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Derivation of Schrödinger equation from a variational principle

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Abstract: The aim of this research is to derive Schrödinger equation from calculus of variations (variational principle), so we use the methodology of calculus of variations. The variational principle one of great scientific significance as they provide a unified approach to various mathematical and physical problems and yield fundamental exploratory ideas.

Keyword: Schrödinger Equation, Variatinal Principle, Hamiltonian-Jacobi Equation

1. Introduction

The calculus of variations is a field of mathematical analysis that deals with maximizing or minimizing functional, which are mappings from a set of functions to the real numbers. Functional are often expressed as definite integrals involving functions and their derivatives. The interest is in extremal functions that make the functional attain a maximum or minimum value or stationary functions, those where the rate of change of the functional is zero. In quantum mechanics, the Schrödinger equation is a partial differential equation that describes how the quantum state of some physical system changes with time. It was formulated in late 1925, and published in 1926, by the Austrian physicist Schrödinger. In classical mechanics, the equation of motion is Newton's second law, and equivalent formulations are the Euler–Lagrange equations and Hamilton's equations. In all these formulations, they are used to solve for the motion of a mechanical system, and mathematically predict what the system will do at any time beyond the initial settings and configuration of the system. In quantum mechanics, the analogue of Newton's law is Schrödinger's equation for a quantum system, usually atoms, molecules, and subatomic particles; free, bound, or localized. It is not a simple algebraic equation, but (in general) a linear partial differential equation. The differential equation describes the wave function of the system, also called the quantum state or state vector. In this research we deduced Schrödinger equation from varitional principle so we introduce Schrödinger equation, canonical equations and variational problems and the Hamiltonian-Jacobi equation

1.1. 1-Canonical Equations and Variational problems

In several problems of physics and mechanics it is convenient to recast Euler's equations in canonical form, which makes possible a general approach to variational problems. Further, the new variable introduced in the process admit of a simple physical interpretation.

Consider the extremum of the functional

$$I[y_1, y_2, ..., y_n] = \int_{x_1}^{x_2} F(x.y_1, y_2, ..., y_n, y_1', y_2', ..., y_n')dx \quad (1)$$

Where $y_1(x),..., y_n(x)$ satisfy certain boundary conditions at x_1 and x_2. The Euler equations are

$$F_{y_i} - \frac{d}{dx}F_{y_i'} = 0 \quad i = 1.2,...,n \quad (2)$$

Which constitute a system of n ordinary differential equation in $y_1(x),..., y_n(x)$. We introduce

$$p_i = F_{y_i'}(x, y_1, ..., y_1', ..., y_n') \quad i = 1.2,...,n \quad (3)$$

Which together with $y_i(i = 1.2,...,n)$ are called canonical variables for the above functional. The variables y_i and p_i are known as canonically conjugate variables. Then (2) gives

$$\frac{dp_i}{dx} = \frac{\partial F}{\partial y_i} \quad i = 1.2,...,n \tag{4}$$

Now, if the Jacobian

$$\frac{D(F_{y_1'}, F_{y_2'},..., F_{y_n'})}{D(y_1', y_2',..., y_n')} \neq 0,$$

Then the system of equation (3) can be solved as

$$y_i' = \omega_i\left(x, y_1,..., y_n, p_1,..., p_n\right)$$

When these are substituted into (4) ,we get a system of first-order equations as

$$\frac{dy_i}{dx} = \omega_i(x, y_1,..., y_n, p_1,..., p_n), \ \frac{dp_i}{dx} = \frac{\partial F}{\partial y_i} \text{ with } i = 1.2,...,n. \tag{5}$$

Henceforward the parentheses in the second equation of (5) signify that y_i' in F are replaced by ω_i .We now introduce the Hamiltonian function

$$H(x, y_1,..., y_n, p_1,..., p_n) = \sum_{i=1}^{n} \omega_i p_i - F \tag{6}$$

Then the system (6) can be written as

$$\frac{dy_i}{dx} = \frac{\partial H}{\partial p_i}, \ \frac{dp_i}{dx} = -\frac{\partial H}{\partial y_i} \qquad i = 1.2,...,n \tag{7}$$

This system is referred to as the Hamiltonian (canonical) system of Euler's equations and of 2n-ordinary equations in 2n unknown functions $y_i(x)$ and p_i.

1.2. 2-The Hamiltonian-Jacobi Equation

Consider the functional in (1), the Euler equation for this functional admit of solutions involving 2n arbitrary constants. Here specification of two points A and B in the space of variables $x, y_1,.., y_n$ through which an extremal must pass gives precisely 2n equations for determining these constants. Hence in the general case there appears a discrete set of extremals joining these points .Let I_{AB} be the value of the functional on each of these extremal,A being regarded as the initial and B as the terminal point. Let A be fixed while $B(x, y_1, y_2,..., y_n)$ is regarded as a movable point. Then I_{AB} is a function of $(x, y_1, y_2,..., y_n)$ and we write

$$I_{AB} = S(x, y_1, y_2,..., y_n) \tag{8}$$

If B changes its position (6) gives

$$dS = -Hdx + \sum_{i=1}^{n} p_i dy_i$$

Which in turn leads to

$$\frac{\partial S}{\partial x} = -H \quad , \frac{\partial S}{\partial y_i} = p_i \ \ i = 1.2,...,n$$

It then follows that S satisfies the following partial differential equation of first order

$$\frac{\partial S}{\partial x} + H\left(x, y_1, y_2,.., y_n, \frac{\partial S}{\partial y_1},..., \frac{\partial S}{\partial y_n}\right) = 0 \tag{9}$$

Which is known as Hamiltonian –Jacobi equation.

1.3. 3-Schrödinger Equation and Variatinal principle

Now we derive the fundamental equation of quantum mechanics (Schrödinger equation) from a variational principle.

First we define an operator known as the Hamiltonian operator as follows:

$$H \equiv -k\nabla^2 + V(x, y, z) \tag{10}$$

Here $k = h^2/(8\pi^2 m)$, where h and m stand for the Plank's constant the mass of the principle whose motion is considered in a field of potential energy V .We now seek a ware function Ψ

Possibly complex extremize the functional

$$\iiint \Psi^*(H\Psi)dxdydz \tag{11}$$

Subject to the constraint

$$\iiint \Psi^*\Psi dxdydz = 1, \tag{12}$$

Where Ψ^* is the complex conjugate of Ψ .The integration is over a fixed domain of x, y and z , We further assume that the admissible function Ψ and Ψ^* either vanish at corresponding points on opposite boundaries. As a consequence

$$\iiint \Psi^*\nabla^2\Psi dxdydz = -\iiint \nabla\Psi^* \cdot \nabla\Psi dxdydz$$

Introducing Lagrange multiplier λ , we then find the extremum of the functional

$$\iiint Kdxdydz = \iiint \left[k\left(\Psi_x^*\Psi_x + \Psi_y^* + \Psi_z^*\Psi_z\right) + V\Psi^*\Psi - \lambda\Psi^*\Psi\right]dxdydz$$

The Euler equation are

$$\frac{\partial K}{\partial \Psi} - \frac{\partial}{\partial x}\left(\frac{\partial K}{\partial \Psi_x}\right) - \frac{\partial}{\partial y}\left(\frac{\partial K}{\partial \Psi_y}\right) - \frac{\partial}{\partial z}\left(\frac{\partial K}{\partial \Psi_z}\right) = 0,$$

$$\frac{\partial K}{\partial \Psi^*} - \frac{\partial}{\partial x}\left(\frac{\partial K}{\partial \Psi_x^*}\right) - \frac{\partial}{\partial y}\left(\frac{\partial K}{\partial \Psi_y^*}\right) - \frac{\partial}{\partial z}\left(\frac{\partial K}{\partial \Psi_z^*}\right) = 0,$$

Which reduce to

$$-k\nabla^2\Psi + V\Psi = \lambda\Psi \quad (13)$$

This is written as $H\Psi = \lambda\Psi$

If we multiply this by Ψ^* and integrate over the domain of x, y, z, the left side becomes the stationary integral (11) which depend by E .Hence by (12) we have $\lambda = E$, so (13) reduces to Schrödinger equation. It is worth pointing out here that there is an interesting and important connection between Hamiltonian-jacobi equation for classical system and the Schrödinger equation for a quantum mechanical system .In fact ,if we put the wave function $\Psi = e^{(i/h)S}$,where S is the action function of the classical system (8),then the Schrödinger equation reduces to the Hamiltonian –Jacobi equation(9) provided S is much larger than Plank's constant h .Thus in the limit of large values of action and energy ,the surfaces of constant phase for the wave function Ψ reduce to surfaces of constant action S for the corresponding classical system. In this case, wave mechanics reduces to classical mechanics just as wave optics reduces to geometrical optics in the limit of very small wavelength. It may be noted that the Klein-Gordon equation

$$\nabla^2\Psi - \frac{1}{c^2}\frac{\partial^2\Psi}{\partial t^2} - \left(\frac{mc}{h}\right)^2\Psi = 0,$$

(c=velocity of light) representing a possible wave equation for a relativistic particle (though it is not correct for an electron or proton)can be constructed in

$$L = -\frac{h^2}{2m}\left[\nabla\Psi^* \cdot \nabla\Psi - \frac{1}{c^2}\left(\frac{\partial\Psi}{\partial t}\right)^2 + \left[\frac{mc}{h}\right]^2\Psi^*\Psi\right].$$

2. Conclusion

The main result of this research we deduced Schrödinger equation by using variational principle and additional result we deduced Schrödinger equation is reduces to the Hamiltonian –Jacobi equation.

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Biography

Dr. Sami Hajazi Mustafa: received his PhD degree in Differential Geometry from Alneelain University, Sudan in 2007. He was a head of Department of Mathematics in Academy of Engineering Sciences in Sudan. Now he is Assistant Professor of Mathematics, University college of Alqunfudha, Umm Al Qura University, Saudi Arabia.