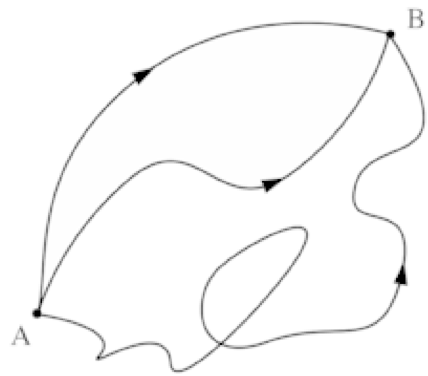
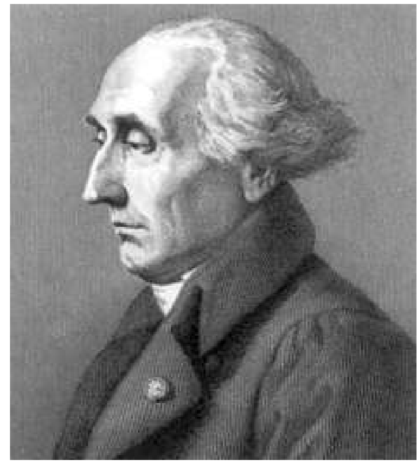
Hamilton's Principle and Lagrangian Mechanics

by Daniel Barker



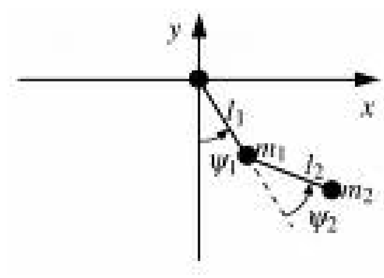


In 1834, William Hamilton hypothesized that particles follow paths that minimize the integral $J = \int_{t_1}^{t_2} L dt$

From this postulate, the equations of Lagrangian mechanics, $\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0$, can be derived.

Problems that would be impossible in Newtonian mechanics can be attacked using these equations.

For example:



Finding the path of motion of a particle is a fundamental physical problem. Inside an inertial frame – a coordinate system that moves with constant velocity – the motion of a system is described by Newton's Second Law: $\mathbf{F} = \dot{\mathbf{p}}$, where $\mathbf{F}$ is the total force acting on the particle and $\dot{\mathbf{p}}$ is the time derivative of the particle's momentum.[1] Provided that the particle's motion is not complicated and rectangular coordinates are used, then the equations of motion are fairly easy to obtain. In this case, the equations of motion are analytically solvable and the path of the particle can be found using matrix techniques.[2] Unfortunately, situations arise where it is difficult or impossible to obtain an explicit expression for all forces acting on a system. Therefore, a different approach to mechanics is desirable in order to circumvent the difficulties encountered when applying Newton's laws.[3]

The primary obstacle to finding equations of motion using the Newtonian technique is the vector nature of **F**. We would like to use an alternate formulation of mechanics that uses scalar quantities to derive the equations of motion. Lagrangian mechanics is one such formulation, which is based on Hamilton's variational principle instead on Newton's Second Law.[4] Hamilton's principle – published in 1834 by William Rowan Hamilton – is a mathematical statement of the philosophical belief that the laws of nature obey a principle of economy. Under such a principle, particles follow paths that are extrema for some associated physical quantities.[5]

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[1] J.B. Marion and S.T. Thornton, Classical Dynamics of Particles and Systems, 4th. ed. (Saunders College Publishing, Fort Worth, PA), p. 232-279.

[2] ibid.
[3] ibid.
[4] G.R. Fowles and G.L. Cassiday, Analytical Mechanics, 7th. ed. (Thomson Brooks/Cole, Belmont, CA), p. 417-459.
[5] ibid.

Hamilton's variational principle states that the integral $J = \int_{t_1}^{t_2} L dt$ taken along a path of possible motion of a physical system is an extremum when evaluated along the path actually taken."[6] $L = T - V$ is the Lagrangian of the system, where T is the kinetic energy and V is the potential energy. Also, note that the system's state at both endpoints of the integral is known. Out of all the ways in which the system could change during the time interval $t_2 - t_1$, the change that occurs is the one that minimizes J.[7] Mathematically, this can be expressed as $\delta J = \delta \int_{t_1}^{t_2} L dt = 0$, where δ represents the perturbation of any particular system parameter about the value attained by that parameter when J is an extremum.[8] Now, we must identify the parameters necessary to uniquely determine the state of the system.

Since T is a function of velocities and V is a function of the coordinates, L must be a function of velocities and coordinates.[9] Thus, the parameters needed are just a set of coordinates that uniquely specify the state of the system and their time derivatives. A free particle's position is uniquely described by the three Cartesian coordinates x, y, and z. We could also use these coordinates to describe the motion of a pendulum. However, in doing so we would have ignored two geometrical constraints on the pendulum's motion. First, the motion is restricted to the xz-plane ($y = 0$) and, second, the pendulum must move along an arc of length l ($l^2 - (x^2 + z^2) = 0$). Using these two equations, two of the coordinates can be eliminated. Thus, only one scalar coordinate is needed to completely specify the pendulum's motion.[10]

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[6] ibid.
[7] ibid.
[8] ibid.
[9] Marion and Thornton, pp. 232-279.
[10] Fowles and Cassiday, pp.417-459.

The choice of coordinate is dictated by the ease of use in the problem at hand. In the case of the pendulum, the angle θ that the pendulum makes with the vertical is the least awkward.[11] In general, a scalar coordinate is needed for each degree of freedom that the system possesses. The number of degrees of freedom is given by $s = 3n - m$, where $3n$ is the number of coordinates that specify the positions of all *n* particles in the system and *m* is the number of holonomic constraints that exist between them.[12] A holonomic constraint has form

$$f_j(x_i, y_i, z_i, t) = 0 \qquad i = 1,2,\ldots,n \qquad j = 1,2,\ldots,m \qquad (*)$$

Using such constraints it is possible to construct a set of *s* generalized coordinates – not connected by equations of constraint – that just suffice to determine the system's state (these coordinates are denoted q_i).[13] Again, the choice of coordinates is arbitrary and should be made based on the applicability to the system in question.

Now, *T* and *V* (and thus *L*) must be written in terms of the q_i's and the $\dot{q}_i$'s.[14] Substituting the resulting expression into Hamilton's variational principle yields

$$\delta J = \delta \int_{t_1}^{t_2} L dt = \int_{t_1}^{t_2} \delta L dt = \int_{t_1}^{t_2} \sum_i \left[\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right] dt = 0 \qquad (1)$$

The last step is an application of the chain rule of differentiation.[315] Further, the variation in the parameters δq_i and $\delta \dot{q}_i$ must vanish at the endpoints of the integral since the initial and final states are specified. An application of the product rule shows that the second term in brackets is

[11] ibid.
[12] Marion and Thornton, pp. 232-279.
[13] Fowles and Casiday, pp. 417-459.
[14] ibid.
[15] C.R. MacCluer, Calculus of Variations: Mechanics, Control, and Other Applications, 1st. ed. (Pearson Prentice Hall, Upper Saddle River, NJ), p. 45-58.

$$\int_{t_1}^{t_2}\sum_i\left[\frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\right]dt=\int_{t_1}^{t_2}\sum_i\left[\tfrac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\delta q_i\right)-\left(\tfrac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right)\delta q_i\right]dt=\sum_i\left[\frac{\partial L}{\partial \dot{q}_i}\delta q_i\right]_{t_1}^{t_2}-\int_{t_1}^{t_2}\sum_i\left[\left(\tfrac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right)\delta q_i\right]dt \quad (2)$$

The integrated term must vanish due to the restriction on the δq_i's outlined above.[2,3] So, substituting (2) into (1) gives

$$\int_{t_1}^{t_2}\sum_i\left[\frac{\partial L}{\partial q_i}-\tfrac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\right]\delta q_i\,dt=0 \quad (3)$$

All variations are completely arbitrary and independent of the others. The generalized coordinates are similarly independent. Therefore, only way to ensure that the integral equals zero is for each of the terms in the sum to vanish independently.[16] Thus,

$$\frac{\partial L}{\partial q_i}-\tfrac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)=0 \quad \mathrm{i}=1,2,...,\mathrm{s} \quad (4)$$

This can also be seen by sequentially setting all but one variation equal to zero.[17] Equation (4) contains the Lagrangian equations of motion for a conservative system with only holonomic constraints. This formulation of mechanics was derived by Joseph Louis de Lagrange (1736-1813) and is named in his honor.[18]

In order to show that (4) leads to the equations of motion that would otherwise result from Newton’s Second Law, let us return to the example of the pendulum and follow the discussion contained in Marion and Thornton. Having selected θ as the single generalized coordinate, we must write the Langrangian in terms of θ. First, write L as a function of x and z:

$$\begin{aligned}T&=\tfrac{1}{2}m\dot{x}^2+\tfrac{1}{2}m\dot{z}^2\\ V&=mgz \qquad\qquad (5)\\ L&=T-V=\tfrac{1}{2}m\dot{x}^2+\tfrac{1}{2}m\dot{z}^2-mgz\end{aligned}$$

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[16] Fowles and Cassiday, pp. 417-459.
[17] MacCluer, pp. 45-48.
[18] Fowles and Cassiday, pp.417-459.

Now, rewrite L in terms of θ and $\dot{\theta}$ using the relations:

$$\begin{aligned} x &= l\sin\theta \\ z &= -l\cos\theta \\ \dot{x} &= l\dot{\theta}\cos\theta \\ \dot{z} &= l\dot{\theta}\sin\theta \end{aligned} \quad (6).$$

Substituting (6) into the last line of (5) yields

$$L = \frac{m}{2} l^2 \dot{\theta}^2 + mgl\cos\theta \quad (7)$$

At this point, the most difficult part of the process is complete. The generalized coordinates have been selected and L has been written in terms of them. Now, we can apply (4) to find the equations of motion:

$$\begin{aligned} \frac{\partial L}{\partial \theta} &= -mgl\sin\theta \\ \tfrac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) &= ml^2\ddot{\theta} \\ \frac{\partial L}{\partial \theta} - \tfrac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}}\right) &= -ml^2\ddot{\theta} - mgl\sin\theta = 0 \end{aligned} \quad (8)$$

After some algebra, this yields

$$\ddot{\theta} + \tfrac{g}{l}\sin\theta = 0 \quad (9),$$

which is the familiar equation of motion for a pendulum derived using Newton's laws.[19] The equivalence of the two methods in this example is by no means a proof. However, experiment is the ultimate arbiter of truth in the physical world, and both Newton's and Lagrange's mechanics have passed this test repeatedly.[20]

[19] Marion and Thornton, pp. 232-279.
[20] Fowles and Cassiday, pp. 417-459.

The Lagrangian technique is actually more onerous than the Newtonian one for the pendulum example because the forces on the pendulum are easily recognized. However, as the complexity of the system increases, the tractability of the Newtonian approach decreases and the Lagrangian method becomes far more elegant. Note that Lagrange's formulation can only be used on conservative systems described by coordinates connected by holonomic constraints. The use of Lagrangian mechanics on systems with non-holonomic constraints – constraints that cannot be expressed in form (*) – is quite difficult and beyond the scope of this paper.[21] However, the extension of Lagrange's equations to non-conservative systems will be addressed.

To fully generalize Lagrange's equations, we elect to follow the process used by Lagrange when he developed his mechanics. This work was made possible by the insights of Jean LeRond D'Alembert (1717-1783).[22] First, note that when a system in equilibrium is displaced by an amount $\delta\mathbf{r}$ the net work done on the system is zero ($\delta W = \sum_i \mathbf{F}_i \cdot \delta\mathbf{r}_i = 0$). D'Alembert realized that this statement could be generalized to dynamic systems by considering the $\dot{\mathbf{p}}$ term from Newton's Second Law to be a real force. This led him to posit D'Alembert's principle

$$\sum_i \left(\mathbf{F}_i - \dot{\mathbf{p}}_i\right)\cdot \delta\mathbf{r}_i = 0 \qquad (10)$$

,

which is equivalent to Newton's Second Law with $\dot{\mathbf{p}}$ rewritten as a real force.[23]

The following is a generalization of the remaining discussion in Fowles and Cassiday. Let us assume that the system described by (10) can be expressed using generalized coordinates but has not yet been written in that form. Then, the first term in (10) is the virtual work

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[21] ibid.
[22] ibid.
[23] ibid.

$$\delta W = \sum_i F_i \cdot \delta x_i = \sum_j \left[\sum_i \left(F_i \frac{\partial x_i}{\partial q_j} \right) \right] \delta q_j = \sum_j Q_j \delta q_j \quad (11)$$

$$Q_j = \sum_i \left(F_i \frac{\partial x_i}{\partial q_j} \right),$$

where Q_j is the generalized force on the system. Also, the virtual work is not zero. The full derivation of the second term of (10) is fairly involved. It will only be outlined here, as a full development can be found in Fowles and Cassiday. We use the product rule and the chain rule to find

$$\sum_i \dot{p}_i \delta x_i = \sum_j \left[\sum_i m \ddot{x}_i \frac{\partial x_i}{\partial q_j} \right] \delta q_j = \sum_j \delta q_j \sum_i m \left[\tfrac{d}{dt} \left(\dot{x}_i \frac{\partial x_i}{\partial q_j} \right) - \dot{x}_i \tfrac{d}{dt} \left(\frac{\partial x_i}{\partial q_j} \right) \right] \quad (12)$$

Now, we use the fact that

$$\frac{\partial x_i}{\partial q_j} = \frac{\partial \dot{x}_i}{\partial \dot{q}_j} \quad (13)$$

which follows from the definition of the generalized coordinates. Also, it can be shown that

$$\tfrac{d}{dt} \left(\frac{\partial x_i}{\partial q_j} \right) = \frac{\partial \dot{x}_i}{\partial q_j} \quad (14)$$

Substituting (13) and (14) into (12) yields

$$\sum_i \dot{p}_i \delta x_i = \sum_j \left[\tfrac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \left(\frac{\partial T}{\partial q_j} \right) \right] \delta q_j \quad (15)$$

Next, putting (11) and (15) back into (10) gives

$$\sum_i (F_i - \dot{p}_i) \delta x_i = \sum_j \left\{ Q_j - \left[\tfrac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_j} \right) - \left(\frac{\partial T}{\partial q_j} \right) \right] \right\} \delta q_j = 0 \quad (16)$$

As with the initial derivation from Hamilton's principle, the variations are independent so all the terms in brackets must vanish individually. Now, $Q_j = \overline{Q}_j + Q'_j$ is the total generalized force in the q_j direction, where $\overline{Q}_j$ is the conservative part of this force and Q'_j is the non-conservative part. Recall that

$$\overline{Q}_j = -\frac{\partial V}{\partial q_j} \quad (17)$$

$$\frac{\partial V}{\partial \dot{q}_j} = 0 \quad (18)$$

because $\overline{Q}_j$ is conservative and V does not depend on $\dot{q}_j$. Thus, the requirement that all terms in brackets in (16) must vanish can be written as

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) = Q'_j \quad \mathrm{j} = 1,2,\ldots,\mathrm{s} \quad (19)$$

This is the generalized version of Lagrange's equations of motion that can be applied to non-conservative systems. The generalized coordinates must still be connected with holonomic constraints. Also, the introduction of Q'_j makes the problem significantly more difficult because Q'_j usually must be determined independently. This means that it is often more practical to use the Newtonian approach when dealing with non-conservative systems.[24]

Having completed this development of Lagrangian mechanics, we comment briefly on the philosophical differences between Newton's and Lagrange's formulations. Newtonian mechanics describes motion in terms of outside influences (forces) acting on the system. The notion of cause and effect is inherent to this approach.[25] Lagrangian mechanics, on the other hand, works only with scalar quantities intrinsic to the system (energies). The derivation from

[24] Marion and Thornton, pp. 232-279; Fowles and Cassiday, pp. 417-459.
[25] Marion and Thornton, pp. 232-279.

Hamilton's principle also implies that nature is trying to achieve a certain purpose with the motion of a system, the minimization of *J*.[26] Remember that, ultimately, Lagrangian and Newtonian mechanics are physically equivalent. There can be no difference between their results for a particular physical problem.

Next, we turn to another formulation of classical mechanics developed by William Rowan Hamilton in conjunction with his variational principle. This formulation is of particular interest because Hamilton worked on it after developing a similar theory based on the variational principle for geometrical optics.[27] The theories for mechanics and optics are analogous to each other, and because of this, Hamiltonian mechanics has found many applications in the realm of quantum mechanics.[28]

We begin the derivation of Hamilton's canonical equations of motion by assuming that $T = T(\dot{q}) > 0$ is a quadratic function and that V is a function only of q. Thus, L has no explicit time dependence. In this case, we can apply Euler's formula to find that

$$H = \sum_i \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} - L = 2T - L = T + V \qquad (20)$$

,

where H is called the Hamiltonian of the system and is equal to the total energy.[29] Let $p_i = \frac{\partial T}{\partial \dot{q}_i}$ be the generalized momenta of the system. Now Lagrange's equations can be expressed as

$$\dot{p}_i = \frac{\partial L}{\partial q_i} \qquad (21)$$

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[26] Marion and Thornton, pp. 232-279.
[27] T.L. Hankins, <u>Sir William Rowan Hamilton</u>, 1st. ed. (Johns Hopkins University Press, Baltimore, MD), p. 172-199.
[28] ibid.
[29] MacCluer, pp. 45-58.

Under this change of variables, the total differential of the Hamiltonian is[30]

$$dH = \sum_i \left[dq_i \frac{\partial H}{\partial q_i} + dp_i \frac{\partial H}{\partial p_i} \right] + dt \frac{\partial H}{\partial t} \qquad (22)$$

However, according to (20), the total differential can also be written in the form[31]

$$dH = \sum_i \left[\dot{q}_i dp_i + d\dot{q}_i p_i - dq_i \frac{\partial L}{\partial q_i} - d\dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right] - dt \frac{\partial L}{\partial t} \qquad (23)$$

If the definition of the generalized momenta and (21) are substituted into (23), we find

$$dH = \sum_i \left[\dot{q}_i dp_i - d\dot{q}_i p_i \right] - dt \frac{\partial L}{\partial t} \qquad (24)$$

Equating coefficients with (22) yields

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \qquad (25)$$

$$\frac{\partial H}{\partial \dot{q}_i} = -\dot{p}_i \qquad (26)$$

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \qquad (27)$$

(25) and (26) are known as the canonical equations of motion.[32] In Hamiltonian mechanics the equations of motion are found using 2*s* first-order equations rather than the *s* second-order equations of the Lagrangian method. Because forming the Hamiltonian as a function of p_i and $\dot{q}_i$ can be more complicated than finding the Lagrangian of the same system, Hamiltonian mechanics have more limited applicability than Lagrangian mechanics. The main strength of

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[30] Marion and Thornton, pp.232-279.
[31] ibid.
[32] Fowles and Cassiday, pp. 417-459.

Hamilton mechanics is the ease with which it can be extended to other fields such as optics and quantum mechanics.[33]

We conclude with a discussion of the applications of Hamilton's variational principle and the Hamiltonian to quantum mechanics. The Hamiltonian occurs as an energy operator in quantum mechanics. This operator occurs when the time-evolution of a quantum system is of interest. The time-evolution operator is given by

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} \qquad (28),$$

where $\hat{H}$ is the Hamiltonian and $\hbar$ is Planck's constant. Thus, the Hamiltonian is a time-translation operator.[5] Also, the fundamental equation of quantum mechanics, Schrödinger's equation, can be written in terms of the Hamiltonian and is defined in terms of the Hamiltonian in some textbooks (Townsend, for example). In this form, the Schrödinger is

$$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi \qquad (29),$$

where ψ is the wave-function.[34] The main point here is that Hamiltonian mechanics is the formulation of classical mechanics that can be translated most easily into quantum mechanics. In fact, Hamilton's work on optics had been largely unknown until Erwin Schrödinger repopularized it. In hindsight, the analogy between optics and classical mechanics present in Hamiltonian mechanics and the variational principle was almost foreboding.[35]

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[33] Marion and Thornton, pp. 232-279.

[34] J.S. Townsend, A Modern Approach to Quantum Mechanics, 1st. ed. (University Science Books, Sausalito, CA), p.93-116, p. 216-233.

[35] T.L. Hankins, Sir William Rowan Hamilton, 1st. ed. (Johns Hopkins University Press, Baltimore, MD), p. 172-199.

Another application of Hamilton's work in quantum mechanics was developed by Richard Feynman.[36] Feynman constructed an integral formulation of quantum mechanics based on a quantum version of the variational principle. This approach involves evaluating a path integral over every possible path that the particle can take, which sounds (and is) rather difficult — in fact, the path integral formulation is only worth using in quantum field theory. Evaluation of the integral leads to a transition amplitude for each path that the particle could take, allowing a formulation of quantum mechanics without the need for operator notation.[37] Interestingly, Feynman's method also allows us to recover Hamilton's principle as a special case of the path-based quantum mechanics. On large scales, the transition amplitudes far from the extremum required by Hamilton's principle interfere destructively and the transition amplitudes near the extremum interfere constructively.[38] This interference causes particles and systems that we experience on the classical scale to follow paths that minimize J.

Finally, we have described and formulated Lagrangian mechanics for conservative as a method to treat problems that are intractable using Newtonian methods. The approach was then extended to systems under the influence of non-conservative forces, although Newton's laws are often more suited to such systems. Another method for finding the equations of motion, Hamiltonian mechanics, was also explored. Of particular interest is the applicability of Hamilton's principle to optics and quantum mechanics. Specifically, the path integral formulation of quantum mechanics allows us to recover the variational principle as a special case. This is reassuring because one of the fundamental postulates of quantum mechanics is its

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[36] Fowles and Cassiday, pp.417-459.
[37] Townsend, pp. 216-233.
[38] ibid.

equivalence to classical mechanics on large scales. However, the primary result is that we now have a simpler, more elegant approach to physical phenomena.

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