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Generalized Ehrenfest Theorem for Nonlinear Schrödinger Equations

T. G. Bodurov[1]

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It is shown that the Ehrenfest theorem can be generalized so that it is valid also for all space-localized solutions ψ of the nonlinear Schrödinger equations (in one or more space dimensions). Then it is shown that as a consequence, the motion of the localized ψ-field as a whole obeys the laws of classical mechanics and those of classical electrodynamics if the interaction of the ψ-field with an external electromagnetic field is defined by the rules of quantum mechanics applied to the nonlinear Schrödinger equation for ψ (in exactly the same manner as to the linear Schrödinger equation). This establishes the existence of a deep link between the nonlinear Schrödinger equations and classical mechanics and electrodynamics.

1. INTRODUCTION

The adjective *space-localized* will appear many times in this paper. The meaning assigned to it for the present purposes is given by the following:

Definition. A singularity-free function $\psi = \psi(\mathbf{x}, t)$ of the coordinates x_i and the time t will be called *space-localized* (or localized) if $|\psi(\mathbf{x}, t)| \to 0$ sufficiently fast when $|\mathbf{x}| \to \infty$, so that its Hermitian norm $\langle\psi, \psi\rangle$ remains finite for all time:

$$\langle\psi, \psi\rangle = \int \psi^*\psi \, d^3x < \infty \tag{1.1}$$

It is known that certain *nonlinear complex field equations* in one or more dimensions possess space-localized solutions (Berestycki and Lions, 1983), including *solitons* (in the one-dimensional case). Several authors have concluded, with various degrees of generality, that if *interaction terms* are introduced in those equations according to the rule

[1] Eugene, Oregon, USA; e-mail: bodt@efn.org.

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$$\frac{\partial}{\partial x^{\mu}} \to \frac{\partial}{\partial x^{\mu}} + igA_{\mu}, \qquad \mu = 0, 1, 2, 3 \tag{1.2}$$

where g is an arbitrary, real constant; then (under certain conditions) the motion of the localized ψ-field, as a discrete entity, is identical to that of a point charge in an electromagnetic field whose 4-potential is A_{μ}.

The first to reach the above conclusion appears to have been Rosen (1939, p. 98). His argument is based on field energy considerations.

Bialynicki-Birula and Mycielski (1976), investigating a *nonlinear Schrödinger* (NLS) equation with a logarithmic nonlinear term, found that this equation admits closed-form localized solutions, which they called *gaussons.* In the same paper they demonstrated that if the logarithmic NLS equation is modified with the substitution (1.2), then "in every electromagnetic field, sufficiently small gaussons move like classical particles."

I showed in a recent paper (Bodurov, 1996) that the same result is valid for a large class of nonlinear complex field equations, which includes the NLS equations. Thus, one is led to the following conjecture: If there is a generalization of the Ehrenfest theorem from quantum mechanics to the NLS equations, then such results can be viewed as its consequences.

The purpose of this paper is to show that, indeed, the statement of Ehrenfest theorem can be extended to all NLS equations for which $\langle\psi, \psi\rangle$ is finite. The only modification is that the integrals in the pertinent expectation values must be explicitely "normalized," and not the solutions $\psi(\mathbf{x}, t)$.

2. A GENERALIZATION OF EHRENFEST THEOREM

Consider the family of all nonlinear Schrödinger equations

$$i\hbar \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2\psi + \Omega(\psi^*\psi)\psi \tag{2.1}$$

where ψ^* is the complex conjugate of ψ and $\Omega = \Omega(\psi^*\psi)$ is any real function of $\psi^*\psi$ such that equation (2.1) admits *space-localized* solutions. The various constants of proportionality which appear in the Schrödinger equation proper have been retained in (2.1), so that a comparison with the classical Ehrenfest theorem can be made most conveniently.

Since (2.1) contains no interaction terms with external fields, the NLS equations of this form will be called *free.* When electromagnetic interaction terms are included in (2.1) according to the quantum mechanics prescription

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - e\Phi \qquad \text{and} \qquad -i\hbar\nabla \to -i\hbar\nabla - e\mathbf{A} \qquad (c=1) \tag{2.2}$$

the resulting equations (with $\boldsymbol{p} = -i\hbar\nabla$)

$$i\hbar\frac{\partial\psi}{\partial t} = \left(\frac{1}{2m}(\boldsymbol{p} - e\mathbf{A})\cdot(\boldsymbol{p} - e\mathbf{A}) + e\Phi + \Omega(\psi^*\psi)\right)\psi \tag{2.3}$$

will also possess space-localized solutions if the potentials Φ and $\mathbf{A}$ are constant in space and in time. This is seen by applying to equation (2.3) the following transformation:

$$\psi'(\mathbf{x}, t) = \mathbf{e}^{i\vartheta}\,\psi(\mathbf{x}, t)$$

where $\vartheta = e(\Phi t - \mathbf{A}\cdot\mathbf{x})/\hbar$. The result is a free NLS equation for ψ' like (2.1). Then, by observing that $\langle\psi', \psi'\rangle = \langle\psi, \psi\rangle$, the above claim follows.

Here, we will consider solutions which remain localized not only when the potentials are constant, but also when the potential variations within the region of localization are sufficiently small. This condition can be adopted for a definition of a *stable solution* of a free NLS equation. The stability of NLS solutions will not be discussed here, since it is not directly related to this paper's topic, and since the stability of nonlinear wave equations in general has been treated elsewhere (e.g., Grillakis *et al.*, 1987; Straus, 1989, Chapter 7). The stability of the logarithmic NLS solutions is discussed in Bialynicki-Birula and Mycielski (1976).

The simplest means to define the position of any space-localized distribution ρ *as a discrete entity* is to give its "center of gravity." Setting $\rho = \psi^*\psi$, one gets for the coordinates of the ψ-field position

$$\mathrm{X}_i(t) = \frac{1}{\langle\psi, \psi\rangle}\int \psi^*\psi\, x_i\, d^3x, \qquad i = 1, 2, 3 \tag{2.4}$$

where ψ is a localized solution of the NLS equation and x_i are the space coordinates. Here, the term "ψ-field position" will always mean the set of values of the above three functionals. Clearly, the definition (2.4) is completely independent of the equation for ψ as long as $\langle\psi, \psi\rangle$ remains finite. These functionals, of course, are identical with the expectation values of the *position operators* x_i in quantum mechanics (QM). However, no probabilistic interpretation will be attached to them or to any other expectation values. Here, such would be entirely unnecessary, since there is no stochastic data involved.

In addition, it should be noted that a solution ψ cannot be normalized and remain a solution of the same nonlinear equation. Instead, the various expectation values and functionals must be "normalized" by dividing them by $\langle\psi,\psi\rangle$. If ψ is a solution of (2.3), with any Φ and $\mathbf{A}$, then its norm $\langle\psi, \psi\rangle$ given by (1.1) is a constant. The proof is exactly the same as for the linear Schrödinger equation, hence it is omitted.

Generalized Ehrenfest Theorem. The second time-derivative of the position-vector functional $\mathbf{X}(t)$ given by (2.4) is proportional to the expectation value of the Hermitian operator $\mathbf{E} + \frac{1}{2}((\boldsymbol{p} - e\mathbf{A}) \times \mathbf{B} - \mathbf{B} \times (\boldsymbol{p} - e\mathbf{A}))$ if they are evaluated with a space-localized solution of the NLS equation (2.3). That is,

$$\frac{d^2}{dt^2}\mathbf{X}(t) = \frac{e}{m\langle\psi, \psi\rangle}\int \psi^*\left(\mathbf{E} + \frac{1}{2}(\boldsymbol{v} \times \mathbf{B} - \mathbf{B} \times \boldsymbol{v})\right)\psi\, d^3x \tag{2.5}$$

where $\mathbf{E} = -\nabla\Phi - \partial\mathbf{A}/\partial t$ and $\mathbf{B} = \nabla \times \mathbf{A}$ are the electric and magnetic fields, respectively, and $\boldsymbol{v} = (\boldsymbol{p} - e\mathbf{A})/m = -(i\hbar\nabla + e\mathbf{A})/m$ is the velocity operator of quantum mechanics.

Proof. For convenience, the NLS equation (2.3) will be written as

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi + \Omega\psi \tag{2.6}$$

where $H = (\boldsymbol{p} - e\mathbf{A})\cdot(\boldsymbol{p} - e\mathbf{A})/2m + e\Phi$ is the Schrödinger operator. With this notation, the first time-derivative of the functional X_i is

$$\begin{aligned}
\mathrm{V}_i = \frac{d\mathrm{X}_i}{dt} &= \frac{1}{\langle\psi, \psi\rangle}\int\left(\psi^* x_i\frac{\partial\psi}{\partial t} + \frac{\partial\psi^*}{\partial t}x_i\psi\right)d^3x \\
&= \frac{1}{i\hbar\langle\psi, \psi\rangle}\int \psi^*\left([x_i, H] + x_i\Omega - \Omega\, x_i\right)\psi\, d^3x \\
&= \frac{1}{m\langle\psi, \psi\rangle}\int \psi^*(p_i - eA_i)\psi\, d^3x
\end{aligned}$$

since obviously the function $\Omega(\psi^*\psi)$ commutes with x_i and the evaluation of the commutator $[x_i, H]$ is a routine result in QM. Thus, the velocity $\mathbf{V}(t)$ of the localized ψ-field is identical with the expectation value of the QM velocity operator $\boldsymbol{v}$ (even in the presence of a magnetic field)

$$\mathbf{V}(t) = \frac{d\mathbf{X}}{dt} = -\frac{1}{m\langle\psi, \psi\rangle}\int \psi^*(i\hbar\nabla + e\mathbf{A})\psi\, d^3x = \frac{1}{\langle\psi, \psi\rangle}\int \psi^*\boldsymbol{v}\psi\, d^3x \tag{2.7}$$

With the same notation, the second time-derivative of $\mathbf{X}(t)$ is

$$\frac{d^2\mathbf{X}}{dt^2} = \frac{d\mathbf{V}}{dt} = \frac{1}{\langle\psi, \psi\rangle} \int \left(\psi^* \boldsymbol{v} \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \boldsymbol{v}\psi + \psi^* \frac{\partial \boldsymbol{v}}{\partial t} \psi \right) d^3x$$

$$= \frac{1}{\langle\psi, \psi\rangle} \int \psi^* \left(\frac{1}{i\hbar} [\boldsymbol{v}, H] - \frac{e}{m} \frac{\partial \mathbf{A}}{\partial t} \right) \psi \, d^3x$$

$$+ \frac{1}{i\hbar m \langle\psi, \psi\rangle} \int \psi^* (\boldsymbol{p}\Omega - \Omega\, \boldsymbol{p}) \psi \, d^3x \qquad (2.8)$$

For any space-localized function ψ the integral containing the nonlinear term is zero, as seen from the following:

$$\int \psi^* (\boldsymbol{p}\Omega - \Omega\, \boldsymbol{p}) \psi \, d^3x = i\hbar \int (\psi^* \Omega \nabla \psi - \psi^* \nabla(\Omega\psi)) \, d^3x$$

$$= i\hbar \int \Omega \nabla (\psi^* \psi) \, d^3x = 0$$

To evaluate the commutator

$$[\boldsymbol{v}, H] = \frac{m}{2} [\boldsymbol{v}, \boldsymbol{v} \bullet \boldsymbol{v}] + e[\boldsymbol{v}, \Phi] = \frac{m}{2} [\boldsymbol{v}, \boldsymbol{v} \bullet \boldsymbol{v}] - \frac{ie\hbar}{m} \nabla\Phi \qquad (2.9)$$

we apply the commutator identity $[L, JK] = J[L, K] + [L, J]K$ to the ith component of the first term

$$[v_i, \boldsymbol{v} \bullet \boldsymbol{v}] = \sum_{i=1}^{3} [v_i, v_j v_j] = \sum_{i=1}^{3} (v_j [v_i, v_j] + [v_i, v_j] v_j) \qquad (2.10)$$

The commutator of any two components of the velocity operator is

$$[v_i, v_j] = \frac{1}{m^2} \left[\left(i\hbar \frac{\partial}{\partial x_i} + eA_i \right), \left(i\hbar \frac{\partial}{\partial x_j} + eA_j \right) \right]$$

$$= \frac{ie\hbar}{m^2} \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) = \frac{ie\hbar}{m^2} (\nabla \times \mathbf{A})_k = \frac{ie\hbar}{m^2} B_k$$

where the values of the indexes i, j, k are the cyclic permutations of 1, 2, 3. Inserting the last into (2.10) yields

$$[v_i, \boldsymbol{v} \bullet \boldsymbol{v}] = \frac{ie\hbar}{m^2} \sum_{\substack{j \neq i,k \\ k \neq i,j}} (v_j B_k + B_k v_j) = \frac{ie\hbar}{m^2} (\boldsymbol{v} \times \mathbf{B} - \mathbf{B} \times \boldsymbol{v})_i$$

when it is observed that now the values of the indexes i, j, k are all permutations of 1, 2, 3, and that the terms corresponding to the odd permutations enter the sum with a negative sign. Substituting this expression into (2.9) and then the result into the first integral of (2.8) produces

$$\frac{d^2\mathbf{X}}{dt^2} = \frac{e}{m\langle\psi, \psi\rangle} \int \psi^* \left(\frac{1}{2} (\boldsymbol{v} \times \mathbf{B} - \mathbf{B} \times \boldsymbol{v}) - \nabla\Phi - \frac{\partial \mathbf{A}}{\partial t} \right) \psi \, d^3x$$
$$= \frac{e}{m\langle\psi, \psi\rangle} \int \psi^* \left(\mathbf{E} + \frac{1}{2} (\boldsymbol{v} \times \mathbf{B} - \mathbf{B} \times \boldsymbol{v}) \right) \psi \, d^3x$$

which completes the proof. ■

It is clear from the preceding that:

(a) An alternative statement of the above theorem could be: *The nonlinear term* $\Omega(\psi^*\psi)$ *does not contribute to the second time-derivatives of the position functionals* X_i.

(b) When the interaction is given only by a scalar potential $U = U(\boldsymbol{x})$ the statement of the same theorem reduces to

$$\frac{d^2\mathbf{X}}{dt^2} = -\frac{1}{m\langle\psi, \psi\rangle} \int \psi^*\psi\nabla U \, d^3x \tag{2.11}$$

This is identical with the statement of the classical Ehrenfest theorem, except that the integral is divided by $\langle\psi, \psi\rangle$, since the solutions ψ are not normalized, as noted earlier. However, the consequences of the two theorems, even in this case, are not the same. This is due to the well-known fact that the linear Schrödinger equation with no external interaction, unlike the nonlinear ones, does not possess space-localized solutions. Note that the *wave packets* of quantum mechanics do not qualify for space-localized solutions. A remarkable consequence of the generalized Ehrenfest theorem is stated as the following:

Corollary. If the potentials Φ and $\mathbf{A}$ change sufficiently slowly in space, then the equation of motion of the localized ψ-field, as a discrete entity, is identical to that of a point-charge e placed in the same electromagnetic field, and is a manifestation of a "Lorentz-force action" exerted on the ψ-field by the electric $\mathbf{E}(\mathbf{X})$ and magnetic $\mathbf{B}(\mathbf{X})$ fields. This equation is

$$m\frac{d^2\mathbf{X}}{dt^2} = e\mathbf{E}(\mathbf{X}) + e\frac{d\mathbf{X}}{dt} \times \mathbf{B}(\mathbf{X}) \tag{2.12}$$

where the ψ-field position $\mathbf{X}$ is given by the functionals (2.4), and the ψ-field mass by the constant m which appears in the corresponding NLS equation (2.3).

Proof. The criterion for the condition "Φ and $\mathbf{A}$ change sufficiently slowly in space" is that the variations of the potentials Φ and $\mathbf{A}$ within the spatial extent of the ψ-field must be negligibly small, so that they can be treated as constant in that region. A quantitative criterion is derived in Bodurov (1996). When this condition is met, we see that a change of the integration variables $x_i = r_i + X_i$ in (2.5) gives for the ith component of the first term

$$\int E_i\,\psi^*\psi\, d^3x = -\int \left(\frac{\partial \Phi(\boldsymbol{r} + \mathbf{X})}{\partial X_i} + \frac{\partial A_i(\boldsymbol{r} + \mathbf{X})}{\partial t}\right)\psi(\boldsymbol{r} + \mathbf{X})^*\psi(\boldsymbol{r} + \mathbf{X})\, d^3r$$

$$= -\left(\frac{\partial \Phi(\mathbf{X})}{\partial X_i} + \frac{\partial A_i(\mathbf{X})}{\partial t}\right)\int \psi(\boldsymbol{r} + \mathbf{X})^*\psi(\boldsymbol{r} + \mathbf{X})\, d^3r$$

$$= \langle \psi, \psi \rangle\, E_i(\mathbf{X})$$

since by the above assumption $\Phi(\boldsymbol{r} + \mathbf{X})$ and $\mathbf{A}(\boldsymbol{r} + \mathbf{X})$ can be replaced with $\Phi(\mathbf{X})$ and $\mathbf{A}(\mathbf{X})$ in the region of localization. Similarly, with the same change of variables, the second term of (2.5) becomes

$$\frac{1}{2}\int \psi^*(\boldsymbol{v} \times \mathbf{B} - \mathbf{B} \times \boldsymbol{v})\psi\, d^3x = -\mathbf{B}(\mathbf{X}) \times \int \psi^*\boldsymbol{v}\psi\, d^3x$$

$$= \langle \psi, \psi \rangle\, \frac{d\mathbf{X}}{dt} \times \mathbf{B}(\mathbf{X})$$

in accordance with (2.7). Inserting the last two results into (2.5) completes the proof. ■

This corollary is a special case of a more general result, obtained by an entirely different approach in Bodurov (1996).

3. CONCLUSIONS

The generalized Ehrenfest theorem and its corollary establish a deep link between the nonlinear Schrödinger equations and classical mechanics and electrodynamics. This is additional evidence that the space-localized solutions of certain nonlinear wave equations can be used to represent *elementary charges* (*particles*). This paper contains results which indicate that such a representation is on a level deeper than classical field theory, namely:

(a) The motion of the ψ-field as a discrete entity obeys the laws of classical mechanics and those of classical electrodynamics (2.12) if the interaction of the ψ-field with an external electromagnetic field is defined by the rules of quantum mechanics applied to the corresponding NLS equation.

(b) The relation of the velocity $\mathbf{V}$ and momentum $\mathbf{P}$ of a localized ψ-field is the same as that for a classical point charge, $\mathbf{P} = m\mathbf{V} + e\mathbf{A}$, as seen from (2.7), if **P** is calculated as the expectation value of the QM momentum operator and the interaction with the external electromagnetic field is defined according to the rules of quantum mechanics.

(c) The fact that the above correspondences hold only when the external fields are of sufficiently low intensity is qualitatively correlated with the result of high-energy physics that particles lose their identity when subjected to very high intensity fields.

It was shown that physically meaningful results, with remarkable generality, are obtained if the interaction between the nonlinear ψ-field and the electromagnetic field is defined according to rule (1.2). We think it is very significant that such results have not been derived, and most likely cannot be derived, from any other definition of the above interaction.

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