

“Schrödinger’s Purloined Hypothesis”

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RÉSUMÉ. Le passage de la mécanique quantique vers la mécanique classique est bien établi et réalisé en faisant tendre la constante de Planck vers zéro. L’opération inverse allant de la mécanique classique vers la mécanique quantique est elle, pour le moins, couverte par un épais brouillard. Nous allons montrer que cette situation provient de l’omission d’une hypothèse implicite dans les toutes premières lignes de la démonstration originale de l’article de Schrödinger où il obtient l’équation stationnaire des ondes. Cette hypothèse n’est pas à proprement parler dissimulée, mais elle n’a pas été explicitée, tout comme dans la nouvelle d’E.A. Poe “la lettre volée” ou “lettre cachée” où les enquêteurs ne trouvent pas la lettre parce qu’elle est sous leurs yeux et au bon endroit. L’amplitude de la fonction d’onde joue le rôle “d’hypothèse cachée” qui permet à Schrödinger la transition de l’équation de Hamilton-Jacobi à son équation de Schrödinger. Cette hypothèse est un élément essentiel qui permet de comprendre où et comment la mécanique de Schrödinger va au delà de “l’ancienne théorie des quanta” de Planck. Le rôle joué par les intuitions de L. de Broglie sur les ondes pour décrire sinon les particules elles-mêmes, leurs mouvements se trouve ainsi explicité.

ABSTRACT. *The transition from quantum wave mechanics to classical mechanics is well established and can be obtained with vanishing Planck’s constant. The reverse operation from classical mechanics to quantum wave mechanics is covered by a misty fog. It will be shown that this situation originates from the omission of one implicit hypothesis in the first lines of Schrödinger’s original derivation of the stationary wave equation. This hypothesis is not concealed but it was made without explicit mention, as in the “Purloined Letter” novel of E.A. Poe, where the detective has trouble to find the letter, simply because it was at the very place it has to be. In this note the role played by the amplitude of the wave function is the purloined hypothesis that allows*

Schrödinger to make the transition from the Hamilton-Jacobi equation to the Schrödinger equation. This hypothesis is an essential clue to understand how and where Schrodinger's wave mechanics goes far beyond Planck's "old quantum theory". It emphasizes the role played by de Broglie's insight on the introduction of waves to describe, if not particles, particles motions.

1 Introduction

The transition from quantum wave mechanics to classical mechanics with vanishing Planck's constant has been amply discussed. The reverse one from classical mechanics to quantum wave mechanics is far less addressed, among the few one can find B. Liebowitz [1, 2, 3, 4]. The main issue is the starting point where the transition from classical to quantum mechanics was performed by E. Schrödinger [5]. It is still an obscure point that we will address in this note. The "magics" of variational equation often invoked by the physicists is by no way shared by mathematicians who have insistently written that no intrinsically new pre-existing equation can result from a change of parametrization or from a variational principle [6]. In the first lines of E. Schrödinger derivation one can extract an hypothesis which was not explicitly stressed at that time. In order to understand where this hypothesis can be found we review the hypotheses of the original E. Schrödinger derivation. Note that in this original paper there are no use of complex numbers or functions. In a second part the original derivation of E. Schrödinger is slightly reformulated and we discuss how the amplitude-phase separation was known to be irrelevant since the very beginning of quantum mechanics and we remind the non-linear equation which was introduced by E. Milne [7] and discussed by L.A. Young [8, 9]. In a third part the first consequences of this hidden hypothesis are stressed. The note concludes with discussing the opportunities open on L. de Broglie unitary wave mechanics theory [10] in connection with the Born-sided unitary particle theory heralded by A. Landé [11, 12]. The motivation of this study is related to recent works on the foundations of quantum mechanics [13, 16, 17, 15, 14], as the search of non linear equations to describe quantum phenomena [18] or vibrating bubbles [19] associated with de Broglie double solution or pilot wave concepts. They emphasize the need for more studies of the classical to quantal transition that may allow to design classical devices showing quantum properties. The present note follows a preceding one on the tentative "Modified Wave Mechanics" of Planck [20, 21, 22, 23].

2 E. Schrödinger’s original derivation of the stationary “wave equation”

- (a) In the original 1926 paper [5] E. Schrödinger considers, for a particle of mass m in a field of forces deriving from a potential $U(\vec{r}) = \frac{-e^2}{r}$, whose dynamics is governed by a Hamiltonian $H(\vec{r}, \vec{\nabla}_{\vec{r}}S)$, the time independent Hamilton-Jacobi equation for the action $S(\vec{r})$. His equation (1) is :

$$H(\vec{r}, \vec{\nabla}_{\vec{r}}S) - E = \frac{1}{2m} \left(\vec{\nabla}S \right)^2 + U(\vec{r}) - E = 0 \quad (1)$$

then he proposes a parametrization for $S(\vec{r})$, adapted to separable problems, which also reminds formally the entropy definition in statistical mechanics, his equation (2)

$$S(\vec{r}) = K \text{Log} \Psi(\vec{r}) \quad (2)$$

K having the dimension of an action. This original derivation did not make use of complex or imaginary numbers neither needs them. Whence his equation quoted (1’)

$$\frac{K^2}{2m} \left(\vec{\nabla} \Psi(\vec{r}) \right)^2 + U(\vec{r}) \Psi(\vec{r})^2 - E \Psi(\vec{r})^2 = 0 \quad (3)$$

He wrote that he does not want to solve this equation and instead sets the variation on the function $\Psi(\vec{r})$, his variational equation (3) :

$$\delta \int_{\Omega} d\vec{r} \left[\frac{K^2}{2m} \left(\vec{\nabla} \Psi(\vec{r}) \right)^2 + U(\vec{r}) \Psi(\vec{r})^2 - E \Psi(\vec{r})^2 \right] \quad (4)$$

Ω standing for the whole domain where the solution is to be found and gets, using the conventional method with by parts integration, his equation (5) :

$$\Delta \Psi(\vec{r}) + \frac{2m}{K^2} [E - U(\vec{r})] \Psi(\vec{r}) = 0 \quad (5)$$

and the surface integral, his equation (6) :

$$\int_{\partial\Omega} d\vec{A} \cdot \vec{\nabla} \Psi(\vec{r}) \delta \Psi(\vec{r}) = 0 \quad (6)$$

with the condition of vanishing $\Psi(\vec{r})$ at the boundaries of Ω . Then the “success story” begins with the computation of the energy levels and the wave functions for the hydrogen atom. It is often introduced as if the variation method has worked “by magic” making the Hamilton Jacobi equation become the Schrödinger equation.

- (b) The point is that a “purloined” hypothesis is to be found between equations (1) and (3, 4). Indeed parametrization (2) leads straightforwardly to :

$$\frac{K^2}{2m} \frac{(\vec{\nabla}\Psi(\vec{r}))^2}{\Psi(\vec{r})^2} + U(\vec{r}) - E = 0 \quad (7)$$

not to (3). And in (4) the variation is not made on $\Psi(\vec{r})$ function of the Hamilton-Jacobi equation (3) but, as remarked but not emphasized by Trkal, who played in a sense the role of an unadvertised “Dupin”, in his very careful analysis [24]. The quantity :

$$\Psi(\vec{r})^2 \left[\frac{K^2}{2m} \frac{(\vec{\nabla}\Psi(\vec{r}))^2}{\Psi(\vec{r})^2} + U(\vec{r}) - E \right] \quad (8)$$

assuming

$$\rho(\vec{r}) = \Psi(\vec{r})^2 = e^{2S(\vec{r})/K} \quad (9)$$

can be re-written as

$$\rho(\vec{r}) \left\{ \frac{1}{2m} (\vec{\nabla}S)^2 + U(\vec{r}) - E \right\} \quad (10)$$

And this shows that the variation is not performed on the S function of the original Hamilton-Jacobi equation (3). It is performed on a function that enters in an averaged Hamilton-Jacobi equation, with a density function $\rho(\vec{r})$ designed such as to match with $\Psi(\vec{r})^2 = e^{2S(\vec{r})/K}$.

This is Schrödinger’s purloined hypothesis. Without this hypothesis one can not derive the wave equation from the Hamilton-Jacobi equation.

In this derivation Schrödinger obtained the wave equation he was searching for. It is remarkable to note that he discussed the validity of his result in terms of the de Broglie connection between

geometrical optics and particle mechanics [25, 26, 27]. It appears to be the same for all the followers. The variational method which is considered by mathematicians as a mere “equation maker” is always presented by physicists, in this context, as a kind of magic that encompass the whole quantum mechanics.

3 Hamilton-Jacobi theory and the transition from Lagrangian to Eulerian Dynamics

Hamilton-Jacobi representation for an ensemble of trajectories .

For a given non-relativistic dynamical system, Hamilton-Jacobi theory considers ensembles of motions from which one specific motion can be deduced. Let a one-particle dynamical system be characterized by mass m , position $\vec{r}(t)$, velocity $\vec{v}(t)$. Following S.A. Rashkovskiy [28], one can consider these ensembles of motions as a whole with a density distribution $\rho(\vec{r}, t)$. The conservation of the motions within a definite volume in space leads to the well known condition :

$$\frac{\partial \rho}{\partial t} + \text{div} [\rho \vec{v}(\vec{r}, t)] = 0 \quad (11)$$

with

$$\vec{v}(\vec{r}, t) = \frac{\vec{\nabla} S(\vec{r}, t)}{m} \quad (12)$$

introduces the velocity field $\vec{v}(\vec{r}, t)$ associated to the function $S(\vec{r}, t)$ which is a complete integral or solution of the Hamilton-Jacobi equation for the motion in a field of force $U(\vec{r}, t)$

$$\frac{\partial S(\vec{r}, t)}{\partial t} + \frac{1}{2m} \left| \vec{\nabla} S(\vec{r}, t) \right|^2 + U(\vec{r}, t) = 0 \quad (13)$$

Finally one recovers

$$\int_{t_0}^t d\vec{r} dt \rho(\vec{r}, t) \left[\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\vec{\nabla} S \right)^2 + U(\vec{r}) \right] = 0 \quad (14)$$

and one can write

$$\delta \int_{t_0}^t d\vec{r} dt \rho(\vec{r}, t) \left[\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\vec{\nabla} S \right)^2 + U(\vec{r}) \right] = 0$$

very close to one of initial Schrödinger’s variational equations in a time dependent version. Nevertheless since $\rho(\vec{r}, t)$ and $S(\vec{r}, t)$ are different

physical quantities, any variation of the previous integral, which is but “an equation maker” has to consider both $\rho(\vec{r}, t)$ and $S(\vec{r}, t)$ independently. Variation over $\rho(\vec{r}, t)$ leads to the Hamilton Jacobi equation (13) and variation over $S(\vec{r}, t)$ leads to motions conservations (11) with a velocity field given by (12).

At this point of the description there is no achievable wave mechanics outcome and S.A. Rashkovskiy has to consider an Hamilton-Jacobi equation including a quantum potential term to recover the time dependent Schrödinger equation [28] in the following of his paper. Indeed, if one links the two quantities as one unique dynamical variable as de Broglie [25], one gets the hydrodynamical representation of the Schrödinger equation which has been extensively studied by de Broglie collaborators [30].

4 Another insight on the significance of $\rho(\vec{r}, t)$

In Rashkovskiy derivation $\rho(\vec{r}, t)$ appears as the normalized density distribution of an ensemble of possible motions for the system. This distribution obeys to conservation equation (11,12) as its only constraint. In Schrödinger derivation $\rho(\vec{r}) = \Psi(\vec{r})^2$ (9) is now constrained by the stationary Schrödinger equation (5) and is no longer a physical quantity separated from the action $S(\vec{r})$. So $\rho(\vec{r})$ can be taken as the density distribution of possible motions compatible, or coherent, with $S(\vec{r})$ that represents the dynamics of the system. In that alternative point of view $\rho(\vec{r})$ is related to the density of a coherent set of possible motions but not directly with the probability density of finding the particle around the location \vec{r} . Indeed some ergodic assumption [31] has to be made to go from the density probability of a motion to the density probability of presence of the particle itself. This tentative interpretation of $\rho(\vec{r})$ is very close to the description of a Gibbsean ensemble by Schrödinger [32], apart from the constraint that makes this density probability in coherence with the dynamics. From this stand point, *Schrödinger wave function describes an ensemble of possible motions for a point particle.* The spatial extension of $\rho(\vec{r})$ is by no means to be linked with the size of the particle. The theory of the electron of Abraham or Lorentz is a theory *of a particle*, where the particle has a size, a radius, Schrödinger’s theory is a theory *with a particle.*

5 Waves versus phase-waves

With standard complex time independent formalism, the wave function parameterization separating real phase and real amplitude functions :

$$\Psi(\vec{r}) = a(\vec{r}) e^{i \varphi(\vec{r})/\hbar}$$

is a convenient one, where the dynamics of the system can be deduced from a non-linear differential equation for the amplitude term [7, 8]. The “phase wave” parameterization

$$\Psi(\vec{r}) = e^{i \phi(\vec{r})/\hbar}$$

leads to complex phase functions in order to recover the unescapable amplitude term.

- (a) The need for the amplitude part as a dynamical variable, non separated from the phase part, is easily demonstrated in EBKM (Einstein Brillouin Keller Maslov [33, 34, 35, 36]) quantization, because it is an essential ingredient in order to get the half, or fractional, quantum numbers. This was one of the success of wave mechanics with respect to the old quantum mechanics constrained to the quantum conditions, n being an integer :

$$\int pdq = nh$$

on a close circuit and Brillouin’s use of $\Psi(\vec{r}) = e^{i S(\vec{r})/\hbar}$, $S(\vec{r})$ being a real function leads also for single valued solutions to

$$\Delta_{12}S(\vec{r}) = S_2(\vec{r}) - S_1(\vec{r}) = nh$$

for any two possible solutions of the Hamilton-Jacobi equation. Single valued solutions for Schrödinger’s equation [37] requires

$$\Delta_{12}S(\vec{r}) = \left[n + \frac{i}{2\pi} \Delta_{12} \text{Log}(a(\vec{r})) \right]$$

the familiar example of of two solutions differing in sign gives :

$$\Delta_{12} \text{Log}(a(\vec{r})) = -i \pi$$

and finally

$$\Delta_{12}S(\vec{r}) = \left[n + \frac{1}{2} \right] h$$

as for the harmonic oscillator motions.

- (b) The quantity $\rho(\vec{r}) = a(\vec{r})^2$ can be considered genuinely as a density distribution. The quantity $S(\vec{r})$ can be considered as an auxiliary quantity from which it is possible to deduce the parameters of the motion for instance position and impulsion of the particle. In the semi-classical limit of modified wave mechanics this quantity can be computed as an Hamilton-Jacobi action. In Schrödinger-Eckart's [38] wave mechanics the dynamical parameters can be defined on each point of space by the rule :

$$\vec{p}(\vec{r}) = \frac{-i\hbar}{\psi} \frac{\partial}{\partial \vec{r}} \psi = \frac{-i\hbar}{a(\vec{r}) e^{iS(\vec{r})/\hbar}} \frac{\partial}{\partial \vec{r}} a(\vec{r}) e^{iS(\vec{r})/\hbar}$$

$$\text{and } \vec{r} = \frac{1}{\psi} \vec{r} \psi$$

Only the quantum mean values have to be real, they are given by an average over a density distribution and one can understand the origin of the term "mean values", for instance :

$$\langle \vec{p} \rangle = \int d\vec{r} \rho(\vec{r}) \vec{p}(\vec{r}) = \int d\vec{r} |\psi|^2 \frac{-i\hbar}{\psi} \frac{\partial}{\partial \vec{r}} \psi$$

$$= \int d\vec{r} \psi^* (-i\hbar) \frac{\partial}{\partial \vec{r}} \psi$$

These formula can be extended in curvilinear coordinates systems :

$$\vec{p}(\vec{r}) = \frac{-i\hbar}{\psi} \frac{\partial}{\partial \vec{r}} \psi \quad \vec{p}^\dagger(\vec{r}) = \frac{i\hbar}{J\psi^*} \frac{\partial}{\partial \vec{r}} J\psi^*$$

J being the Jacobian. And if the self conjugation seems to be lost the two representations give the same mean value :

$$\langle \vec{p} \rangle = \int d\vec{r} J |\psi|^2 \frac{-i\hbar}{\psi} \frac{\partial}{\partial \vec{r}} \psi$$

$$= \int d\vec{r} J \psi^* (-i\hbar) \frac{\partial}{\partial \vec{r}} \psi = -(-i\hbar) \int d\vec{r} J \psi (-i\hbar) \frac{1}{J} \frac{\partial}{\partial \vec{r}} J \psi^*$$

- (c) The phase-amplitude parametrization was reduced as a one physical quantity problem since the beginning of quantum mechanics [7, 8, 9] for the time independent wave equation (5) in one dimension.

Milne’s wave function parametrization is a known mathematical procedure that focusses on the amplitude part of the wave function

$$\psi(x) = Cw(x) \sin \left\{ a \int_{x_0}^x w(x)^{-2} dx - \alpha \right\} \quad (15)$$

($a \neq 0$ is related to the boundary conditions, α and C arbitrary constants) and the associated “image” non linear equation :

$$\frac{d^2w(x)}{dx^2} + \frac{2m}{\hbar^2} (E - U(x))w(x) - \frac{a^3}{w(x)^3} = 0 \quad (16)$$

whence the compatibility relation :

$$\frac{a}{\pi} \int_{-\infty}^{+\infty} w(x)^{-2} dx = n \quad (17)$$

n being an integer, which acts as a quantum condition. Young [8, 9] parametrization is based on a more physical intuition where the wave function is parametrized as

$$\psi(x) = C P(x)^{-1/2} \cos \left\{ \int_{x_0}^x P(s) ds + \alpha \right\} \quad (18)$$

and the associated “image” non-linear equation

$$P(x)^{1/2} \frac{d^2P(x)^{-1/2}}{dx^2} + \frac{2m}{\hbar^2} (E - U(x)) + P(x)^2 = 0 \quad (19)$$

where the compatibility condition

$$\int_{-\infty}^{+\infty} P(x) dx = n\pi \quad (20)$$

is written in a form more close to Planck’s quantum conditions. Young names $P(x)$ the local momentum. If this formulation looks “more physical” it is not easy to link $P(x)$, to the classical momentum $p_{cl}(x) = \pm \sqrt{\frac{2m}{\hbar^2} (E - U(x))}$ or with any of the two other local momenta $\bar{p}(x) = -i\hbar\psi(x) \frac{\partial}{\partial x} \psi(x)$ or with $p(x) = \frac{-i\hbar}{\psi(x)} \frac{\partial}{\partial x} \psi(x)$. The two preceding ways are mathematically equivalent to the Bohm-deBroglie treatment of the wave equation, the quantum potential problem being solved by elimination of either the amplitude or the phase function. They nevertheless emphasize that the amplitude and the phase functions represent a same physical quantity which is the condition seen in (4) required to get coherent assemblies of motions.

6 Remarks on the interpretation of Schrödinger's mechanics

- (a) The wave function is established for a dynamical system, say one particle. The wave function is a summary of the possible dynamical characteristics of the motion of this particle : it describes an ensemble of motions whose partition is given by the structure of density distribution. By its very construction Schrödinger wave function cannot represent a particle "in itself". What Schrödinger built is not the theory of the wave function *of* a particle, this is the theory of the wave function *with* one particle *and* a distribution density. The naive arguments towards a all-wave interpretation are based on the heuristic consideration that the wave group velocity can be identified with the particle velocity of the associated classical problem. This holds only if one disregards the wave packet dispersion and it presents problems even for a particle inside a one-dimensional box.
- (b) The superposition principle concerns Schrödinger's wave function. It is associated to the linearity of the wave equation. We need waves in order to reproduce the experimental interference patterns. The phase amplitude parameterization leads to non-linear equations, but they rely on *the Schrödinger equation which describes essentially families of point-like particles motions*. This framework is unable to describe the characteristics of the particle (internal parameters such that the size, the form, etc).

7 Conclusion : Unitary Wave Theory versus Unitary Particle Theory

- (a) The above remarks indicate that de Broglie waves are still a program [25, 29, 10, 16]. In the whole one has to construct wave functions which satisfy Schrödinger's equation and superposition principle. Each elementary Schrödinger's wave function has to describe the density distribution of the motions. They have to be reconstructed by combining de Broglie's waves of the singular or non-linear kind, in order to describe both the motions and the form factors related to the particle described as a very tiny domain in space. The very ingenious attempts that have made use of Schrödinger's equation and Madelung's hydrodynamic interpretation to describe elementary particles as waves have been unsuccessful because the

Schrödinger equation is not the suitable one [20, 21, 22]. Nevertheless it has to be considered as a constraint for any more refined description.

- (b) As a first trial a Schrödinger wave function could be constructed as a sum of products of 2 functions, one for the particle de Broglie wave has to describe the wave singularity in motion, the other function has to describe the distribution of each of these singularities. The difficult issue is that one has to guess the wave equation for the singularities and that is clearly not an easy task. The following task is the matching of Schrödinger’s equation with the equation for the density distribution. The very point is to understand the physical significance of Planck’s constant h , which is the reason why we can but consider a wave description, in the de Broglie way, for particles.

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