Ehrenfest's Theorem and Nonclassical States of Light

1. Ehrenfest's Theorem in Quantum Mechanics

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When it was first enunciated, Ehrenfest's Theorem provided a necessary and important link between classical mechanics and quantum mechanics. Today, the content of the theorem is understood to be a natural and immediate consequence of the equation of motion for operators when quantum mechanics is formulated in the Heisenberg picture. Nevertheless, the theorem leads to useful approximations when systems with Hamiltonians of higher than quadratic order in the dynamical variables are considered. In this two-part article, we use it to provide a convenient illustration of the differences between so-called classical and nonclassical states of radiation.


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1. Paul Ehrenfest and the Quantum–Classical Connection

The Austrian-Dutch physicist Paul Ehrenfest (1880–1933) stands out among those who worked in the grey area of semiclassical physics straddling quantum mechanics (QM) and classical mechanics (CM). His work provided a tangible correspondence between the quantum and classical worlds, through the Ehrenfest theorem. This theorem brought comfort to the practitioners of physics at a time in history when glimpses of the quantum world and its laws left them uneasy, in marked contrast to the familiar terrain of classical physics. It connects the dynamics of the expectation values of operators representing the physical observables of a quantum system to the dynamics of their classical counterparts. The purpose of this article is to illustrate this theorem in action with the help of a simple model in quantum optics, and to bring out precisely how nonclassical effects show up in the case of certain experimentally realizable states of quantized radiation.

As several diverse concepts are involved in this task, this article is written in two parts. In this first part, we focus on the Ehrenfest theorem and its implications in QM. In the second part, we shall consider the instructive illustration of the theorem (in its general form) provided by the dynamics of some states of a single-mode radiation field.

In CM, the state of a particle moving in one dimension is completely determined if the instantaneous values of its position and momentum are known through direct or indirect measurement. QM, on the other hand, is inherently probabilistic. We can only speak of the *probability amplitude* for the position of the particle to lie in the range (x, x + d x), when it is in a certain state at time *t.*

We first set the stage with a brief recapitulation of some standard material in elementary QM. Even the simplest quantum mechanical system, a trailer to the quantum world, turns the strictly deterministic approach to physics on its head. In CM, the state of a particle moving in one dimension is completely determined if the instantaneous values of its position and momentum are known through direct or indirect measurement. QM, on the other hand, is inherently probabilistic. We can only speak of the *probability amplitude* for the position of the particle to lie in the range $(x\,,\,x + \mathrm{d}x)$, when it is in a certain state at time t. The latter is specified by a *state vector* $|\Psi(t)\rangle$ in an appropriate Hilbert space. The probability amplitude required is defined as the *overlap* of the state vector with the position eigenstate $|x\rangle$, and is given by $\langle x|\Psi(t)\rangle$. It is precisely this quantity that is called the position-space wave function $\psi(x,t)$. Alternatively, one may consider the probability amplitude for the particle to have a momentum in the range $(p\,,\,p+\mathrm{d}p)$ when it is in the same state $|\Psi(t)\rangle$. This is given by the overlap of the state vector with the momentum eigenstate $|p\rangle$, namely, the momentum-space wave function $\langle p|\Psi(t)\rangle \equiv \widetilde{\psi}(p,t)$. Both these wave functions are generally complex-valued functions of their arguments. They yield the probability densities $|\psi(x,t)|^2$ and $|\widetilde{\psi}(p,t)|^2$ in the position and momentum, respectively. The normal-

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ization

$$\langle\Psi(t)|\Psi(t)\rangle = \int_{-\infty}^{\infty} |\psi(x,t)|^2\, \mathrm{d}x = \int_{-\infty}^{\infty} |\widetilde{\psi}(p,t)|^2\, dp = 1 \tag{1}$$

ensures that the total probability (of the existence of the particle) is unity, as required. In what follows, we shall assume that the states we deal with are always normalized to unity.

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$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle, \tag{2}$$

where $\hat{H}$ is the Hamiltonian operator, assumed to be hermitian (more precisely, self-adjoint). An overhead caret will be used to denote operators. The adjoint of $|\Psi(t)\rangle$, namely, the bra vector $\langle\Psi(t)|$, satisfies the equation

$$-i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi(t)| = \langle\Psi(t)|\,\hat{H}(t). \tag{3}$$

Note that we have allowed for a possible explicit time-dependence of the Hamiltonian. In the special case of an isolated system, $\hat{H}$ is t-independent. In that case the formal solution of the Schrödinger equation, for a given initial state $|\Psi(0)\rangle$, is

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle. \tag{4}$$

The operator $e^{-i\hat{H}t/\hbar}$ is unitary. This means that the state of the system evolves by the gradual unfolding of a unitary transformation of the initial state. The last statement remains true even when $\hat{H}$ has an explicit t-dependence, although the unitary time-development operator is then more complicated than the simple exponential $e^{-i\hat{H}t/\hbar}$. The unitarity of the time-development operator ensures the conservation of total probability, i.e., $\langle\Psi(t)|\Psi(t)\rangle = 1$ at all times.

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The values of physical quantities such as the position and momentum of the particle in any given state are the outcomes of measurements of the corresponding quantum observables. The latter are operators that act on the states of a system. The measurement problem in QM is closely linked to the interpretation of QM and other foundational questions. We do not enter into these matters here, but rather, restrict ourselves to the standard, conventional view. In contrast to a classical system, a measurement of any observable $\hat{A}$ of a quantum mechanical system will, in general, change the state of the system. The result of the measurement can be any one of the eigenvalues of the operator $\hat{A}$. An amazing feature of quantum physics is that the outcome of a measurement does not imply that the observable had that same value just prior to the measurement. In general, no definitive statement can be made about the value of an observable before a measurement of that observable. What QM does yield, unambiguously, is complete information of a *statistical* nature about any physical observable. For instance, it provides us with an elegant formula for the average value, or *expectation value* $\langle\hat{A}\rangle$, of a quantum observable. It also gives us definite formulas for the *scatter* about this average value, in terms of the expectation values of all the powers $\hat{A}^n$, where $n = 2, 3, \ldots$.

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We have stated that a single measurement of an observable $\hat{A}$ yields any one of the eigenvalues of that operator. In order to obtain its expectation value $\langle\hat{A}\rangle$, the same measurement has to be made, in principle, on each member of an infinite number of identical copies of the quantum system, all prepared in the same state. $\langle\hat{A}\rangle$ is the arithmetic average of the results of all the measurements. As mentioned already, this quantity is calculable in QM. For example, the expectation values of the position and momentum of a particle moving in one dimension, when it is in the normalized state $|\Psi(t)\rangle$, are given by

$$\langle\hat{x}\rangle(t) = \langle\Psi(t)|\hat{x}|\Psi(t)\rangle \quad \text{and} \quad \langle\hat{p}\rangle(t) = \langle\Psi(t)|\hat{p}|\Psi(t)\rangle, \tag{5}$$

respectively. We will use the somewhat loose but better-looking notation $\langle\hat{x}(t)\rangle$ and $\langle\hat{p}(t)\rangle$ for these expectation values. (It is, in fact, precisely the notation we would use if we worked in the Heisenberg picture. See the remarks in *Box* 1.) In order to find the actual numerical values from these formal expressions, we need to choose a specific *basis* in the Hilbert space, and also work in a specific *representation* – much as we choose, in solving a problem in CM, a frame of reference as well as a coordinate system in that frame. As you know, calculations in QM involve mathematical tools from linear vector spaces, probability theory, matrix methods and differential equations. Against this backdrop, it is easy to appreciate why, in the early days of QM, the need was so acutely felt for a vital link between the familiar classical world and the puzzling quantum world. It was precisely this link that was supplied by Ehrenfest in his theorem.

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2. Ehrenfest's Theorem

Consider an isolated quantum mechanical system in the (normalized) state $|\Psi(t)\rangle$. Let $\hat{A}(t)$ be the operator representing an arbitrary observable of the system, where we have allowed for a possible explicit time dependence. Its expectation value is $\langle\hat{A}(t)\rangle = \langle\Psi(t)|\hat{A}(t)|\Psi(t)\rangle$. Differentiating this formula with respect to t and using the Schrödinger equation (2) for $|\Psi(t)\rangle$ and (3) for its adjoint $\langle\Psi(t)|$, we get

$$\mathrm{d}\langle\hat{A}(t)\rangle/\mathrm{d}t = (i\hbar)^{-1} \; [\hat{A}(t)\,,\,\hat{H}(t)]\rangle + \; \partial\hat{A}(t)/\partial t\rangle. \tag{6}$$

Here, $[\hat{A}\,,\,\hat{H}] \equiv \hat{A}\,\hat{H} - \hat{H}\,\hat{A}$ is the commutator of $\hat{A}$ and $\hat{H}$. Observe that (6) is reminiscent of the equation of motion of a *classical* dynamical variable $A(t)$ in a

Box 1. Ehrenfest's Theorem in Hindsight

We have stated that the general form of Ehrenfest's Theorem is that given by equation (6). With the benefit of the hindsight provided by more than 85 years of quantum mechanics, it may be argued that this is no 'theorem' at all; rather, it is simply the formula for the rate of change of the expectation value of any operator (or observable) in QM. This becomes quite obvious if we work in the Heisenberg picture instead of the Schrödinger picture. Remember that the two pictures are 'unitarily equivalent'. That is, (i) they are connected by a unitary transformation, and (ii) the physical content is exactly the same in either of the two pictures. The second condition above is met by requiring that every expectation value be exactly the same when computed in the two pictures. In the Heisenberg picture, it is the operators that carry the burden of time evolution. The Heisenberg equation of motion for any observable is

$$\mathrm{d}\hat{A}(t)/\mathrm{d}t = (i\hbar)^{-1}\,[\hat{A}(t)\,,\,\hat{H}(t)] + \partial\hat{A}(t)/\partial t\,, \tag{A}$$

where all the operators are now those in the Heisenberg picture. Taking the expectation value of both sides of this equation in any state $|\Psi\rangle$, we obtain precisely (6).

As stated in the text, however, it is in the sense of the approximation in equation (10) (or a similar approximation in more general cases, amounting to the neglect of fluctuations about the mean or expectation values of observables) that the term 'Ehrenfest's Theorem' is most commonly used. The question of interest, then, is the extent to which the approximation is a good one, and the conditions under which this is so.

Hamiltonian system, namely,

$$\mathrm{d}A(t)/\mathrm{d}t = \{A(t)\,,\,H(t)\} + \partial A(t)/\partial t. \tag{7}$$

$\{A, H\}$ is the Poisson bracket of A with the classical Hamiltonian H. As is well known, the QM $\rightarrow$ CM correspondence says that commutators divided by $i\hbar$ go over into the corresponding Poisson brackets in the limit $\hbar \rightarrow 0$. Thus (6) goes over into (7) in the classical limit. This immediately raises several interesting and important issues, such as the precise form of the mapping between operators on Hilbert space and functions in classical phase space[1], the extent to which different quantum states differ from 'classicality', and so on.

[1] This aspect is discussed further in Mallesh *et al*, *Resonance*, Vol.16, No.3, p.254, 2011.

Equation (6) is, in fact, the Ehrenfest Theorem in its general form, although this term is often used to refer to the relationship in certain special cases – notably, that of a particle moving in one dimension in a time-independent potential. Setting its mass equal to unity, the Hamiltonian of the particle is $\hat{H} = \frac{1}{2}\hat{p}^2 + V(\hat{x})$. Using the canonical commutation relation $[\hat{x}\,,\,\hat{p}] = i\hbar\hat{I}$ where $\hat{I}$ is the identity (or unit) operator, equation (6) immediately gives

$$\mathrm{d}\langle\hat{x}\rangle/\mathrm{d}t = \langle\hat{p}\rangle \quad \text{and} \quad \mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t = -\langle V'(\hat{x})\rangle \equiv \langle F(\hat{x})\rangle \tag{8}$$

in *any* state of the particle. Here V' denotes the derivative of the function V with respect to its argument. For instance, if $V(\hat{x}) = k\,\hat{x}^n$ (where k is a constant), then $V'(\hat{x})$ stands for the operator $nk\,\hat{x}^{n-1}$. We have also written the function $-V'$ as F in analogy with the classical case, where the negative gradient of the potential is the force on the particle. The equations of motion (8) for the expectation values of the position and momentum are so well-known and so often used in quantum physics, that they are sometimes referred to (somewhat imprecisely) as the *general* form of the Ehrenfest relation itself.

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Something very special happens when the potential is a quadratic function of the position, as in the case of the linear harmonic oscillator, for which $V(\hat{x}) = \frac{1}{2}\omega^2\,\hat{x}^2$. Equations (8) then reduce to

$$\mathrm{d}\langle\hat{x}\rangle/\mathrm{d}t = \langle\hat{p}\rangle \quad \text{and} \quad \mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t = -\omega^2\,\langle\hat{x}\rangle. \tag{9}$$

But these are precisely the equations satisfied by the dynamical variables x and p of a *classical* linear harmonic oscillator. This is why the Ehrenfest theorem is sometimes stated in the form: 'Quantum mechanical expectation values satisfy the classical equations of motion.' Clearly, this statement is rigorously true only in the very special case of a particle moving in a quadratic potential. The crucial point is that $\langle\hat{x}^n\rangle$ *is not the same as* $\langle\hat{x}\rangle^n$ *except for* $n = 1$. Over and above this problem, going from CM to QM also leads to ambiguities in

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the ordering of non-commuting variables. A little more generally, the theorem as stated above is *approximately* true for an arbitrary potential $V(\hat{x})$ under the following circumstances. Suppose the state of the particle is such that its position-space probability density $|\psi(x,t)|^2$ is essentially concentrated in the vicinity of the expectation value $\langle\hat{x}(t)\rangle$ at all times. This means that the variance of the position and all its higher cumulants are always very small, and the approximation $F(\hat{x})\rangle \simeq F(\langle\hat{x}\rangle)$ is a good one. In that case equations (8) for the time evolution of the expectation values of $\hat{x}$ and $\hat{p}$ become

$$\mathrm{d}\langle\hat{x}\rangle/\mathrm{d}t = \langle\hat{p}\rangle \quad \text{and} \quad \mathrm{d}\langle\hat{p}\rangle/\mathrm{d}t \simeq F(\langle\hat{x}\rangle). \tag{10}$$

Clearly, these are the same as the classical equations of motion for the position and momentum, $\mathrm{d}x/\mathrm{d}t = p$ and $\mathrm{d}p/\mathrm{d}t = F(x)$. It is in *this* sense that the Ehrenfest theorem is invoked most often. Note, however, that the validity of this statement depends strongly on the state of the system at all times.

There is another noteworthy point about equations (9) for $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ in the case of potentials that are no more than quadratic in $\hat{x}$. The equations are *closed*, in the sense that they do not involve the expectation values of any other functions of $\hat{x}$ and $\hat{p}$. Thus the dynamics of the pair $(\langle\hat{x}\rangle, \langle\hat{p}\rangle)$ is not coupled to that of the expectation values of higher powers of $\hat{x}$ and $\hat{p}$ and their combinations. *This is no longer true for nonquadratic potentials.* In the latter case, the higher moments of $\langle\hat{x}\rangle$ play an important role in determining how $\langle\hat{p}\rangle$ changes with time. The expectation values of $\hat{x}$ and $\hat{p}$ and their higher powers vary in time in a complicated manner, indicative of the complex distortion and spread of the quantum state from its original form (e.g., in the position representation). At the quadratic level, the dynamical variables concerned are $\hat{x}^2$, $\hat{p}^2$, $\hat{x}\,\hat{p}$ and $\hat{p}\,\hat{x}$. The equation of motion for $\hat{p}^2$, for instance, reads

$$\mathrm{d}\langle\hat{p}^2\rangle/\mathrm{d}t = F(\hat{x})\,\hat{p}\rangle + \hat{p}\,F(\hat{x})\rangle. \tag{11}$$

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Therefore, unless $F(\hat{x})$ is a linear function of its argument, the system of equations for quadratic functions of $\hat{x}$ and $\hat{p}$ is not closed: higher moments than the second appear on the right-hand sides of these equations. When $\hat{H}$ is nonquadratic in the momentum as well, the dynamics is even more complicated. This is demonstrated in the spreading of a wave packet passing through a nonlinear optical medium called a Kerr medium: the effective Hamiltonian in this case involves terms up to fourth powers of $\hat{x}$ and $\hat{p}$. We shall discuss this example in the second part of this article. Under certain specific circumstances, a dispersing wave packet can even resurrect itself at definite instants of time (leading to so-called *revivals* of the wave packet).

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For a wide variety of initial states, the wave function can display significant changes from its original form during time evolution *even in a quadratic potential*. We shall refer to some of these states as *nonclassical states*, for reasons which will become clear in the sequel. The dynamics of the variance and the higher moments, governed essentially by the commutator $[\hat{p}\,,\,V(\hat{x})] = -i\hbar\,V'(\hat{x})$, becomes important in these cases.

It must be emphasized that expectation values are the objects in quantum physics that can be compared with the results of measurements. In contrast, the state vector of the system is not an observable. As a result, an exact reconstruction of the state from expectation values can be done only if the mean values and all the higher moments and cross-correlators of all relevant observables of the system are known. In general, this is an infinite set of expectation values, impossible to obtain in practice. *Quantum state reconstruction* is a challenging aspect of quantum physics.

Several interesting quantum states have been proposed and studied, especially in the context of quantum optics. The experimental realization of these states is a continuing endeavour. Many of these states exhibit properties which have no classical counterparts. In the second part of this article we shall examine the departures from 'classicality' exhibited by certain quantum states of radiation. This exercise will illustrate the various points made above regarding Ehrenfest's theorem and its applicability in different situations.

Suggested Reading

[1] **The article on Paul Ehrenfest in *Wikipedia*.**

[2] **M J Klein, *Paul Ehrenfest: The Making of a Theoretical Physicist*, Vol.1, 2nd Edition, Elsevier, Amsterdam, 1985.**

[3] **J J Sakurai, *Modern Quantum Mechanics*, International Student Edition, Addison Wesley Longman, Reading, Massachusetts, 1999.**

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