Derivation of the Nonlinear Schrödinger Equation

from First Principles

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ABSTRACT. The generic form of the nonlinear Schrödinger (NLS) equations is derived from two assumptions which are entirely independent from the postulates of quantum mechanics. This derivation is not possible if the particles are assumed to be point-like. Regarding the Schrödinger equation proper as a special case of the NLS equations, we argue that the results of this paper imply that the probabilistic interpretation of quantum mechanics is not necessary.

1. Introduction

It is a common understanding that the fundamental equations of physics cannot be derived, they can only be deduced. This is also the case with the Schrödinger's equation which was deduced from the de Broglie relations and from certain correspondences between optics and mechanics which are found in Jacobi's equation [1], [2], [3]. However, the generic form of the nonlinear Schrödinger (NLS) equations can be derived.

This paper treats the Schrödinger equation proper as a special case of the NLS equations, for the complex field $\psi = \psi(x, t)$, whose form is

$$i\,\frac{\partial \psi}{\partial t} = -\,\mu \nabla^2 \psi + G(\psi^* \psi, x)\psi \;. \tag{1.1}$$

Here μ is a positive constant and $G(\psi^*\psi, x)$ is a real-valued function (which needs not be continuous) of the density $\psi^*\psi$ and the coordinates $x = (x_1, \ldots, x_n)$. We show that the form (1.1) the NLS equations, and hence that of the Schrödinger equation proper, can be derived from two

assumptions which are completely independent of the postulates of quantum mechanics. This derivation is presented as a new evidence that the probabilistic interpretation of quantum mechanics is not necessary. The discussion of this topic is left for the last section. In addition, the fact that such derivation is possible shows that there is a well defined mathematical connection between classical field theory / classical mechanics, on one hand, and quantum mechanics on the other. We maintain that this quantitative connection is far more specific than the qualitative correspondence principle of Bohr.

For the convenience of the reader we give the following outline of the derivation:

a. The first assumption is: the sought equation for the *spatially localized* field ψ belongs to the family of *Complex Hamiltonian Evolution* (CHE) equations.

b. A set of n functionals of ψ are defined whose values give the n coordinates of the field's localization center.

c. The velocity of the localization region is obtained by differentiating the above position functionals with respect to time and using the field equation to eliminate the time derivatives of ψ. The values of the resulting functionals, called the velocity functionals, cannot depend on the choice of the coordinate system 's origin. This requirement is met only if the Hamiltonian functional satisfies certain identity. When this is the case, two consequences follow: the Hamiltonian density is Gauge type I invariant and the norm of ψ is constant in time.

d. Next, we find an expression for the field's linear momentum density using the appropriate components of the energy-momentum 4-tensor.

e. The second assumption is: The linear momentum densities are proportional to the integrands of the corresponding velocity functionals. The constant of proportionality is the field's mass. This assumption leads to a set of $2n$ simple partial differential equations for the Hamiltonian density. When their solution is inserted into the generic form of the CHE equations the result is the NLS equation, in the nonlinear case, and the Schrödinger equation in the linear case.

2. The Derivation

According to the standard approach to quantum mechanics atomic systems and, in particular, elementary particles can be *represented* by

wave-functions which are solutions of the Schrödinger equation. This implies that a particle and its wave-function are two distinct entities. Here, following the views of Louis de Broglie and Albert Einstein we adopt an alternative approach, which is: *the particle is a spatially localized wave-function or field.* Consequently, this field must be endowed with energy and momentum densities. The simplest, if not the only, way to do this is via the energy-momentum 4-tensor of the classical field theory, which requires a Lagrangian density for the field.

Thus, our objective is to find an evolution equation for the scalar complex field $\psi = \psi(x_1 \ldots, x_n, t)$ for which there exists a Lagrangian density. This motivates the following

Assumption 1. *The sought field equation is a Complex Hamiltonian Evolution (CHE) equation, i.e., it is of the form*

$$i\,\frac{\partial\psi}{\partial t} = \frac{\delta H}{\delta\psi^*} \tag{2.1}$$

where $H = H[\psi^*\psi]$ is the Hamiltonian functional

$$H = \int_{I\!R^n} \mathcal{H}(\psi, \psi^*, \partial\psi, \partial\psi^*)\, d^n x \tag{2.2}$$

with $\partial\psi = \partial\psi/\partial x$ and

$$\frac{\delta H}{\delta\psi^*} = \frac{\partial\mathcal{H}}{\partial\psi^*} - \frac{d}{dx_j}\frac{\partial\mathcal{H}}{\partial(\partial_j\psi^*)}$$

is the variational derivative of H with respect to ψ^*. The summation convention of repeated indeces is adopted in this paper. For a discussion of the CHE family of equations see Bodurov [4]. Equation (2.1) is meaningful if H is finite, hence ψ must be *spatially localized* field since the integration domain in (2.2) is always the entire $I\!R^n$.

In what follows we will need n functionals of ψ whose values are the n coordinates X_k of the center of the localization region of the density $\psi^*\psi$. The candidates are

$$(X_k)^s = \frac{1}{N}\int_{I\!R^n} (x_k)^s \psi^*\psi\, d^n x \;, \qquad k = 1, \ldots, n$$

where s is a positive odd integer and

$$N = \int_{I\!R^n} \psi^* \psi \, d^n x \qquad (2.3)$$

is the norm of ψ. However, the natural requirement that the localization center of any spherically symmetric density $\psi^* \psi$ must coincide with the center of symmetry is satisfied only for $s = 1$. This justifies the following

Definition 1. *The coordinates of the center of the localization region of* ψ *are given by*

$$X_k = \frac{1}{N} \int_{I\!R^n} x_k \, \psi^* \psi \, d^n x \, , \qquad k = 1, \ldots, n \, . \qquad (2.4)$$

One can find the velocity of the localization region of ψ by simply differentiating the position functional (2.4) with respect to time. The result, called the *velocity functional*, is a functional of ψ and ψ^*

$$
\begin{aligned}
V_k = \frac{dX_k}{dt} &= \frac{1}{N} \int x_k \frac{d(\psi^* \psi)}{dt} \, d^n x - \frac{1}{N^2} \frac{dN}{dt} \int x_k \, \psi^* \psi \, d^n x \\
&= \frac{i}{N} \int \left(\psi \frac{\partial \mathcal{H}}{\partial \psi} - \psi^* \frac{\partial \mathcal{H}}{\partial \psi^*} + \partial_j \psi \frac{\partial \mathcal{H}}{\partial(\partial_j \psi)} - \partial_j \psi^* \frac{\partial \mathcal{H}}{\partial(\partial_j \psi^*)} \right) x_k \, d^n x \\
&+ \frac{i}{N} \int \left(\psi \frac{\partial \mathcal{H}}{\partial(\partial_k \psi)} - \psi^* \frac{\partial \mathcal{H}}{\partial(\partial_k \psi^*)} \right) d^n x - \frac{1}{N^2} \frac{dN}{dt} \int x_k \, \psi^* \psi \, d^n x \quad (2.5)
\end{aligned}
$$

where $\partial_j \psi$ stands for $\partial \psi / \partial x_j$. In the above, equation (2.1) was used to eliminate the $\partial \psi / \partial t$ and $\partial \psi^* / \partial t$ and then integration by parts was applied to the appropriate terms.

We see that the first and the third integrands in (2.5) contain the factor x_k which makes the velocity of the localization region dependant on our choice of the coordinate system origin. This, certainly, cannot be the case. Therefore, the first and the third integrals in the above expression must be zero. Moreover, they must vanish separately since the first depends on derivatives of ψ and ψ^* while the third does not. The vanishing of the first integral requires that the Hamiltonian density $\mathcal{H}$ identically satisfies the condition

$$\psi \frac{\partial \mathcal{H}}{\partial \psi} - \psi^* \frac{\partial \mathcal{H}}{\partial \psi^*} + \partial_j \psi \frac{\partial \mathcal{H}}{\partial(\partial_j \psi)} - \partial_j \psi^* \frac{\partial \mathcal{H}}{\partial(\partial_j \psi^*)} = 0 \, . \qquad (2.6)$$

Next, using equ. (2.1) we calculate the time derivative of $\psi^*\psi$

$$\frac{d}{dt}(\psi^*\psi) + i\frac{d}{dx_j}\left(\psi\frac{\partial\mathcal{H}}{\partial(\partial_j\psi)} - \psi^*\frac{\partial\mathcal{H}}{\partial(\partial_j\psi^*)}\right)$$
$$= i\left(\psi\frac{\partial\mathcal{H}}{\partial\psi} - \psi^*\frac{\partial\mathcal{H}}{\partial\psi^*} + \partial_j\psi\frac{\partial\mathcal{H}}{\partial(\partial_j\psi)} - \partial_j\psi^*\frac{\partial\mathcal{H}}{\partial(\partial_j\psi^*)}\right) .$$

Taking (2.6) into account we see that the density $\psi^*\psi$ obeys the conservation law

$$\frac{d}{dt}(\psi^*\psi) + i\frac{d}{dx_j}\left(\psi\frac{\partial\mathcal{H}}{\partial(\partial_j\psi)} - \psi^*\frac{\partial\mathcal{H}}{\partial(\partial_j\psi^*)}\right) = 0 . \tag{2.7}$$

Hence, the norm N is constant, i.e.

$$\frac{dN}{dt} = \int\frac{d}{dt}(\psi^*\psi)\,d^nx = 0 \tag{2.8}$$

and the third integral in (2.5) also vanishes. Thus, the velocity functional (2.5) reduces to

$$V_k = \frac{i}{N}\int\left(\psi\frac{\partial\mathcal{H}}{\partial(\partial_k\psi)} - \psi^*\frac{\partial\mathcal{H}}{\partial(\partial_k\psi^*)}\right)d^nx , \qquad k = 1,\ldots,n . \tag{2.9}$$

Observe that the integrand of (2.9) is equal to the flux density in (2.7) divided by N.

A second consequence of (2.6) is that the Hamiltonian density $\mathcal{H}$ is Gauge type I invariant [5], that is, invariant under the transformations

$$\psi' = \psi\,e^{i\varepsilon} , \qquad \psi'^* = \psi^*\,e^{-i\varepsilon} \tag{2.10}$$

where ε is the parameter of the transformation. To see this, denote the transformed Hamiltonian density by

$$\mathcal{H}' = \mathcal{H}(\psi', \psi'^*, \partial\psi', \partial\psi'^*) .$$

Then, the invariance condition

$$\frac{d\mathcal{H}'}{d\varepsilon}\bigg|_{\varepsilon=0} = i\left(\psi\frac{\partial\mathcal{H}}{\partial\psi} - \psi^*\frac{\partial\mathcal{H}}{\partial\psi^*} + \partial_j\psi\frac{\partial\mathcal{H}}{\partial(\partial_j\psi)} - \partial_j\psi^*\frac{\partial\mathcal{H}}{\partial(\partial_j\psi^*)}\right) = 0$$

is fulfilled if and only if the condition (2.6) is fulfilled.

In order to determine the field's linear momentum we follow a common practice in classical field theory, that is, we identify the densities of the field's linear momentum $\mathcal{P}_k$ with the entries $-\mathcal{T}_{k0}$ of the *energy-momentum 4-tensor* for the field ψ

$$\mathcal{P}_k = -\mathcal{T}_{k0} = -\frac{\partial \psi}{\partial x_k} \frac{\partial \mathcal{L}}{\partial(\partial_t \psi)} - \frac{\partial \psi^*}{\partial x_k} \frac{\partial \mathcal{L}}{\partial(\partial_t \psi^*)} \qquad (2.11)$$

where $\partial_t \psi$ stands for $\partial \psi / \partial t$ and

$$\mathcal{L} = \frac{i}{2}\left(\psi^* \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \psi\right) - \mathcal{H} \qquad (2.12)$$

is the Lagrangian density for the field equations (2.1). Inserting (2.12) into (2.11) produces for the components of the linear momentum density

$$\mathcal{P}_k = \frac{1}{2i}\left(\psi^* \frac{\partial \psi}{\partial x_k} - \frac{\partial \psi^*}{\partial x_k} \psi\right) , \qquad k = 1, \ldots, n . \qquad (2.13)$$

Consequently, the components of the field's linear momentum are given by the functionals

$$P_k = \frac{1}{2i} \int_{\mathbb{R}^n} \left(\psi^* \frac{\partial \psi}{\partial x_k} - \frac{\partial \psi^*}{\partial x_k} \psi\right) d^n x = -i \int_{\mathbb{R}^n} \psi^* \frac{\partial \psi}{\partial x_k} d^n x. \qquad (2.14)$$

It is remarkable that the last functional, obtained from purely classical arguments, differs from the *expectation value* of the linear momentum in quantum mechanics only by the multiplicative constant $\hbar/N$ (note that ψ is not normalized).

Assumption 2. *The linear momentum density (2.13) is proportional to the integrand of the velocity functional (2.9) for any spatially localized solution ψ of (2.1), i.e.*

$$\frac{1}{2i}\left(\psi^* \frac{\partial \psi}{\partial x_k} - \frac{\partial \psi^*}{\partial x_k} \psi\right) = m\frac{i}{N}\left(\psi \frac{\partial \mathcal{H}}{\partial(\partial_k \psi)} - \psi^* \frac{\partial \mathcal{H}}{\partial(\partial_k \psi^*)}\right) . \qquad (2.15)$$

Integrating both sides of the above equation produces

$$P_k = mV_k , \qquad k = 1, \ldots, n$$

which shows that the constant of proportionality m should be interpreted to be the *mass* of the field ψ. It follows from (2.15) that $\mathcal{H}$ satisfies the partial differential equations

$$\frac{\partial \mathcal{H}}{\partial(\partial_k \psi^*)} = \frac{N}{2m}\frac{\partial \psi}{\partial x_k}\ , \qquad \frac{\partial \mathcal{H}}{\partial(\partial_k \psi)} = \frac{N}{2m}\frac{\partial \psi^*}{\partial x_k} \qquad (2.16)$$

in which x_k, ψ, ψ^*, $\partial_k \psi$ and $\partial_k \psi^*$ are the independent variables. The general solution of the first set of equations is

$$\mathcal{H} = \frac{N}{2m}\frac{\partial \psi^*}{\partial x_k}\frac{\partial \psi}{\partial x_k} + \mathcal{G}(\psi, \psi^*, \partial\psi, x)$$

where $\mathcal{G}(\psi, \psi^*, \partial\psi, x)$ is the integration "constant". When the last expression is inserted into the second set of equations (2.16) one finds

$$\frac{\partial \mathcal{G}}{\partial(\partial_k \psi)} = 0\ , \qquad k = 1, \ldots, n\ .$$

Finally, we take into account that $\mathcal{G}$ is Gauge type I invariant, i.e. invariant under the transformations (2.10), since $\mathcal{H}$ is such according to (2.6). Consequently, $\mathcal{G}$ is a function of only x and $\psi^*\psi$. Thus, the Hamiltonian density becomes

$$\mathcal{H} = \frac{N}{2m}\frac{\partial \psi^*}{\partial x_k}\frac{\partial \psi}{\partial x_k} + \mathcal{G}(\psi^*\psi, x) = \frac{N}{2m}\nabla\psi^* \cdot \nabla\psi + \mathcal{G}(\psi^*\psi, x)\ . \quad (2.17)$$

Inserting expression (2.17) into the CHE equation (2.1) yields the NLS equation (1.1)

$$i\frac{\partial \psi}{\partial t} = -\frac{N}{2m}\nabla^2\psi + G(\psi^*\psi, x)\psi \qquad (2.18)$$

with $\mu = N/2m$ and $G(\rho, x) = \partial\mathcal{G}(\rho, x)/\partial\rho$. If ψ does not interact with any external fields then $\mathcal{H}$, and hence $\mathcal{G}$, cannot depend explicitly on the coordinates x. In this case, the field is spatially localized due to the self-interaction potential $G(\psi^*\psi)$ which makes the equation nonlinear. For spatially localized solutions of nonlinear field equations see [6].

Alternatively, if the field equation is linear $\mathcal{G}$ must be proportional to $\psi^*\psi$, and at the same time, depend explicitly on x in order to insure localization

$$\mathcal{G}(\psi^*\psi, x) = U(x)\,\psi^*\psi\ .$$

Thus, the Hamiltonian density in the linear case is

$$\mathcal{H} = \frac{N}{2m}\nabla\psi^* \cdot \nabla\psi + U(x)\,\psi^*\psi \;. \qquad (2.19)$$

When this is inserted into the CHE equation (2.1) one obtains the linear Schrödinger equation

$$i\,\frac{\partial\psi}{\partial t} = -\,\frac{N}{2m}\nabla^2\psi + U(x)\,\psi \qquad (2.20)$$

in which N appears in place of $\hbar$ and $U(x)$ is the potential (of the external interaction) divided by $\hbar$.

3. A Concluding Discussion

There are several implications of the above derivation. First of all, it should be observed that this derivation is not possible with the standard approach to quantum mechanics for the following reasons:

a. In the conventional quantum mechanics the wave-function of a *free* particle is a complex plane wave. This wave, as a field, cannot be the carrier of the particle's attributes since the energy and momentum densities will, then, be constant in space making the energy and momentum functionals either infinite or zero, and hence, meaningless. In this case, one is forced to regard the wave-function merely as a calculational device.

b. The ψ-field can be spatially localized either by a self-interaction (represented by a nonlinearity in the field equation) or by an interaction with an external field. If the equation is linear only the second alternative remains. Then, the position of the localization center is determined by the position of the external field in space. Hence, the velocity functionals are not meaningful unless the linear Schrödinger equation is considered as a special (or a limiting) case of the NLS equation.

c. The ψ-field cannot be a measure of the probability of a particle being found in certain space region and at the same time the carrier of definitive energy and momentum densities for the same particle. Thus, the probabilistic interpretation of ψ is neither compatible with nor needed for the present derivation.

The second observation is that this derivation is clearly not meaningful if the particles are assumed to be point-like. On the other hand,

the probabilistic interpretation is meaningful only for point-like particles. This is so because probability density cannot be defined for an ensemble of objects with finite dimensions. Indeed, the number of such objects in a given volume element is not defined when the volume element is smaller than the objects. Hence, the limit of the ratio [*number of objects*]/[*volume*], when [*volume*] → 0 does not exist. Again, there are two alternatives to choose from. We believe that this paper demonstrates that choosing the alternative *all particles are spatially extended entities* opens up possibilities which the other alternative prohibits.

The fundamental rule of quantum mechanics is: the equations governing the quantum counterpart of a classical system are found by replacing the linear momenta p_k with the operators $-i\hbar\,\partial/\partial x_k$ and treating all functions of the coordinates as multiplication operators. This rule has produced an immense number of wonderful results. On the other hand, the number of those who ask *"why does this rule work so well?"* is continuously diminishing. The answer is needed not to give us more confidence in the rule, but rather to tell us how and where to look for the next "magic rule". This paper should have demonstrated that the question is meaningful and its answer can be fruitful. For example, the functional (2.14) is identical with the expectation value of the linear momentum operator of quantum mechanics except that N appears in place of $\hbar$ (note that ψ in (2.14) is not normalized). This functional was derived from commonly accepted principles of classical field theory and not postulated as in quantum mechanics. The assumptions on which such derivations are based constitute, at least, partial answers to the above question.

It was already observed that in equation (2.20) the norm N of ψ appears in place of Planck's constant $\hbar$. This correspondence cannot be dismissed as some peculiar coincidence because the same correspondence is obtained from several other completely unrelated arguments. See Bodurov [7], [8].

In conclusion, let us recall that the empirical laws of Kepler describe the motions of the planets very accurately. For some time after Kepler's discovery, apparently, no one asked *"why Kepler's laws work so well?"* Newton asked this question and answered it by showing that these laws can be derived from a few assumptions which became the foundations of classical astronomy and mechanics.

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