Abstract

We address a mathematical and physical status of exotic (like e.g. fractal) wave packets and their quantum dynamics. To this end, we extend the formal meaning of the Schrödinger equation beyond the domain of the Hamiltonian. The dynamical importance of the finite mean energy condition is elucidated.

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1 Motivation

For a simple Hamiltonian system whose energy operator $\hat{H}$ has a countably infinite spectrum \{\(E_n\}\} and normalized eigenvectors \{|n\rangle\}, so that $\hat{H}|n\rangle = E_n|n\rangle$ and $\langle m|n\rangle = \delta_{mn}$, any general pure state of the system is defined in terms of a normalized superposition $|\psi,0\rangle = \sum c_n|n\rangle$, $\sum |c_n|^2 = 1$. Its unitary time evolution follows:

$$|\psi,t\rangle = \sum c_n \exp \left( - \frac{i E_n t}{\hbar} \right) |n\rangle \doteq \exp \left( - \frac{i \hat{H} t}{\hbar} \right) |\psi,0\rangle.$$  (1)

Since $\hat{H}$ typically is an unbounded Hilbert space operator, we need a number of precautions concerning its domain properties, to infer the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi,t\rangle = \hat{H} |\psi,t\rangle$$  (2)

while it is often taken for granted, that the operator identity

$$\left( \hat{H} - i\hbar \frac{\partial}{\partial t} \right) |\psi,t\rangle = 0$$  (3)

unquestionably holds true for all states of the system, even most exotic like e.g. fractal wave packets of Refs. 1-3.

The two manifestations, 2 and 3, of the Schrödinger picture quantum dynamics are inequivalent for all states which are not in the domain of the Hamiltonian. A particular example of this situation is provided in 4: the time evolution of a fractal quantum state, represented by a continuous but
nowhere differentiable function \(|\psi, t\rangle\), can per force be related to the Schrödinger equation, but in a weak sense, by demanding that:

\[ E_n \langle n|\psi, t\rangle = \frac{i\hbar}{\partial t} \langle n|\psi, t\rangle \] (4)

hold true for all \(n\). The left-hand-side may be interpreted as a scalar product of two Hilbert space vectors \(\hat{H}|n\rangle\) and \(|\psi, t\rangle\), but surely cannot be rewritten as \(\langle n|\hat{H}|\psi, t\rangle\).

The present paper is devoted to a deeper discussion of deceivingly simple formulas (2), (3), (4) and their mutual relationships. Since domain problems are encountered while evaluating mean values of unbounded observables, we pay particular attention to the importance of the finiteness of mean energy condition.

If this restriction is violated, one encounters "infinite mean energy" states, \([1, 3]\). On the physical grounds they are irrelevant (nonexistent), since one would need an infinite energy to create (prepare) them. As well, by considering such states as a limiting case of an approximation procedure, in terms of a sequence of states with increasing finite energy, one ends up with a standard mathematical non-existence problem for the mean value.

The finite mean energy condition is known to be an important technical input that entails a trajectory interpretation of the Schrödinger picture quantum dynamics, in terms of sample paths of a Markov diffusion-type process, \([4]\). Since there appeared published claims, \([3]\), that standard trajectory interpretations fail for a certain class of wave functions that have well defined quantum evolutions, we indicate why evolutions considered in \([3]\) are in fact ill-defined.

## 2 Schrödinger equation

Let \(\mathcal{U}(\mathcal{H})\) denote a family of functions of a real variable \(t \in \mathbb{R}\) with values in \(\mathcal{H} = L^2(\mathbb{R}^n; dx)\), such that:

(i) functions \(\psi(t)\) are continuous i.e. \(\lim_{t \to t_0} \|\psi(t) - \psi(t_0)\| = 0\)

(ii) we have \(\|\psi(t_1)\| = \|\psi(t_2)\|\) for all \(t_1, t_2 \in \mathbb{R}\).

A function \(\psi(t)\) is called strongly differentiable if for each value \(t \in \mathbb{R}\) there exists \(\psi'(t) \in \mathcal{H}\) obeying:

\[ \lim_{t' \to t} \frac{\|\psi(t') - \psi(t)\|}{t' - t} - \psi'(t) \| = 0. \] (5)

Then we write \(\psi'(t) = \frac{d}{dt} \psi(t)\).

Let \(\hat{H}\) be a self-adjoint operator with the dense domain \(D(\hat{H}) \subset \mathcal{H}\). We say that \(\psi(t)\) obeys the Schrödinger equation (set \(\hbar = 1\))

\[ \hat{H}\psi(t) = i \frac{d\psi(t)}{dt} \] (6)
if the following three conditions are valid:
(a) $\psi(t) \in D(\hat{H})$ for all $t \in \mathbb{R}$,
(b) $\psi(t)$ is strongly differentiable,
(c) the equality in Eq. (6) is verified to hold true.

Let us notice that to handle the left-hand-side of (6) the condition (a) is both necessary and sufficient. As far as the right-hand-side is concerned, we only need to know that $\psi(t)$ is strongly differentiable, which has nothing in common with the condition (a). Once we have a strongly differentiable function $\psi(t)$ for which - additionally - (a) holds true, we are ultimately allowed to check (c). If so, we can tell that $\psi(t)$ actually is a solution of the Schrödinger equation.

Let us denote $E_\lambda, \lambda \in \mathbb{R}$ a resolution of unity for $\hat{H}$ i.e. $\hat{H} = \int_{-\infty}^{+\infty} \lambda dE_\lambda$. If $\phi$ is a continuous function of a real variable (continuity is presumed for convenience, but it is not a must), then we define a "function of an operator" $\phi(\hat{H}) = \int_{-\infty}^{+\infty} \phi(\lambda) dE_\lambda$. Its domain is $\{ f \in \mathcal{H}; \int_{-\infty}^{+\infty} |\phi(\lambda)|^2 d(f, E_\lambda f) < \infty \}$.

If $\phi$ is bounded, then $\phi(\hat{H})$ is a bounded operator. In particular, if we take $a < b$ in $\mathbb{R}$ and $\psi \in \mathcal{H}$, then the function
\[
\psi_{a,b}(t) = \int_{a}^{b} \exp(-i\lambda t) d(E_\lambda \psi) = \int_{-\infty}^{+\infty} \exp(-i\lambda t) d(E_\lambda [E_b - E_a] \psi) = \exp(-\hat{H}t)[E_b - E_a] \psi
\] (7)
fulfills conditions (a), (b) and (c), that is solves the Schrödinger equation.

We have a strong convergence $\lim_{b \to +\infty, a \to -\infty} [E_b - E_a] \psi$ and also
\[
\lim_{b \to +\infty, a \to -\infty} \psi_{a,b}(t) = \int_{-\infty}^{+\infty} \exp(-i\lambda t) d(E_\lambda \psi) = \exp(-i\hat{H}t) \psi = \psi(t)
\] (8)
where however $\psi(t)$ needs not to belong to the domain of $\hat{H}$. In such case one cannot even attempt to verify the equality (6). Nonetheless $\exp(-i\hat{H}t) \psi = \psi(t)$ is well defined.

3 Quantum evolution beyond the domain of $\hat{H}$

We shall give a rigorous meaning to the formula (3) when extended to functions not belonging to the domain of $\hat{H}$. Let $\mathcal{E}$ denote a family of continuous functions $u$ of a real variable, taking values in $\mathbb{R}$ and such that $\lambda - u(\lambda)$ is a bounded function. By $\mathcal{E}_{\hat{H}}$ we denote a family of functions with values in the Hilbert space $\mathcal{H}$ defined as follows:
\[
\mathcal{E}_{\hat{H}} = \{ \psi^u(t) = \int_{-\infty}^{+\infty} \exp[iu(\lambda)t] d(E_\lambda \psi) = \exp[-iu(\hat{H})t] \psi \} \] (9)
where $u \in \mathcal{E}$, $\psi \in \mathcal{H}$. Clearly, $\mathcal{E}_{\hat{H}} \subset \mathcal{U}(\mathcal{H})$.

Some care is needed to extend the formula (3) beyond the domain of $\hat{H}$. To this end, let us define an operation $\hat{S}$ with the domain $\mathcal{E}_{\hat{H}}$ and values in $\mathcal{U}(\mathcal{H})$, which will be a extension of $(\hat{H} - i \frac{d}{dt})$. We
Indeed, we infer that \( \hat{\psi} \) on \( Q \) function \( \psi \) take actually have \( \hat{\psi} \) take both (a) and (b). Consequently, \( \hat{\psi} \) is well defined and we have

\[
(\hat{H} - i \frac{d}{dt})\psi_{a,b}(t) = \int_{-\infty}^{\infty} [\lambda - u(\lambda)] \exp[-iu(\lambda)t]d(E_{\lambda}[E_b - E_a]\psi).
\]

Because of

\[
\|(\hat{H} - i \frac{d}{dt})\psi_{a,b}(t)\|^2 \leq \int_{-\infty}^{\infty} [\lambda - u(\lambda)]^2 d(\psi, E_{\lambda}^2) \leq M \int_{-\infty}^{\infty} d(\psi, E_{\lambda}^2) = M\|\psi\|^2
\]

where \( M = \sup_{\lambda} |\lambda - u(\lambda)|^2 \), it is possible to extend \( (\hat{H} - i \frac{d}{dt}) \) to an operator \( \hat{S} \) whose action on a function \( \psi(t) = \int_{-\infty}^{\infty} \exp[-iu(\lambda)t]d(E_{\lambda}\psi) \) reads as follows:

\[
\hat{S}\psi(t) = \int_{-\infty}^{\infty} [\lambda - u(\lambda)] \exp[-iu(\lambda)t]d(E_{\lambda}\psi).
\]

Indeed, we infer that \( (\hat{H} - i \frac{d}{dt})\psi_{a,b}(t) \) converges strongly in \( \mathcal{H} \) and uniformly in \( t \) to \( \int_{-\infty}^{\infty} [\lambda - u(\lambda)] \exp[-iu(\lambda)t]d(E_{\lambda}\psi) \). Thus, we can define \( \hat{S}\psi_{a,b}(t) = (\hat{H} - i \frac{d}{dt})\psi_{a,b}(t) \) and in view of Eq. (12) the operator \( \hat{S} \) is an extension of \( (\hat{H} - i \frac{d}{dt}) \) to the whole of \( \mathcal{E}_{\mathcal{H}} \).

In connection with the above extension notion, let us recall that if we have operators \( A \) and \( B \) defined on their respective domains \( Q_A \) and \( Q_B \) such that \( Q_A \subset Q_B \) and if an operator \( B \) is defined on \( Q_B \) so that \( Ax = Bx \) for all \( x \in Q_A \), then we call \( B \) an extension of \( A \) and denote \( A \subset B \). We actually have \( (\hat{H} - i \frac{d}{dt}) \subset \hat{S} \).

At this point, we may consider

\[
\hat{S}\psi(t) = 0
\]

which is clearly an equation solved by any function \( \psi(t) \) with \( u(\lambda) = \lambda \). This equation is a rigorous version of (3), the fact which if often disregarded in the literature, c.f. (3). It is clear that (13) cannot be directly rewritten in the form (3), unless with an obvious abuse of notation.

4 Finite energy condition and Hilbert space scale

A necessary condition for the equation (2) to make sense is the condition denoted previously by (a): \( \psi(t) \in D(\hat{H}) \) for all \( t \). We relate this property to the so-called finite mean energy condition, which according to (4) is a limitation upon wave functions, necessary to ensure the existence of a stochastic counterpart of the Schrödinger picture evolution (i.e. well defined Markovian diffusion-type processes).

We are here motivated by (4). The statement of Ref. (3) is: there exist pure quantum states for which the mean energy is finite, but no consistent Schrödinger evolution (2) can be defined (in fact, our condition (a) does not hold true). A complementary statement of (3) and (4) is that: there exist wave functions which ”have infinite mean energy”.
In contrast to the reasoning of Ref. [3], in [1] the pertinent (fractal) wave function is derived in a controlled way, through a well defined limiting procedure. Since the mean energy diverges in this limit, it is more correct to say about the "nonexistence" of the mean value, instead of invoking a state with an "infinite mean energy". Let us discuss in some detail the background and validity of these claims.

We assume that $\hat{H}$ is defined in $\mathcal{H}$ and is: (i) self-adjoint, (ii) is bounded from below, (iii) is unbounded from above. In view of (ii), we may always replace a given Hamiltonian by a strictly positive operator, hence we assume: (iv) $\hat{H}$ is strictly positive i. e. there is $m > 0$ such that for all $\psi \in D(\hat{H})$ we have $(\psi, \hat{H}\psi) \geq m\|\psi\|^2$.

The domain $D(\hat{H}) \subset \mathcal{H}$ is a linear space with the scalar product of $\mathcal{H}$.

However, $D(\hat{H})$ is not a Hilbert space: $D(\hat{H}) \neq \mathcal{H}$ and $D(\hat{H})$ is dense in $\mathcal{H}$. Thence $D(\hat{H})$ is not complete, [5].

In the linear space $D(\hat{H})$ we introduce a new scalar product:

$$ (f, g)_2 = (\hat{H}f, \hat{H}g) \quad (14) $$

where $f, g \in D(\hat{H})$ and $(\cdot, \cdot)$ is the scalar product in $\mathcal{H}$. Since $\hat{H}$ is strictly positive, one can prove that the hitherto incomplete linear space $D(\hat{H})$ becomes complete in the new norm inferred from $(\cdot, \cdot)_2$.

With this scalar product $D(\hat{H})$ actually is a Hilbert space which we denote $\mathcal{H}_2$. We have the set inclusion $\mathcal{H}_2 \subset \mathcal{H}$ and $\|f\| \leq \|f\|_2$ for all $f \in \mathcal{H}_2$.

We can define a number of other scalar products on $D(\hat{H})$, like e g.

$$ (f, g)_k = (H^{k/2}f, H^{k/2}g) \quad (15) $$

with $k = 2, 1, 0, -1, -2$. The case of $k = 2$ we have just considered, while $k = 0$ corresponds to the standard Hilbert space scalar product in $\mathcal{H}$. Each of these scalar products defines a corresponding norm in $D(\hat{H})$ according to $\|f\|_k = \|H^{k/2}f\|$, for $f \in D(\hat{H})$.

Let us stress that $D(\hat{H})$ is complete exclusively in the norm $\|\cdot\|_2$. However, we can complete $D(\hat{H})$ to respective Hilbert spaces in each of the considered norms, so arriving at the Hilbert space scale (the set inclusion $\subset$ means also $\neq$):

$$ \mathcal{H}_2 \subset \mathcal{H}_1 \subset \mathcal{H}_0 = \mathcal{H} \subset \mathcal{H}_{-1} \subset \mathcal{H}_{-2} \quad (16) $$

which is paralleled by a chain of norm inequalities $\|f\|_2 \geq \|f\|_1 \geq \|f\|_0 = \|f\| \geq \|f\|_{-1} \geq \|f\|_{-2}$ for all $f \in D(\hat{H}) \equiv \mathcal{H}_2$.

Let us consider $\mathcal{H}_1$ as a set of vectors which, by definition, contains $D(\hat{H})$ as a dense subset. Therefore for all $f \in D(\hat{H})$ we have:

$$ \|f\|^2 = (f, f)_1 = (\hat{H}^{1/2}f, \hat{H}^{1/2}f) = (f, \hat{H}f) = \langle \hat{H} \rangle f \quad (17) $$
where in addition one can demonstrate that $\mathcal{H}_1 = D(\hat{H}^{1/2})$.

If $\psi \in D(\hat{H})$, we traditionally call $(\psi, \hat{H}\psi)$ the mean energy of the quantum system in the pure state $\psi$. The mean value coincides with an $\mathcal{H}$-scalar product of two legitimate Hilbert space vectors: $\psi$ and $\hat{H}\psi$.

Perhaps it is worthwhile to spell out the meaning of mean energy states $\psi$ which do not belong to $D(\hat{H})$. The previously mentioned claims of Ref. [3, 1] appear to ignore the problem of how to handle the “mean value” with $\psi$ which is not in the domain of $\hat{H}$. The relevant statement in Sect. 3 of Ref. [3] reads: ”one can arrange $\hat{H}\psi$ to diverge (as the series) almost everywhere, while keeping the average energy $\langle \hat{H} \rangle$ finite”.

Let us come back to the formula (17). If $g \in \mathcal{H}_1$ but $g$ is not an element of $D(\hat{H})$, it is not allowed to infer uncritically $\|g\|^2 = (g, \hat{H}g)$, because $\hat{H}g$ is not defined. Nevertheless, since we have in hands a consistent definition of $\|g\|^2 = (\hat{H}^{1/2}g, \hat{H}^{1/2}g)$, in view of Eq. (17) the formula $(\hat{H}^{1/2}g, \hat{H}^{1/2}g)$ may possibly be interpreted as a straightforward generalization of the mean energy notion ($\langle \hat{H} \rangle_g$, c.f. Eq. (17)). Then $\mathcal{H}_1$, with $\mathcal{H}_2 \subset \mathcal{H}_1 \subset \mathcal{H}$, would stand for a natural extension of the set of states with a finite mean energy beyond the domain $\mathcal{H}_2$ of $\hat{H}$.

For states beyond $\mathcal{H}_1$ we may expect infinite values for $\|g\|^2$ to occur. Since $\|g\|^2$ is not defined, one may interpret any $g \in \mathcal{H} \setminus \mathcal{H}_1$ as an infinite energy state, in the sense that $\langle \hat{H} \rangle_{E_\alpha g} = (E_\alpha g, \hat{H}E_\alpha g) \to \infty$ as $\alpha \to \infty$.

We have considered a selfadjoint, unbounded, strictly positive operator $\hat{H}$ in a Hilbert space $\mathcal{H}$. $\hat{H}$ is invertible and the inverse operator $\hat{H}^{-1}$ is bounded in $\mathcal{H}$. Notice that for any $f \in \mathcal{H}$, we have $\hat{H}^{-1}f \in D(\hat{H})$ and consequently:

$$\hat{H}D(\hat{H}) = \mathcal{H}$$

(18)

and

$$\hat{H}^{-1}\mathcal{H} = D(\hat{H}).$$

(19)

Therefore, for the operator $\hat{H}^{-1}$ we need not to bother about domain properties and for any $f \in \mathcal{H}$ we have the well defined mean value (a scalar product of two Hilbert space vectors) $(f, \hat{H}^{-1}f)$. Since any $f \in \mathcal{H}$ can be represented in the form $f = \hat{H}\psi$ where $\psi \in D(\hat{H})$, we have:

$$(f, \hat{H}^{-1}f) = (\psi, \hat{H}\psi)$$

(20)

which ultimately reduces the finite mean energy definition exclusively to vectors from $D(\mathcal{H})$. The mean energy notion appears not to have meaning beyond $D(\hat{H})$, unless carefully generalized.
5 Trajectory-based interpretations of quantum motion

The original purpose of Ref. [3] has been a critique of "trajectory-based interpretations of quantum mechanics" with two targets: Nelson’s stochastic mechanics and so-called Bohmian mechanics. The point is that those two targets refer to the Schrödinger picture quantum dynamics and not the full-fledged formalism of quantum theory with varied experimental connotations.

A well founded fact is that at least two different "trajectory pictures" can be related to the very same mathematical model based on the Schrödinger wave packet evolution: deterministic Bohmian paths [6, 7] and random paths of (basically singular) diffusion-type processes, [4, 8]. Additionally, under suitable restrictions (free motion, harmonic attraction) classical deterministic phase-space paths are supported by the associated with $\psi(x,t)$ positive Wigner distribution function and its spatial marginal distribution, c.f. [9] for a related discussion.

However, none of the above derived trajectory "pictures" deserves the status of an underlying physical "reality" for quantum phenomena, although each of them may serve as more or less adequate pictorial description of the wave-packet dynamics, [6, 10].

It is in view of Born’s statistical interpretation postulate, that the the Schrödinger picture dynamics sets a well defined transport problem for a probability density $\rho(x,t) = |\psi(x,t)|^2$ which one is tempted to resolve in terms of stochastic processes and their sample paths. A direct interpretation in terms of random "trajectories" of a Markovian diffusion-type process is here in principle possible under a number of mathematical restrictions, but may happen to be non-unique and not necessarily global in time. The nontrivial boundary data, like the presence of wave function nodes, create additional problems although the nodes are known to be never reached by the pertinent processes. The main source of difficulty lies in guaranteeing the existence of a process per se i.e. of the well defined (and unique, if possible) Markovian transition probability density function, which in its full generality still remains a profound mathematical problem, [8]. A related issue of the global existence of Bohmian trajectories has been addressed in [7].

Both stochastic and causal (Bohmian) trajectory interpretations, need the solvability of the Schrödinger equation, hence conditions a), b) and c) of Section 2 must be respected. Accordingly, with $\psi(t)$ belonging to the domain of $\hat{H}$, we infer from the formula (20) that the finite energy condition automatically follows. This state of affairs hardly one can interpret as "incomplete", formally or physically, on the basis of Ref. [3].

There is no doubt that states not in the domain of $\hat{H}$ are not amenable to a straightforward trajectory interpretation, but this feature was rather obvious from the outset, in rigorous formulations of the pertinent theories, [4, 7]. The real point is whether those "outer" states can be termed "physical", i.e. compatible with well defined experimental procedures and their mathematical (quantum...
mechanical) imaging, see e.g. Refs. [11, 12]. This issue has been left untouched in ref. [3].

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