Section 5.5: Schrodinger Equation from a Lagrangian

The quantum theory relies primarily on the Schrodinger wave equation to describe the dynamics of quantum particles. The present section shows one method by which the Lagrangian formulation leads to the Schrodinger wave equation. The companion volume on quantum and solid state shows the beautiful connection with the Feynman path integral. Subsequent sections in the present volume explore the meaning of the Hamiltonian and the Schrodinger wave equation in more detail.

As a mathematical exercise, we start with the Lagrange *density*

$$\mathscr{L} = i\hbar\psi^*\dot{\psi} - \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi - V(r)\,\psi^*\psi \tag{5.5.1a}$$

or equivalently

$$\mathscr{L} = i\hbar\psi^*\dot{\psi} - \frac{\hbar^2}{2m}\sum_j \partial_j\psi^*\partial_j\psi - V(r)\,\psi^*\psi \tag{5.5.1b}$$

where $j = x, y, z$ the Lagrangian is

$$L = \int d^3x\,\mathscr{L} \tag{5.5.1c}$$

The Lagrange density is a functional of the independent coordinates ψ, ψ^* and their derivatives $\partial_j\psi, \partial_j\psi^*$ where $j = x, y, z$.

The variation of L leads to the Euler-Lagrange equations of the form

$$\frac{\partial\mathscr{L}}{\partial\phi} - \sum_a \partial_a \frac{\partial\mathscr{L}}{\partial(\partial_a\phi)} = 0 \tag{5.5.2a}$$

where $a = x, y, z, t$ and $\phi = \psi$ or ψ^*. Setting $\phi = \psi^*$ provides

$$\frac{\partial\mathscr{L}}{\partial\psi^*} - \sum_a \partial_a \frac{\partial\mathscr{L}}{\partial(\partial_a\psi^*)} = 0 \tag{5.5.2b}$$

Evaluating the first term produces

$$\frac{\partial\mathscr{L}}{\partial\psi^*} = \frac{\partial}{\partial\psi^*}\left[i\hbar\psi^*\dot{\psi} - \frac{\hbar^2}{2m}\sum_j \partial_j\psi^*\partial_j\psi - V(r)\,\psi^*\psi\right] = i\hbar\dot{\psi} - V(r)\,\psi$$

The argument of the second term in Equation 5.5.2b produces

$$\frac{\partial\mathscr{L}}{\partial(\partial_a\psi^*)} = \frac{\partial}{\partial(\partial_a\psi^*)}\left\{i\hbar\psi^*\partial_t\psi - \frac{\hbar^2}{2m}\sum_j \partial_j\psi^*\partial_j\psi - V(r)\,\psi^*\psi\right\} = \begin{cases} 0 & a = t \\ -\dfrac{\hbar^2}{2m}\partial_j\psi & a = j \end{cases}$$

Equation 5.5.2b becomes

$$i\hbar\dot{\psi} - V(r)\,\psi + \frac{\hbar^2}{2m}\sum_j \partial_j\partial_j\psi = 0$$

Therefore, we find the Schrodinger wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\,\psi = i\hbar\dot{\psi} \tag{5.5.3}$$

We can find the classical Hamiltonian density (energy per unit volume)

$$\mathscr{H} = \pi\dot{\psi} - \mathscr{L} \tag{5.5.4a}$$

where π is the momentum conjugate to ψ and the total energy is

$$H = \int d^3x \ \mathscr{H} \tag{5.5.4b}$$

The conjugate momentum is defined by

$$\pi = \frac{\partial \mathscr{L}}{\partial \dot{\psi}} \tag{5.5.5}$$

For the Lagrange density in Equation 5.5.1, we find

$$\pi = \frac{\partial \mathscr{L}}{\partial \dot{\psi}} = \frac{\partial}{\partial \dot{\psi}} \left\{ i\hbar \psi * \dot{\psi} - \frac{\hbar^2}{2m} \sum_j \partial_j \psi * \partial_j \psi - V(r) \ \psi * \psi \right\} = i\hbar \psi *$$

The classical Hamiltonian density becomes

$$\mathscr{H} = \pi \dot{\psi} - \mathscr{L} = i\hbar \psi * \dot{\psi} - \left\{ i\hbar \psi * \dot{\psi} - \frac{\hbar^2}{2m} \nabla \psi * \cdot \nabla \psi - V(r) \ \psi * \psi \right\} = \frac{\hbar^2}{2m} \nabla \psi * \cdot \nabla \psi + V(r) \ \psi * \psi$$

Often times the Lagrange density is stated as

$$\mathscr{L} = i\hbar \psi * \dot{\psi} + \frac{\hbar^2}{2m} \psi * \nabla^2 \psi - V(r) \ \psi * \psi = \psi * \left(i\hbar \partial_t + \frac{\hbar^2}{2m} \nabla^2 - V \right) \psi \tag{5.5.6}$$

This last equation comes from Equations 5.5.1 by partially integrating and assuming the surface terms are zero. The Hamiltonian density then has the form

$$\mathscr{H} = \pi \dot{\psi} - \mathscr{L} = \psi * \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi \tag{5.5.7}$$

In terms of the quantum theory, the classical Hamiltonian is most related to the average energy

$$H = \int d^3x \ \psi * \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = \langle \psi | H_{sch} | \psi \rangle \tag{5.5.8a}$$

where

$$H_{sch} = -\frac{\hbar^2}{2m} \nabla^2 + V \tag{5.5.8b}$$