International Review of Physics (IREPHY)

Managing Editor:

Santolo Meo
Department of Electrical Engineering
FEDERICO II University
21 Claudio - I80125 Naples, Italy
santolo@unina.it

The ***International Review of Physics (IREPHY)*** is a publication of the **Praise Worthy Prize S.r.l.**.
The Review is published bimonthly, appearing on the last day of February, April, June, August, October, December.

Published and Printed in Italy by **Praise Worthy Prize S.r.l.**, Naples, December 31, 2007.

On the First Schrödinger Paper on Quantum Mechanics

L. Skála[1,2], V. Kapsa[1]

Abstract – *In his first paper on quantum mechanics, Schrödinger made attempt to derive his famous stationary equation from the Hamilton-Jacobi equation of classical mechanics. The ansatz he made in the relation between the classical action and the wave function is analyzed and reformulated in a way consistent with the standard interpretation of quantum mechanics.* ***Copyright © 2007 Praise Worthy Prize S.r.l. - All rights reserved.***

***Keywords**: classical mechanics, quantum mechanics, Hamilton-Jacobi equation, Schrödinger equation*

Nomenclature

H	Hamilton function
q	coordinate
$S(q)$	classical action
E	energy
ψ	wave function
$V(q)$	potential energy
e	elementary charge
m	mass of the electron
x, y, z	coordinates
$\hbar$	Planck konstant
p	momentum
i	imaginary unit
$\hat{\mathbf{p}}$	momentum operator

I. Introduction

In his first paper on quantum mechanics [1] entitled "Quantisierung als Eigenwertproblem", Schrödinger introduced his famous equation and applied it successfully to the hydrogen atom.

The starting point of his discussion was the time independent Hamilton-Jacobi equation:

$$H\left(q,\frac{\partial S}{\partial q}\right)=E \quad (1)$$

He then introduced a new real function ψ by the equation:

$$S=K\ln\psi \quad (2)$$

where K is a positive constant and obtained a new equation for ψ:

$$H\left(q,\frac{K}{\psi}\frac{\partial\psi}{\partial q}\right)=E \quad (3)$$

For the hydrogen atom with the potential energy $V=-e^2/r$ he derived the following equation:

$$\frac{K^2}{2m}\left[\left(\frac{\partial\psi}{\partial x}\right)^2+\left(\frac{\partial\psi}{\partial y}\right)^2+\left(\frac{\partial\psi}{\partial z}\right)^2\right]+(V-E)\psi^2=0 \quad (4)$$

Further, Schrödinger searched for a finite single-valued real function $\psi=\psi(x,y,z)$ with the continuous second derivatives for which the integral of the left hand side of Eq. (4) over the whole space is extremal:

$$\delta J=\delta\iiint\left\{\frac{K^2}{2m}\left[\left(\frac{\partial\psi}{\partial x}\right)^2+\left(\frac{\partial\psi}{\partial y}\right)^2+\left(\frac{\partial\psi}{\partial z}\right)^2\right]+(V-E)\psi^2\right\}dxdydz=0 \quad (5)$$

Performing integration by parts in the last equation he obtained the result:

$$\frac{\delta J}{2}=\int\delta\psi\frac{\partial\psi}{\partial n}dS+-\iiint\delta\psi\left[\frac{K^2}{2m}\Delta+(E-V)\right]\psi\,dxdydz=0 \quad (6)$$

Assuming that the first integral over the fixed surface at infinity equals zero (condition valid for the motion in a finite volume) he derived the equation:

$$-\frac{K^2}{2m}\Delta\psi+V\psi=E\psi \quad (7)$$

Comparing the energy spectrum of the hydrogen atom following from this equation and the Bohr theory Schrödinger obtained $K=\hbar$.

Manuscript received and revised November 2007, accepted December 2007

The resulting equation is known now as the stationary Schrödinger equation. The physical meaning of ψ, namely the probability amplitude, was not known in 1926.

II. Problems

To illustrate problems related to Eq. (2) we consider first the wave function of a free particle in one dimension:

$$\psi = e^{ipx/\hbar}/N \tag{8}$$

where N is a normalization constant. The motion of a free particle is not quantized and classical and quantum mechanics should agree in this case. Equations (2) and (8) lead to:

$$S = K(ipx/\hbar - \ln N) \tag{9}$$

while the definition of the classical action yields:

$$S = \int_{x_0}^{x} p dx' = p(x - x_0) \tag{10}$$

Comparing the x-dependent parts in the last two equations we see that the relation (2) between S and ψ with a real constant K cannot be fulfilled. We can try to obey Eq. (2) by taking the imaginary constant K=-$i\hbar$. Then the x-dependent parts of Eqs. (9) and (10) are equal, however, incorrect sign of the kinetic energy operator in Eq. (7) is obtained. It indicates that relation (2) between S and ψ is not suitable.

One could argue that the two cases described above cannot be compared since the wave function (8) describes a free particle that is not localized in the space while the classical free particle moves along the straight line trajectory. The plane wave function (8) can be replaced by a more general wave function describing a localized wave packet (see also [2]-[8]):

$$\psi = e^{(iS_1 - S_2)/\hbar} \tag{11}$$

where S_1 and S_2 are real functions and the function ψ obeys the normalization condition:

$$\int |\psi|^2 dxdydz = \int e^{-2S_2/\hbar} dxdydz = 1 \tag{12}$$

For the sake of compatibility with [2]-[4] the minus sign in front of the S_2 function is used here. Different roles of S_1 and S_2 in Eq. (11) can be illustrated in the following way. For S_1=0, the wave function ψ is real and the mean momentum is equal zero for the functions obeying the condition $|\psi|^2 = \psi^2 \to 0$ for $x,y,z \to \infty$:

$$\begin{aligned}\langle \hat{p}_x \rangle &= -i\hbar \iiint \psi(\partial\psi/\partial x) dxdydz = \\ &= -i\hbar/2 \iiint (\partial\psi^2/\partial x) dxdydz = \\ &= -i\hbar/2 \iint \psi^2\Big|_{x=-\infty}^{x=\infty} dydz = 0\end{aligned} \tag{13}$$

It is seen that the probability density current:

$$\mathbf{j} = \frac{\hbar}{2mi}\left(\psi^* \nabla\psi - \psi\nabla\psi^*\right) = \frac{1}{m}|\psi|^2 \nabla S_1 \tag{14}$$

is equal to zero for the real wave function ψ. These well-known results show that in order to describe the motion with a nonzero momentum, the function S_1 must be different from zero and ψ cannot be real. On the other hand, the function S_2 gives the probability density $|\psi|^2$=exp(-2$S_2/\hbar$) and should not appear in the limit of classical mechanics.

Discussion given above shows that relation (2) between the real functions S and ψ assumed by Schrödinger cannot be used as the starting point for a mathematically consistent heuristic transition from the Hamilton-Jacobi equation to the stationary Schrödinger equation.

III. From Quantum to Classical Mechanics

Now we show that the transition from the Schrödinger equation to the Hamilton-Jacobi equation, i.e., transition inverse to that discussed by Schrödinger, can easily be done if Eq. (2) is replaced by Eq. (11). The stationary Schrödinger equation has the usual form:

$$\frac{\hat{\mathbf{p}}^2}{2m}\psi + V\psi = E\psi\ ,\ \hat{\mathbf{p}} = -i\hbar\nabla \tag{15}$$

Now, we multiply this equation by the complex conjugate function ψ^* and integrate over the whole space. Taking into account that the momentum operator is self-adjoint we can then write:

$$\frac{1}{2m}\int |-i\hbar\nabla\psi|^2 dxdydz + \int (V-E)|\psi|^2 dxdydz = 0 \tag{16}$$

Using Eq. (11) in the last equation we get:

$$\begin{aligned}&\int \frac{(\nabla S_1)^2}{2m} e^{-2S_2/\hbar} dxdydz + \\ &\int \frac{(\nabla S_2)^2}{2m} e^{-2S_2/\hbar} dxdydz + \\ &\int (V-E) e^{-2S_2/\hbar} dxdydz = 0\end{aligned} \tag{17}$$

To perform a transition to the classical mechanics, we assume that the probability density:

$$|\psi|^2 = e^{-2S_2/\hbar} \tag{18}$$

has very small values everywhere except for the close vicinity of the classical trajectory $\mathbf{r}_{cl}$, where it achieves its maximum and the gradient of S_2 at $\mathbf{r}_{cl}$ is equal to zero:

$$\nabla S_2\big|_{\mathbf{r}=\mathbf{r}_{cl}} = 0 \tag{19}$$

In such a case, the probability density can be replaced by the δ-function:

$$|\psi|^2 = \delta(\mathbf{r} - \mathbf{r}_{cl}) \tag{20}$$

and the probabilistic character of the theory disappears. Therefore, the function S_2 describing the form of the probability distribution $|\psi|^2$ does not appear in classical mechanics. We note also that Eq. (20) corresponds to the limit $\hbar \to 0+$ in Eq. (18). Then, the straightforward use of Eqs. (17)-(20) leads to the Hamilton-Jacobi equation:

$$\frac{\left[\nabla S(\mathbf{r}_{cl})\right]^2}{2m} + (V - E) = 0 \tag{21}$$

for the classical action S that can be obtained from S_1 in the limit:

$$S = \lim_{\hbar \to 0+} S_1 \tag{22}$$

IV. From Classical to Quantum Mechanics

Finally, we discuss the transition from the Hamilton-Jacobi equation to the Schrödinger equation that can replace the original Schrödinger discussion. First we modify Eq. (2) by using the imaginary unit i in the relation between S and ψ:

$$iS = K \ln\psi \tag{23}$$

or:

$$\psi = e^{iS/K} \tag{24}$$

where S is the classical action. Classical trajectories with exact position and momentum measurements are mathematical abstraction only, and the real description of physical measurements must take into account their probabilistic character. For this reason, we write the Hamilton-Jacobi equation (21) in the form:

$$\iiint \left[\frac{(\nabla S)^2}{2m} + (V - E)\right] \delta(\mathbf{r} - \mathbf{r}_{cl}) dxdydz = 0 \tag{25}$$

in which the integration in the probability space instead physically unclear integration in Eq. (5) is used. At this point corresponding to the classical limit, the probability distribution has the form δ($\mathbf{r}$-$\mathbf{r}_{cl}$), where the variables in the corresponding Hamilton-Jacobi equation are $\mathbf{r}_{cl}$. In the following step, we go closer to quantum mechanics and replace the δ-function by a very narrow probability distribution exp(-2S_2/K), where K>0 is a small constant. Then, the last equation can be generalized as:

$$\iiint \left[\frac{(\nabla S_1)^2}{2m} + (V - E)\right] e^{-2S_2/K} dxdydz = 0 \tag{26}$$

Here, new functions S_1 and S_2 describe the motion close to the classical limit and S_1 equals S in this limit. Assuming that the probability distribution exp(-2S_2/K) achieves its maximum at $\mathbf{r}_{cl}$ we can also presume:

$$\nabla S_2\big|_{\mathbf{r}=\mathbf{r}_{cl}} = 0 \tag{27}$$

It is possible to generalize Eq. (26) again:

$$\iiint \left[\frac{(\nabla S_1)^2 + (\nabla S_2)^2}{2m} + (V - E)\right] e^{-2S_2/K} dxdydz = 0 \tag{28}$$

Here, derivatives of both the functions S_1 and S_2 are taken in the same way with a chance to describe classical as well as probabilistic aspects of the motion. This generalization means that the kinetic energy is attributed not only to the motion with $\nabla S_1 \neq 0$ leading to the nonzero probability density current (14) (it can be denoted as the kinetic energy with respect to the coordinate system in which the measurement is performed) but also to cases when ∇S_1=0 and the form of the probability distribution $|\psi|^2$=exp(-2S_2/K) is characterized by the gradient $\nabla S_2 \neq 0$ (kinetic energy related to the form of the probability distribution). In a general case, both contributions to the kinetic energy have to be taken into account. It is seen that a new function ψ instead S_1 and S_2 can be now introduced:

$$iS_1 - S_2 = K \ln\psi \tag{29}$$

or:

$$\psi = e^{(iS_1 - S_2)/K} \tag{30}$$

Then, Eq. (28) can be written in terms of the function ψ:

$$\iiint \left[\frac{|-iK\nabla\psi|^2}{2m} + (V-E)|\psi|^2\right] dxdydz = 0 \qquad (31)$$

We note that the imaginary unit in Eqs. (29)-(30) is important from the point of view of transforming the expression $[(\nabla S_1)^2+(\nabla S_2)^2]$ to $|-iK\nabla\psi|^2$ in the last equation. Supposing that the operator $(-iK\nabla)$ is self-adjoint we get:

$$\iiint \psi^* \left[-\frac{K^2}{2m}\Delta\psi + (V-E)\psi\right] dxdydz = 0 \qquad (32)$$

It is seen from this result that we can assume validity of the equation:

$$\left(-\frac{K^2}{2m}\Delta + V\right)\psi = E\psi \qquad (33)$$

which, except for the numerical factor K^2, has the form of the stationary Schrödinger equation. The value of K can be found in a similar way as it was one by Schrödinger, namely, by comparing solutions of the last equation with known experimental or theoretical results and concluding that $K=\hbar$.

V. Conclusions

In our discussion given in the last section, we were inspired by the original Schrödinger approach and the transition from the Schrödinger equation to the Hamilton-Jacobi equation performed in Section III.

Comparing our discussion with that of Schrödinger we see that the original equation (2) between the classical action S and the wave function ψ was replaced by a more complex relation (29). This relation contains not only the imaginary unit i but also two new functions S_1 and S_2. The function S_1 contains information about the motion in space and tends to the classical action S in the limit $\hbar\to 0+$ (see Eq. (22)). The function S_2 gives the probability density $|\psi|^2=\exp(-2S_2/K)$ which becomes the δ-function for $\hbar\to 0+$ (see Eqs. (25)-(28)). This interpretation of the wave function is a natural way of describing the probabilistic character of measurements. In our approach, the probabilistic interpretation of the wave function is introduced before the Schrödinger equation is obtained.

One of important points in the above discussion is the integration over the whole space performed in Eq. (5). In Eq. (25) and the following equations, we interpreted it as an integration over probabilities to find the particle in different parts of the space. Such probabilistic interpretation of measurements (see also [2]-[4]) seems to be physically reasonable, however, other interpretations like that used by Bohm are also possible [6]-[7]. On the other hand, our approach does not indicate that it is necessary to assume that particles move along trajectories with well-defined positions obeying the classical equation of motion with a quantum potential as assumed by Bohm. For this reason, the standard interpretation of quantum mechanics has been used here.

Transition from the time-dependent Hamilton-Jacobi equation to the time-dependent Schrödinger equation can be performed in an analogous way and will not be discussed here. The inverse transition was discussed e.g. in [2]-[4].

We can conclude that the transition from the time-independent Hamilton-Jacobi equation to the stationary Schrödinger equation discussed above is not straightforward and can be made only in a few successive steps, in which a new concept, namely the probabilistic description of the motion, is introduced. Despite the fact that Eq. (2) is not from the point of view of the present knowledge correct, ideas introduced by Schrödinger were very fruitful and the celebrated Schrödinger equation opened a new era in physics.

Acknowledgements

This work was supported by the MSMT grant No. 0021620835 of the Czech Republic.

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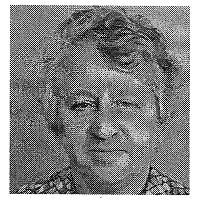
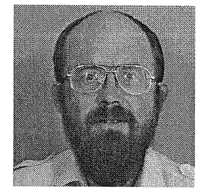
Authors' information

[1]Charles University,
Faculty of Mathematics and Physics,
Ke Karlovu 3,
121 16 Prague 2,
Czech Republic.

[2]University of Waterloo,
Department of Applied Mathematics,
Waterloo, Ontario N2L 3G1,
Canada



L. Skala was borned in 1947 in Ash, Czech Republic. He is professor of theoretical physics at the Charles University in Prague, Czech Republic and adjunct professor of applied mathematics at the University of Waterloo, Canada.
He published more than 100 papers and three textbooks in theoretical physics.
Prof. Skala is a member of the American Physical Society, Institute of Physics (England) and Union of Czech Mathematicians and Physicists.



V. Kapsa was borned in 1961 in Pisek, Czech Republic. He is research worker at the Charles University in Prague, Czech Republic.
He published more than 15 papers in theoretical chemical physics.
Dr. Kapsa is a member of the Union of Czech Mathematicians and Physicists.