Analele Universităţii de Vest din Timişoara
Vol. LVI, 2012
Seria Fizică

NOTE ON THE SCHRÖDINGER EQUATION

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Article Info
Received: 28 December 2011
Accepted: 22 January 2012

Keywords: Lagrangian and Hamiltonian formalisms, Schrödinger equation.

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

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

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

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

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

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

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

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

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

Now, we start with the Hamiltonian

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

from which we derive the Hamilton equations[2]

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

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

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

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

Regarding the equations (9-12) we choose the initial conditions[3]

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

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

[3]It is obvious that the initial conditions (13-14) imply the relations $\psi^*(\mathbf{x},t_0) = \psi_0^*(\mathbf{x})$, $\pi^*(\mathbf{x},t_0) = -\frac{i}{2\hbar}\left(\frac{\hbar^2}{2m}\partial_i\partial_i - V\right)\psi_0(\mathbf{x})$.

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

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

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

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

which lead to

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

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

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

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

such that (17-18) lead to

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

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

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

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

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

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

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

Acknowledgment

The work of M. M. Bârcan was partially supported by the strategic grant POSDRU/88/1.5/S/49516, Project ID 49516 (2009), co-financed by the European Social Fund-Investing in People, within the Sectorial Operational Programme Human Resources Development 2007-2013.

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