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Ehrenfest theorem, Galilean invariance and nonlinear Schrödinger equations

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Abstract

We prove that Galilean invariant Schrödinger equations derived from Lagrangian densities necessarily obey the Ehrenfest theorem for velocity-independent potentials. The conclusion holds as well for Lagrangians describing nonlinear self-interactions. An example of Doebner and Goldin motivates the result.

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1. Ehrenfest theorem breaking

Nonlinear Schrödinger equations such as the Gross-Pitaevskii equation [1] describe Bose–Einstein condensates (BEC) of alkali gases. The equation is effective, derivable from a field theory by taking condensate expectation values. Another widespread application of nonlinear Schrödinger equations is in density functional phenomenological models. In these theories, the Schrödinger equation reads

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

where $O(|\psi|^2)$ is a nonlinear and sometimes nonlocal [2] functional of the density $\rho = |\psi|^2$. The Ehrenfest equation for the average velocity, including the nonlinear term of equation (1), reads

$$m \frac{d}{dt} \langle \vec{v}(t) \rangle = - \int d^3x \rho(\vec{r}) \vec{\nabla} [U(\vec{r}) + O(\rho)]. \quad (2)$$

Since

$$\int d^3x \rho \vec{\nabla} [O(\rho)] = 0 \quad (3)$$

we arrive at the usual Ehrenfest equation for the velocity. If the external interaction is coupled nonlinearly to the density, through a potential $U(\rho, \vec{r})$, then the Ehrenfest theorem is still satisfied, but this time with a nonlinear force¹

$$\vec{F}(t) = - \int d^3x |\psi(\vec{r})|^2 \vec{\nabla} U(\rho, \vec{r}). \quad (4)$$

The vanishing of equation (3) is due to the dependence of $O(\rho)$ solely on ρ and not on the phase of ψ . Consider now the Schrödinger equation proposed by Doebner and Goldin [4], without the diffusive term²

$$i \frac{\partial \psi}{\partial t} = - \frac{\vec{\nabla}^2 \psi}{2m} + \lambda \vec{\nabla} \cdot \left(\frac{\vec{J}}{|\psi|^2} \right) \psi + U(\vec{r}) \psi \quad (5)$$

where λ is a coupling constant and $\vec{J} = \frac{i}{2m} (\vec{\nabla} \psi^* \psi - \vec{\nabla} \psi \psi^*)$. Galilean transformations are given by [5]

$$\vec{r} \rightarrow \vec{r} - \delta \vec{v} t \quad \frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t} - \delta \vec{v} \cdot \vec{\nabla} \quad \psi \rightarrow e^{i\phi} \psi \quad \phi = \frac{1}{2} m (\delta \vec{v})^2 - m \delta \vec{v} \cdot \vec{r} \quad (6)$$

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

$$\frac{\vec{J}}{|\psi|^2} \rightarrow \frac{\vec{J}}{|\psi|^2} + \delta \vec{v}. \quad (7)$$

Equation (5) is then Galilean invariant. However, the Ehrenfest theorem is not satisfied:

$$m \frac{d}{dt} \langle \vec{v}(t) \rangle = \vec{F}(t) + \lambda \int d^3x \vec{\nabla} |\psi|^2 \cdot \vec{\nabla} \left(\frac{\vec{J}}{|\psi|^2} \right). \quad (8)$$

Identity (3) is of no use now, since the last term in equation (8) depends both on derivatives of the modulus and derivatives of the phase of the wavefunction. We shall show that failure to obey the Ehrenfest theorem for the case of space-dependent external potentials, including nonlinear self-interactions is due either to the absence of a Lagrangian from which the equations are derivable, or to the Galilean noninvariance of the equation when a Lagrangian is present.

2. Ehrenfest theorem as a consequence of Galilean invariance

Consider a generic Schrödinger Lagrangian density

$$\mathcal{L}(\psi, \psi_t, \psi_i) = \mathcal{L}(S_t, S_i, R, R_t, R_i) \quad \psi = R e^{iS} \quad (9)$$

where suffixes denote partial derivatives with respect to time t and with respect to the spatial coordinate x_i . Space translations are generated by the transformations $\vec{r} \rightarrow \vec{r} + \vec{\epsilon}$, with $\vec{\epsilon}$ a constant parameter. Invariance of the action engenders the law of conservation for the linear momentum density

$$0 = \frac{\partial p_j}{\partial t} + \frac{\partial T_{ij}}{\partial x_i} \quad \vec{p} = - \frac{\partial \mathcal{L}}{\partial S_t} \vec{\nabla} S - \frac{\partial \mathcal{L}}{\partial R_t} \vec{\nabla} R \quad T_{ij} = \delta_{ij} \mathcal{L} - \frac{\partial \mathcal{L}}{\partial S_i} S_j - \frac{\partial \mathcal{L}}{\partial R_i} R_j. \quad (10)$$

As the Lagrangian (9) is independent of S , flux is conserved

$$0 = \frac{\partial J_0}{\partial t} + \vec{\nabla} \cdot \vec{J} \quad J_0 = - \frac{\partial \mathcal{L}}{\partial S_t} \quad \vec{J} = - \frac{\partial \mathcal{L}}{\partial \vec{\nabla} S}. \quad (11)$$

¹ This is analogous to the results found in soliton models [3].

² A sizeable body of literature on related topics may be traced by citations to [4].

In equations (10) and (11), the only conditions imposed are that the Lagrangian is a real scalar dependent on the complex wavefunction and, independent of spatial coordinates except through the wavefunction and its derivatives. We also assume that there are no derivatives of higher order, although this is not an essential ingredient.

The connection with the Ehrenfest theorem now follows from Galilean invariance of the Schrödinger equation, or covariance of the action for finite Galilean boosts. Covariance, not invariance, is appropriate, as a boost modifies the kinetic energy and consequently changes the action. Applying an infinitesimal Galilean transformation as specified in equations (6), to the Lagrangian \mathcal{L} , i.e. dropping the term quadratic in the velocity, the variation of the Lagrangian becomes

$$\begin{aligned}\delta\mathcal{L} &= -\frac{\partial\mathcal{L}}{\partial S_t}\delta\vec{v}\cdot\vec{\nabla}S - \frac{\partial\mathcal{L}}{\partial R_t}\delta\vec{v}\cdot\vec{\nabla}R + \frac{\partial\mathcal{L}}{\partial\vec{v}S}\cdot m\delta\vec{v} \\ &= \delta\vec{v}\cdot\vec{p} - m\delta\vec{v}\cdot\vec{J}\end{aligned}\quad (12)$$

where we have used the definitions of \vec{p} and \vec{J} in equations (10) and (11). For the action to be covariant, which is equivalent to being invariant for infinitesimal Galilean boosts, equation (12) implies

$$\vec{p} = m\vec{J} + \vec{\nabla}f(\vec{r}, t). \quad (13)$$

Galilean invariance thus requires the probability flux to differ from the conserved linear momentum density by at most a total divergence. We can also proceed backwards from equation (13) and reconstruct the Galilean invariance.

We are now ready to show the validity of the Ehrenfest theorem for a generic Lagrangian as in equation (9), to which we add a scalar potential term $\mathcal{L}_U = -U(\vec{r})|\psi|^2$.

The Lagrangian is no longer invariant under translations, but the action still is. Equation (10) is now modified to

$$0 = \frac{\partial p_j}{\partial t} + \frac{\partial T_{ij}}{\partial x_i} + \frac{\partial U(\vec{r})}{\partial x_j}|\psi|^2. \quad (14)$$

Integrating over space for asymptotically vanishing wavefunctions, we find

$$\frac{d}{dt}\int d^3x p_j(\vec{r}, t) = -\int d^3x \frac{\partial U(\vec{r})}{\partial x_j}|\psi|^2. \quad (15)$$

This is the second law of Newton for the ‘field’ momentum \vec{p} , but it is not yet related to the Ehrenfest theorem.

Using equation (11), we have as usual

$$\begin{aligned}\frac{d}{dt}\langle\vec{r}\rangle &= \int d^3x \vec{r}\frac{\partial J_0}{\partial t} \\ &= -\int d^3x \vec{r}\vec{\nabla}\cdot\vec{J} \\ &= \int d^3x \vec{J}.\end{aligned}\quad (16)$$

Then from equations (13) and (15)

$$\begin{aligned}m\frac{d^2}{dt^2}\langle\vec{r}\rangle &= m\frac{d}{dt}\int d^3x \vec{J} \\ &= \frac{d}{dt}\int d^3x \vec{p} \\ &= -\int d^3x \vec{\nabla}[U(\vec{r})]|\psi|^2 \\ &= \langle\vec{F}\rangle.\end{aligned}\quad (17)$$

3. Conclusion

We have shown that the requirement of Galilean invariance imposed on a real scalar local Lagrangian describing a Schrödinger field, including spatially dependent interactions and nonlinear self-interactions, implies the Ehrenfest theorem. The conditions are sufficient, but we have not shown they are necessary. Equivalently, if a Schrödinger equation with such interactions violates the Ehrenfest theorem then either it is not derivable from a Lagrangian, or it is not Galilean invariant. The key step in the proof is the connection between the flux vector and the field momentum of equation (13).

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