Ehrenfest theorem, Galilean invariance and nonlinear Schrödinger equations

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Abstract

Galilean invariant Schrödinger equations possessing nonlinear terms coupling the amplitude and the phase of the wave function can violate the Ehrenfest theorem. An example of this kind is provided.

The example leads to the proof of the theorem: A Galilean invariant Schrödinger equation derived from a lagrangian density obeys the Ehrenfest theorem. The theorem holds for any linear or nonlinear lagrangian.

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1 Introduction

The linear Schrödinger equation for a pointlike object interacting with an external force derived from a potential $U(\vec{r})$,

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2} m \nabla^2 \psi + U(\vec{r}) \psi$$

obeys the Ehrenfest theorem[1]. The theorem is expressed as an equation for the velocity and an effective second law of Newton. The probability function for the averaging procedure is taken to be the absolute value squared of the wave function that solves the pertaining Schrödinger equation.

The Ehrenfest equations read

$$<\vec{v}> = \frac{d}{dt} <\vec{r}>$$

$$<\vec{r}> = \int d^3x |\psi(\vec{r}, t)|^2 \vec{r}$$

(2)

and

$$m \frac{d}{dt} <\vec{v}> = \vec{F}(t)$$

$$\vec{F}(t) = -\int d^3x |\psi(\vec{r}, t)|^2 \nabla U(\vec{r})$$

(3)

The theorem states that the quantum expectation values of position and velocity of a suitable quantum system obey the classical equations of motion. This observation supports the choice of Born[2] of the amplitude squared as a probability weight factor. According to the present interpretation of quantum mechanics [3], the outcome of measurements of the motion of identically prepared pointlike systems, their location and speed when subjected to so-called 'external' forces, will be, on average, the same as the sharp values of their classical counterparts.

In classical deterministic mechanics, the sources of randomness are twofold, statistical fluctuations and extreme sensitivity to initial conditions. Statistical fluctuations can be minimized by bringing the system in contact with a reservoir at very low temperature, near absolute zero. The sensitivity to initial conditions causing chaotic behavior are not omnipresent. They arise for nonlinear systems. Hence, the outcome of the measurement of a point particle is in principle, predetermined. Eqs.(1) tell us that besides the statistical fluctuations, quantum systems possess an extra source of indeterminacy, that is regulated in a very definite way by the complex wave function. This is in some sense better for the
experimenter than classical thermal fluctuations that are hidden completely. Even in the limit of zero temperature, at which the classical fluctuations vanish and a deterministic outcome is expected, the macroscopic variables position and velocity are still fuzzy. The fuzziness is prescribed by the Schrödinger equation. Hence, only averages obey deterministic equations.

Ehrenfest theorem can be extended to many point particle systems without difficulty. The theorem embodies Bohr’s correspondence principle. As such, the dynamics dictated by eq.(1) ought to be independent of Planck’s quantum of action \( \hbar \). A failure of the ehrenfest theorem would carry on to the behavior of quantum particles in external fields such as gravitational fields. A system that is assumed to obey a nonlinear Schrödinger equation of the kind described below, displays an inherent nonclassical behavior, even on the average.

In section 2 we single out the kind of nonlinearities that violate with Ehrenfest theorem. In section 3 we prove a theorem that connects Galilean invariance, and the existence of a lagrangian density whose Euler-Lagrange equation is the Schrödinger equation, to the fulfillment of the Ehrenfest theorem. The proof hinges upon the existence of a lagrangian density. The existence of this density guarantees the existence of a conserved energy and a conserved linear momentum for the free particle, even when the particle is allowed to self-interact. Galilean invariance then inforces a connection between the Ehrenfest average velocity and the conserved momentum.
2 Ehrenfest theorem breaking

The linear Schrödinger equation for a pointlike quantum particle whose configuration wave function is \( \psi(\mathbf{r}) \), in interaction with an external potential \( U(\mathbf{r}) \), can be derived from the lagrangian

\[
\mathcal{L} = -\frac{i}{2} \left( \frac{\partial \psi^*}{\partial t} \psi - \frac{\partial \psi}{\partial t} \psi^* \right) - \frac{1}{2m} \mathbf{\nabla} \psi^* \cdot \mathbf{\nabla} \psi - |\psi|^2 U(\mathbf{r}) \tag{4}
\]

The lagrangian is a real scalar. A global phase transformation on the wave function leaves the lagrangian invariant. The Noether current for the symmetry becomes\[4\]

\[
\begin{align*}
 j_0 &= \psi^* \psi \\
 \mathbf{j} &= \frac{i}{2m} \left( \mathbf{\nabla} \psi^* \psi - \mathbf{\nabla} \psi \psi^* \right) \tag{5}
\end{align*}
\]

Born\[2\] interpreted this current as a probability current. \( j_0 \), the probability density, and, \( \mathbf{j} \), the probability flux. For waves whose amplitude decreases fast enough at infinity, current conservation

\[
\frac{\partial j_0}{\partial t} + \mathbf{\nabla} \cdot \mathbf{j} = 0 \tag{6}
\]

implies that the norm \( N = \int d^3x \ |\psi|^2 \) is independent of time. By rescaling the wave function to unit norm, the modified norm is in Born’s view the total probability to have the particle anywhere in space.

Ehrenfest\[1\], before Born, found that there is a way to define a privileged location whose dynamics follows the classical equations of motion. After Born’s interpretation, it becomes clear that the definition

\[
\langle \mathbf{r} \rangle = \int d^3x \ |\psi|^2 \mathbf{r} \tag{7}
\]

is a sound one for the averaged position variable or packet centroid. Derivation with respect to time of eq.(7), application of eq.(6), and integration by parts for well behaved wave functions yields eq.(2) with

\[
\langle \mathbf{v}(t) \rangle = \int d^3x \ \mathbf{j} \tag{8}
\]

Further derivation of the latter and use of the Schrödinger equation of eq.(1), yields the eq.(3).
Consider now nonlinear Schrödinger equations. Such equations as the Gross-Pitaevskii equation\(^5\) are frequently used for the description of Bose-Einstein condensates (BEC) of Alkali gases. The equation is an effective equation, derivable from a field theory by taking condensate expectation values, and it has found quite success in the description of the BEC setup. Starting from a linear field theory of particles, it is possible to arrive at a nonlinear Schrödinger equation in which the interactions are of zero range to lowest order. In this sense the effective theory is merely an approximation to the actual complicated dynamics ruling the behavior of the particles in interaction. As an effective theory, it has found a fair amount of predictive power. It is logical then, to ask the question whether this effective theory still obeys the Ehrenfest theorem. If the answer is in the affirmative, then, the averaging procedure that lead to the Schrödinger equation for the condensate did not break the connection to classical physics. If not, then, either this breaking is a falsification due to the approximations, or else, it really reflects an observable feature of these systems. In our opinion, only experiment can answer this question.

Another widespread application of nonlinear Schrödinger equations is that of density functional phenomenological models. In these models, the self-interaction of the particles, is nonlinear in the density. This approach yields stational and dynamical properties of systems, ranging from electron transport in solids\(^7\), electronic excitations\(^8\), soft condensed matter\(^9\) phase transitions in liquid crystals\(^10\), phonons in solids \(^{11,12}\), colloids\(^{13}\), liquids and nuclei \(^{14}\), atoms and molecules \(^{15}\), quantum dots\(^{16}\), etc. In these theories, the Schrödinger equation becomes

\[
i \frac{\partial \psi}{\partial t} = - \frac{1}{2m} \mathbf{\nabla}^2 \psi + \left[ O(|\psi|^2) + U(\mathbf{r}) \right] \psi \tag{9}\]

where \(O(|\psi|^2)\) is a nonlinear and sometimes nonlocal\(^6\) functional of the density \(\rho = |\psi|^2\). Calculating the time derivative of the velocity of eq.(8), with the nonlinear term of eq.(9) included, we find

\[
m \frac{d}{dt} < \mathbf{\nabla}(t) > = - \int d^3x \, \rho(\mathbf{r}) \frac{1}{2} \mathbf{\nabla} \left[ U(\mathbf{r}) + O(\rho) \right] \tag{10}\]

Using the trivial property

\[
\int d^3x \, \rho \, \mathbf{\nabla}[O(\rho)] = 0 \tag{11}\]

we arrive at the same Ehrenfest equation as that of eq.(2, 3). Nonlinear Schrödinger equations with nonlinearities such as that of eq.(9) obey the Ehrenfest relations. Perhaps this is expected as the nonlinear terms are essentially classical, depending on the density \(\rho\) and not on the wave function itself. If the external interaction is itself nonlinear such as \(U(\rho, x)\), then the Ehrenfest therem is still satisfied, but this time with a nonlinear force \(^1\)

\(^1\)This is analogous to the results found in soliton models\(^{17}\)
\[ \mathbf{F}(t) = - \int d^3 x |\psi(\mathbf{r})|^2 \mathbf{\nabla} U(\rho, \mathbf{r}) \]

In the following we will show that nonlinear Schrödinger equations of a different type, for which the nonlinearity depends on the phase also, do not obey the Ehrenfest equations. The trivial property of eq.(11) is the clue to the construction of the desired equations. The vanishing of eq.(11) is due to the dependence of \( O(\rho) \) solely on \( \rho \). It is easy to show, that an operator that depends on gradients of the phase for instance, will yield extra terms to the Ehrenfest equations.

Consider the Schrödinger equation proposed by Doebner and Goldin[18], without the diffusive term

\[
i \frac{\partial \psi}{\partial t} = -\frac{\mathbf{\nabla}^2 \psi}{2m} + \lambda \mathbf{\nabla} \cdot \left( \frac{\mathbf{j}}{|\psi|^2} \right) \psi + U(\mathbf{r}) \psi
\]

where \( \lambda \) is a coupling constant and \( \mathbf{j} \) is defined in eq.(5). Current conservation still holds as in eq.(6). The definition of the velocity is still given by eq.(2). Equation (13 is Galilean invariant. Galilean invariance is effected by means of the transformations [19, 4, 20]

\[
\begin{align*}
\mathbf{r} & \rightarrow \mathbf{r} - \delta \mathbf{v} t \\
\frac{\partial}{\partial t} & \rightarrow \frac{\partial}{\partial t} - \delta \mathbf{v} \cdot \mathbf{\nabla} \\
\psi & \rightarrow e^{i\phi} \psi \\
\phi & = \frac{1}{2} m (\delta \mathbf{v})^2 - m \delta \mathbf{v} \cdot \mathbf{r}
\end{align*}
\]

with \( \delta \mathbf{v} \) a constant velocity parameter. Under these substitutions, the free Schrödinger equation is invariant, while

\[
\frac{\mathbf{j}}{|\psi|^2} \rightarrow \frac{\mathbf{j}}{|\psi|^2} + \delta \mathbf{v}
\]

Eq.(13) is then Galilean invariant. However the Ehrenfest theorem is not satisfied

\[
m \frac{d}{dt} \langle \mathbf{v}(t) \rangle = \mathbf{F}(t) + \lambda \int d^3 x \mathbf{\nabla} |\psi|^2 \cdot \mathbf{\nabla} \left( \frac{\mathbf{j}}{|\psi|^2} \right)
\]

The identity (11) is of no use now. The last term in eq.(16) depends on derivatives of the amplitude and derivatives of the phase of the wave function, and not on \( \rho \) solely as in eq.(11).

\(^2\)A sizeable body of literature on related topics may be traced by citations to the ref.[18]
The failure to satisfy the Ehrenfest theorem may by traced back to the absence of a lagrangian density for which eq.(13) is its Euler-Lagrange equation of motion. This remark will be put in the form of a theorem in the next section.
3 Ehrenfest theorem as a consequence of Galilean invariance

The proof of the theorem proceeds by the following steps. The Schrödinger lagrangian for a free particle including self-interactions of any nonlinear nature, but no explicit dependence on the space or time coordinates is introduced. The corresponding action is then invariant under spatial coordinate translations. By Noether’s theorem there arises a conserved current and the physical law of conservation of linear momentum. The lagrangian is also demanded to be a real scalar. It depends on the phase of the wave function only through its derivatives. Phase transformations will then induce the law of conservation of probability identified as the modulus squared of the wave function.

Galilean invariance of the lagrangian then determines a connection between the probability current and the linear momentum. Finally, this connection insures the validity of the Ehrenfest theorem.

Consider a lagrangian density

\[ L(\psi, \psi_t, \psi_i) = L(S_t, S_i, R, R_t, R_i) \]

where suffixes denote partial derivatives, with respect to time \(t\) and with respect to the coordinate \(x_i\). As we are in the nonrelativistic domain, we do not differentiate between covariant and contravariant indices.

Space translations are generated by the transformations \( \vec{r} \rightarrow \vec{r} + \vec{\epsilon} \), with \( \vec{\epsilon} \) a constant parameter. As the lagrangian is independent of the coordinates, it is invariant under this transformation. When the parameter \( \vec{\epsilon} \) is promoted to be space-time dependent \([4]\), the law of conservation of linear momentum appears as a condition on the invariance of the action for arbitrary \( \vec{\epsilon} \).

The variation of the action reads

\[
\delta A = \delta \int d^3x \, dt \, L \\
= \int d^3x \, dt \left[ L \, \vec{\nabla} \cdot \vec{\epsilon} - \frac{\partial L}{\partial S_t} \vec{\nabla} S \cdot \vec{\epsilon} - \frac{\partial L}{\partial R_t} \vec{\nabla} R \cdot \vec{\epsilon} \\
- \frac{\partial L}{\partial S_i} \vec{\nabla} S \cdot \vec{\epsilon}_i - \frac{\partial L}{\partial R_i} \vec{\nabla} R \cdot \vec{\epsilon}_i \right]
\]

The invariance of the action then engenders the law of conservation of linear momentum

\[
0 = \frac{\partial p_j}{\partial t} + \frac{\partial T_{ij}}{\partial x_i}
\]
where

\[
\begin{align*}
\vec{p} &= -\frac{\partial L}{\partial S_t} \nabla S - \frac{\partial L}{\partial R_t} \nabla R \\
&= -\frac{\partial L}{\partial \psi_t} \nabla \psi - \frac{\partial L}{\partial \psi^*_t} \nabla \psi^*_t \\
T_{ij} &= \delta_{ij} L - \frac{\partial L}{\partial S_i} S_j - \frac{\partial L}{\partial R_i} R_j \\
&= \delta_{ij} L - \frac{\partial L}{\partial \psi_i} \psi_j - \frac{\partial L}{\partial \psi^*_i} \psi^*_j
\end{align*}
\]

(20)

As the lagrangian (17) is independent of \(S\), a transformation of the form \(S \to S + \theta(x,t)\), will generate the law of conservation of probability. Straightforward manipulations lead to

\[
0 = \frac{\partial J_0}{\partial t} + \nabla \cdot \vec{J}
\]

(21)

where

\[
\begin{align*}
J_0 &= -\frac{\partial L}{\partial S_t} \\
&= i \frac{\partial L}{\partial \psi^*_t} \psi^* - i \frac{\partial L}{\partial \psi^*_t} \psi \\
\vec{J} &= -\frac{\partial L}{\partial \nabla S} \\
&= i \frac{\partial L}{\partial \nabla \psi^*} \psi^* - i \frac{\partial L}{\partial \nabla \psi} \psi
\end{align*}
\]

(22)

In both equations (20,22) we do not specify the dynamics, by replacing the lagrangian with the free Schrödinger lagrangian. The only conditions imposed are, the very existence of a lagrangian that is a real scalar dependent on a complex wave function and independent of spatial coordinates except through the wave function and its derivatives. We also assumed that there do not appear derivatives of higher order, although this is not an essential ingredient. Both eqs.(19,21) may be obtained also by means of the Euler-Lagrange equations[21, 22]. It is easy to check that they are mere identities when the Euler-Lagrange equations are used.

The connection to Ehrenfest theorem now proceeds through the demand of Galilean invariance of the Schrödinger equation or covariance of the action for finite Galilean boosts.
Covariance, and not invariance, as a boost modifies the kinetic energy, and consequently changes the action. Applying an infinitesimal galilean transformation to the lagrangian \( L \) as specified in eqs.(14), i.e. dropping the term quadratic in the velocity, the variation of the lagrangian becomes

\[
\delta L = - \frac{\partial L}{\partial S_t} \delta \vec{v} \cdot \vec{E} S - \frac{\partial L}{\partial R_t} \delta \vec{v} \cdot \vec{E} R + \frac{\partial L}{\partial \nabla S} \cdot m \delta \vec{v}
\]

where we have used the definitions of \( \vec{p} \) and \( \vec{J} \) in eqs.(20,22). For the action to be covariant, which is equivalent to being invariant for infinitesimal Galilean boosts, eq.(23) implies

\[
\vec{p} = m \vec{J} + \vec{\nabla} f(\vec{r}, t)
\]  

Galilean invariance requires the probability flux to differ from the conserved linear momentum by at most a total divergence. For all practical purposes both vectors are one and the same up to the factor of the mass.

The existence of a real scalar lagrangian, even including nonlinear self-interaction terms, and the requirement of independence on coordinates for the free self-interacting is necessary and sufficient for the equivalence between \( m \vec{J} \) and \( \vec{p} \). Necessary, as we can proceed backwards from eq.(24) and reconstruct Galilean invariance.

We are now ready to show the validity of Ehrenfest theorem for a generic lagrangian as in eq.(17).

We add a scalar potential term \( \mathcal{L}_u = -U(\vec{r}) |\psi|^2 \) to the lagrangian. Use of different types of potentials, such as velocity dependent vector potentials, do not change the conclusions. Moreover, nonlinear potentials will generate forces as in eq.(12).

The lagrangian is no longer invariant under translations, but the action still is. Equation (19) is now modified to

\[
0 = \frac{\partial p_j}{\partial t} + \frac{\partial T_{ij}}{\partial x_i} + \frac{\partial U(\vec{r})}{\partial x_j} |\psi|^2
\]

Integrating over space for asymptotically vanishing wave functions, we find

\[
\frac{d}{dt} \int d^3x \ p_j(\vec{r}, t) = - \int d^3x \frac{\partial U(\vec{r})}{\partial x_j} |\psi|^2
\]

This is the second law of Newton for the 'field' momentum \( \vec{p} \). It bears no relation to the Ehrenfest theorem at this stage.

\( ^3 \)This method is straightforward for our purposes, use of the Noether method yields a tautology.
Consider now the definition of \(<\vec{r}>\) of eq.(2). Using eq.(21) we find

\[
\frac{d}{dt} <\vec{r}> = \int d^3x \vec{r} \frac{dJ_0}{dt} \\
= - \int d^3x \vec{r} \nabla \cdot \vec{J} \\
= \int d^3x \vec{J} \tag{27}
\]

Using eqs.(24,26) we find the second law of Newton for the centroid of the packet \(<\vec{r}>\), the Ehrenfest theorem

\[
m \frac{d^2}{dt^2} <\vec{r}> = m \frac{d}{dt} \int d^3x \vec{J} \\
= \frac{d}{dt} \int d^3x \vec{p} \\
= - \int d^3x \vec{\nabla}[U(\vec{r})] |\psi|^2 \\
= <\vec{F}> \tag{28}
\]

4 Conclusions

We have shown that the demand of Galilean invariance on a scalar real local lagrangian pertaining to a Schrödinger field, linear or nonlinear in the wave functions, implies the validity of the Ehrenfest theorem. The same does not hold for Schrödinger equations that are not derivable from an action principle. Among the terms that fulfill the requirements of Galilean invariance, and can serve as viable nonlinear self inter-actions, we can mention the function \(g(q)\), with \(q = R_t + \vec{j} \cdot \vec{\nabla}ln(R)\).
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