

NOTE ON THE SCHRÖDINGER EQUATION

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Abstract

A second-order formalism leading to an equation describing the same dynamics as the Schrödinger one is developed under some compatible initial conditions.

It is well-known that the Euler-Lagrange [1] and Hamilton [2] equations are involved in many aspects of theoretical physics. On the one hand, the Schrödinger equation [3]-[4] can be derived from the first-order Lagrangian

$$\Lambda_0 = \frac{i\hbar}{2}(\psi^* \dot{\psi} - \dot{\psi}^* \psi) - \frac{\hbar^2}{2m}(\partial_i \psi^*)(\partial_i \psi) - V\psi^* \psi. \quad (1)$$

On the other hand, the Hamiltonian formulation of the Schrödinger equation was involved in many applications of quantum mechanics [5]-[9].

In this paper we develop a second-order formalism leading to an equation that describes the same dynamics as the Schrödinger one under some compatible initial conditions. In the sequel, we restrict ourselves to the one-particle Schrödinger equation with a time independent potential $V(\mathbf{x})$.

From the canonical approach of (1), one infers the second-class constraints

$$\chi \equiv \pi - \frac{i\hbar}{2}\psi^* \approx 0, \quad \chi^* \equiv \pi^* + \frac{i\hbar}{2}\psi \approx 0, \quad (2)$$

and the canonical Hamiltonian

$$H_0(t) = \int d^3x \left(\frac{\hbar^2}{2m}(\partial_i \psi^*)(\partial_i \psi) + V\psi^* \psi \right). \quad (3)$$

The notations π and π^* signify the canonical momenta conjugated with ψ , respectively ψ^*

$$[\psi(\mathbf{x}, t), \pi(\mathbf{y}, t)] = \delta^3(\mathbf{x} - \mathbf{y}) = [\psi^*(\mathbf{x}, t), \pi^*(\mathbf{y}, t)], \quad (4)$$

where the symbol $[\]$ denotes the Poisson bracket. Thus, the Hamiltonian equations of motion can be written as

$$\dot{F}(\mathbf{x}, t) = [F(\mathbf{x}, t), H_0(t)]^\bullet, \quad (5)$$

where the Dirac bracket [10]-[12] takes the form

$$\begin{aligned} [F_1(\mathbf{x}, t), F_2(\mathbf{y}, t)]^\bullet &= [F_1(\mathbf{x}, t), F_2(\mathbf{y}, t)] - \\ &- \frac{i}{\hbar} \int d^3 z [F_1(\mathbf{x}, t), \chi(\mathbf{z}, t)] [\chi^*(\mathbf{z}, t), F_2(\mathbf{y}, t)] + \\ &+ \frac{i}{\hbar} \int d^3 z [F_1(\mathbf{x}, t), \chi^*(\mathbf{z}, t)] [\chi(\mathbf{z}, t), F_2(\mathbf{y}, t)]. \end{aligned} \quad (6)$$

After eliminating the second-class constraints (the independent co-ordinates of the reduced phase-space are ψ and ψ^*), with the help of (5) we find that the dynamics is governed by the equations of motion

$$\dot{\psi} = \frac{i\hbar}{2m} \partial_i \partial_i \psi - \frac{i}{\hbar} V \psi, \quad \dot{\psi}^* = -\frac{i\hbar}{2m} \partial_i \partial_i \psi^* + \frac{i}{\hbar} V \psi^*, \quad (7)$$

which are nothing but the Schrödinger equations for ψ and ψ^* .

Now, we start with the Hamiltonian

$$\bar{H}_0(t) = \int d^3 x \left(\pi^* + \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi - V \psi \right) \right) \left(\pi - \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi^* - V \psi^* \right) \right) \quad (8)$$

from which we derive the Hamilton equations¹

$$\dot{\psi} = \pi^* + \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi - V \psi \right), \quad (9)$$

$$\dot{\psi}^* = \pi - \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi^* - V \psi^* \right), \quad (10)$$

$$\dot{\pi} = -\frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \left(\pi - \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi^* - V \psi^* \right) \right), \quad (11)$$

$$\dot{\pi}^* = \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \left(\pi^* + \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi - V \psi \right) \right). \quad (12)$$

Regarding the equations (9-12) we choose the initial conditions²

¹It is easy to see that the Hamiltonian (8) describes a non-degenerate system.

²It is obvious that the initial conditions (13-14) imply the relations $\psi^*(\mathbf{x}, t_0) = \psi_0^*(\mathbf{x})$,

$$\pi^*(\mathbf{x}, t_0) = -\frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi_0(\mathbf{x}).$$

$$\psi(\mathbf{x}, t_0) = \psi_0(\mathbf{x}), \quad (13)$$

$$\pi(\mathbf{x}, t_0) = -\frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi_0^*(\mathbf{x}). \quad (14)$$

Substituting (9) in (12) and (10) in (11) we derive the equations

$$\frac{\partial}{\partial t} \left(\pi^* - \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi - V \psi \right) \right) = 0, \quad (15)$$

$$\frac{\partial}{\partial t} \left(\pi + \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i \psi^* - V \psi^* \right) \right) = 0, \quad (16)$$

which lead to

$$\pi^*(\mathbf{x}, t) - \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi(\mathbf{x}, t) = k(\mathbf{x}), \quad (17)$$

$$\pi(\mathbf{x}, t) + \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi^*(\mathbf{x}, t) = k^*(\mathbf{x}), \quad (18)$$

where $k(\mathbf{x})$ and $k^*(\mathbf{x})$ are some functions determined by the initial conditions. Writing down (17-18) for $t = t_0$ and using the initial conditions, we deduce the relations

$$k(\mathbf{x}) = 0 = k^*(\mathbf{x}), \quad (19)$$

such that (17-18) lead to

$$\pi^* = \frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi, \quad \pi = -\frac{i}{2\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi^*. \quad (20)$$

Inserting (20) in (9-10) we arrive at (7). In consequence, we have proved the next result: c_1) $(\psi(\mathbf{x}, t), \psi^*(\mathbf{x}, t), \pi(\mathbf{x}, t), \pi^*(\mathbf{x}, t))$ are solutions of equations (9-12) subject to the initial conditions (13-14) if and only if $(\psi(\mathbf{x}, t), \psi^*(\mathbf{x}, t))$ are solutions of equations (7) subject to the initial conditions (13).

It is easy to show that the Hamiltonian (8) comes from the non-degenerate second-order Lagrangian

$$\bar{\Lambda}_0 = \dot{\psi}^* \dot{\psi} - \frac{i}{2\hbar} \dot{\psi}^* \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi + \frac{i}{2\hbar} \dot{\psi} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi^*, \quad (21)$$

which is different from that used in [13]. At the Lagrangian level the initial conditions (13-14) take the form

$$\psi(\mathbf{x}, t_0) = \psi_0(\mathbf{x}), \quad (22)$$

$$\dot{\psi}(\mathbf{x}, t_0) = \frac{i}{\hbar} \left(\frac{\hbar^2}{2m} \partial_i \partial_i - V \right) \psi_0(\mathbf{x}). \quad (23)$$

Due to the fact that the Lagrangian (21) is non-degenerate the following standard result holds:
 $c_1)$ $(\psi(\mathbf{x},t), \psi^*(\mathbf{x},t))$ are solutions to the Euler-Lagrange equations $\delta\bar{\Lambda}_0/\delta\psi = 0$, $\delta\bar{\Lambda}_0/\delta\psi^* = 0$ subject to the initial conditions (22-23) if and only if $(\psi(\mathbf{x},t), \psi^*(\mathbf{x},t), \pi(\mathbf{x},t), \pi^*(\mathbf{x},t))$ are solutions of equations (9-12) in the presence of the initial conditions (13-14).

Thus, results $c_1)$ and $c_2)$ lead to the following conclusion: *the solutions to the Euler-Lagrange equations $\delta\bar{\Lambda}_0/\delta\psi = 0$, $\delta\bar{\Lambda}_0/\delta\psi^* = 0$ subject to the initial conditions (22-23) coincide with the solutions to the equations (7) corresponding to the initial conditions (13).*

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