Derivation of generalized Schrödinger equation

Classically any single particle system can be describe through the use of the Lagrangian formalism. The Lagrangian can be written as

$$\mathcal{L}(t, x(t), \dot{x}(t)) = \frac{1}{2}m\dot{x}^2 - V(x) \tag{1}$$

with $(x, \dot{x})$ a pair of generalized coordinates and $V(x)$ a generic potential.

By applying the calculus of variations to minimize the action, we derive the Euler-Lagrange equations, which govern the dynamics of the system:

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} \tag{2}$$

These equations provide the equations of motion for the system in terms of the generalized coordinates.

By applying the Euler-Lagrange equations to the generic Lagrangian form used in Eq.(1) we get

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{dp}{dt} \tag{3}$$

where the generalized momentum is defined as $p = m\dot{x}$.

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{dp}{dt} \tag{4}$$

We can use the generalized momentum to rewrite the Lagrangian in function fo a new set of generalized coordinates (x, p) finding

$$\mathcal{L}(t, x(t), p(t)) = \frac{1}{2m}p^2 - V(x) \tag{5}$$

By differentiating the Lagrangian with respect to the generalized momentum, we obtain the Hamiltonian formulation of mechanics.

$$\frac{\partial \mathcal{L}}{\partial p} = \frac{p}{m} = \frac{dx}{dt} \tag{6}$$

By looking at Eq.(3) and (6), we see a correspondence between variations in x and p: at fixed time a change in the Lagrangian with respect to position corresponds to (generate) a change in momentum over time and a change in the Lagrangian with respect to momentum in the momentum corresponds to (generate) a change in position over time. By analogy with quantum mechanics, we define the momentum p as the generator of translations in space and x as the generator of momentum evolution.

This can be further generalized by looking at a change of the Lagrangian with respect to time

$$\begin{aligned}\frac{d\mathcal{L}(t,x(t),\dot{x}(t))}{dt} &= \frac{\partial\mathcal{L}}{\partial t} + \frac{\partial x}{\partial t}\frac{\partial\mathcal{L}}{\partial x} + \frac{\partial\dot{x}}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{x}} \\ &= \frac{\partial\mathcal{L}}{\partial t} + \dot{x}\frac{d}{dt}(\frac{\partial\mathcal{L}}{\partial\dot{x}}) + \frac{\partial\dot{x}}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{x}} \\ &= \frac{\partial\mathcal{L}}{\partial t} + \frac{d}{dt}(\frac{\partial\mathcal{L}}{\partial\dot{x}}\dot{x})\end{aligned} \tag{7}$$

where in the second line we have used the Euler-Lagrange equation. We notice that

$$\mathcal{L} - \frac{\partial\mathcal{L}}{\partial\dot{x}}\dot{x} = -(\frac{1}{2}m\dot{x}^2 + V(x)) = E$$

with E the energy.

Finally we can rewrite Eq.(7) as

$$\frac{\partial\mathcal{L}}{\partial t} = -\frac{dE}{dt} \tag{8}$$

Hence, in analogy what previously done we say that the energy E is the generator of time evolution.

We will now use this finding to derive the Schrödinger equation in quantum mechanics.

Given a time dependent state $|\psi(t)\rangle$ we define the time evolution operator $\hat{U}(t)$ as

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle \tag{9}$$

There are two physical constraints that we need to impose upon the time evolution operator $\hat{U}$

1. Probability is conserved through time
2. Time evolution is reversible

The first constraint implies that the evolution operator needs to be unitary $\hat{U}^\dagger U = \mathbb{1}$.

To derive the form of $\hat{U}(t)$ we start by studying a small time variation dt. In this case, we can develop $\hat{U}(t)$ in series up to first order an Eq.() takes the form

$$|\psi(dt)\rangle = (\mathbb{1} + \dot{\hat{U}}(0)dt + \mathcal{O}(dt^2))|\psi(0)\rangle \tag{10}$$

with $\mathbb{1}$ the identity operator and $\hat{U}(0)$ the time evolution operator at time $t = 0$.

Rewriting Eq.(10) we get

$$\frac{|\psi(dt)\rangle - |\psi(0)\rangle}{dt} = \frac{d|\psi\rangle}{dt} = \dot{\hat{U}}(0)|\psi\rangle \tag{11}$$

where $\dot{\hat{U}}(t)$ is the time derivative of the evolution operator.

Using the unitary of $\hat{U}$ we get $\dot{\hat{U}}^\dagger(0) = -\dot{\hat{U}}(0)$, which means that the $\dot{\hat{U}}$ operator is anti-hermitian. We define an hermitian operator $\hat{H} = i\dot{\hat{U}}(0)$. Then Eq.(13) can be written as

$$i\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle \tag{12}$$

In analogy with what we have previosuly done in the Lagrangian formalism, we identify $\hat{H}$ as the Hamiltonian of the system and recognize that it is the generator of time evolution.

One final step remains: both sides of Eq. (12) must have the same units. Using dimensional analysis, we can rewrite it as

$$i\hbar\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle \tag{13}$$

where $\hbar$ is the reduced Planck constant.

There are three key points to note about our derivation of the Schrödinger equation:

- The Planck constant h appears as a consequence of dimensional analysis.
- The presence of the imaginary unit i, and thus the inherent complexity of the equation, follows directly from the requirement that time evolution be unitary, Moreover to preserve probability, the time evolution generator must be Hermitian.
- The Hamiltonian $\hat{H}$ rises from the analogy with the generator of time evolution in classical mechanics..