A path of Quantum Mechanics from classical mechanics: An elegant way of introducing Quantum Mechanics

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ABSTRACT

The classical Newtonian equation will be written in terms of the Lagrangian equations of motion and the Hamilton Function H will be defined in terms of momenta and velocity in the generalised coordinate and the Lagrangian L. It will be seen that Hamilton's function represents the total of kinetic and potential energy, T + V, for a conservative system. Hamilton's function will then be written in the form of the Hamiltonian operator by using the appropriate postulate of Schrödinger to arrive at the Schrödinger Wave Equation and thus the path to Quantum Mechanics from classical mechanics will be traced.

1. Introduction

One popular way of introducing Quantum Mechanics to the readers of the subject is to start with the experiment of Lummer and Pringsheim [1] (1899) with black body (cavity) radiation and Planck's formulation [2] of his epoch-making equation for the interpretation of the entire spectral range of the curve in the year 1900. The subsequent development is very fascinating [3,4]. Planck's brilliant idea was extended by Einstein to explain the photoelectric effect [5], Einstein's equation for variation of heat capacity of solids at low temperature [6] which indicated a breakdown of classical equipartition theorem, Bohr's theory of hydrogen spectra [7], the Compton effect [8], the de Broglie hypothesis for wave particle duality [9], Heisenberg's uncertainty principle [10], Niels Bohr's Gadenken [11] (Thought) Experiment providing justification for the Heisenberg's uncertainty principle and finally developing the wave equation for the de Broglie matter wave emerging to the Schrödinger Wave Equation [12] and ultimately led to the Schrödinger Wave Mechanics [12].

An alternative elegant way of introducing the subject is to start with classical Newtonian equations of motion. This methodology is developed in the following section [12,13].

2. Methodology

Since mechanics is the science which deals with motion and Quantum Mechanics deals with motion of atomic and subatomic particles with much lower mass and very high velocity compared to that of a heavier body and lower velocity whose motion is dealt in classical mechanics, it is an elegant way to start from the Newtonian classical equations of motion to trace the path to Quantum Mechanics from Classical Mechanics.

Newton's equation of motion for the i^{th} component of a body in the X-direction may be represented as

$$F_{x_i} = m_i \ddot{x}_i \tag{1}$$

Where, $\dot{x}_i = \frac{dx_i}{dt}$ and $\ddot{x}_i = \frac{d}{dt}\frac{dx_i}{dt}$

With similar expressions for Fy_i and Fz_i

Again, from definition

$$F_{x_i} = -\frac{\partial V}{\partial x_i} \tag{2}$$

Where V is the potential energy, with similar expressions for Fy_i and Fz_i

So, equating (1) and (2), one can write

$$m_i \ddot{x}_i + \frac{\partial V}{\partial x_i} = 0 \tag{3}$$

With i = 1, 2, 3, ... for a body with n particles.

Now, the total kinetic energy T is expressed as

$$T = \frac{1}{2}\sum_{i=1}^{n} m_i (\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2)$$

Then, the partial derivative

$$\frac{\partial T}{\partial \dot{x}_i} = m_i \dot{x}_i \text{ and } \frac{d}{dt}\frac{\partial T}{\partial \dot{x}_i} = m_i \ddot{x}_i \tag{4}$$

From equations (3) and (4)

$$\frac{d}{dt}\frac{\partial T}{\partial \dot{x}_i} + \frac{\partial V}{\partial x_i} = 0 \tag{5}$$

With similar expressions for the Y and Z directions. Equation (5) is Newton's equation of motion. Equation (5) contains two functions T and V. At this stage, Lagrange introduced a function L, given by

$$L = T - V \tag{6}$$

Then equation (5) may be written as

$$\frac{d}{dt}\frac{\partial (L+V)}{\partial \dot{x}_i} + \frac{\partial (T-L)}{\partial x_i} = 0 \tag{7}$$

Since, T and V are independent of x_i and $\dot{x}_i$ respectively

One can write equation (7) as

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} - \frac{dL}{\partial x_i} = 0 \tag{8}$$

With similar expressions for Y and Z directions. Equation (8) is the Lagrangian equation of Motion. The advantage of this form of equation is this that the equation is invariant under any coordinate transformation. So, in the generalized coordinate system, one can express the Lagrangian's equation in the form

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

With $j = 1, 2, \ldots\ldots, 3n$

Since $q_j = f(x_i, y_i, z_i)$

In equation (9), $\dot{q}_j$ is the generalized velocity and $\frac{\partial L}{\partial q_j}$ is the generalized force.

The generalized momenta is given by

$$p_j = \frac{\partial L}{\partial \dot{q}_j}$$

Then equation (9) yields

$$\dot{p}_j = \frac{\partial L}{\partial q_j}$$

Lagranje's equation is a second order differential equation which is converted to a coupled first order differential equation as shown below. It is seen that

$$L = f(q_j, \dot{q}_j) \tag{10}$$

$$dL = \Sigma_j \left(\frac{\partial L}{\partial q_j} dq_j + \frac{\partial L}{\partial \dot{q}_j} d\dot{q}_j\right)$$

$$= \Sigma_j (\dot{p}_j dq_j + p_j d\dot{q}_j) \tag{11}$$

Now, if one considers the differential of $\Sigma_j p_j \dot{q}_j$ which has the dimension of energy as dL, then

$$d\Sigma_j p_j \dot{q}_j = \Sigma_j (\dot{q}_j dp_j + p_j d\dot{q}_j) \tag{12}$$

Subtracting equation (11) from equation (12)

$$d(\Sigma_j p_j \dot{q}_j - L) = \Sigma_j (\dot{q}_j dp_j + \dot{p}_j dq_j) \tag{13}$$

At this stage, a very important substitution is made:

$$(\Sigma_j p_j \dot{q}_j - L) = H \tag{14}$$

Where H is Hamilton's function.

Then equation (13) yields

$$dH = \Sigma_j (\dot{q}_j dp_j + \dot{p}_j dq_j)$$

Thus

$$\frac{\partial H}{\partial p_j} = \dot{q}_j \text{ and } \frac{\partial H}{\partial q_j} = -\dot{p}_j \tag{15}$$

Equations (15), a coupled first order differential equation, known as, Hamilton's equation of Motion now replaces Lagrange's equations of motion.

The definition of H as given in equation (14) has got two very important consequences:

(i)

$$\frac{dH}{dt} = \frac{d}{dt}(\Sigma_j p_j \dot{q} - L)$$

$$= \Sigma\left(p_j \ddot{q}_j + \dot{p}_j \dot{q}_j - \frac{\partial L}{\partial q_j}\frac{dq_j}{dt} - \frac{\partial L}{\partial \dot{q}_j}\frac{d\dot{q}_j}{dt}\right)$$

$$= \Sigma(p_j \ddot{q}_j + \dot{p}_j \dot{q}_j - \dot{p}_j \dot{q}_j - p_j \ddot{q}_j)$$

$$= 0$$

That is H is a constant of motion, since it does not change with time

(ii)

$$\Sigma_j p_j \dot{q}_j = \Sigma \frac{\partial L}{\partial \dot{q}_j} \dot{q}_j = \Sigma \frac{\partial T}{\partial \dot{q}_j} \dot{q}_j \tag{16}$$

By definition, kinetic energy, T, is a quadratic function of velocity and T is given by

$$T = \Sigma_{ij} a_{ij} \dot{q}_i \dot{q}_j$$

$$\frac{\partial T}{\partial \dot{q}_j} = 2\Sigma_i a_{ij} \dot{q}_i \tag{17}$$

(Since j contains one value j = i)

From equations (16) and (17)

$$\Sigma_j p_j \dot{q}_j = 2\Sigma_{ij} a_{ij} \dot{q}_i \dot{q}_j = 2T$$

Therefore,

$$H = (\Sigma_j p_j \dot{q}_j - L) = 2T - L$$

$$= T + T - L = T + V \tag{18}$$

Thus, Hamilton's function H represents the total energy.

Now, it is convenient to apply Schrödinger's appropriate postulates [14] for the foundation of wave mechanical form of quantum mechanics.

If Ψ be a mathematical function representing the state of a particle, then Ψ would satisfy the operator equation for a conservative system.

$$\hat{H}\Psi(q) = E\Psi(q) \tag{19}$$

Here $\hat{H}$ is the Hamiltonian operator. This is a simple case of time independent Schrödinger equation. In equation (19) E is a constant independent of time and coordinate and is known as eigen value of the Hamiltonian operator $\hat{H}$ and Ψ is known as eigen function.

Now, the following rule is followed

The classical Hamilton's function H or total energy is written in terms of coordinates and momenta (q_j and p_j). The corresponding Quantum Mechanical Operator $\hat{H}$ is obtained by keeping coordinates q_j's unchanged and representing the momenta p_j by

$$\frac{h}{2\pi i} \frac{\partial}{\partial q_j}$$

For example, Hamilton's function for an electron may be given by

$$H = T + V \tag{20}$$

$$T = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} \tag{21}$$

(For simplicity, cartesian coordinate system is used)

From equation (20)

$$H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V$$

Therefore, the Hamiltonian operator

$$\hat{H} = \frac{1}{2m}[-\frac{h^2}{4\pi^2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V] \tag{22}$$

Substituting in equation (19)

$$-\frac{h^2}{8\pi^2 m}\nabla^2\Psi(q) + V\Psi(q) = E\Psi(q)$$

$$\nabla^2\Psi(q) + \frac{8\pi^2 m}{h^2}(E - V)\Psi(q) = 0 \tag{23}$$

This is the Schrödinger wave equation.

Solving for Ψ in equation (23) and evaluating the expectation (average) value of E with the help of Schrödinger postulate is the prime objective of studying Quantum Mechanics.

$$\langle H \rangle = \langle E \rangle = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{24}$$

$$= \frac{\int \Psi^* \hat{H} \Psi \, dv}{\int \Psi^* \Psi \, dv} \tag{25}$$

Schrödinger formulated this wave mechanics in 1926. In 1925, Heisenberg provided the matrix formulation, known as Matrix Mechanics in 1925 and the two together constitute Quantum Mechanics.

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Professor Mukherjee has supervised the Ph.D. work of fifteen students and published about 120 research articles in internationally reputed journals. He completed sixty years of his academic life in 2020 and one Special Issue of the Journal of the Indian Chemical Society, 2021 has been published in his honour.

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