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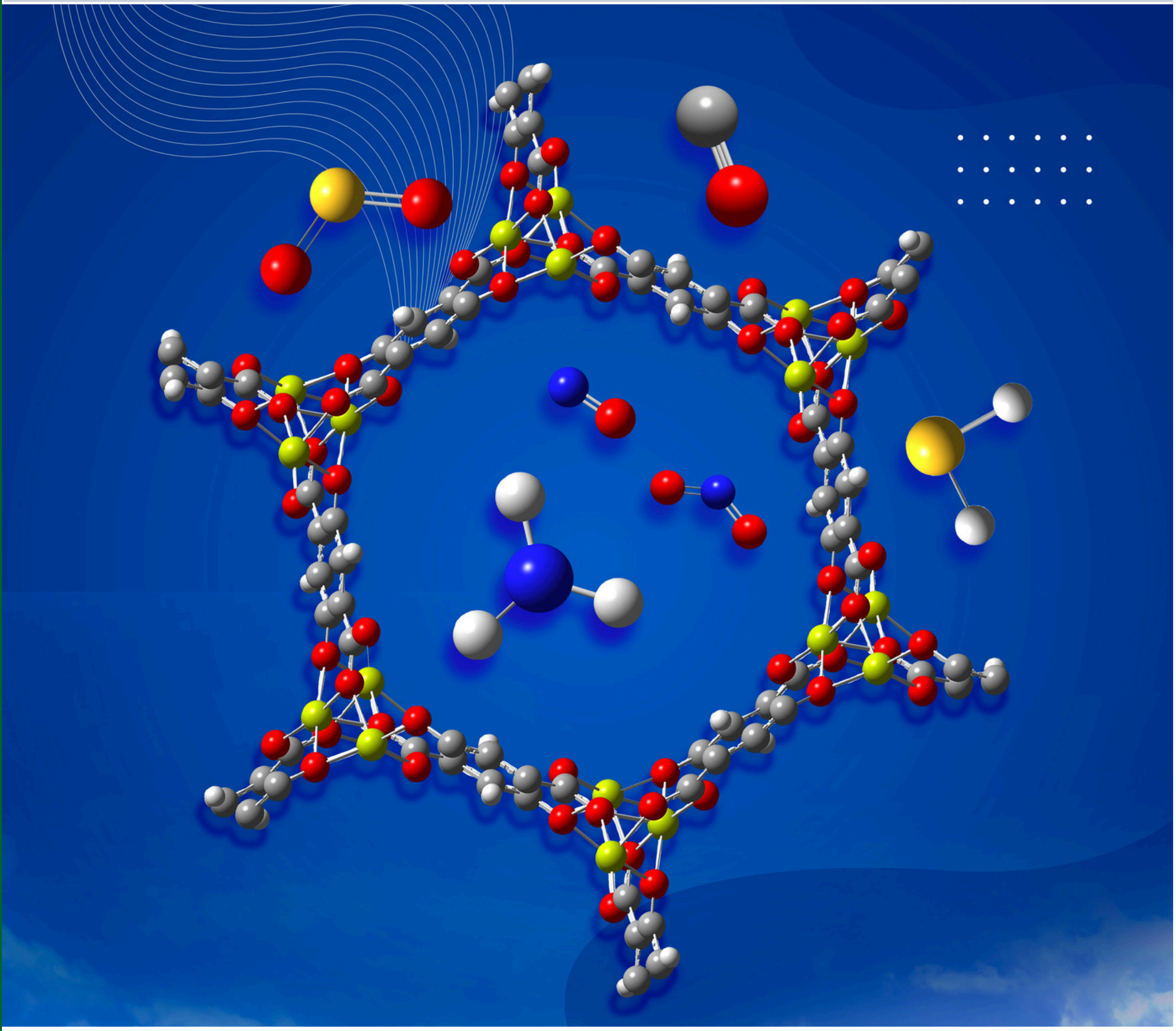

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Chief Editor

Aabiskar Bhusal

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TABLE OF CONTENTS

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Him. Phys. **11** 21-27, (2024)

Himalayan Physics

From the Hamilton-Jacobi equation to the Schrödinger equation and vice versa, without additional terms and approximations

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Abstract: In this article, we will answer a question posed in the book Classical Mechanics by H. Goldstein: "*Is the Hamilton-Jacobi equation the short wavelength limit of the Schrödinger equation*?" But, before that, we will identify an essential element that will take us from the Hamilton-Jacobi equation to the dynamic equation of non-relativistic quantum mechanics for a function Ψ through an exact procedure. This element is the linear independence of the functions Ψ and Ψ^* (their complex conjugate). Their independence is demonstrated for physical systems where the acting physical potential does not explicitly depend on time. Proceeding in reverse, from the Schrödinger equation, we obtain the Hamilton-Jacobi equation, exactly, without additional terms.

Keywords: Hamilton-Jacobi equation • Schrödinger equation • Linear independence of functions • Quantum Hamilton-Jacobi equation

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I. Introduction

The significant contribution of Prof. E. Schrödinger in the form of a differential equation that determines the dynamics of a quantum particle, through a complex function Ψ, based on Prof. L. De Broglie on the wave behavior of what was previously considered "true" microscopic particles (electrons[1], neutrons[2], atoms, and neutral molecules[3]) is known as wavefunction [1–4]. Schrödinger's work, which occurred more

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[1] *Physicists C. Davisson and L. Germer discovered electron diffraction in 1927. Later, in 1928, P.S. Tartakovski and, independently, G. Thomson, also observed such diffraction. In 1949, physicist V. Fabrikant and collaborators observed the diffraction of individual electrons, launched one after another.*

[2] *Diffraction and thermal neutrons were observed using beams generated in a nuclear reactor braked by graphite blocks.*

[3] *In 1929, physicist O. Stern and his collaborators discovered the wave properties of a beam of neutral atoms and molecules, separately.*

or less parallel to Prof. W. Heisenberg's matrix mechanics, identified the ansatz $\Psi(x,t) = exp\{\frac{i}{\hbar}S(x,t)\}$, which would correspond to a wave behavior, which had the action $S(x,t)$, divided by the constant of Planck $\hbar$, in its phase angle. The nonlinear Hamilton-Jacobi equation [3], as it is an equation for action, which in the particular case of a spatial variable x and a variable t, independent of each other, is written as,

$$\frac{\partial S}{\partial t}(x,t) + \frac{1}{2m}\left(\frac{\partial S}{\partial x}(x,t)\right)^2 + U(x) = 0, \tag{1}$$

where $U(x)$ is the potential, m is the mass parameter and $(\partial S/\partial x)^2$ is the nonlinear term, was used by Schrödinger [5] to test the mathematical consistency of his ansatz, leading him to modify this equation so that it is compatible internally [2]. In the case of a spatial variable, the "modified H-J" equation is written as,

$$\frac{1}{2}\left(\left(\frac{\partial S(x,t)}{\partial t}\right)^* + \frac{\partial S(x,t)}{\partial t}\right) + \frac{1}{2m}\left(\frac{\partial S(x,t)}{\partial x}\right)\left(\frac{\partial S(x,t)}{\partial x}\right)^* + U(x) = 0, \tag{2}$$

In [2], using expression (2), the construction of the Schrödinger equation is shown. In reference [3], starting from the Schrödinger equation, we arrive at an equation similar to the Hamilton-Jacobi one, which differs from it by an additional term, which disappears in the limit $\hbar \to 0$. It addresses the same subject [4, 6, 7].

In this article, an element was identified that is absent in the deductions that led from the "modified Hamilton-Jacobi" equation, as in (2), to the Schrödinger equation (for a field Ψ) [2] and from the Schrödinger equation for the "Hamilton-Jacobi (with additional term)" equation [3] which, if it had been included, would allow obtaining the Schrödinger equation, from the same Hamilton-Jacobi equation, and vice versa, without additional term and without approach, through exact procedures. Such a missing element is the linear independence of Ψ and Ψ^*, the complex conjugate of Ψ.

A complementary aspect

When the action is evaluated on a curve $q = x(t)$, it is clear that x and t are no longer independent, and so $S(x,t) \ \to \ S_q(t)$.

From [3], in the case of a spatial coordinate x, we have that its expression (10.12) is written explicitly as follows (here another notation is used),

$$p\mathcal{V}(x,p,t) - \mathcal{H}(x,p,t) = \mathcal{L}(x,t,\mathcal{V}(x,p,t)), \tag{3}$$

where, unlike [3], the independent variable v (written as $\dot{x}_i$ in [3]) it does not appear in the leftmost term, as this must be isolated[4] from its expression (8.2), the same as, in the 1-dimensional case, is written as,

$$p = \frac{\partial}{\partial v}\mathcal{L}(x,v,t), \tag{4}$$

---

[4] *Which is always possible because any standard Lagrangian is a convex function on the variable v.*

Thus, we obtain v from (4) in terms of the other independent variables x, p, t:

$$v = \mathcal{V}(x, p, t) \tag{5}$$

Note that $\mathcal{V}$ acquires a specific expression for each specific Lagrangian. Then, for the total time derivative of the action, in the 1-dimensional version of (10.12), in [3], we write, for a trajectory $q = x(t)$,

$$\frac{d}{dt}S_q(t) = \mathcal{L}\Big(x(t), \mathcal{V}\Big(x(t), p(t), t\Big), t\Big), \tag{6}$$

which in general literature appears written in a simplified way as,

$$\frac{d}{dt}S_q(t) = \mathcal{L}\Big(x(t), \dot{x}(t), t\Big), \tag{7}$$

II. Development

In this section we obtain the Schrödinger equation, for a spatial variable x, from the Hamilton-Jacobi equation, following an exact procedure. Conversely, we obtain the Hamilton-Jacobi equation from the Schrödinger equation, without making any approximations.
The ansatz considered by Schrödinger [2–4, 6, 7] is written as,

$$\Psi(x, t) = exp\Big\{\frac{i}{\hbar}S(x, t)\Big\}, \tag{8}$$

Let us see below a characteristic that the functions Ψ, given above, and Ψ^*, the complex conjugate of Ψ, present.
(i) Are the functions Ψ and Ψ^* linearly dependent?
These functions have two independent variables, x and t, so we should calculate the corresponding generalized Wronskians, as it is known that the values, all null, of these Wronskians constitute a necessary condition for linear dependence of the functions considered [8]. Here, however, it will be enough to calculate one of these Wronskians:

$$W_1 = \begin{vmatrix} \Psi & \Psi^* \\ \partial_t\Psi & \partial_t\Psi^* \end{vmatrix} = \begin{vmatrix} exp\{\frac{i}{\hbar}S(x,t)\} & exp\{-\frac{i}{\hbar}S(x,t)\} \\ \frac{i}{\hbar}(\partial_t S)exp\{\frac{i}{\hbar}S(x,t)\} & -\frac{i}{\hbar}(\partial_t S)exp\{-\frac{i}{\hbar}S(x,t)\} \end{vmatrix}$$

$$\Longrightarrow \quad W_1 = -\frac{2i}{\hbar}\,\partial_t S(x, t). \tag{9}$$

It can be shown that W_1, in (9), admits non-zero values for each physical system in which the acting potential does not explicitly depend on time. In fact, it can be seen from equation (1) that if the potential

U does not present an explicit dependence on time, one can expect a solution of this equation that is of the separable[5] type in its variables x and t, or be, in the form,

$$S(x,t) = a\,t + g(x), \quad a \neq 0, \quad (a = \text{constant}), \tag{10}$$

Note that the separability of S is independent of the dimensionality of the physical system considered. Thus, from (9) and (10), we have that, for the case considered, $W_1 \neq 0$; therefore, the functions Ψ and Ψ^* are linearly independent.

(ii) The calculation of the derivatives of (8), with respect to x and t, separately, is straightforward. It can be seen that the non-linear term in (1), previously multiplied by $exp\{iS(x,t)/\hbar\}$, can be obtained from the second partial spatial derivative of Ψ, multiplied by $\hbar^2/2m$. Thus, we find:

$$\underbrace{\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 exp\left\{\frac{i}{\hbar}S(x,t)\right\}} = \frac{i\hbar}{2m}\left(\frac{\partial^2 S}{\partial x^2}\right)exp\left\{\frac{i}{\hbar}S(x,t)\right\} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(exp\left\{\frac{i}{\hbar}S(x,t)\right\}\right) \tag{11}$$

From Hamilton-Jacobi to Schrödinger

We multiply the Hamilton-Jacobi equation, in (1), by $exp\{iS(x,t)/\hbar\}$. In the resulting expression we substitute (11). Thus, we obtain,

$$exp\left\{\frac{i}{\hbar}S(x,t)\right\}\left(\frac{\partial S}{\partial t}\right) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(exp\left\{\frac{i}{\hbar}S(x,t)\right\}\right) + U(x)\; exp\left\{\frac{i}{\hbar}S(x,t)\right\} +$$

$$+\frac{i\hbar}{2m}\left(\frac{\partial^2 S}{\partial x^2}\right)exp\left\{\frac{i}{\hbar}S(x,t)\right\} = 0. \tag{12}$$

Substituting (8) and the partial derivative of Ψ (with respect to t) into (12), we have,

$$\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} - \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(x)\Psi + \underbrace{\frac{i\hbar}{2m}\left(\frac{\partial^2 S}{\partial x^2}\right)}\Psi = 0, \tag{13}$$

The term in expression that differs from the Schrödinger equation, in the 1-dimensional case is highlighted. In the following subsection , making use of the linear independence of Ψ and Ψ^*, we manage to “eliminate” exactly this term.

---

[5] *The function $g(x)$ is found by solving the equation that results from substituting (10) into (1).*

The consequence of Ψ and Ψ^* being linearly independent

As already mentioned, we can eliminate exactly the term highlighted in (13) to arrive at the same Schrödinger equation. Let's look at this.

Let us multiply (13) by the complex conjugate of Ψ, that is, by Ψ^*. On the other hand, multiply the complex conjugate of the equation in (13) by Ψ. Adding these two equations and arranging the terms we can write,

$$\Psi^*\bigg\{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+U(x)\Psi+\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}\bigg\}+\Psi\bigg\{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+U(x)\Psi^*-\frac{\hbar}{i}\frac{\partial\Psi^*}{\partial t}\bigg\}=0 \tag{14}$$

In the homogeneous expression in (14) we use the fact that Ψ and Ψ^* are linearly independent, so it must be fulfilled that the terms in braces assume null values for any x and t in the domain of $\Psi(x,t)$. So, we have,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+U(x)\Psi+\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}=0 \qquad \& \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+U(x)\Psi^*-\frac{\hbar}{i}\frac{\partial\Psi^*}{\partial t}=0, \tag{15}$$

obtaining, precisely, the Schrödinger equation and its complex conjugate equation.

The reverse procedure: from Schrödinger to Hamilton-Jacobi

Starting from the equations in (15), we multiply each of them, separately, from left to right, by Ψ^* and by Ψ, arriving at (14). In equation (14) the terms can be arranged to obtain the following expressions: "$\Psi^*(\partial\Psi/\partial t)-\Psi(\partial\Psi^*/\partial t)$", "$\Psi^*(\partial^2\Psi/\partial x^2)+\Psi(\partial^2\Psi^*/\partial x^2)$" and "$2U(x)\Psi\Psi^*$"; besides, we add and subtract the term "$(i\hbar/2m)(\partial^2S/\partial x^2)\Psi^*\Psi$", and after rearranging the terms, we have,

$$\Psi^*\bigg\{+\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+U(x)\Psi+\frac{i\hbar}{2m}\left(\frac{\partial^2S}{\partial x^2}\right)\Psi\bigg\}+$$

$$\Psi\bigg\{-\frac{\hbar}{i}\frac{\partial\Psi^*}{\partial t}-\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+U(x)\Psi^*-\frac{i\hbar}{2m}\left(\frac{\partial^2S}{\partial x^2}\right)\Psi^*\bigg\}=0. \tag{16}$$

hence, by the linear independence argument of Ψ and Ψ^*, we have that the terms between braces must be null. Thus, we arrive, separately, at expression (13) and its complex conjugate. Using the expression of the partial time derivative of Ψ, of the second partial spatial derivative of Ψ, and (8), which we substitute into (13), we have,

$$\frac{\hbar}{i}\left(\frac{i}{\hbar}\right)\left(\frac{\partial S}{\partial t}\right)exp\bigg\{\frac{i\hbar}{2m}S(x,t)\bigg\}-\frac{\hbar^2}{2m}\bigg\{-\frac{1}{\hbar^2}\left(\frac{\partial S}{\partial x}\right)^2+\frac{i}{\hbar}\left(\frac{\partial^2S}{\partial x^2}\right)\bigg\}exp\bigg\{\frac{i\hbar}{2m}S(x,t)\bigg\}+$$

$$+U(x)\;exp\bigg\{\frac{i\hbar}{2m}S(x,t)\bigg\}+\frac{i\hbar}{2m}\left(\frac{\partial^2S}{\partial x^2}\right)exp\bigg\{\frac{i\hbar}{2m}S(x,t)\bigg\}=0. \tag{17}$$

and, factoring the exponential term and since the oscillatory factor is not zero, we arrive at the Hamilton-Jacobi equation,

$$\left(\frac{\partial S}{\partial t}\right)+\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2+U(x)=0. \tag{18}$$

through an exact procedure. In [3], where the 3-dimensional case is considered, starting from the Schrödinger equation, we arrive at an equation that is modified in relation to the Hamilton-Jacobi equation, as it includes an additional term given by $i\hbar/2m\nabla^2 S$. This equation is called "quantum Hamilton-Jacobi", which recovers the Hamilton-Jacobi equation only after taking the limit $\hbar\to 0$.

III. Discussion

Based on what was developed here, we know that starting solely from the Schrödinger equation, as in [3, 4, 6] it would not be possible to arrive at the Hamilton-Jacobi equation through an exact procedure (as it would be necessary also to use the complex version conjugate of the Schrödinger equation and the linear independence of the functions Ψ and Ψ^*), but, in [3, 4, 6], we arrive at the so-called "Quantum Hamilton-Jacobi equation" (HJQ), which becomes the same Hamilton-Jacobi equation in the limit $\hbar\to 0$, which eliminates the additional term that appears in the HJQ equation [6]. Thus, the question posed in [3], which says: "*Is the Hamilton-Jacobi equation the short wavelength limit of the Schrödinger equation*?", will have an answer that will depend on the context considered. In this work, which identifies the exact procedure to obtain the Hamilton-Jacobi equation from the Schrödinger equation, and vice versa, the answer would be negative, different from that for the context in which this specific question was originally defined in [3].

IV. Conclusion

In this article, in the case of a 1-dimensional physical system, with spatial coordinate x, in which a potential that does not explicitly depend on time acts, it was possible to make the transition from the Hamilton-Jacobi equation to the Schrödinger equation and, vice versa, through exact procedures. We have seen two cases. We first started with the Schrödinger ansatz $\Psi(x,t)=e^{(i/\hbar)S(x,t)}$, given in (8), we used the Hamilton-Jacobi equation and obtained (13), which would be a "Schrödinger" type equation (with additional term), which, however, later gave way to the same Schrödinger equation, in subsection 2.2, where we made use, in addition to (13), of its conjugate equation complex and the mathematical fact that the functions Ψ and Ψ^* are linearly independent, which was demonstrated in section 2. With this, we obtained both the Schrödinger equation and its conjugated complex equation, in (15). In the second case, seen in subsection 2.3, with the Schrödinger ansatz, given in (8), we simultaneously use the Schrödinger equations and their complex conjugate to obtain an expression that contains the following terms: “$\Psi^*(\partial\Psi/\partial t) - \Psi(\partial\Psi^*/\partial t)$”, “$\Psi^*(\partial^2\Psi/\partial x^2) + \Psi(\partial^2\Psi^*/\partial x^2)$” and “$2U(x)\Psi\Psi^*$”. Subsequently, using the linear independence of the functions Ψ and Ψ^*, we arrive at equation (13), and then, by simple manipulations, we arrive at the Hamilton-Jacobi equation. In both cases the procedures used were exact.

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