How to generalize the Ehrenfest theorem and the uncertainty principle

Klaus Renziehausen, Ingo Barth

Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany
Email: ksrenzie@mpi-halle.mpg.de, barth@mpi-halle.mpg.de

April 15, 2019

Abstract

The Ehrenfest theorem and the Robertson uncertainty relation are well-known basic equations in quantum mechanics. In both equations a commutator of two operators occurs, where for the Ehrenfest theorem one of these two operators is the Hamiltonian. For the correctness of the derivation of the Ehrenfest theorem, there arise problems if we use the azimuthal angle in polar or spherical coordinates as the other operator in this commutator. In addition, similar problems may occur for the derivation of the Robertson uncertainty relation if we use the azimuthal angle as one of the two operators in the commutator. As a consequence, there exist problematic cases, where the Ehrenfest theorem and the Robertson uncertainty relation are not correct. The purpose of this paper is to present and discuss a generalized Ehrenfest theorem and a generalized uncertainty relation being still valid for these problematic cases. Hereby, we define and use a mathematical operation called expectation commutator.

1 Introduction

In 1927, Paul Ehrenfest derived two differential equations being well-known as the Ehrenfest theorems that describe the time rate of change of the quantum mechanical expectation values of position and momentum [1]. In addition, there is another version of the Ehrenfest theorem that describes the time rate of change for the quantum mechanical expectation value for nearly any observable [2]. However, for the azimuth angle in cylindrical or spherical coordinates, this version of the Ehrenfest theorem is not valid because for this observable, mathematical difficulties occur for the calculation of the commutator of the azimuth angle and the $z$ component of the angular momentum [3–5]. Since the Hamilton operator of the system may contain the operator for the $z$ component of the angular momentum, these mathematical difficulties then appear for the calculation of the commutator of this Hamilton operator and the azimuth angle as well. As a consequence, we are confronted with the same problem as above for the application of the Ehrenfest theorem for the azimuth angle. At least, it is possible to circumvent this problem by considering a periodic function of the azimuth angle instead of the azimuth angle itself [6]. But we found a method to generalize the Ehrenfest theorem given in [2] so that this generalized Ehrenfest theorem is valid for this problematic case, too: Therefore, we define a new commutator type called expectation commutator and add a new term in the Ehrenfest theorem using this expectation commutator. As a result, the generalized Ehrenfest theorem found this way can be used to calculate the time rate of change of the expectation values for all observables including the azimuth angle. We discuss this in detail for a model system where we focus our analysis on...
the dependency of the Hamiltonian and the wave function on the azimuth angle.

Another well-known context in quantum mechanics is the Robertson uncertainty relation [7]. This is a relation for the product of the uncertainties of two observables, and it is a further development of the uncertainty relation of Heisenberg, who discussed in [8] the special case of the uncertainty relation of position and momentum. Now, as an additional point, for the Robertson uncertainty relation [7] the problems mentioned for the Ehrenfest theorem occur as well [3–5]. However, we can solve these problems by generalizing the Robertson uncertainty relation in an analogous manner like the Ehrenfest theorem, and in doing so, this generalized uncertainty relation can be applied for the $z$ component of the angular momentum and the azimuth angle, too. For the above-mentioned model system, we demonstrate this application of the generalized uncertainty relation.

2 The generalization of the Ehrenfest theorem

The time-dependent Schrödinger equation (TDSE)

$$i\hbar \frac{\partial \Psi}{\partial t} = H \Psi$$

with the Hamilton operator $H$ describes the time evolution of the wave function $\Psi$. In addition, for an observable with an associated operator $O$, its expectation value is given by:

$$\langle O \rangle = \langle \Psi | O | \Psi \rangle.$$  \hspace{1cm} (2)

Now, an equation for the time derivative of this expectation value $\langle O \rangle$ is derived. Therefore, we use the TDSE (1) and find:

$$\frac{d\langle O \rangle}{dt} = \frac{d}{dt} \langle \Psi | O | \Psi \rangle$$

$$= \left( \frac{\partial \Psi}{\partial t} \right) \langle O | \Psi \rangle + \langle \Psi | O \frac{\partial \Psi}{\partial t} \rangle + \langle \Psi \frac{\partial O}{\partial t} | \Psi \rangle$$

$$\quad = \frac{i}{\hbar} \left( \langle H\Psi | O\Psi \rangle - \langle \Psi | OH\Psi \rangle \right) + \left( \langle O \frac{\partial \Psi}{\partial t} \rangle \right)$$

$$\quad = \frac{i}{\hbar} \left( \langle H\Psi | O\Psi \rangle - \langle \Psi | HO\Psi \rangle + \langle \Psi | HO\Psi \rangle - \langle \Psi | OH\Psi \rangle \right) + \left( \langle \Psi \frac{\partial O}{\partial t} \rangle \right).$$  \hspace{1cm} (3)

As the next step, a mathematical operation is defined which we call the expectation commutator and designate with the symbol $\#$. For two operators $A$ and $B$, we apply the expectation commutator by the evaluation of

$$A\#B := \langle A\Psi | B\Psi \rangle - \langle \Psi | AB\Psi \rangle.$$  \hspace{1cm} (4)

Note that the term $A\#B$ is a complex number, while the result of the evaluation of an usual commutator

$$[A, B] := AB - BA$$  \hspace{1cm} (5)

is itself an operator. Then, using the Eqs. (4) and (5), we rewrite the Eq. (3) and find:

$$\frac{d\langle O \rangle}{dt} = \frac{i}{\hbar} \left( H\#O + \langle [H, O] \rangle \right) + \left( \langle \frac{\partial O}{\partial t} \rangle \right).$$  \hspace{1cm} (6)
On the other hand, the time derivative of an expectation value is described by the Ehrenfest theorem given by [2]:

\[
\frac{d\langle O \rangle}{dt} = \frac{i}{\hbar} \langle [H, O] \rangle + \left\langle \frac{\partial O}{\partial t} \right\rangle.
\]  

(7)

We realize that there is a difference between the Eq. (6) and the Ehrenfest theorem (7): In Eq. (6), an extra term

\[
\frac{i}{\hbar}(H \# O) = \frac{i}{\hbar} \left( \langle H \Psi | O \Psi \rangle - \langle O | H \Psi \rangle \right).
\]  

(8)

appears. Because of this context, we call Eq. (6) the generalized Ehrenfest theorem. Now, the question arises why this extra term appears in the generalized Ehrenfest theorem, and for which cases is it not zero?

To discuss this question, we take into account that the Hamilton operator \(H\) is a self-adjoint operator, and the wave functions in its domain \(H\) of Hilbert space describe quantum mechanical systems. Then, for two of these wave functions \(\Psi \in H\) and \(\Phi \in H\) holds:

\[
\langle H \Phi | \Phi \rangle = \langle \Phi | H \Phi \rangle.
\]  

(9)

Now, if we could assign the term \(O \Psi\) appearing in the extra term (8) to such a wave function \(\Phi\) in Eq. (9), so that \(O \Psi \in H\) is true, then it is trivial to show that the extra term (8) vanishes and the Ehrenfest theorem (7) is valid.

However, there are cases for which this assignment cannot be made, i.e. \(O \Psi \notin H\), and the extra term (8) does not vanish. Then, the Ehrenfest theorem (7) is not valid, and only the generalized Ehrenfest theorem (6) is correct. We will discuss such a concrete case in Sec. 4.

3 The generalization of the uncertainty principle

In the previous section, we explained the generalization of the Ehrenfest theorem. As an additional point, a similar analysis can be made for the uncertainty principle: Analyzing Robertson’s derivations about the uncertainty principle [27], one finds as an intermediate result of a straightforward calculation the following uncertainty relation for the uncertainties \(\Delta A\) and \(\Delta B\) of two observables with associated operators \(A\) and \(B\):

\[
\Delta A \Delta B \geq \frac{1}{2} |\langle A \Psi | B \Psi \rangle - \langle B \Psi | A \Psi \rangle|.
\]  

(10)

Then, we make the following transformation using both Eq. (1) for the expectation commutator and Eq. (5) for the normal commutator:

\[
\langle A \Psi | B \Psi \rangle - \langle B \Psi | A \Psi \rangle = A \# B - B \# A + \langle [A, B] \rangle.
\]  

(11)

Inserting this result into Eq. (10), we find:

\[
\Delta A \Delta B \geq \frac{1}{2} |A \# B - B \# A + \langle [A, B] \rangle|.
\]  

(12)

Now, we compare the result above with the well-known Robertson uncertainty relation [7]

\[
\Delta A \Delta B \geq \frac{1}{2} |\langle [A, B] \rangle|,
\]  

(13)

and find that two extra expectation commutators appear in Eq. (12). Thus, we call Eq. (12) the generalized uncertainty relation.

So, as an analogy to the situation for the generalized Ehrenfest theorem (6) and the Ehrenfest theorem (7), there are cases where the Robertson uncertainty relation (13) is not correct. For these cases, the term \(A \# B - B \# A\) does not vanish. In the next section, we will explain an example where this applies.
4 Applications

For the following applications, we analyze square-integrable wave functions \( \Psi(\varphi) \in \mathcal{H} \) of the azimuthal angle \( \varphi \) describing the quantum mechanical system. So, the domain for the azimuthal angle \( \varphi \) for these wave functions \( \Psi(\varphi) \) is restricted to the interval \([0, 2\pi]\), and since such wavefunctions \( \Psi(\varphi) \) are continuously differentiable \[9\], they fulfill the boundary conditions

\[
\Psi(0) = \Psi(2\pi) \quad \text{and} \quad \frac{\partial \Psi(\varphi)}{\partial \varphi} \bigg|_{\varphi=0} = \frac{\partial \Psi(\varphi)}{\partial \varphi} \bigg|_{\varphi=2\pi}.
\]  

(14)

For simplicity, we focus only on the coordinate \( \varphi \) and do not consider other coordinates in more detail. When we refer to the boundary conditions \[14\] in the text below using functions designated with other symbols than \( \Psi \), then \( \Psi \) has to be substituted in Eq. \[14\] by the symbols for these other functions.

For our system, we consider the following Hamilton operator

\[
H(\varphi) = \frac{1}{2I_z} L_z^2 + V(\varphi),
\]  

(15)

where \( L_z \) is the usual angular momentum operator \(-i\hbar \frac{\partial}{\partial \varphi}\) and \( I_z \) is the according moment of inertia being independent of \( \varphi \). Moreover, \( V(\varphi) \) is the potential. Here, this potential is just regarded because it appears typically in such a Hamilton operator describing the rotation around the \( z \) axis but it has no impact on the results of all further calculations.

For this model, we evaluate now the expectation commutator of the Hamiltonian with a real-valued function \( f(\varphi) \). Hereby, the domain of the function \( f(\varphi) \) does not need to be restricted to the interval \([0, 2\pi]\) and, in general, \( f(\varphi) \) does not fulfill the boundary conditions \[14\]. Using Eq. \[4\], we find:

\[
H(\varphi) \# f(\varphi) = \int_0^{2\pi} d\varphi \left[ (H(\varphi) \Psi(\varphi))^* f(\varphi) \Psi(\varphi) - \Psi^*(\varphi) H(\varphi) (f(\varphi) \Psi(\varphi)) \right]
\]

\[
= \frac{\hbar^2}{2I_z} \left[ \frac{2}{i} \left( f(0) - f(2\pi) \right) \triangle \left( \Psi^*(0) \frac{\partial \Psi(0)}{\partial \varphi} \right) \right]
\]

\[
+ \left( \frac{\partial f(\varphi)}{\partial \varphi} \bigg|_{\varphi=2\pi} - \frac{\partial f(\varphi)}{\partial \varphi} \bigg|_{\varphi=0} \right) |\Psi(0)|^2.
\]  

(16)

The result \[16\] shows that in general, the term \( H(\varphi) \# f(\varphi) \) does not vanish because \( f(\varphi) \) does not fulfill the boundary conditions \[14\]. Thus, in these general cases, it is the generalized Ehrenfest theorem \[6\], which has to be applied for the calculation of the time derivative \( \frac{df(\varphi)}{dt} \) and not the Ehrenfest theorem \[7\].

For this calculation, we evaluate the expectation value of the commutator \( [H(\varphi), f(\varphi)] \), too:

\[
\langle [H(\varphi), f(\varphi)] \rangle = \frac{\hbar^2}{2I_z} \left[ \frac{2}{i} \int_0^{2\pi} d\varphi \frac{\partial f(\varphi)}{\partial \varphi} \triangle \left( \Psi^*(\varphi) \frac{\partial \Psi(\varphi)}{\partial \varphi} \right) \right]
\]

\[
- \left( \frac{\partial f(\varphi)}{\partial \varphi} \bigg|_{\varphi=2\pi} - \frac{\partial f(\varphi)}{\partial \varphi} \bigg|_{\varphi=0} \right) |\Psi(0)|^2.
\]  

(17)

Then we find for the time derivative \( \frac{df(\varphi)}{dt} \) using the generalized Ehrenfest theorem \[6\]:

\[
\frac{d}{dt} \langle f(\varphi) \rangle = \frac{\hbar}{I_z} \left[ \left( f(0) - f(2\pi) \right) \triangle \left( \Psi^*(0) \frac{\partial \Psi(0)}{\partial \varphi} \right) \right] + \int_0^{2\pi} d\varphi \frac{\partial f(\varphi)}{\partial \varphi} \triangle \left( \Psi^*(\varphi) \frac{\partial \Psi(\varphi)}{\partial \varphi} \right).
\]  

(18)
The reason why the term $H(\varphi)\# f(\varphi)$ does not vanish generally can be analyzed using a context concerning the Eq. (10), which we explained in Sec. 2. As a consequence of this context, the term $H(\varphi)\# f(\varphi)$ would vanish if the function $\Phi(\varphi) := f(\varphi)\Psi(\varphi)$ could be interpreted as a wave function $\Phi(\varphi) \in \mathcal{H}$ describing the quantum mechanical system. But since the function $f(\varphi)$ does not fulfill the boundary conditions (14) generally, the function $\Phi(\varphi)$ does not fulfill the boundary conditions (14) generally, either, and cannot be related to a wave function describing the quantum mechanical system, i.e. $\Phi(\varphi) \notin \mathcal{H}$. However, for the special case of functions $f(\varphi)$ being $2\pi$ periodic like $\sin \varphi$ or $\cos \varphi$ the boundary conditions (14) hold for $f(\varphi)$. In this case, $\Phi(\varphi) \in \mathcal{H}$ is true and the term $H(\varphi)\# f(\varphi)$ given in Eq. (10) vanishes. So, for these periodic functions $f(\varphi)$, the Ehrenfest theorem (7) is valid again. This validity of the Ehrenfest theorem for $2\pi$ periodic functions $f(\varphi)$ was discussed already in (6).

In addition, in (10) one-dimensional wave functions are analyzed which fulfill periodic boundary conditions (14) generally, either, and cannot be related to a wave function describing the system. But since this term generally violates the Robertson uncertainty relation (13) if $L_z$ is not chosen appropriately, the application of the generalized uncertainty relation (12) for our system and the related results given in (10) are equivalent to a discussion of our system for a function $f(\varphi) = \varphi$. Beyond that context, it is discussed here that a generalized Ehrenfest theorem (9) exists which can be used to calculate the time derivative $\frac{d}{dt} f(\varphi)$ for all functions $f(\varphi)$, no matter if the expectation commutator $H(\varphi)\# f(\varphi)$ vanishes or not. In addition, the generalized Ehrenfest theorem (9) has a form for which it is clear that it turns into the Ehrenfest theorem (13) if the term $H(\varphi)\# f(\varphi)$ vanishes. As an additional detail, we mention that functions $f(\varphi)$ exist being not $2\pi$ periodic, but the expectation commutator $H(\varphi)\# f(\varphi)$ disappears for these functions $f(\varphi)$, too – for instance, this applies for the function $f(\varphi) = \varphi^2(\varphi - 2\pi)^2$ which is not $2\pi$ periodic but it fulfills already the boundary conditions (14). Thus, for this special function, the time derivative $\frac{d}{dt} f(\varphi)$ can be calculated within the Ehrenfest theorem (7), too.

In addition, we discuss now the application of the generalized uncertainty relation (12) for our system and the two operators $A = L_z$ and $B = f(\varphi)$. For this application, there are the two expectation commutators $f(\varphi)\# L_z$ and $L_z\# f(\varphi)$ in Eq. (12). While $f(\varphi)\# L_z$ vanishes trivially, we find for $L_z(\varphi)\# f(\varphi)$ the following result, which does not vanish generally:

$$L_z\# f(\varphi) = \int_0^{2\pi} d\varphi \left[ \left( \frac{\partial}{\partial \varphi} \right)^* f(\varphi) \Psi(\varphi) - \Psi^*(\varphi) L_z f(\varphi) \Psi(\varphi) \right] \right]$$

$$= \frac{\hbar}{i} \left( f(0) - f(2\pi) \right) |\Psi(0)\rangle^2.$$

(19)

So, for these general cases where $L_z\# f(\varphi) \neq 0$, the Robertson uncertainty relation (13) is not correct, but the generalized uncertainty relation (12) has to be applied instead. For this application of Eq. (12), we use the expectation value of the commutator $[L_z, \varphi]$

$$\langle [L_z, f(\varphi)] \rangle = \frac{\hbar}{i} \left\langle \frac{\partial f(\varphi)}{\partial \varphi} \right\rangle$$

(20)

and find

$$\Delta L_z \Delta f(\varphi) \geq \frac{\hbar}{2} \left| \left( f(0) - f(2\pi) \right) |\Psi(0)\rangle^2 + \left\langle \frac{\partial f(\varphi)}{\partial \varphi} \right\rangle \right|.$$

(21)

The explanation why the term $L_z\# f(\varphi)$ does not vanish in general cases, can be given in an analogous manner like we discussed the term $H(\varphi)\# f(\varphi)$ above: Being related to an observable, the operator $L_z$ is a self-adjoint operator. So, analogously to Eq. (9), for two wave functions $\Psi \in \mathcal{H}$ and $\Phi \in \mathcal{H}$ describing the system holds:

$$\langle L_z \Psi | \Phi \rangle = \langle \Psi | L_z \Phi \rangle.$$

(22)

Thus, the expectation commutator $L_z\# f(\varphi)$ would vanish if the term $f(\varphi)\Psi(\varphi)$ could be related to a wave function $\Phi(\varphi) \in \mathcal{H}$ describing the system. But since this term generally violates the
boundary conditions (14), that means \( f(\varphi)\Psi(\varphi) \not\in \mathcal{H} \), this is not possible \([5, 6]\). However, for \(2\pi\) periodic functions \( f(\varphi) \) the boundary conditions (14) are fulfilled by \( f(\varphi)\Psi(\varphi) \), so the expectation commutator \( L_z \# f(\varphi) \) is zero for this case, and the Robertson uncertainty relation (13) is valid again.

In literature, the problem that the application of the Robertson uncertainty relation (13) is problematic for the choice \( A = L_z \) and \( B = f(\varphi) \) is already discussed: In \([3,5]\), it is shown that if \( f(\varphi) \) is a \(2\pi\) periodic function, then the Robertson uncertainty relation (13) is valid again. In addition, in \([3,4]\) a generalized uncertainty relation for the special case \( f(\varphi) = \varphi \) is given. Beyond these results, we have derived here the Eq. (21) being valid for all functions \( f(\varphi) \), and we have derived a generalized uncertainty relation (12) for which it is transparent that it turns into the Robertson uncertainty relation (13) if the term \((A\#B - B\#A)\) vanishes.

5 Summary

In this paper, we have derived and discussed a generalized Ehrenfest theorem and a generalized uncertainty relation. Our motivation for this work is that the Ehrenfest theorem [2] and the Robertson uncertainty relation [7] are not valid generally. However, the Ehrenfest theorem turns out to be wrong when applied for the calculation of the time derivative of the expectation value for the azimuthal angle \( \varphi \) [6]. In addition, the Robertson uncertainty relation turns out to be wrong, too, when applied for the calculation of a lower boundary for the product of the uncertainties \( \Delta L_z \) and \( \Delta \varphi \) \([3,5]\). The deeper reason for this problem is the following context: In these cases, the function \( \Phi(\varphi) := \varphi\Psi(\varphi) \), where \( \Psi(\varphi) \) is a wave function describing the system, is not inside the domain of functions for which \( L_z \) is a self-adjoint operator \([3,5,6]\).

So, we had the idea to derive a generalized Ehrenfest theorem and a generalized uncertainty relation, where these mathematical problems do not appear anymore. Therefore, we defined an expectation commutator, and these generalized equations could be derived using this mathematical operator. There is a transparent connection of these generalized equations to the Ehrenfest theorem and the Robertson uncertainty relation:

In the generalized Ehrenfest theorem, there is an extra term which is calculated using the expectation commutator. If this extra term vanishes, the generalized Ehrenfest theorem turns into the Ehrenfest theorem given in textbooks. Analogously, in the generalized uncertainty relation, there is another extra term being calculated using the expectation commutator, too. Moreover, if this other extra term vanishes, the generalized uncertainty relation turns into the Robertson uncertainty relation.

References

[1] P. Ehrenfest, Z. Phys. 45, 455–457 (1927).
[2] F. Schwabl, Quantum Mechanics, (Springer-Verlag, Berlin, 2007), 4th ed., pp. 28 – 31, 97 – 99.
[3] P. Carruthers and M. M. Nieto, Rev. Mod. Phys. 40, 411 (1968).
[4] K. Kraus, Am. J. Phys. 38, 1489 (1970).
[5] L. C. Biedenharn and J. D. Louck, The Racah-Wigner Algebra in Quantum Theory, (Cambridge University Press, Cambridge, 1985), pp. 313 – 323.
[6] D. H. Kobe, Am. J. Phys. 51, 912 (1983).
[7] H. P. Robertson, Phys. Rev. 34, 163 (1929).
[8] W. Heisenberg, Z. Phys. 43, 172 (1927).

[9] W. Nolting, *Theoretical Physics 6, Quantum Mechanics - Basics*, (Springer Nature, Cham, 2017), pp. 236 – 238.

[10] R. N. Hill, Am. J. Phys. 41, 736 (1973).