Conceptual Inconsistencies of Finite-dimensional Quantum and Classical Dynamics

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(Dated: December 19, 2011)

By attempting to derive the finite-dimensional quantum and classical mechanics within the recently develop technique of Ehrenfest quantization \([\text{D. I. Bondar \textit{et al.}} (2011) \text{arXiv:1105.4014}]\), we demonstrate that no finite-dimensional quantum and classical dynamics satisfy the Ehrenfest theorems. Non-Hermitian dynamics is shown to suffer from the same problems. Other peculiarities, such as the non-existence of the free particle case and the ambiguity in defying potential forces, are exposed.

PACS numbers: 03.65.-w

\textbf{Introduction.} Quantum mechanics in a finite-dimensional Hilbert space is experiencing renewed interest in the light of many applications in quantum information science, quantum optics, numerical methods, and physics of the Plank length. In the current paper, by attempting to derive finite-dimensional quantum and classical mechanics within the Ehrenfest quantization, we will reveal their fundamental inconsistencies in describing dynamics.

The Ehrenfest quantization is a novel method for derivation of dynamical equations from average values’ evolution. In Ref. \([22]\), along with many other applications, we utilized this technique to infer the classical Liouville and Schrödinger equations from the Ehrenfest theorems

\[
m \frac{d}{dt} \langle \Psi(t) | \hat{\dot{x}} | \Psi(t) \rangle = \langle \Psi(t) | \hat{\dot{p}} | \Psi(t) \rangle, \tag{1}
\]

\[
d \langle \Psi(t) | \hat{p} | \Psi(t) \rangle = \langle \Psi(t) | -U'(\hat{x}) | \Psi(t) \rangle, \tag{2}
\]

by only assuming that the coordinate \(\hat{x}\) and momentum \(\hat{p}\) operators commute in the former case and obey the canonical commutation relation in the latter. (We consider systems with one spatial coordinate throughout the paper even though the reached conclusions are valid for any number of spatial coordinates.) However, this derivation breaks down within a finite-dimensional Hilbert space because no finite-dimensional operators obey the canonical commutation relation \([1]\).

What is the finite-dimensional analog of the coordinate and momentum operators? To answer this question, we recall the physical origin of the canonical commutation relation. Utilizing group-theoretic arguments, Wely demonstrated \([1]\) (see also Ref. \([3]\)) that

\[
| \langle x | p \rangle |^2 = \text{const} \iff [\hat{x}, \hat{p}] = i\hbar \tag{3}
\]

(an alternative derivation of this correspondence was put forth in Ref. \([23]\)). Contrary to the r.h.s., the l.h.s. of Eq. \((3)\) is meaningful in a finite-dimensional setting. Thus, in the literature on finite-dimensional quantum mechanics, the coordinate and momentum operators are unanimously defined as ones whose eigenvectors obey

\[
\langle x_n | p_k \rangle = \exp(i2\pi nk/N)/\sqrt{N}, \tag{4}
\]

where \(n, k = -j, -j+1, \ldots, j-1, j, j = 2N+1, \hat{x}|x_n\rangle = an|x_n\rangle, \hat{p}|p_k\rangle = 2\pi \hbar k/(aN)|p_k\rangle, \) and \(N\) is the Hilbert space’s dimension (for a detailed description of the notation see tutorial \([15]\)). The eigenvectors of these coordinate and momentum operators form mutually unbiased bases. The adjective “unbiased” physically means that if a system is prepared in a state belonging to one of the bases, then all outcomes of the measurement with respect to the other basis occurs with equal probabilities.

The finite-dimensional Schrödinger equation is of the form

\[
\frac{i\hbar}{d} \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle, \tag{5}
\]

where the Hamiltonian \(\hat{H}\) needs to be defined. There are at least two independent ways of introducing \(\hat{H}\). First, the following Hamiltonian

\[
\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x}), \tag{6}
\]

is adapted with the specification that the coordinate and momentum operators are defined by Eq. \((4)\). Such a choice is nearly a tacit definition of the Hamiltonian in finite-dimensional quantum mechanics. Second, in the infinite-dimensional coordinate representation, the first term of the Hamiltonian \(\hat{H}\) is proportional to the second derivative. An alternative definition of \(\hat{H}\) is achieved once this term is approximated by a finite difference. This is a widely used approach in numerical calculations (see, e.g., Ref. \([24]\)). Evidently that the listed two forms of \(\hat{H}\) are drastically different even though they share the same limit when \(N \to \infty\).

Which definition is more fundamental? The Ehrenfest quantization is a well-suited framework for addressing such a question. We shall demonstrate that all finite-dimensional representations of quantum and classical dynamics are plagued with inconsistencies; in particular, Eq. \((2)\) is always violated while Eq. \((1)\) may...
or may not be satisfied. This conclusion is valid in spite of finite-dimensional formulations providing arbitrary accurate numerical approximations for the infinite-dimensional case.

**Inconsistencies of Finite-dimensional Mechanics.** First and foremost, we apply the Ehrenfest quantization [22] to Eqs. (1) and (2) bearing in mind that \( \hat{x} \) and \( \hat{\rho} \) are some matrices of a finite size. Stone’s theorem (see, e.g., Ref. [22, 23]) guarantees the uniqueness of the Hermitian operator \( \hat{H} \) in Eq. (3). Applying the chain rule to the l.h.s. of Eqs. (1–2) and then utilizing Eq. (5), one obtains

\[
i \hat{H}, \hat{x} = i \hbar \hat{\rho}, \quad \hat{i} \hat{H}, \hat{\rho} = -\hbar U'(\hat{x}). \tag{7}
\]

We shall demonstrate below that Eqs. (7) and (8) cannot be satisfied by non-trivial finite-dimensional operators leading to the invalidity of the Ehrenfest theorems. The root of all the problems is the nonexistence of finite-dimensional operators obeying the canonical commutation relation.

**Theorem 1.** Assume that \( \hat{\rho} \) and \( \hat{H} \) are non-zero finite-dimensional Hermitian operators. If \( [\hat{H}, \hat{\rho}] = 0 \) then there is no finite-dimensional linear operator \( \hat{x} \) such that \( \hat{i}[\hat{H}, \hat{x}] = \hat{\rho} \).

**Proof.** Let \( |E_n\rangle \) denote an eigenvector of \( \hat{H} \) such that \( \hat{H} |E_n\rangle = E_n |E_n\rangle \). Since the operators \( \hat{H} \) and \( \hat{\rho} \) commute, \( \hat{\rho} |E_n\rangle = p_n |E_n\rangle \). Assuming that \( \hat{i}[\hat{H}, \hat{x}] = \hat{\rho} \), one obtains

\[
i \langle E_n | \hat{H}, \hat{x} | E_m \rangle = i \langle E_n - E_m | \langle E_n | \hat{x} | E_m \rangle = p_m \langle E_n | E_m \rangle, \tag{9}
\]

\( \forall n, m \). The special case of this identity, when \( n = m \), reads \( p_n = 0 \), \( \forall m \). This contradicts the assumption that \( \hat{\rho} \) is a non-zero matrix.

The physical meaning of Theorem 1 is that there is no notion of the free particle in finite-dimensional quantum mechanics. This statement is also a consequence of the probability conservation, which is closely linked to Stone’s theorem. If the wave function’s normalization is constant in time and \( \hat{x} \) is finite-dimensional, then particle’s motion is confined to the interval bounded by the smallest and largest eigenvalues of \( \hat{x} \). This confinement must be realized by a force. Since standalone Eq. (7) is solvable with respect to \( \hat{H} \) [see Eq. (13) below], then \( \hat{i}[\hat{H}, \hat{\rho}] / \hbar \) from Eq. (10) can be considered as the definition of the confining force. Note that the Ehrenfest theorems do not hold for a particle in a box in the infinite-dimensional case as well [27].

The following statement demonstrates that the finite-dimensional classical mechanics is more complicated than quantum one:

**Theorem 2.** Let \( \hat{x} \) and \( \hat{\rho} \) be non-zero finite-dimensional Hermitian operators with \([\hat{x}, \hat{\rho}] = 0 \). There is no finite-dimensional operator \( \hat{L} \) such that \( \hat{i}[\hat{L}, \hat{x}] = \hat{\rho} \).

**Proof.** Let \( |n\rangle \) denote a common eigenvector for the operators \( \hat{x} \) and \( \hat{\rho} \) : \( \hat{x} |n\rangle = x_n |n\rangle \), \( \hat{\rho} |n\rangle = \rho_n |n\rangle \). “Sandwiching” the identity \( \hat{i}[\hat{L}, \hat{x}] = \hat{\rho} \) between these eigenstate, we obtain

\[
i \langle n | \hat{L} | k \rangle (x_k - x_n) = \rho_n \langle n | k \rangle. \tag{10}
\]

If \( n = k \), then \( \rho_n = 0 \), \( \forall n \), i.e., \( \hat{\rho} \) is a zero matrix. This contradicts the assumption of the theorem.

**Theorem 3.** There are no finite-dimensional operators \( \hat{A} \) and \( \hat{B} \) such that

\[
[f(\hat{A}), \hat{B}] = f'(\hat{A}), \tag{11}
\]

for any “good” function \( f(z) \).

**Proof.** Let a function of an operator be defined as

\[
f(\hat{A}) := \int g(k)e^{ik\hat{A}} dk, \quad f'(\hat{A}) := \int ikg(k)e^{ik\hat{A}} dk,
\]

where \( g(k) \) is the Fourier transform of a function \( f(z) \). The correctness of Eq. (11) implies that

\[
[e^{ik\hat{A}}, \hat{B}] = ike^{ik\hat{A}}. \tag{12}
\]

Differentiating the last identity with respect to \( k \) and setting \( k = 0 \), we reach the contradiction \( [\hat{A}, \hat{B}] = 1 \).

This theorem implies that Eq. (8) never has a solution. Furthermore, theorem 3 indicates that contrary to the infinite-dimensional case, there are two nonequivalent ways \( \hat{F} = -U'(\hat{x}) \) and \( \hat{F} = i[U(\hat{x}), \hat{\rho}] / \hbar \) to introduce the notion of a potential force \( \hat{F} \) in a finite-dimensional setting. Taking into account the comment after Theorem 1 the latter definition should be preferred.

**Illustrations.** Assuming \( \hat{x} \) is Hermitian and has a non-degenerate spectrum, a solution of Eq. (7) reads

\[
\langle x_k | \hat{H}^* | x_l \rangle = \begin{cases} 
U(x_k) + C & \text{if } k = l \\
\frac{i}{m} \left( \delta_{k,k+1} - \delta_{k,k-1} \right) & \text{otherwise}
\end{cases}
\]

where \( \hat{x} |x_k\rangle = x_k |x_k\rangle \) and \( C \) is an arbitrary real constant. For any definition of the momentum operator \( \hat{\rho} \), Eq. (13) provides the most general form of a Hamiltonian satisfying the first Ehrenfest theorem [Eq. (10)].

The simplest finite-difference approximation of derivative is \( d\Psi(x_k)/dx \approx [\Psi(x_{k+1}) - \Psi(x_{k-1})] / (2a) \). We choose the equally spaced eigenvalues (with step \( a \)) of the coordinate operator, then \( (x_k | \hat{p} | x_l) = -i\hbar (\delta_{l,k+1} - \delta_{l,k-1}) / (2a) \). From Eq. (13), one obtains

\[
\langle x_k | \hat{H}_{fd} | x_l \rangle = \frac{-\hbar^2}{2ma^2} (\delta_{l,k+1} + \delta_{l,k-1}) + [U(x_k) + C] \delta_{l,k}, \tag{14}
\]

which is the well known finite-difference approximation of the operator: \( -\hbar^2 / (2m) a^2 \partial^2 / dx^2 + U(x) \). Therefore, the
The simplest finite-difference approximation for the Hamiltonian indeed obeys Ehrenfest theorem [1]. The Hamiltonian $\hat{H}_{mub}$ from Eq. (13) with $\hat{p}$ from Eq. (4) also satisfies Eq. (1). However, the finite-dimensional Hamiltonian $\hat{H}_{mub}$ from Eq. (6) with $\hat{p}$ from Eq. (4) does not satisfy the Ehrenfest theorems.

Considering the example of the singular Harmonic oscillator,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{\omega^2}{8} x^2 + \frac{g}{4x^2}, \quad 0 \leq x < \infty,$$

which has a convenient analytic solution [28], we demonstrate in Figs. 1 and 2 that the accuracy of numerical calculations does not depend on whether an approximate finite-dimensional Hamiltonian obeys Ehrenfest theorem [1]. In the case of the Hamiltonian $\hat{H}_{mub}^*$ and $\hat{H}_{mub}$, the values for the coordinate step size, $a$, are selected to minimize the largest eigenvalues of $\hat{H}_{mub}^*$ and $\hat{H}_{mub}$, respectively. Such a choice of the step size gives the best fit between the approximate spectra and the exact results [see Figs. 1(b) and 1(c)]. However, this does not work in the case of the Hamiltonian $\hat{H}_{fd}^*$. The value of $a$ for $\hat{H}_{fd}^*$ needs to be manually adjusted to achieve the best fit. The purpose of this fitting is to demonstrate [see Fig. 2(a)] that the Hamiltonian $\hat{H}_{fd}^*$ is not suited for calculating highly excited states despite reproducing the spectrum better than $\hat{H}_{mub}^*$ and $\hat{H}_{mub}$. Finally, note that the Hamiltonian $\hat{H}_{mub}^*$, which satisfies Ehrenfest theorem [1], provides the same quality results as the Hamiltonian $\hat{H}_{mub}$ that does not obey Eq. (1).

A Non-Hermitian Hamiltonian as an Unsuccessful Attempt to Fix the Inconsistencies. Non-Hermitian Hamiltonians are widely employed in physics to model resonant and unbound states (see, e.g., Refs. [29, 30] and references therein) and as a handy trick to avoid numerical artifacts related to the finiteness of spatial grids (see, e.g., Ref. [31]). Despite tremendous practical advantages, we shall demonstrate that non-Hermitian Hamiltonians do not resolve the unveiled conceptual difficulties.

If the wave function’s normalization is permitted to decreased in time, then a quantum particle may leave the interval bounded by the coordinate operator’s smallest and largest eigenvalues. Therefore, one may anticipate that at least the notion of a free particle can be introduced for non-Hermitian Hamiltonians. Nevertheless, it is not the case.

First, redoing the Ehrenfest quantization of Eqs. (1) and (2) by assuming that $\hat{H} \neq \hat{H}^\dagger$, we obtain the following generalizations of Eqs. (4) and (5):

$$im(\hat{H}^\dagger \hat{x} - \hat{x} \hat{H}) = \hbar \hat{p}, \quad i(\hat{H}^\dagger \hat{p} - \hat{p} \hat{H}) = -\hbar U^\prime(\hat{x}).$$

We shall utilize a well developed theory of the operator equation $\Delta \tilde{X} - \tilde{X} \hat{B} = \tilde{Y}$, reviewed in Ref. [32], to disprove the existence of the free particle. Let $\sigma(\tilde{A})$ denote the spectrum of an operator $\tilde{A}$.

**Lemma 1.** Assume that $\tilde{x}, \tilde{p}$, and $\tilde{H}$ are bounded. If $\sigma(\hat{H}^\dagger) \cap \sigma(\hat{H}) = \emptyset$ and

$$im(\hat{H}^\dagger \tilde{x} - \tilde{x} \hat{H}) = \hbar \tilde{p}, \quad \hat{H}^\dagger \tilde{p} = \tilde{p} \hat{H},$$

then $\tilde{p} = \tilde{x} = 0$.

**Proof.** First, we employ the Rosenblum theorem [33] (see Theorem 9.3 in Ref. [32]) to Eq. (17) and then employ Eq. (18) to show

$$im \tilde{x} = \frac{\hbar}{2\pi i} \int_{\Gamma} d\xi (\hat{H}^\dagger - \xi)^{-1} \tilde{p} (\hat{H} - \xi)^{-1} \approx \frac{\hbar}{2\pi i} \int_{\Gamma} d\xi (\hat{H} - \xi)^{-2} = 0,$$

where $\Gamma$ denotes a union of closed contours in the complex plane with total winding numbers 1 around $\sigma(\hat{H}^\dagger)$ and 0 around $\sigma(\hat{H})$. \qed
Assume i) Theorem 4. Assume i) $\hat{H}$, $\hat{x}$, and $\hat{p}$ are finite-dimensional operators satisfying Eqs. (17) and (18); ii) $\lim_{t \to +\infty} |\langle \Psi(t) | \hat{\Psi}(t) \rangle| < \infty$, where $|\Psi(t)\rangle$ is a solution of Eq. (1); iii) the eigenvectors $\{ |E_n\rangle \}_{n=1}^{N}$ of $\hat{H} |E_n\rangle = E_n |E_n\rangle$, $n \in I := \{1, 2, \ldots, N\}$ span the entire Hilbert space. Then, $\hat{p} = 0$.

Proof. Suppose that $\hat{p} \neq 0$. According to the Lyapunov stability theory [14], the second assumption implies that $\Im(E_n) \leq 0$, $\forall n \in I$. Lemma 1 guarantees that $\hat{H}$ has at least one single real eigenvalue. Introduce $R := \{ n \in I : \Im(E_n) = 0 \} \neq \emptyset$ – the set of indices of the real eigenvalues. “Sandwiching” Eqs. (17) and (18) leads to

$$\langle E_k^* - E_l, \hat{\Psi} | \hat{\Psi} \rangle = \hbar \langle E_k | \hat{p} | E_l \rangle ,$$

$$\langle E_k^* - E_l, \hat{\Psi} | \hat{p} | E_l \rangle = 0, \quad \forall k, l \in I . \quad (21)$$

According to Eq. (21), $\langle E_k | \hat{p} | E_l \rangle$ may be non-zero only for $(k, l) \in Q := \{(k, l) \in R \times R | E_k = E_l\}$. However, Eq. (20) enforces $\langle E_k | \hat{p} | E_l \rangle = 0, \forall (k, l) \in Q$. Therefore, we reached the contradiction $\hat{p} = 0$.

Theorem 4, being a generalization of Theorems 1 and 2, disproves the existence of free-particle quantum and classical mechanics in the non-Hermitian setting.

Conclusions. We demonstrated that all finite-dimensional representation of quantum and classical dynamics violate the second Ehrenfest theorem [Eq. (2)], and only specially constructed representations satisfy the first Ehrenfest theorem [Eq. (1)]. The non-existence of the free particle case and the ambiguity in defying potential forces were also demonstrated.

Acknowledgments. The authors thank Michael Spanner and Serguei Patchkovskii for valuable discussions. Financial support from DARPA and NSF is acknowledged.
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