Geometry, Topology, and Physics Chapter 1: Quantum Physics

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1 Introduction

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2 1.1: Analytical Mechanics

2.1 1.1.1: Newtonian Mechanics

Let $\mathbf{x}(t)$ denote the position of a mass m at time t. Suppose the particle is moving under an external force $\mathbf{F}(\mathbf{x})$. Then $\mathbf{x}(t)$ satisfies the second-order differential equation

$$m\frac{d^2\mathbf{x}(t)}{dt^2} = \mathbf{F}(\mathbf{x}(t)) \tag{1}$$

called **Newton's equation** or simply the **equation of motion**.

A **conserved force** is one that can be expressed as the gradient of a scalar function: $\mathbf{F}(\mathbf{x}) = -\nabla V(\mathbf{x})$ (the negative sign is present simply in order to use the physically-realized force $\mathbf{F}$ and scalar potential V – mathematically it could be absorbed into V, and we'd recover the definition of a conservative vector field). An example of a non-conserved force is friction: $F = -\eta\frac{dx}{dt}$.For a conserved force, the following scalar quantity is also conserved:

$$E = \frac{m}{2}\left(\frac{d\mathbf{x}}{\mathbf{t}}\right)^2 + V(\mathbf{x}) \tag{2}$$

In order to see this fact, we simply take the derivative of (2) with respect to time and use the equation of motion (1):

$$\frac{dE}{dt} = \sum_{k=1,2,3}\left[m\frac{dx_k}{dt}\frac{d^2x_k}{dt^2} + \frac{\partial V}{\partial x_k}\frac{dx_k}{dt}\right] = \sum_k\left(m\frac{d^2x_k}{dt^2} + \frac{\partial V}{\partial x_k}\right)\frac{dx_k}{dt} = 0 \tag{3}$$

where the last equality comes from (1). Of course, we can now *define* the quantity E as the (mechanical) energy.

2.2 Lagrangian Formalism

As students of physics, we already know of the many difficulties working in the Newtonian formalism: vectors are difficult to work with (especially in a non-orthogonal coordinate system), second-order ODEs are not ideal if we can solve the problem with a first-order ODE, constraints are difficult to systematically take into account, etc. Perhaps the only convincing we need that we must search for a formalism beyond the

Newtonian scheme is that quantum physics can't be directly derived from Newtonian mechanics. Thus, here we introduce the Lagrangian and Hamiltonian formalisms, starting with the former.

Consider a system whose state[1] is described by N paramters $\{q_i\}_{i=1}^N$ in some space (really, manifold) M. M is referred to as the **configuration space** of the **generalized coordinates** $\{q_i\}$.

Suppose a particle has a trajectory described by $q(t)$, $t \in [t_i, t_f]$ with $q(t_i) = q_i$ and $q(t_f) = t_f$. Then we can consider the functional

$$S[q(t), \dot{q}(t)] = \int_{t_i}^{t_f} L(q, \dot{q})dt \tag{4}$$

which we will define as the **action**. Nakahara makes the odd choice to define S before we've defined the **Lagrangian** L which shows up in the integrand of (4), but following his style, I will simply choose to state that the Lagrangian must be chosen such that **Hamilton's principle** (otherwise known as the **principle of least action**) is satisfied. This principle states that the physically realized trajectory[2] corresponds to an extremum of the action.

Let's see if we can get any mathematics to come from Hamilton's principle. Let $q(t)$ be a path that realizes the extremum of S (this is, therefore, the physically-realized path). Consider now a variation $\delta q(t)$ of this trajectory such that $\delta q(t_i) = \delta q(t_f) = 0$ (i.e., q_i and q_f do not change). The reason for imposing this condition will become clear later. The action therefore changes under this variation by:

$$\begin{aligned}\delta S &= \int_{t_i}^{t_f} L(q + \delta q, \dot{q} + \delta \dot{q})dt - \int_{t_i}^{t_f} L(q, \dot{q}) \\ &= \int_{t_i}^{tf} \delta L \\ &= \int_{t_i}^{t_f} \Big(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q}\Big)dt \end{aligned} \tag{5}$$

Anticipating the result we wish to obtain, we will now use integration by parts on the second term in (5):

$$\int_{t_i}^{t_f} \frac{\partial L}{\partial \dot{q}}\delta \dot{q}dt = \delta q \frac{\partial L}{\partial \dot{q}}\bigg|_{t_i}^{t_f} - \int_{t_i}^{t_f} \delta q \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}dt = -\int_{t_i}^{t_f} \delta q \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}dt \tag{6}$$

We therefore see the reasoning behind that nebulous demand that $\delta q(t_i) = \delta q(t_f) = 0$: it is what gives the second equality in (6) so that we can plug this into (5) and recover:

$$\delta S = \int_{t_i}^{t_f} \Big(\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\Big)\delta q dt \tag{7}$$

If you've never done this calculation, you may be wondering why equation (7) is so special. Here's the kicker: $q(t)$ realizes an extremum of S, so (7) must vanish. We therefore have derived the all-important **Euler-Lagrange equation**:

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0 \tag{8}$$

which can be generalized to N degrees of freedom indexed by k in the obvious way:

$$\frac{\partial L}{\partial q_k} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_k} = 0 \tag{9}$$

[1] The term *state* here is not well-defined. More often than not, generalized coordinates describe position in some way (whether that's linear displacement x, angular displacement θ, or otherwise). The precise definition here is not as important as recognizing that generalized coordinates allow us to very easily and systematically eliminate the use of Cartesian coordinates (which can be inconvenient in certain contexts).

[2] It is worthwile mentioning that the action S can in fact be defined for *any* trajectory, and this fact becomes relevant later.

A physicist may be inclined to write that $\frac{\delta S}{\delta q}$ is equivalent to the Euler-Lagrange equations. Indeed this is correct to some degree, but in order to make this notion rigorous, we employ the **functional derivative**. It is defined via

$$\frac{\delta f(t_2)}{\delta f(t_1)} = \delta(t_1 - t_2) \tag{10}$$

For our purposes, we have

$$\frac{\delta S[q,\dot{q}]}{\delta q(s)} \stackrel{\text{def}}{=} \lim_{\varepsilon\to 0} \frac{S[q(t)+\varepsilon\delta(t-s), \dot{q}(t)+\varepsilon\frac{d}{dt}\delta(t-s)] - S[q(t),\dot{q}(t)]}{\varepsilon} \tag{11}$$

where

$$\begin{aligned}
S[q(t)+\varepsilon\delta(t-s), \dot{q}(t)+\varepsilon\frac{d}{dt}\delta(t-s)] &= \int dt L\Big(q(t)+\varepsilon\delta(t-s), \dot{q}+\varepsilon\frac{d}{dt}\delta(t-s)\Big) \\
&= \int dt L(q,\dot{q}) + \varepsilon\int dt\Big(\frac{\partial L}{\partial q}\delta(t-s) + \frac{\partial L}{\partial \dot{q}}\frac{d}{dt}\delta(t-s)\Big) + \mathcal{O}(\varepsilon^2) \\
&= S[q,\dot{q}] + \varepsilon\Big(\frac{\partial L}{\partial q}(s) - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}(s)\Big) + \mathcal{O}(\varepsilon^2)
\end{aligned} \tag{12}$$

Thus we indeed see that the Euler-Lagrange equation may be written as

$$\frac{\delta S}{\delta q(s)} = \frac{\partial L}{\partial q}(s) - \frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}}\Big)(s) = 0 \tag{13}$$

Define the **conjugate momentum** as $\frac{\partial L}{\partial \dot{q}}$. A coordinate q_k of which the Lagrangian is independent is called **cyclic**. The conjugate momentum to a cyclic coordinate is conserved. That is, if q_k is cyclic, then

$$\frac{dp_k}{dt} = \frac{\partial L}{\partial q_k} = 0 \tag{14}$$

One last quick remark before we move onto Hamiltonians: If $Q(q)$ is an arbitrary function of q, then the Lagrangians L and $L + dQ/dt$ yield the same Euler-Lagrange equation. I don't show this here, but Nakahara makes this very explicitly clear.

2.3 Hamiltonian Formalism

The Hamiltonian formalism discussed in this section offers several advantages over the Lagrangian formalism, most of which will be apparent later. Suffice to say that anyone with an elementary understanding of quantum mechanics understands the importance of the Hamiltonian.

Suppose a Lagrangian L is given. Then the **Hamiltonian** (as a function of momentum p and coordinate q) is defined by the Legendre transform:

$$H(q,p) \stackrel{\text{def}}{=} \sum_k p_k\dot{q}_k - L(q,\dot{q}) \tag{15}$$

Formally, note that we must require that the Jacobian satisfies

$$\det\Big(\frac{\partial p_i}{\partial \dot{q}_j}\Big) \neq 0 \tag{16}$$

Just as before with Hamilton's principle, we will consider an infinitesimal change (this time both in q_k and p_k) in order to obtain some useful differential equations. In this case (excluding terms second-order in infinitesimal changes):

$$\begin{aligned}
H(q+\delta q, p+\delta p) - H(q,p) &= \sum_k \big(\dot{q}_k\dot{p}_k + \dot{q}_k\delta p_k + \delta\dot{q}_k p_k\big) + L(q,\dot{q}) - L(q+\delta q, \dot{q}+\delta\dot{q}) \\
&= \sum_k \Big(\dot{q}_k\delta p_k + \delta\dot{q}_k p_k - \frac{\partial L}{\partial q_k}\delta q_k - \frac{\partial L}{\partial \dot{q}_k}\delta\dot{q}_k\Big)
\end{aligned}$$

We could then go through the rigorous functional derivative calculations of (11)-(12) in order to show that

$$\frac{\partial H}{\partial p_k} = \dot{q}_k \tag{17}$$

$$\frac{\partial H}{\partial q_k} = -\frac{\partial L}{\partial q_k} = -\dot{p}_k \tag{18}$$

which are **Hamilton's equations of motion**.

Note that we define the space with coordinates (q_k, p_k) as the **phase space**. Let $A(q,p)$ and $B(q,p)$ be two functions defined on the phase space of a Hamiltonian H. Then the Poisson bracket[3] is defined by

$$[A,B] \stackrel{\text{def}}{=} \sum_k \Big(\frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial q_k}\Big) \tag{19}$$

The Poisson bracket is a **Lie bracket**, meaning it satisfies linearity, skew-symmetry, and the **Jacobi identity**:

$$[[A,B],C] + [[B,C],A] + [[C,A],B] = 0 \tag{20}$$

as a general note: don't memorize this! Each term here is just one of the three cyclic permutations of $\{A, B, C\}$.

Clearly, the fundamental Poisson brackets are

$$[p_i, p_j] = [q_i, q_j] = 0 \tag{21}$$
$$[q_i, p_j] = \delta_{ij} \tag{22}$$

since in phase space, q and p are independent coordinates.

Let $A(q,p)$ be a physical quantity. Then its time derivative is given by

$$\begin{aligned}\frac{dA}{dt} &= \sum_k \Big(\frac{dA}{dq_k}\frac{dq_k}{dt} + \frac{dA}{dp_k}\frac{dp_k}{dt}\Big) \\ &= \sum_k \Big(\frac{dA}{dq_k}\frac{\partial H}{\partial p_k} - \frac{dA}{dp_k}\frac{\partial H}{\partial q_k}\Big) \\ &= [A, H]\end{aligned} \tag{23}$$

That is to say, **if** $[A,H] = 0$, **then** A **is conserved**.

Theorem 1 (Noether's Theorem)**.** *Let $H(q_k, p_k)$ be a Hamiltonian that is invariant under the infinitesimal coordinate transformation $q_k \to q'_k = q_k + \varepsilon f_k(q)$. Then*

$$Q = \sum_k p_k f_k(q) \tag{24}$$

is conserved.

Proof. The Jacobian Λ_{ij} (up to $\mathcal{O}(\varepsilon)$) associated with the $q_k \to q'_k$ is

$$\Lambda_{ij} = \frac{\partial q'_i}{\partial q_j} \simeq \delta_{ij} + \varepsilon\frac{\partial f_i(q)}{\partial q_j} \tag{25}$$

The momentum transforms as

$$p_i \to \sum_j p_j \Lambda^{-1}_{ji} \simeq p_i - \varepsilon \sum_j p_j \frac{\partial f_j}{\partial q_i} \tag{26}$$

[3] I generally prefer to use {} to denote the Poisson bracket since it gets promoted to the commutator [] in quantum mechanics, and I don't like to confuse the two (then again, {} could also be easily confused with the anticommutator which becomes much more important in quantum field theory).

Therefore:

$$\begin{aligned}
0 &= \delta H \\
&= \frac{\partial H}{\partial q_k}\varepsilon f_k(q) - \frac{\partial H}{\partial p_j}\varepsilon p_i \frac{\partial f_i}{\partial q_j} \\
&= \varepsilon\Big[\frac{\partial H}{\partial q_k} f_k(q) - \frac{\partial H}{\partial p_j} p_i \frac{\partial f_i}{\partial q_j}\Big] \\
&= \varepsilon[H, Q] = \varepsilon \frac{dQ}{dt} \qquad (27)
\end{aligned}$$

which shows that Q is conserved. ■

Maybe what we've just done doesn't seem significant, but it is arguably the greatest discovery in mathematical physics. Putting it simply: **conserved quantities leave the Hamiltonian invariant**. What's more is that the conserved quantity Q is the **generator of the transformation** that leaves the Hamiltonian invariant. To see what we mean:

$$\begin{aligned}
[q_i, Q] &= \sum_k \Big[\frac{\partial q_i}{\partial q_k}\frac{\partial Q}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial Q}{\partial q_k}\Big] \\
&= \sum_k \delta_{ik} f_k(q) = f_i(q) \qquad (28)
\end{aligned}$$

In other words, $\delta q_i = \varepsilon f_i(q) = \varepsilon[q_i, Q]$.

Perhaps this is a little too abstract, and you're having trouble visualizing what Q would be in a physical example. Consider a particle m moving in a two-dimensional plane with an axial symmetric potential $V(r)$. The Lagrangian (which, again, is simply defined so far as being the function which allows the action S to satisfy the Euler-Lagrange equations in (9)) is

$$L(r, \theta) = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) - V(r) \qquad (29)$$

and the conjugate momenta are

$$\begin{aligned}
p_r &= m\dot{r} \\
p_\theta &= mr^2\dot{\theta} \qquad (30)
\end{aligned}$$

so the Hamiltonian is

$$H = p_r\dot{r} + p_\theta\dot{\theta} - L = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + V(r) \qquad (31)$$

Because H is independent of θ, it is invariant under the (infinitesimal) transformation

$$\theta \to \theta + \varepsilon \cdot 1 \qquad (32)$$

which leaves p_θ invariant. Notice that $f(\theta) = 1$ in this case, so by Noether's Theorem, the quantity

$$Q = p_\theta \cdot 1 = mr^2\dot{\theta} \qquad (33)$$

is conserved. Indeed, this quantity is the angular momentum.