



Quantum Field Theory
M.Sc. 4th Semester
MPHYEC-1: Advanced Quantum Mechanics
Unit III (Part 4)
Topic: Quantization of Schrodinger Equation

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Quantization of Schrödinger Equation

The name Schrodinger field is used for a field $\Psi(r, t)$ satisfying the Schrodinger equation.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \quad \dots (1)$$

Eqn. (1) is quantized equation of motion of particle of mass m moving in a potential V . Here $\Psi(r, t)$ is thought of as a classical field, which can be quantized by converting it into an operator. Since it is the second time the equation being quantized, it is referred to as second quantization.

The Lagrangian density \mathcal{L} taken in the form:

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

reduces to classical field equation,

$$\frac{\partial \mathcal{L}}{\partial \Psi} - \sum_{x,y,z} \frac{\partial}{\partial x} \left(\frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \Psi}{\partial x} \right)} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\Psi}} \right) \quad \dots (3)$$

to the familiar Schrodinger equation, eq. (1) Ψ & Ψ^* in Eqn. (2) can be considered as independent fields giving the Lagrange's equation of motion. The variation with respect to Ψ^* in Eqn. (3) directly gives Eqn. (1) while variation with respect to Ψ gives the complex conjugate of Eqn. (1):

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V\Psi^* \quad \dots (4)$$

the momentum canonically conjugate to Ψ is:

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} = i\hbar \Psi^* \quad \dots (5)$$

where, we have used the expression for \mathcal{L} given in Eqn. (2). Using Eqn. (2) and Eqn. (5) the Hamiltonian density H now becomes

$$\begin{aligned} H &= \pi \dot{\Psi} - \mathcal{L} \\ &= \frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + V(r, t) \Psi^* \Psi \quad \dots (6a) \end{aligned}$$

$$= -\frac{i\hbar}{2m} \nabla \pi \cdot \nabla \Psi - \frac{i}{\hbar} V \pi \Psi \quad \dots (6b)$$

Using Eqn. (6a) the Hamiltonian H is given by

$$H = \int_V \left(\frac{\hbar^2}{2m} \nabla \Psi^* \cdot \nabla \Psi + V(r, t) \Psi^* \Psi \right) d^3r \quad \dots (7)$$

The classical field equation in Hamiltonian form are given by

$$\dot{\Psi} = \frac{\partial H}{\partial \pi} \quad \text{and} \quad \dot{\pi} = -\frac{\partial H}{\partial \Psi}$$

It follows from the discussion of functional derivatives,

$$\dot{\Psi} = \frac{\partial X}{\partial \pi} = \frac{\partial H}{\partial \pi} - \nabla \cdot \frac{\partial H}{\partial (\nabla \pi)} = \frac{\partial H}{\partial \pi} \quad \dots (8)$$

$$\dot{\pi} = \frac{\partial H}{\partial \psi} = - \left(\frac{\partial H}{\partial \psi} - \nabla \cdot \frac{\partial H}{\partial (\nabla \psi)} \right) = - \frac{\partial H}{\partial \psi} \quad \dots (9)$$

These equations can be expressed in the familiar form by substituting the value of H from Eqn. (6b). Now,

$$\dot{\Psi} = -\frac{i}{\hbar} V\Psi + \frac{i\hbar}{2m} \nabla^2 \Psi$$

Multiplying by $i\hbar$,

$$i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \quad \dots (10)$$

Replacement of H in Eqn. (9) gives

$$\dot{\pi} = \frac{i}{\hbar} V\pi - \frac{i\hbar}{2m} \nabla^2 \pi$$

Since $\pi = i\hbar\Psi^*$ (Eqn. 5), this eqn. becomes

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V\Psi^* \quad \dots (11)$$

Eqns. (10) & (11) are the familiar classical equation and its complex conjugate for the Schrodinger field. This validates the expression for Lagrangian density, Eqn. (2) and the Hamiltonian density derived from it, Eqn. (6).

Since Ψ is now an operator, Ψ^* is to be interpreted as the Hermitian adjoint of Ψ rather than its complex conjugate and is usually denoted by Ψ^\dagger .

Now, H is Hermitian and the quantized HAMILTONIAN is the operator that represents the total energy of the field. The quantum condition reduces to

$$[\Psi(r, t), \Psi^\dagger(r', t)] = \delta(r - r') \quad \dots (12)$$

Assignment

1. Describe the process of Quantisation of field and Schrödinger Equation.
2. Derive the commutation relation satisfied by complex scalar field.
3. Derive the commutation relation satisfied by Hamiltonian.
4. Describe the Poisson bracket formulation of Field variables.

Reference:

1. An Introduction to Quantum Field Theory by Mrinal Dasgupta
2. QUANTUM FIELD THEORY A Modern Introduction by Michio Kaku
3. First Book of Quantum Field Theory by Amitabha Lahiri & P. B. Pal
4. Quantum mechanics by G.S. Chaddha