

LAGRANGIAN FOR THE SCHRÖDINGER EQUATION

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References: W. Greiner & J. Reinhardt, *Field Quantization*, Springer-Verlag (1996), Chapter 3, Section 3.1.

As a prelude to 'proper' quantum field theory, we'll look first at turning the non-relativistic quantum theory based on the Schrödinger equation into a field theory. Before we develop a *quantum* field theory of the Schrödinger equation, we'll first look at this equation treating the wave function $\psi(\mathbf{x}, t)$ as a *classical* (that is, non-quantum) field. The Schrödinger equation is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{x}, t) \psi \quad (1)$$

where $V(\mathbf{x}, t)$ is, as usual, the potential function.

In order to apply the techniques of classical field theory, we need a Lagrangian density \mathcal{L} . There doesn't seem to be any way of actually deriving Lagrangian densities; presumably they are found through trial and error, with perhaps a bit of physical intuition. In any case, the Lagrangian density for the Schrödinger equation turns out to be

$$\mathcal{L}(\psi, \nabla \psi, \dot{\psi}) = i\hbar \psi^* \dot{\psi} - \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi - V(\mathbf{x}, t) \psi^* \psi \quad (2)$$

As ψ is a complex function, it has real and imaginary parts, so we can treat ψ and ψ^* as independent fields. As we saw earlier, we can derive the Euler-Lagrange equations for multiple fields from the principle of least action and end up with

$$\frac{\partial \mathcal{L}}{\partial \phi^r} - \frac{\partial}{\partial q^\mu} \left(\frac{\partial \mathcal{L}}{\partial \phi^r_{,\mu}} \right) = 0 \quad (3)$$

where the ϕ^r are the fields and $q^\mu = (\mathbf{x}, t)$. In this case, the two fields are ψ and ψ^* and we get the two equations

$$\frac{\partial \mathcal{L}}{\partial \psi} - \frac{\partial}{\partial x^i} \frac{\partial \mathcal{L}}{\partial \psi_{,i}} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \frac{\partial \mathcal{L}}{\partial \psi} - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla \psi} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = 0 \quad (4)$$

$$\frac{\partial \mathcal{L}}{\partial \psi^*} - \frac{\partial}{\partial x^i} \frac{\partial \mathcal{L}}{\partial \psi^*_{,i}} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} = \frac{\partial \mathcal{L}}{\partial \psi^*} - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla \psi^*} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} = 0 \quad (5)$$

The second term in each row just introduces the gradient sign ∇ as a shorthand for the $\frac{\partial}{\partial x^i} \frac{\partial \mathcal{L}}{\partial \psi_i}$ and $\frac{\partial}{\partial x^i} \frac{\partial \mathcal{L}}{\partial \psi_i^*}$ terms.

We can plug 2 into these two equations to verify that we recover the original Schrödinger equation 1 and its complex conjugate. From 4 we have

$$\frac{\partial \mathcal{L}}{\partial \psi} = -V(\mathbf{x}, t) \psi^* \quad (6)$$

$$\nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla \psi} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* \quad (7)$$

$$\frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\hbar \psi^* \quad (8)$$

$$\frac{\partial \mathcal{L}}{\partial \psi} - \nabla \cdot \frac{\partial \mathcal{L}}{\partial \nabla \psi} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = -i\hbar \psi^* + \frac{\hbar^2}{2m} \nabla^2 \psi^* - V(\mathbf{x}, t) \psi^* = 0 \quad (9)$$

$$-i\hbar \psi^* = \frac{\hbar^2}{2m} \nabla^2 \psi^* - V(\mathbf{x}, t) \psi^* \quad (10)$$

which is the complex conjugate of 1. Plugging 2 into 5 just reproduces 1.

The conjugate momentum density π can be calculated for the two fields ψ and ψ^* . We get

$$\pi_1(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\hbar \psi^*(\mathbf{x}, t) \quad (11)$$

$$\pi_2(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} = 0 \quad (12)$$

The Hamiltonian density is defined as

$$\mathcal{H} = \sum_r \pi_r \dot{\phi}^r - \mathcal{L} \quad (13)$$

$$= i\hbar \psi^* \dot{\psi} - \left[i\hbar \psi^* \dot{\psi} - \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi - V(\mathbf{x}, t) \psi^* \psi \right] \quad (14)$$

$$= \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi + V(\mathbf{x}, t) \psi^* \psi \quad (15)$$

The total Hamiltonian is the integral of this over 3-d space:

$$H = \int d^3x \mathcal{H} \quad (16)$$

$$= \int d^3x \left[\frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi + V(\mathbf{x}, t) \psi^* \psi \right] \quad (17)$$

We can integrate the first term by parts, by integrating the $\nabla \psi^*$ term and invoking the usual assumption that $\psi^* \rightarrow 0$ fast enough at infinity that the integrated term is zero. We then get

$$H = \int d^3x \left[-\frac{\hbar^2}{2m} \psi^* \nabla^2 \psi + V(\mathbf{x}, t) \psi^* \psi \right] \quad (18)$$

$$= \int d^3x \psi^* \left[-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{x}, t) \psi \right] \quad (19)$$

Referring back to quantum mechanics for a moment, we see that this last integral is just $\langle \psi | \hat{H} | \psi \rangle$, that is, the expectation value of the Hamiltonian operator, which is the total energy of the system.

Finally, we can write down the Poisson brackets, since these are general results for any field ψ and its conjugate momentum π :

$$\{ \psi(\mathbf{x}, t), \pi(\mathbf{x}', t) \}_{PB} = \delta^3(\mathbf{x} - \mathbf{x}') \quad (20)$$

$$\{ \phi(\mathbf{x}, t), \phi(\mathbf{x}', t) \}_{PB} = 0 \quad (21)$$

$$\{ \pi(\mathbf{x}, t), \pi(\mathbf{x}', t) \}_{PB} = 0 \quad (22)$$

These brackets will be used later when we quantize the theory.

PINGBACKS

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