

A sharp version of Ehrenfest's theorem for general self-adjoint operators

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We prove the Ehrenfest theorem of quantum mechanics under sharp assumptions on the operators involved.

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1. Introduction

While we know a great deal about analytical properties of the commutative algebra generated by a single unbounded self-adjoint operator (via a continuous or measurable functional calculus), much less is known mathematically about the non-commutative algebra generated by more than one such operator.

This note is concerned with Ehrenfest's theorem in quantum mechanics, which naturally involves pairs of non-commuting unbounded self-adjoint operators. For a quantum system that evolves via the time-dependent Schrödinger equation

$$i \frac{d}{dt} \psi(t) = H \psi(t), \quad (1.1)$$

Ehrenfest's theorem asserts that the time evolution of the quadratic forms

$$\langle \psi(t), A \psi(t) \rangle = \langle \psi(0), e^{iHt} A e^{-iHt} \psi(0) \rangle$$

is governed by the equation

$$\frac{d}{dt} \langle A \rangle_{\psi(t)} = i \langle [H, A] \rangle_{\psi(t)}. \quad (1.2)$$

Here, $\psi(t)$ belongs to a complex Hilbert space X , H and A are unbounded self-adjoint operators on X , $[H, A]$ denotes the commutator $HA - AH$ and $\langle A \rangle_{\varphi}$ stands for the quadratic form $\langle \varphi, A \varphi \rangle$. Of course, at the moment, the terms in the above equation are only formal, as it is not clear whether and where the required operator compositions are well defined.

Physically, $\psi(t)$ describes the state of the quantum system at time t , H is the Hamiltonian of the system (obtained, e.g. by quantizing an underlying classical Hamiltonian), A is an observable and the value of its quadratic form gives the

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expected value of the observable in a measurement. In Ehrenfest's (1927) original work, H was a Schrödinger operator of form $-\Delta + V(x)$ and A a component of the position or momentum operator. In this case, the left-hand side of equation (1.2) describes the expected value of a position or momentum measurement, and the right-hand side of equation (1.2) turns out to be the expected value of velocity respectively force, linking quantum mechanics to classical mechanics. Rigorous versions are not difficult to obtain in the context of classical, rapidly decaying solutions for smooth potentials (Blank *et al.* 1994) or when A is relatively bounded with respect to H , and play an important role in the analysis of space-time behaviour of Schrödinger wavefunctions (Hunziker 1966; Radin & Simon 1978) and scattering theory (Sigal & Soffer 1987; Graf 1990; Dereziński 1993; Dereziński & Gerard 1997). For a rigorous treatment of non-relatively bounded A and applications to atomic and molecular systems with Coulomb interactions, see Friesecke & Koppen (2009).

Our goal in this note is to prove the following sharp version of Ehrenfest's theorem for general self-adjoint operators.

Theorem 1.1 (Sharp Ehrenfest theorem). *Let $A : D(A) \rightarrow X$, $H : D(H) \rightarrow X$ be densely defined self-adjoint operators on a Hilbert space X . If e^{-itH} leaves $D(A) \cap D(H)$ invariant for all t , then for any $\psi_0 \in D(A) \cap D(H)$, the expected value $\langle A \rangle_{\psi(t)}$, $\psi(t) := e^{-itH}\psi_0$, is continuously differentiable with respect to t and satisfies equation (1.2), the right-hand side being understood in the inner product sense*

$$\langle [H, A] \rangle_{\psi} := \langle H\psi, A\psi \rangle - \langle A\psi, H\psi \rangle \quad (\psi \in D(A) \cap D(H)). \quad (1.3)$$

(Recall that a linear operator $A : D(A) \rightarrow X$ defined on a subspace $D(A)$ of a Hilbert space X is called hermitean when $\langle A\psi, \varphi \rangle = \langle \psi, A\varphi \rangle$ for all $\psi, \varphi \in D(A)$, and self-adjoint if in addition the domain $D(A)$ is dense and in a suitable sense maximal, e.g. Reed & Simon (1980). Self-adjoint operators H generate a one-parameter unitary group e^{-itH} ; Reed & Simon (1980).) Note that the hypothesis above that $\psi(t) = e^{-itH}\psi_0$ belongs to $D(A)$ for all t is necessary for the element $A\psi(t)$ appearing in the inner product in equation (1.2) to be well defined. Thus, Ehrenfest's theorem always holds when it makes sense in an operator-theoretic setting. (Conceivable abstract extensions of the expressions in equation (1.2) to quadratic form domains are not investigated here.)

From an analysis point of view, an interesting aspect of the result is the automatic higher regularity of the expected value $\langle A \rangle_{\psi(t)}$ in time; *a priori* it is not even clear that $t \mapsto \langle A \rangle_{\psi(t)}$ is continuous.

Self-adjointness of A cannot be weakened to hermiteanity; otherwise, even continuity of $t \mapsto \langle A \rangle_{\psi(t)}$ can fail. See the counterexample at the end of this note. This phenomenon is not obvious, as only H is required to generate a unitary group in order for the expected values appearing in equation (1.2) to be well defined.

Proof. Starting point is the following result of Friesecke & Koppen (2009), which involves a weaker assumption on the operator A (densely defined hermitean instead of self-adjoint) but a stronger assumption on the 'coupling' between the unitary group e^{-itH} and the operator A (see (H3) below).

Proposition 1.2 (Friesecke & Koppen 2009). *Let H and A be two densely defined linear operators on X such that*

- (H1) $H : D(H) \rightarrow X$ is self-adjoint, $A : D(A) \rightarrow X$ is hermitean;
- (H2) e^{-itH} leaves $D(A) \cap D(H)$ invariant for all $t \in \mathbb{R}$;
- (H3) for any $\psi_0 \in D(A) \cap D(H)$, $\sup_{t \in I} \|A e^{-itH} \psi_0\| < \infty$ for $I \subset \mathbb{R}$ bounded.

Then, for $\psi_0 \in D(A) \cap D(H)$, the expected value $\langle A \rangle_{\psi(t)}$, $\psi(t) := e^{-itH} \psi_0$, is continuously differentiable with respect to t and satisfies equation (1.2), the right-hand side being understood in the sense of equation (1.3).

For completeness, we sketch the (simple) proof. Consider the difference quotient

$$\frac{\langle \psi(t+h), A\psi(t+h) \rangle - \langle \psi(t), A\psi(t) \rangle}{h} \\ = \left\langle A\psi(t+h), \frac{\psi(t+h) - \psi(t)}{h} \right\rangle + \left\langle \frac{\psi(t+h) - \psi(t)}{h}, A\psi(t) \right\rangle.$$

As $h \rightarrow 0$, the second term goes to $i\langle H\psi(t), A\psi(t) \rangle$, as $((\psi(t+h) - \psi(t))/h) \rightarrow -iH\psi(t)$ strongly owing to the strong differentiability of the unitary group $\{e^{-itH}\}_{t \in \mathbb{R}}$ on $D(H)$. The first term goes to $-i\langle A\psi(t), H\psi(t) \rangle$ as the first factor $A\psi(t+h)$, being bounded by (H3), converges weakly up to subsequences to a limit $f \in X$, which must equal $A\psi(t)$ as

$$\langle f, \varphi \rangle = \lim_{h_j \rightarrow 0} \langle A\psi(t+h_j), \varphi \rangle = \lim_{h_j \rightarrow 0} \langle \psi(t+h_j), A\varphi \rangle = \langle \psi(t), A\varphi \rangle = \langle A\psi(t), \varphi \rangle$$

for φ 's belonging to the dense subset $D(A)$. Hence, the whole sequence $A\psi(t+h)$ tends weakly to $A\psi(t)$, and so $\langle A \rangle_{\psi(t)}$ is differentiable with respect to t and satisfies equation (1.2). Continuity of the derivative follows by combining the above weak convergence with the strong convergence of $H\psi(t+h)$ to $H\psi(t)$.

Theorem 1.1 is an immediate consequence of proposition 1.2 and the following:

Proposition 1.3. *Let H and A be two densely defined operators on X such that*

- (H1') $H : D(H) \rightarrow X$ is self-adjoint, $A : D(A) \rightarrow X$ is hermitean and closed;
- (H2) $T(t) := e^{-itH}$ leaves $D(A) \cap D(H)$ invariant for all $t \in \mathbb{R}$.

Then, for any $\psi_0 \in D(A) \cap D(H)$, $\sup_{t \in I} \|AT(t)\psi_0\| < \infty$ for $I \subset \mathbb{R}$ bounded.

Proof. Throughout the proof, we fix $\psi_0 \in D(A) \cap D(H)$.

(i) We claim that there exists a non-empty interval $I = (a, b)$ such that $\sup_{t \in I} \|AT(t)\psi_0\| < \infty$.

This can be established with the help of the Baire category theorem, as follows. Consider the sets $E_n := \{t \in \mathbb{R} : \|AT(t)\psi_0\| \leq n\}$, $n \in \mathbb{N}$. Because $T(t)\psi_0 \in D(A)$ for all t , we have $\cup_{n \in \mathbb{N}} E_n = \mathbb{R}$. Moreover, E_n is closed. Namely, suppose $t_j \in E_n$, $t_j \rightarrow t$. Then, $\|AT(t_j)\psi_0\| \leq n$, and so $\{AT(t_j)\psi_0\}$ is a bounded sequence in X . Hence, for a subsequence, again denoted t_j , $AT(t_j)\psi_0 \rightharpoonup \chi$ weakly in X , and by weak lower

semi-continuity of the norm, $\|\chi\| \leq \liminf_{j \rightarrow \infty} \|AT(t_j)\psi_0\|$, whence $\|\chi\| \leq n$. To infer that E_n is closed, it suffices to show that $\chi = AT(t)\psi_0$. But for all $\eta \in D(A)$, using the weak convergence of $AT(t_j)\psi_0$, the hermiteanity of A , and the continuity of $T(t)\psi_0$ in t ,

$$\langle \eta, \chi \rangle = \lim_{j \rightarrow \infty} \langle \eta, AT(t_j)\psi_0 \rangle = \lim_{j \rightarrow \infty} \langle A\eta, T(t_j)\psi_0 \rangle = \langle A\eta, T(t)\psi_0 \rangle = \langle \eta, AT(t)\psi_0 \rangle.$$

As $D(A)$ is dense, $AT(t)\psi_0 = \chi$, as asserted. By the Baire category theorem, the countable union of the E_n cannot be of first category; so, the closure of some E_n must contain an open set. As this E_n is closed, it must contain an open set, and the assertion of Step (i) follows. We remark that this step did not use the closedness of the operator A .

(ii) We claim that there exists an open interval containing 0 such that $\sup_{t \in I} \|AT(t)\psi_0\| < \infty$.

To see this, the idea is to use the group property of $T(t)$ as well as an appropriate norm on $D(A) \cap D(H)$ with respect to which $AT(t)$ is a continuous map into X . Let $t_0 := ((a+b)/2)$ be the midpoint of the interval from Step (i), and let $t \in (a, b)$. Then,

$$\begin{aligned} \|AT(-t_0+t)\psi_0\| &= \|AT(-t_0)T(t)\psi_0\| \\ &\leq \sup_{\eta \in D(A) \cap D(H) \setminus \{0\}} \frac{\|AT(-t_0)\eta\|}{\|\eta\|_E} \cdot \|T(t)\psi_0\|_E, \end{aligned} \quad (1.4)$$

for any norm $\|\cdot\|_E$ on $D(A) \cap D(H) =: E$. The art now is to choose the norm in such a way that the first factor on the right is finite, and the second factor is uniformly bounded for $t \in (a, b)$. A natural candidate for such a norm is $\|\cdot\|_E := \|\cdot\| + \|A \cdot\| + \|H \cdot\|$. By Step (i) and the fact that $\|T(t)\psi_0\|$ and $\|HT(t)\psi_0\|$ are conserved, the second factor satisfies

$$\begin{aligned} \sup_{t \in (a,b)} \|T(t)\psi_0\|_E &= \sup_{t \in (a,b)} \left(\|T(t)\psi_0\| + \|AT(t)\psi_0\| + \|HT(t)\psi_0\| \right) \\ &= \|\psi_0\| + \|H\psi_0\| + \sup_{t \in (a,b)} \|AT(t)\psi_0\| < \infty. \end{aligned} \quad (1.5)$$

To see that the first factor on the r.h.s. of equation (1.4) is finite is less easy.

First, we claim that E with the above norm is a Banach space. This is a variant of the familiar fact that the domain $D(A)$ of a closed operator endowed with the graph norm $\|\psi\| + \|A\psi\|$ is a Banach space, and is straightforward to verify using the closedness of A and H .

Next, we claim that $B := AT(-t_0)$ is a closed operator from E to X . (Clearly, B is defined on all of E , because $T(-t_0)$ maps $D(A)$ into $D(A)$ by (H2).) To prove this, we have to show that if $\psi_j \in E$, $\psi_j \rightarrow \psi$ in E and $B\psi_j \rightarrow \eta$ in X , then $\psi \in D(B)$ and $B\psi = \eta$. As B is defined on all of E , the first condition is satisfied. To show that $B\psi = \eta$, we use that $\|\psi_j - \psi\|_X \leq \|\psi_j - \psi\|_E$, and so $\psi_j \rightarrow \psi$ in X . By the boundedness of $T(-t_0) : X \rightarrow X$, it follows that $T(-t_0)\psi_j \rightarrow T(-t_0)\psi$ in X . Because $AT(-t_0)\psi_j \rightarrow \eta$ in X and A is closed, $T(-t_0)\psi \in D(A)$ and $AT(-t_0)\psi = \eta$. Thus, $B\psi = \eta$, as was to be shown.

Finally, we appeal to the closed graph theorem: $B: E \rightarrow X$ is a closed linear operator between Banach spaces, and must hence be bounded. Consequently,

$$\|AT(-t_0)\|_{L(E,X)} := \sup_{\eta \in E \setminus \{0\}} \frac{\|AT(-t_0)\eta\|}{\|\eta\|_E} < \infty, \quad \text{for all } t_0 \in \mathbb{R}. \quad (1.6)$$

Together with equations (1.4) and (1.5), this establishes the assertion of Step (ii).

(iii) We claim that on any bounded interval $I \subset \mathbb{R}$, $\sup_{t \in I} \|AT(t)\psi_0\| < \infty$.

By Step (ii), there exist $\varepsilon > 0$, $C > 0$ such that $\|AT(t)\psi_0\| \leq C$ for all $|t| \leq \varepsilon$. Next, consider $\varepsilon \leq |t| \leq 2\varepsilon$. For each such t , $T(t)$ can be written as $T(\varepsilon)T(s)$ or $T(-\varepsilon)T(s)$ for some $|s| \leq \varepsilon$. Clearly for $\psi_0 \in D(A) \cap D(H) = E$

$$\|AT(\pm\varepsilon)T(s)\psi_0\| \leq \|AT(\pm\varepsilon)\|_{L(E,X)} \sup_{|s| \leq \varepsilon} \|T(s)\psi_0\|_E \leq \|AT(\pm\varepsilon)\|_{L(E,X)} C, \quad (1.7)$$

the above operator norm being finite owing to equation (1.6). Hence,

$$\|AT(t)\psi_0\| \leq \underbrace{\max\{\|AT(\varepsilon)\|_{L(E,X)}, \|AT(-\varepsilon)\|_{L(E,X)}\}}_{=:M} C, \quad \text{for all } |t| \leq 2\varepsilon.$$

Iterating gives $\|AT(t)\psi_0\| \leq M^{n-1}C$ for all $|t| \leq n\varepsilon$, for any $n \in \mathbb{N}$. This completes the proof of proposition 1.3. \blacksquare

Proposition 1.3 could alternatively be proved by recourse to known but non-trivial results in the theory of C_0 -groups. One first deduces from restriction properties of C_0 -groups (Amrein *et al.* 1996, proposition 3.2.5) that $T(t)$ defines a C_0 -group on $D(A) \cap D(H)$ with respect to the graph norm of the pair of A and H . This, however, requires a considerable amount of machinery, in particular a characterization of C_0 -groups on Banach spaces with separable dual via weak Borel measurability. One then appeals to known locally uniform bounds on norms of C_0 -groups (Amrein *et al.* 1996, proposition 3.2.2) which are related to the fact that measurable solutions to the functional inequality $e^{t+s} \leq e^t e^s$ are locally uniformly bounded. By contrast, the proof given above only uses basic functional analysis.

Observe that in fact it suffices to assume in theorem 1.1 that A be a closed hermitean operator, required to be neither densely defined nor self-adjoint. This can be seen by replacing A by PAP , where P denotes the orthogonal projection from X to $\tilde{X} := \overline{\text{span}}\{\psi(t) : t \in \mathbb{R}\}$, and by applying propositions 1.3 and 1.2 to \tilde{X} instead of X .

Counterexample. The following example shows that the assumption in Ehrenfest's theorem that A be self-adjoint cannot be weakened to hermitean (and that the assumption in proposition 1.3 that A be closed cannot be dropped).

Let $X = L^2(\mathbb{R})$, $H = -i(d/dx)$, so that the unitary group e^{-itH} acts by translation: $e^{-itH}\psi_0(x) = \psi_0(x-t)$. The idea is that the finite linear span of a well-chosen single orbit $\{\psi(t) : t \in \mathbb{R}\}$, $\psi(t) = e^{-itH}\psi_0$, contains infinitely many functions φ_j with disjoint support contained in a single bounded interval. The φ_j can be constructed such that $\psi(t)$ becomes 'resonant' with the projectors $P_j = |\varphi_j\rangle\langle\varphi_j|$ at particular times t_j , whereas at these times it is annihilated by all the other projectors. One then takes A to be a suitable linear combination of these projectors P_j on $\text{span}\{\psi(t) : t \in \mathbb{R}\}$, extended by 0 on the orthogonal complement.

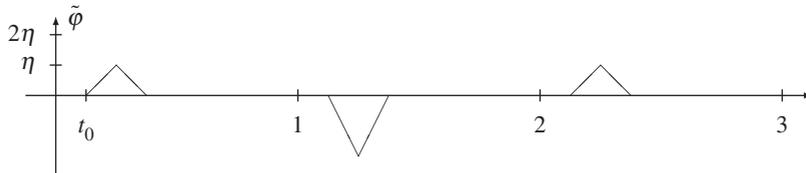


Figure 1. $\tilde{\varphi}$.

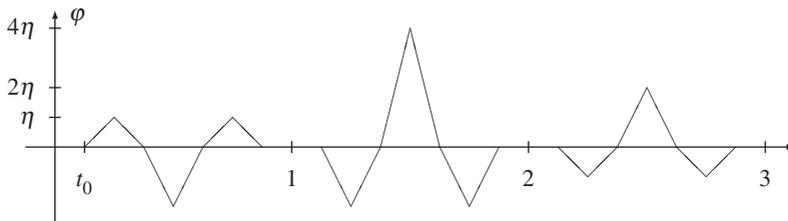


Figure 2. φ .

Let $\psi_0 \in D(H) = H^1(\mathbb{R})$ be the ‘tent’ function with $\psi_0(0) = \psi_0(2) = 0$, $\psi_0(1) = 1$ and such that ψ_0 is linear on each of the intervals $(-\infty, 0)$, $(0, 1)$, $(1, 2)$, $(2, \infty)$.

(i) If I is any open subinterval of $(0, 1)$, we can choose $\varphi \in \text{span}\{\psi(t) : t \in I\} \setminus \{0\}$ (meaning finite linear combinations) such that $\varphi \perp \text{span}\{\psi(t) : t \notin I + \mathbb{Z}\}$ in the following way. Let $t_0, t_0 + 6\eta \in I$ and in order to achieve small support consider the second difference $\tilde{\varphi} := \psi(t_0) - 2\psi(t_0 + \eta) + \psi(t_0 + 2\eta) = \psi_0(\cdot - t_0) - 2\psi_0(\cdot - (t_0 + \eta)) + \psi_0(\cdot - (t_0 + 2\eta))$. Then, $\tilde{\varphi} \neq 0$ is supported on $[t_0, t_0 + 2\eta] + \{0, 1, 2\}$. In fact, on $(0, 1)$ $\tilde{\varphi}$ is the piecewise linear interpolation of $\tilde{\varphi}(t_0) = 0$, $\tilde{\varphi}(t_0 + \eta) = \eta$, $\tilde{\varphi}(t_0 + 2\eta) = 0$ and $\tilde{\varphi}(t + 1) = -2\tilde{\varphi}(t)$, $\tilde{\varphi}(t + 2) = \tilde{\varphi}(t)$ for $t \in [0, 1]$, see figure 1.

Now, to achieve orthogonality to affine functions, take again a second difference, $\varphi := \tilde{\varphi} - 2\tilde{\varphi}(\cdot - 2\eta) + \tilde{\varphi}(\cdot - 4\eta) = \psi(t_0) - 2\psi(t_0 + \eta) - \psi(t_0 + 2\eta) + 4\psi(t_0 + 3\eta) - \psi(t_0 + 4\eta) - 2\psi(t_0 + 5\eta) + \psi(t_0 + 6\eta)$, see figure 2. Then, $\varphi \in \text{span}\{\psi(t) : t \in I + \mathbb{Z}\} \setminus \{0\}$, and φ is supported on $[t_0, t_0 + 6\eta] + \{0, 1, 2\}$ and one easily sees that $\int_{t_0+k}^{t_0+6\eta+k} x\varphi(x) dx = 0$ for all $k \in \mathbb{Z}$. Now, if $t \notin I + \mathbb{Z}$, then $\psi(t)$ is linear on each interval $(t_0 + k, t_0 + 6\eta + k)$, and so we obtain that indeed $\langle \psi(t), \varphi \rangle = 0$.

(ii) Now, choose infinitely many pairwise disjoint open intervals $I_j \subset (0, 1)$, $j \in \mathbb{N}$. Choosing vectors corresponding to the interval I_j as described in step (i) and normalizing, we obtain an orthonormal system (φ_j) . To each $\varphi_j \in \text{span}\{\psi(t) : t \in I_j\}$, we may also choose $t_j \in I_j$ and $a_j \in \mathbb{R}$ such that $a_j |\langle \varphi_j, \psi(t_j) \rangle|^2 > j$. We then define the hermitean operator A on $D(A) := \text{span}\{\psi(t) : t \in \mathbb{R}\} \oplus \text{span}\{\psi(t) : t \in \mathbb{R}\}^\perp$ by

$$A\psi := \sum_{j \in \mathbb{N}} a_j \langle \varphi_j, \psi \rangle \varphi_j$$

on $\text{span}\{\psi(t) : t \in \mathbb{R}\}$ and zero on its orthogonal complement. (Note that by construction, the sum in this definition is in fact finite.) Then, A is a densely defined hermitean operator such that $D(A) \cap D(H)$ is invariant under e^{-itH} . But

$\langle A \rangle_{\psi(t)}$ is not bounded on $(0, 1)$ because on I_j

$$\langle \psi(t), A\psi(t) \rangle = \langle \psi(t), \sum_{j \in \mathbb{N}} a_j \langle \varphi_j, \psi(t) \rangle \varphi_j \rangle = a_j |\langle \psi(t), \varphi_j \rangle|^2,$$

in particular, $\langle \psi(t_j), A\psi(t_j) \rangle > j$.

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