Variational Principles in Physics (Particularly in Quantum Mechanics)

— Dan Styer, © 18 March 2014; minor correction 9 January 2015; additions 6 February 2015 and 4 December 2020

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Classical motion of one particle

A classical particle of mass m moves in one dimension, subject to potential energy V(x), from initial time t_a to final time t_b . The position $x_0(t)$ changes from $x_0(t_a) = x_a$ to $x_0(t_b) = x_b$. How does the real path $x_0(t)$ differ from all other functions x(t) with $x(t_a) = x_a$ to $x(t_b) = x_b$? Here's one way:

Calculate the *action* $S\{x(t)\}$ for each such function:

$$S\{x(t)\} \equiv \int_{t_a}^{t_b} \left[\frac{1}{2}m\dot{x}^2(t) - V(x(t))\right] dt.$$
 (1)

The real path $x_0(t)$ is the function that extremizes this action. (That is, it minimizes or maximizes it. Usually it's a minimum, so this principle is often called "the principle of least action". By the way, the term in square brackets above is called "the Lagrangian".)

Starting from this principle we derive a differential equation for $x_0(t)$.

Vary the possible path x(t) about some reference path $x_{ref}(t)$, that is consider paths of the form

$$x(t) = x_{\rm ref}(t) + \lambda \eta(t), \tag{2}$$

where $\eta(t)$ is an arbitrary deviation function with

$$\eta(t_a) = 0 \quad \text{and} \quad \eta(t_b) = 0, \tag{3}$$

and find the difference between $S\{x(t)\}$ and $S\{x_{ref}(t)\}$. If my claim is true, then deviations about the reference path $x_0(t)$ will result in zero change of action to first order in λ . However, before looking at the physical implications, we solve the mathematical problem of finding the difference between $S\{x(t)\}$ and $S\{x_{ref}(t)\}$.

How does the Lagrangian of path x(t) differ from the Lagrangian of path $x_{ref}(t)$?

$$\dot{x}(t) = \dot{x}_{ref}(t) + \lambda \dot{\eta}(t), \quad so \quad \dot{x}^2(t) = \dot{x}_{ref}^2(t) + \lambda 2 \dot{x}_{ref}(t) \dot{\eta}(t) + \lambda^2 \dot{\eta}^2(t).$$
 (4)

Meanwhile,

$$V(x(t)) = V(x_{\rm ref}(t) + \lambda \eta(t)) = V(x_{\rm ref}(t)) + \left. \frac{\partial V}{\partial x} \right|_{x_{\rm ref}(t)} \lambda \eta(t) + \mathcal{O}(\lambda^2), \tag{5}$$

 \mathbf{SO}

$$\begin{bmatrix} \frac{1}{2}m\dot{x}^{2}(t) - V(x(t)) \end{bmatrix} = \begin{bmatrix} \frac{1}{2}m\dot{x}_{ref}^{2}(t) - V(x_{ref}(t)) \end{bmatrix} + \lambda \begin{bmatrix} m\dot{x}_{ref}(t)\dot{\eta}(t) - \frac{\partial V}{\partial x} \Big|_{x_{ref}(t)} \eta(t) \end{bmatrix} + \mathcal{O}(\lambda^{2}).$$
(6)

Thus the action of path x(t) differs from the action of path $x_{ref}(t)$ through

$$S\{x(t)\} = S\{x_{\rm ref}(t)\} + \lambda \int_{t_a}^{t_b} \left[m \dot{x}_{\rm ref}(t) \dot{\eta}(t) - \frac{\partial V}{\partial x} \Big|_{x_{\rm ref}(t)} \eta(t) \right] dt + \mathcal{O}(\lambda^2).$$
(7)

Looking at the left half of the integral above, we use integration by parts to write

$$\int_{t_a}^{t_b} m \dot{x}_{\rm ref}(t) \dot{\eta}(t) \, dt = \left[m \dot{x}_{\rm ref}(t) \eta(t) \right]_{t_a}^{t_b} - \int_{t_a}^{t_b} m \ddot{x}_{\rm ref}(t) \eta(t) \, dt, \tag{8}$$

however because $\eta(t_a) = 0$ and $\eta(t_b) = 0$ (equation 3), the term in square brackets vanishes. Thus the actions differ through

$$S\{x(t)\} = S\{x_{ref}(t)\} + \lambda \int_{t_a}^{t_b} \left[-m\ddot{x}_{ref}(t) - \frac{\partial V}{\partial x} \Big|_{x_{ref}(t)} \right] \eta(t) dt + \mathcal{O}(\lambda^2).$$
(9)

We have solved the mathematical problem.

Now for the physics: The principle of least action claims that if $x_{ref}(t)$ is the true path $x_0(t)$, then deviations about the reference path result in zero change of action to first order in λ . In other words the integral

$$\int_{t_a}^{t_b} \left[-m\ddot{x}_0(t) - \left. \frac{\partial V}{\partial x} \right|_{x_0(t)} \right] \eta(t) \, dt \tag{10}$$

must vanish for any function $\eta(t)$ that vanishes at t_a and t_b . The only way for this to happen is for the expression within square brackets to vanish for all times between t_a and t_b , that is, the true path must satisfy

$$m\ddot{x}_0(t) = -\left.\frac{\partial V}{\partial x}\right|_{x_0(t)},\tag{11}$$

an equation normally written as

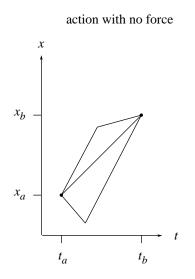
$$m\ddot{x}(t) = F(x(t)). \tag{12}$$

Things are looking good for the principle of least action.

[Normally we solve this equation subject to the initial values $x(t_a) = x_a$ and $\dot{x}(t_a) = v_a$. Here we solve it subject to the boundary values $x(t_a) = x_a$ and $x(t_b) = x_b$.]

What does this mean? What's going on physically?

Think about vertical motion from point x_a at time t_a to some higher point x_b at some later time t_b . For our first consideration, we turn off gravity so there's no potential energy, and the principle of least action is just the principle of least average-kinetic-energy. One way to make this journey is to proceed always at the average speed $V_{ave} = (x_b - x_a)/(t_b - t_a)$. Another way is to go faster than average at the beginning, then slower than average at the end. A third way is to go down at the beginning, then *really* fast at the end.



In the second and third ways, the velocity will deviate from the average velocity — sometimes positively, sometimes negatively, but it has to deviate. Because the velocity in $\frac{1}{2}mv^2$ comes in with a square, these deviations from average will always *increase* the average kinetic energy. Thus the *uniform* velocity case will minimize

$$\int_{t_a}^{t_b} \frac{1}{2} m v^2(t) \, dt. \tag{13}$$

And indeed, we know that in the absence of forces a particle moves uniformly!

Now we turn gravity back on. We still want the smallest possible average kinetic energy, but we also want the largest possible average potential energy. The regions of high potential energy are high up, but to reach them we have to go up at high speed and then come down at high speed. Both of these of course increase the average kinetic energy. So there's a trade-off. As you know, the trade-off minimizes action when the position as a function of time is a parabola as shown here:

x_{b} more (- P.E.) here x_{a} more (+ K.E.) here t_{a} t_{b}

action with gravitational force

John C. Baez writes that "the Lagrangian measures something we could vaguely refer to as the 'activity' or 'liveliness' of a system: the higher the kinetic energy the more lively the system, the higher the potential energy the less lively. So, we're being told that nature likes to minimize the total of 'liveliness' over time: that is, the total action. In other words, nature is as lazy as possible!" (*Lectures on Classical Mechanics*, page 7.)

[In his essay "Gravity, Time, and Lagrangians", Elisha Huggins discusses this tradeoff through general relativity: You know that a moving clock ticks slowly, but also (because of gravitational time dilation) a higher clock ticks more rapidly. How can you move a clock from x_a at time t_a to x_b at time t_b , while maximizing the time ticked off by the clock? You want to go slow, but you also want to go high. For this one instance, maximizing the clock time is the same as minimizing the action. I don't know how general this result is, but I've always found it intriguing.]

One classical particle, but more abstractly

We do the same problem, but instead of using the particular Lagrangian

$$\left[\frac{1}{2}m\dot{x}^{2}(t) - V(x(t))\right]$$
(14)

we look more abstractly at the Lagrangian

$$L(x(t), \dot{x}(t), t) \tag{15}$$

where the above means the function

$$L(u, v, w)$$
 evaluated at $u = x(t), v = \dot{x}(t), w = t.$ (16)

Apply the same deviation

$$x(t) = x_{\rm ref}(t) + \lambda \eta(t) \tag{17}$$

as before (equation 2), with the same endpoints condition (3) as before. The more abstract equation analogous to equation (6) is

$$L(x(t), \dot{x}(t), t) = L|_{\text{ref}} + \lambda \left[\frac{\partial L}{\partial u} \Big|_{\text{ref}} \eta(t) + \frac{\partial L}{\partial v} \Big|_{\text{ref}} \dot{\eta}(t) \right] + \mathcal{O}(\lambda^2),$$
(18)

where the notation $f|_{\text{ref}}$ means the function f(u, v, w) evaluated at $u = x_{\text{ref}}(t)$, $v = \dot{x}_{\text{ref}}(t)$, w = t. Integrating with respect to time t, we find the equation analogous to equation (7),

$$S\{x(t)\} = S\{x_{\rm ref}(t)\} + \lambda \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial u} \Big|_{\rm ref} \eta(t) + \frac{\partial L}{\partial v} \Big|_{\rm ref} \dot{\eta}(t) \right] dt + \mathcal{O}(\lambda^2).$$
(19)

Using the "integration by parts trick" of equation (8), we obtain

$$S\{x(t)\} = S\{x_{ref}(t)\} + \lambda \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial u} \Big|_{ref} \eta(t) - \frac{d}{dt} \left(\frac{\partial L}{\partial v} \Big|_{ref} \right) \eta(t) \right] dt + \mathcal{O}(\lambda^2)$$

$$= S\{x_{ref}(t)\} + \lambda \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial u} \Big|_{ref} - \frac{d}{dt} \left(\frac{\partial L}{\partial v} \Big|_{ref} \right) \right] \eta(t) dt + \mathcal{O}(\lambda^2).$$
(20)

We are done with the math and can continue with physics. If $x_{ref}(t)$ is $x_0(t)$, then the principle of least action says that the integral multiplying λ vanishes for any possible function $\eta(t)$, so the term in square brackets must vanish for all times between t_a and t_b :

$$\frac{\partial L}{\partial u}\Big|_{0} - \frac{d}{dt} \left(\frac{\partial L}{\partial v}\Big|_{0}\right) = 0.$$
(21)

This is called the Euler-Lagrange equation. It gets tiresome to keep the u and v variables straight, and we always plug x(t) into u and $\dot{x}(t)$ into v, so this equation is usually written as

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0.$$
(22)

This expression leaves the unfortunate impression that you're taking the partial derivative of L with respect to the function $\dot{x}(t)$ — what?!?!?! — but if you realize that it's just shorthand for the correct interpretation (first take the partial derivative of L with respect to the argument v, second plug in $v = \dot{x}(t)$, third take the time derivative of the resulting function) then you'll appreciate its brevity.

This approach generalizes in a straightforward way to functions of several variables (several particles, moving in two or three dimensions), and in a less-straightforward way to the velocity-dependent force of magnetism. You can do this for yourself. There are also interesting mathematical questions: Does every differential equation have an associated minimization principle? Is there a procedure for finding a Lagrangian when presented with an arbitrary differential equation? We will not pursue any of these questions. Instead, we will generalize to a variational principle for fields.

Variational principle for classical fields

A field is a function that depends on both space and time: f(x,t). Suppose we are given an initial and a final value for the field: $f(x,t_a)$ and $f(x,t_b)$. Suppose also that the boundary condition for the field is f(0,t) = 0 and f(L,t) = 0. [The situation to think of is a stretch, clamped string of length L. The function f(x,t) is the height of the string above equilibrium. Normally we solve this problem as an initial value problem, i.e. given

the initial height values $f(x, t_a) = y(t_a)$ and initial vertical velocity values $\frac{\partial f}{\partial t}(x, t_a) = v_y(t_a)$,

but in this case we solve it as a boundary value problem.]

The "Lagrangian density" is some function of the form

$$\mathcal{L}(f(x,t),\frac{\partial f(x,t)}{\partial x},\frac{\partial f(x,t)}{\partial t},t) = \mathcal{L}(f,f_x,f_t,t).$$
(23)

The action is

$$S\{f(x,t)\} = \int_{t_a}^{t_b} \int_0^L \mathcal{L}(f, f_x, f_t, t) \, dx \, dt.$$
(24)

What are the Euler-Lagrange equations that tell us which function $f_0(x,t)$ minimizes $S\{f(x,t)\}$?

In this case I'll be less finicky about the notation, but we proceed in a familiar manner by considering deviations

$$f(x,t) = f_0(x,t) + \lambda \eta(x,t)$$
(25)

where

$$\eta(x,t_a) = 0, \qquad \eta(x,t_b) = 0, \qquad \eta(0,t) = 0, \qquad \eta(L,t) = 0.$$
 (26)

Now

$$\mathcal{L}(f, f_x, f_t, t) = \mathcal{L}(f_0, f_{0,x}, f_{0,t}, t) + \lambda \left[\frac{\partial \mathcal{L}}{\partial f} \eta(t) + \frac{\partial \mathcal{L}}{\partial f_x} \eta_x(x, t) + \frac{\partial \mathcal{L}}{\partial f_t} \eta_t(x, t) \right] + \mathcal{O}(\lambda^2).$$
(27)

Integrating over both space and time,

$$S\{f(x,t)\} = S\{f_0(x,t)\} + \lambda \int_{t_a}^{t_b} \int_0^L \left[\frac{\partial \mathcal{L}}{\partial f}\eta(t) + \frac{\partial \mathcal{L}}{\partial f_x}\eta_x(x,t) + \frac{\partial \mathcal{L}}{\partial f_t}\eta_t(x,t)\right] dx dt + \mathcal{O}(\lambda^2).$$
(28)

Using the integration by parts trick first in space (note the importance of the boundary conditions in space) and then in time,

$$S\{f(x,t)\} = S\{f_0(x,t)\} + \lambda \int_{t_a}^{t_b} \int_0^L \left[\frac{\partial \mathcal{L}}{\partial f}\eta(t) - \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial f_x}\eta(x,t) - \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial f_t}\eta(x,t)\right] dx dt + \mathcal{O}(\lambda^2).$$
(29)

So the Euler-Lagrange equation for the function f(x,t) that minimizes the action is

$$\frac{\partial \mathcal{L}}{\partial f} - \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial f_x} - \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial f_t} = 0.$$
(30)

For example, suppose the Lagrangian density happens to be

$$\mathcal{L} = f_t^2 - A f_x^2. \tag{31}$$

Then

$$\frac{\partial \mathcal{L}}{\partial f} = 0, \qquad \frac{\partial \mathcal{L}}{\partial f_x} = -2Af_x, \qquad \frac{\partial \mathcal{L}}{\partial f_t} = 2f_t,$$
(32)

and the Euler-Lagrange equation is

$$2A\frac{\partial f_x}{\partial x} - 2\frac{\partial f_t}{\partial t} = 0 \tag{33}$$

 or

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{A} \frac{\partial^2 f}{\partial t^2}.$$
(34)

This is the wave equation with wave speed $\sqrt{A}!$

Once again, you can think of straightforward generalizations to functions of many variables, and to vector fields, and to multiple fields. (For example, if you were write down the Lagrangian density for the electromagnetic field, so that the Maxwell equations would come from minimizing the action, then the Lagrangian density would of course have to depend on both $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$.)

I would like a better physical handle on this result. What exactly are we minimizing and why would nature want it to be that way?

Variational principle for electromagnetic field

In electromagnetism, a given charge density $\rho(\vec{r},t)$ and current density $\vec{j}(\vec{r},t)$ set up electromagnetic fields $\vec{E}(\vec{r},t)$ and $\vec{B}(\vec{r},t)$. The fields can be describe through "potential functions" $V(\vec{r},t)$ and $\vec{A}(\vec{r},t)$ which have the property that

$$\begin{array}{lll} \vec{B}(\vec{r},t) &=& \vec{\nabla} \times \vec{A}(\vec{r},t) \\ \vec{E}(\vec{r},t) &=& -\vec{\nabla} V(\vec{r},t) - \frac{\partial \vec{A}(\vec{r},t)}{\partial t} \end{array}$$

The Lagrangian density for electromagnetism turns out to be

$$\mathcal{L}(\vec{r},t) = -\rho(\vec{r},t)V(\vec{r},t) + \vec{j}(\vec{r},t) \cdot \vec{A}(\vec{r},t) + \frac{\epsilon_0}{2}\vec{E}^2(\vec{r},t) + \frac{1}{2\mu_0}\vec{B}^2(\vec{r},t).$$
(35)

We have to vary with respect to the potentials, not with respect to the fields (the fields are derivatives of the potentials). When we do that, we produce the Maxwell equations.

Another Lagrangian density

Let's just try another Lagrangian density, just for kicks:

$$\mathcal{L} = \frac{\hbar^2}{2m} (f_x^2 + g_x^2) + \hbar (fg_t - gf_t) + V(x)(f^2 + g^2).$$
(36)

Varying relative to f gives:

$$0 = \frac{\partial \mathcal{L}}{\partial f} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial f_x} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial f_t}$$

$$= \hbar g_t + 2V(x)f - \frac{\partial}{\partial x} \left(\frac{\hbar^2}{2m} 2f_x\right) - \frac{\partial}{\partial t} \left(-\hbar g\right)$$

$$= 2\hbar g_t + 2V(x)f - 2\frac{\hbar^2}{2m} f_{xx}$$

$$-\hbar g_t = -\frac{\hbar^2}{2m} f_{xx} + V(x)f$$

$$\frac{\partial g}{\partial t} = -\frac{1}{\hbar} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right] f.$$
(37)

Varying relative to g gives:

$$0 = \frac{\partial \mathcal{L}}{\partial g} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial g_x} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial g_t}$$

$$= -\hbar f_t + 2V(x)g - \frac{\partial}{\partial x} \left(\frac{\hbar^2}{2m} 2g_x\right) - \frac{\partial}{\partial t} (\hbar f)$$

$$= -2\hbar f_t + 2V(x)g - 2\frac{\hbar^2}{2m}g_{xx}$$

$$\hbar f_t = -\frac{\hbar^2}{2m}g_{xx} + V(x)g$$

$$\frac{\partial f}{\partial t} = +\frac{1}{\hbar} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] g.$$
(38)

If you have been listening in this course at all, you will be inspired to define

$$\psi(x,t) = f(x,t) + ig(x,t) \tag{39}$$

and then add equation (38) to *i* times equation (37) to produce

$$\frac{\partial\psi(x,t)}{\partial t} = -\frac{i}{\hbar} \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t).$$
(40)

I will not insult you by giving a name to this equation.

This encourages us to go back and write the Lagrangian density (36) in terms of ψ , resulting in

$$\mathcal{L} = \frac{\hbar^2}{2m} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\hbar}{2i} \left\{ \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right\} + V(x)\psi^*\psi.$$
(41)

Once again, I'd like a better physical picture. To use Baez's terminology, what does this Lagrangian density say about the "liveliness" of quantum mechanics?

The variational method

How is the variational principle described here related to the variational method for the ground state energy?

Take the class of wavefunctions of form

$$\psi(x,t) = e^{-(i/\hbar)E_n t} \eta(x).$$
(42)

In this case

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E_n \,\psi(x,t),\tag{43}$$

 \mathbf{so}

$$\mathcal{L} = \frac{\hbar^2}{2m} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\hbar}{2i} \left\{ \psi^* \left(-\frac{i}{\hbar} E_n \right) \psi - \psi \left(+\frac{i}{\hbar} E_n \right) \psi^* \right\} + V(x) \psi^* \psi$$
$$= \frac{\hbar^2}{2m} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + (V(x) - E_n) \psi^* \psi.$$
(44)

The Lagrangian density is thus independent of time, and the action to be minimized is

$$S = (t_b - t_a) \int_{-\infty}^{+\infty} \frac{\hbar^2}{2m} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + (V(x) - E_n) \psi^* \psi \, dx$$

$$= (t_b - t_a) \int_{-\infty}^{+\infty} \frac{\hbar^2}{2m} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + V(x) \psi^* \psi \, dx - (t_b - t_a) E_n \qquad [[\dots \text{ integrate by parts to get...}]]$$

$$= (t_b - t_a) \int_{-\infty}^{+\infty} \psi^* \left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi^* \psi \, dx - (t_b - t_a) E_n$$

$$= (t_b - t_a) \int_{-\infty}^{+\infty} \psi^* \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi \, dx - (t_b - t_a) E_n$$

$$= (t_b - t_a) \left[\langle \hat{H} \rangle - E_n \right]. \tag{45}$$

But I'm not sure how to interpret this, because of the following worry.

My worry about the variational principle for quantum mechanics and electromagnetism

When we derived the Euler-Lagrange equations I said up front (equation 26): consider deviations with

$$\eta(x, t_a) = 0, \qquad \eta(x, t_b) = 0, \qquad \eta(0, t) = 0, \qquad \eta(L, t) = 0.$$
 (46)

Okay, when we get to quantum mechanics the last two are replaced with

$$\eta(-\infty, t) = 0, \qquad \eta(+\infty, t) = 0,$$
(47)

which is fine. But I don't understand how to make variations subject to a given fixed initial wavefunction plus a given fixed final wavefunction. It was fine for the wave equation, which is second order in time, so it can be solved either as an initial value problem (initial position function fixed plus initial velocity function fixed) or as a boundary value problem (initial position function fixed plus final position function fixed). But the Schrödinger equation is first order in time: once you've fixed the initial wavefunction there's nothing more to fix — you can't also specify the final wavefunction.

The exact same concern holds for electromagnetism, because the Maxwell equations are again first order in time.

This bugs me.