ! But of course we have to make sure that this comes down to a canonical transformation, and then we have to find it. If we find it, we have completely solved the dynamical problem. The idea is now that in order to have nothing move in the new variables, a way that is certain, is to make the new Hamiltonian K vanish. So we're looking for a canonical transformation, generated by a function F_2, such that $K = H + \partial F_2/\partial t = 0$. Taking $F_2(q, P, t)$, then we have:

$$p_i = \frac{\partial F_2}{\partial q_i} \quad (29)$$

and our requirement is:

$$H\left(q_1,...,q_n;\frac{\partial F_2}{\partial q_1},...,\frac{\partial F_2}{\partial q_n},t\right)+\frac{\partial F_2}{\partial t}=0 \tag{30}$$

This equation is know as the **Hamilton-Jacobi equation**. It is a first order partial differential equation in F_2. In the literature, F_2 is actually written S, and is called **Hamilton's Principal Function**. From the theory of partial differential equations, a complete solution to this equation consists of:

$$S=S(q_1,...,q_n;\alpha_1,...,\alpha_{n+1};t) \tag{31}$$

But one constant has to be an additive constant (only derivatives of S appear in the Hamilton-Jacobi equation). After dropping that constant, we can call the n remaining constants simply P_i, and we have:

$$S=S(q_1,...,q_n;P_1,...,P_n;t) \tag{32}$$

The canonical transformation satisfying our request then takes on the form:

$$p_i = \frac{\partial S(q,P,t)}{\partial q_i} \tag{33}$$

$$Q_i = \frac{\partial S(q,P,t)}{\partial P_i} \tag{34}$$

Inverting the transformation yields the original total solution to the dynamical problem:

$$q_j(t) = q_j(Q,P,t) \tag{35}$$

$$p_j(t) = p_j(Q,P,t) \tag{36}$$

where the new coordinates, (Q,P) are to be considered constants that are functions of (q^0,p^0).

The crucial point in all this is of course to find a complete solution to the Hamilton-Jacobi equation.

It is interesting to note the following:

$$\frac{dS}{dt}=\frac{\partial S}{\partial q_i}\dot{q}_i+\frac{\partial S}{\partial t}=p_i\dot{q}_i-H=L \tag{37}$$

so:

$$S=\int L dt \tag{38}$$

3.2 Hamilton's Characteristic Function

In the case the original Hamiltonian does not contain time explicitly, the Hamilton-Jacobi equation takes on the form:

$$H\left(q_1,...,q_n;\frac{\partial S}{\partial q_1},...\frac{\partial S}{\partial q_n}\right)+\frac{\partial S}{\partial t}=0 \tag{39}$$

As the first term doesn't contain time, we can propose the following solution:

$$S(q_i, P_i, t) = W(q_i, P_i) - P_1 t \tag{40}$$

(here, the P_i are supposed to be integration constants). This then leads to the following equation:

$$H\left(q_i, \frac{\partial W}{\partial q_i}\right) = P_1 \tag{41}$$

This is a partial differential equation, not containing time anymore, in the function W, called **Hamilton's Characteristic Function**. Note that one of the constants of integration, namely P_1 is equal to the constant value of the old hamiltonian. If the hamiltonian doesn't contain time, we know that it is a constant of motion. In many cases, this comes down to the constant energy of the system. We can of course stop here, but we can also look at another canonical transformation than the one generated by S; we can look at what canonical transformation W itself generates:

$$p_i = \frac{\partial W}{\partial q_i} \tag{42}$$

$$Q_i = \frac{\partial W}{\partial P_i} \tag{43}$$

Because the generating function, W, doesn't contain explicitly time, the values of the old and the new Hamiltonian are the same. So $K = P_1$. Note that all the new coordinates, Q_i, are cyclic in this system. The solution to the canonical equations are that all P_i are constant, and all Q_i for $i \neq 1$ are constant. We also have:

$$Q_1 = t + t_0 \tag{44}$$

Because the equations for $Q_{2,...,n}$ as a function of the q_i, equations 43, do not involve time explicitly, they are n-1 equations for n variables q_i, and constitute implicit orbit equations.

We could have written S differently:

$$S(q_i, P_i, t) = W(q_i, P_i) - K(P_1, P_2, ..., P_n)t \tag{45}$$

with K just any function of P_i. In this case, the new Hamiltonian would have been $K = K(P_1, P_2, ..., P_n)$. This allows for a more symmetrical treatment: all coordinates Q_i are still cyclic, and the canonical equations specify that:

$$Q_i = \nu_i t + \beta_i \tag{46}$$

with:

$$\nu_i = \frac{\partial K}{\partial P_i} \tag{47}$$

Interesting to note is that:

$$\frac{dW}{dt} = \frac{\partial W}{\partial q_i}\dot{q}_i = p_i \dot{q}_i \tag{48}$$

which leads to:

$$W = \int p_i dq_i \tag{49}$$

Let us consider a simple example, which is needed in quantum mechanics (in the WKB method):

$$H(p,x) = \frac{p^2}{2m} + V(x) \tag{50}$$

We hence have, from the conservation of energy:

$$p = \pm\sqrt{2m(E - V(x))} \tag{51}$$

This allows us to use:

$$W(x,E) = \int p_i dq_i = \int^x \pm\sqrt{2m(E - V(x'))}dx' \tag{52}$$

In this extremely simple example, we found a rather explicit form of W very easily. Usually things don't go so fast!