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Article

On a Unitary Solution for the Schrödinger Equation

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Abstract: For almost 75 years, the general solution for the Schrödinger equation was assumed to be generated by an exponential or a time-ordered exponential known as the Dyson series. We study the unitarity of this solution in case of singular Hamiltonian and provide a new methodology that is not based on the assumption that the underlying space is $L^2(\mathbb{R})$. Then, an alternative operator for generating the time evolution is suggested that is manifestly unitary, regardless of the choice of the Hamiltonian. The new construction involves an additional positive operator that normalizes the wave-function locally and allows us to preserve unitary even on indefinite norm spaces. Our considerations show that Schrödinger's and Liouville's equations are, in fact, two sides of the same coin, and together they become the unified description of quantum systems.

1. Introduction

The Schrödinger equation (named after Erwin Schrödinger, who postulated the equation in 1925) is the fundamental operatorial equation that governs the wave function of a quantum-mechanical system [1]. The discovery of this linear differential equation was a significant landmark in the development of quantum mechanics. In basic terms, if a wave-function of a system is given at some moment t_0 (denoted by $|\Psi(t_0)\rangle$) one can determine the wave-function at all the subsequent moments by solving [2,3]

$$\frac{d}{dt}\,|\Psi(t)\rangle \;=\; -i\hat{H}\,|\Psi(t)\rangle\,. \tag{1}$$

As long as the Hamiltonian of the system $\hat{H}$ is expressible as a bounded[1] self-adjoint[2] operator with no time dependence, the solution of (1) is given by the unitary evolution,

$$|\Psi(t)\rangle \;=\; \hat{U}(t,\,t_0)\,|\Psi(t_0)\rangle\,, \qquad \hat{U}(t,\,t_0) = \exp\left[-i\int_{t_0}^{t} dt'\,\hat{H}\right], \tag{2}$$

regardless the choice of space. In various cases, the Hamiltonian of a quantum system includes a time dependent part, and thus equation (1) is replaced by

$$\frac{d}{dt}\,|\Psi(t)\rangle \;=\; -i\hat{H}(t)\,|\Psi(t)\rangle\,, \qquad or \qquad \frac{d\hat{U}(t,\,t_0)}{dt} \;=\; -i\hat{H}(t)\,\hat{U}(t,\,t_0). \tag{3}$$

1 A linear operator $\hat{\mathcal{O}} : \mathcal{D}(\hat{\mathcal{O}}) \to \mathcal{Y}$ is called bounded if and only if $\sup_{|||\psi\rangle||=1} \|\hat{\mathcal{O}}\,|\psi\rangle\|_{\mathcal{Y}} < \infty$ for any $|\psi\rangle \in \mathcal{D}(\hat{\mathcal{O}})$ where the notation $\|\hat{\mathcal{O}}\,|\psi\rangle\|_{\mathcal{Y}}$ denotes the norm of $\hat{\mathcal{O}}\,|\psi\rangle$ on the space $\mathcal{Y}$ [5].

2 An operator $\hat{\mathcal{O}}$ on the Hilbert space $\mathcal{H}$ is called self-adjoint if it is operatorically identical to its adjoint, $\hat{\mathcal{O}}^\dagger = \hat{\mathcal{O}}$. The equivalence between two operators implies two conditions: $\langle\varphi|\,\hat{\mathcal{O}}^\dagger\,|\psi\rangle = \langle\varphi|\,\hat{\mathcal{O}}\,|\psi\rangle$ for $|\varphi\rangle\,, |\psi\rangle \in \mathcal{H}$, and additionally the domains are identical, $\mathcal{D}(\hat{\mathcal{O}}^\dagger) = \mathcal{D}(\hat{\mathcal{O}})$.

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The widely known general solution for (3) is expressible by using the $\hat{T}$ operator[3] [4],

$$\hat{U}(t, t_0) = \hat{T} \exp\left[-i \int_{t_0}^{t} dt'\, \hat{H}(t')\right]. \tag{4}$$

It is well known that solutions (2) and (4) are unitary on Hilbert spaces for any choice of self-adjoint Hamiltonians. However, as we shall discuss, the property of unitarity can no longer be shown everywhere on more general spaces unless the Hamiltonian is strictly bounded self-adjoint. Our claim in this paper is the following: instead of solutions (2) and (4), one can obtain a universal unitary solution[4],

$$|\Psi(t)\rangle = \hat{\mathcal{P}}(t, t_0)\,|\Psi(t_0)\rangle\,, \qquad \hat{\mathcal{P}}(t, t_0) \equiv \hat{\mathcal{N}}(t, t_0)\,\hat{U}(t, t_0), \tag{5}$$

with

$$\hat{\mathcal{N}}(t, t_0) \equiv \sqrt{\hat{U}^{\dagger-1}(t, t_0)\,\hat{U}^{-1}(t, t_0)}\,. \tag{6}$$

This solution no longer rely on any assumption with regards to the properties of the space or Hamiltonian. As shall later be explained, the only formulation of the Schrödinger equation that is consistent with the probabilistic interpretation [40] is governed by the bounded self-adjoint component[5] $\hat{\mathcal{H}}(t)$ of the general Hamiltonian $\hat{H}(t)$. The resulting equation is solely that of wave mechanics,

$$\frac{d}{dt}\,|\Psi(t)\rangle = -i\hat{\mathcal{H}}(t)\,|\Psi(t)\rangle\,, \qquad or \qquad \frac{d\hat{\mathcal{P}}(t, t_0)}{dt} = -i\hat{\mathcal{H}}(t)\,\hat{\mathcal{P}}(t, t_0). \tag{7}$$

The new operator $\hat{\mathcal{N}}(t, t_0)$ from (6) is known as the *"normalization operator"* or *"jump operator"*. In its defining relation the operator $\hat{U}^{-1}(t, t_0)$ denotes the inverse of $\hat{U}(t, t_0)$, and $\hat{U}^{\dagger-1}(t, t_0)$ is the inverse of its adjoint. The inclusion of the operator $\hat{\mathcal{N}}(t, t_0)$ is, in fact, a promotion of the familiar normalization procedure of a quantum states to operatoric level, such that it becomes a local procedure rather than a global one[6]. In other words, instead of having normalization only as an asymptotic procedure, it is now ensured even at the intermediate times. From definition (6) it is already evident that the introduction of $\hat{\mathcal{N}}$ is not necessary if $\hat{U}$ from (4) is truly an exact unitary operator. In that case the adjoint operator coincides with the inverse operator, $\hat{U}^{\dagger}(t, t_0) = \hat{U}^{-1}(t, t_0)$ and $\hat{U}^{\dagger-1}(t, t_0) = \hat{U}(t, t_0)$, which leads to $\hat{\mathcal{N}}(t, t_0) = \mathbf{1}$. However, as we shall explicitly show, this simplification is generally not valid in various interesting situations, among them is the case of gauge theories.

This paper is organized as follows: in Section 2 we explain for what reason the standard solution cannot always provide a unitary description for quantum systems. In Section 3, we provide a proof for the validity of the new solution, discuss its properties, and compute the new corresponding perturbative construction. In Section 4, we provide a few practical demonstrations in which the new solution differs from the current mainstream approach. In Section 5, we summarize the implications of our result on various aspects. In Appendix A, we discuss the applicability of the iterative method. In Appendix B, the details of the computation of the differential equation for the dynamics of $\hat{\mathcal{N}}$ is provided.

2. Normalization as a Consequence of Unboundedness

In this part we review the standard argument that is considered a proof for the unitarity of $\hat{U}$ in the case of time-dependent Hamiltonian, Equation (4). Our intention is to have a closer look at the necessary mathematical conditions involved there, and then discuss under what circumstances this

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[3] The action of this operator, known as the time-ordering operator, is defined by $\hat{T}\left[\hat{H}(t')\,\hat{H}(t)\right] \equiv \Theta(t'-t)\hat{H}(t')\,\hat{H}(t) + \Theta(t-t')\hat{H}(t)\,\hat{H}(t')$, where $\Theta(t'-t)$ is the Heaviside theta function.

[4] We denote the exact solution by $\hat{\mathcal{P}}$ from the word *pitaron* which means solution in Hebrew.

[5] The definition of this component is later provided in Equation (53).

[6] Note that an operator $\boldsymbol{A}$ is called a square root of operator $\boldsymbol{B}$ if it satisfies $\boldsymbol{A}^2 = \boldsymbol{B}$.

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argument can be invalidated. Afterwards, a new construction is motivated, in which unitarity becomes a robust property and no longer can be broken. And lastly, we characterize from the mathematical perspective the different choices of Hamiltonians for which our considerations become relevant.

2.1. Why Is $\hat{U}$ Not Always Unitary?

Our starting point is a quick reminder for the procedure that has led to the result shown in Equation (4). The central idea is to solve the differential equation (3) by iterations [2]: at first turning the original differential equation to an integral equation, and then substituting the result "inside itself" repeatedly[7] [8],

$$\begin{aligned} \hat{U}(t,t_0) &= \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\,\hat{H}(t')\,\hat{U}(t',t_0) \\ &= \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\,\hat{H}(t')\left[\hat{\mathbf{1}} - i\int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{U}(t'',t_0)\right]. \end{aligned} \tag{8}$$

The applicability of the iterative method is discussed in Appendix A, but for now let us assume the validity of this method[9]. The series that is obtained by this process, known as the Dyson series [4], is given by

$$\hat{U}(t,t_0) = \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\,\hat{H}(t') - \int_{t_0}^{t} dt'\,\hat{H}(t')\int_{t_0}^{t'} dt''\hat{H}(t'') + \dots \tag{9}$$

At this point the terms of the series above should be interpreted as merely a abstract operatoric symbols. The convergence properties of the terms and of the series as a whole are dictated by the choice of the Hamiltonian as well as the time interval of the evolution. Let us now present the familiar argument that currently exist in the literature [2] and regarded as a proof for the unitarity of $\hat{U}(t,t_0)$. By assuming that one can replace the integrations in the iterative form with the productive form,

$$\hat{U}(t,t_0) = \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\,\hat{H}(t') - \int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') + \dots \tag{10}$$

And by assuming $\hat{H}^\dagger(t) = \hat{H}(t)$ along with the validity of the operator simplifications[10]

$$(\hat{O}_1 + \hat{O}_2)^\dagger = \hat{O}_1^\dagger + \hat{O}_2^\dagger, \qquad (\hat{O}_1\,\hat{O}_2)^\dagger = \hat{O}_2\,\hat{O}_1, \tag{11}$$

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7 Therefore, it is clear that the original terms in the perturbative series involving integrations in the iterative form $\int_Y \int_X f(x,y)\,dx\,dy$, and not the productive form $\int_{X\times Y} f(x,y)\,dx\,dy$.

8 The integration over an operator is defined as $\int_{t_0}^{t_1} dt\,\hat{O}(t) \equiv \int_{t_0}^{t_1} dt \int_{\varphi,\psi} |\varphi\rangle\langle\varphi|\,\hat{O}(t)\,|\psi\rangle\langle\psi|$ where the inner integration includes any $|\varphi\rangle, |\psi\rangle \in \mathcal{D}(\hat{O})$. Note that exchanging of the ordering of integrations, $\int_{t_0}^{t_1} dt \int_{\varphi,\psi} \to \int_{\varphi,\psi}\int_{t_0}^{t_1} dt$, is generally permitted only if $\hat{O}(t)$ is a bounded operator.

9 At first sight, the solution (9) seems to satisfy the Schrodinger equation. Indeed, by applying the derivative term-by-term based on $\frac{d}{dx}\left(\int_{x_0}^{x} dx'\,\hat{O}(x')\right) = \hat{O}(x)$, it seems that we arrive at

$$\frac{d\hat{U}(t,t_0)}{dt} = \frac{d}{dt}(\hat{\mathbf{1}}) - \frac{d}{dt}\left(i\int_{t_0}^{t} dt'\,\hat{H}(t')\right) - \frac{d}{dt}\left(\int_{t_0}^{t} dt'\,\hat{H}(t')\int_{t_0}^{t'} dt''\hat{H}(t'')\right) + \dots = -i\hat{H}(t)\,\hat{U}(t,t_0).$$

However, the problem starts when dealing with the regime in which the Leibniz integral rule is not applicable, so the derivative and integration are no longer commutative operations. Moreover, interchanging order of differentiation and summation of infinite terms, $\frac{d}{dt}\sum_{n=0}^{n=\infty} f_n \to \sum_{n=0}^{n=\infty}\frac{d}{dt} f_n$, is generally not permitted []. The series might be non-differentiable, or the series of derivative might not converge, or the series of derivatives converges to something other than the derivative of the series.

10 Essentially, we assume that both $\left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^\dagger = \int_{t_0}^{t} dt'\,\hat{H}(t')$ and $\left(\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'')\right)^\dagger = \int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t')$. These non-trivial simplifications can only be guaranteed for bounded self-adjoint Hamiltonians integrted over a proper domain.

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the expansion conjugate to (10) takes the form

$$\hat{U}^{\dagger}(t,t_0) \,=\, \hat{\mathbf{1}} + i\int_{t_0}^{t} dt'\,\hat{H}(t') - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t') + \ldots \tag{12}$$

It then follows, by taking the product of (10) and (12), that

$$\begin{aligned}\hat{U}^{\dagger}(t,t_0)\,\hat{U}(t,t_0) \,&=\, \hat{\mathbf{1}} + \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^2 - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') \\ &\quad - \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t') + \ldots\end{aligned} \tag{13}$$

The next step, as shown in Figure 1, is to apply an "operatoric version" of the Fubini theorem [9] and exchange of the ordering of the two time integrations in the last term of (13),

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t'')\,\hat{H}(t') \,=\, \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\,\hat{H}(t')\,\hat{H}(t''). \tag{14}$$

Then, after introducing the replacement (14) in the result of (13), the last two terms can be combined together,

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'') + \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\,\hat{H}(t')\,\hat{H}(t'') \,=\, \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^2, \tag{15}$$

what allegedly seems to lead to the inevitable conclusion that $\hat{U}^{\dagger}(t,\,t_0) \,=\, \hat{U}^{-1}(t,\,t_0)$.

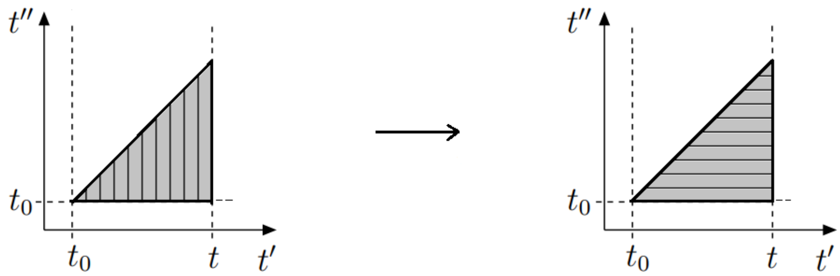

Figure 1. Changing the order of integration via the Fubini theorem. Left: the original integration. This integration was required to be performed on the triangle defined by first integrating the interval $t'' \in [t_0,\, t']$, and only then $t' \in [t_0,\, t]$. Right: the integration after applying the Fubini theorem – the first integration is carried on the interval $t'' \in [t',\, t]$.

Now, let us look again on the argument that has been presented above, but this time adopt a more cautious approach, paying attention to the mathematical conditions involved at each step that we perform. Before we proceed, a wise question to ask ourselves is – is this argument applicable for the case of unbounded Hamiltonian? How does the domain of the Hamiltonian, $D(\hat{H})$, affect the argument?

A detailed discussion about the differences between these two kinds of mathematical constructions can be found in [10,11]. From there we learn that confidently answering the question above is necessary in order to determine the legitimate set of simplification operations that can be performed. For clarity, let us summarize the underlying requirements which took place while

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presenting the unitarity argument above[11]:

◇ **Additivity of integrands**: for operators $\hat{\mathcal{O}}_1$ and $\hat{\mathcal{O}}_2$, and for any t_0, t_1,

$$\int_{t_0}^{t_1} dt\, \hat{\mathcal{O}}_1(t) + \int_{t_0}^{t_1} dt\, \hat{\mathcal{O}}_2(t) = \int_{t_0}^{t_1} dt\, \left(\hat{\mathcal{O}}_1(t) + \hat{\mathcal{O}}_2(t)\right). \tag{16}$$

◇ **Additivity of integration intervals**: for an operator $\hat{\mathcal{O}}$, any t_0, t_2, $t_0 \leq t_1 \leq t_2$,

$$\int_{t_0}^{t_1} dt\, \hat{\mathcal{O}}(t) + \int_{t_1}^{t_2} dt\, \hat{\mathcal{O}}(t) = \int_{t_0}^{t_2} dt\, \hat{\mathcal{O}}(t). \tag{17}$$

Clearly, our argument established unitarity not as a general property that is valid for a general choice of Hamiltonian, but rather only those that are self-adjoint. In fact, our ability to perform operation (16) is mathematically justified only if the domains of the integrated operators on both sides is equivalent throughout the evolution[12]. More importantly, in order to satisfy the property (17), the operator $\hat{\mathcal{O}}(t_1)$ is required to be a bounded operator[13]. A sufficient condition that ensures the validity of the unitarity argument is that the involved operators are satisfying an analogous condition to absolute convergence for any choice of $|\psi\rangle \in \mathcal{D}(\hat{H})$,

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, \left\| \hat{H}(t'')\, \hat{H}(t')\, |\psi\rangle \right\|_{\mathcal{Y}}^2 < \infty. \tag{18}$$

However, various interesting problems (such as gauge theories) we often deal with a situations in which the condition above is violated. That happens since either the time interval under consideration is improper, $\Delta t \equiv t - t_0 = \infty$, or due to integrand containing singularities, as discussed in example 4.3. In these cases the resulting integrals (potentially obtained after regularization procedure) converge only conditionally and demand additional care.

What about Stone's Theorem?

In case that the Hamiltonian is time-independent, the theorem that allows us to regard (2) as a unitary operator is given by Stone's theorem [12]. This theorem provides a one-to-one correspondence between self-adjoint and unitary operators as stated below.

• ***Stone's theorem:*** *let* $\hat{H} : \mathcal{D}(\hat{H}) \to \mathcal{H}$ *be a possibly unbounded self-adjoint operator, the map* $\hat{U}(\Delta t) = e^{-i\Delta t\, \hat{H}}$ *is a strongly-continuous one-parameter unitary operator.*

However, there are three saddle situations in which one cannot any longer rely on this theorem, all connected with the necessity of careful treatment of the element ∞.

◇ **Infinitely dimensional Hilbert spaces**: as discussed in example 4.1, a self-adjoint operator satisfy an additional condition on its domain that an Hermitian operator does not. In case that

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11 An additional operation that is not listed is the Fubini theorem, as mentioned in (14). However, it can be shown that this operation is redundant in terms of the mathematical requirements, as its validity is ensured if (17) is satisfied. In any case, it is clear that applying simplification (14) is not universal, and cannot be guaranteed to yield a correct transition if the integrand is conditionally convergent.

12 Contrary to the case of bounded operators, unbounded operators on a given space do not form an algebra, nor even a complete linear space [5]. Each unbounded operator is defined on its own domain, so that if $\hat{\mathcal{O}}_1$ and $\hat{\mathcal{O}}_2$ are two unbounded operators defined on the domains $\mathcal{D}(\hat{\mathcal{O}}_1)$ and $\mathcal{D}(\hat{\mathcal{O}}_2)$ respectively, then the domain of operator $\hat{\mathcal{O}}_1 + \hat{\mathcal{O}}_2$ is $\mathcal{D}(\hat{\mathcal{O}}_1) \cap \mathcal{D}(\hat{\mathcal{O}}_2)$. Note that two operators which act in the same way are to be considered as different if they are not defined on the same subspace of Hilbert space. According to Hellinger-Toeplitz theorem [5], if a self-adjoint operator is well defined on the entire Hilbert space it has to be bounded.

13 It is worth mentioning that one can 'save additivity' by replacing the standard Riemann integral with a modified definition of integral, but obviously, this will not cure the fundamental problem, but rather just hide it inside the integrals definitions.

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$\mathcal{D}(\hat{H}^\dagger) \neq \mathcal{D}(\hat{H})$ it can be said that the Hamiltonian is Hermitian but not self-adjoint. Note that this type of space is fundamental to QM, since in order satisfy the relation, $[\hat{x}, \hat{p}] = i\hbar$, either the position $\hat{x}$ or momentum operators $\hat{p}$ must be an unbounded operator[14]. Since in order to apply Stone's theorem the property of Hermiticity alone is an insufficient condition, one should not be surprised that establishing unitarity cannot be done.

♢ **Singular potentials**: these type of potentials are defined only on a densly defined domain, but not everywhere. An example for this choice of Hamiltonian is explicitly discussed in example 4.2,

$$\hat{H}(x) = \frac{1}{\|\hat{x} - \hat{x}_0\|}, \tag{19}$$

which is defined on the domain $\mathcal{D}(\hat{H}) = \{\|\hat{H}\,|\psi\rangle\| < \infty\}$. It is common to consider this problem on an inadequate space, $\mathcal{H} = L^2(\mathbb{R})$, in which the value of the Hamiltonian on the singular location is replaced by 0. However, this cannot be done for a general choice of space, such as indefinite norm spaces. In that case the Stone theorem cannot imply unitarity in the region outside the domain of the Hamiltonian,

$$\mathcal{E}(\hat{H}) \equiv \mathcal{H} \setminus \mathcal{D}(\hat{H}) = \{\|\hat{H}\,|\psi\rangle\| = \infty\}. \tag{20}$$

In other words, unitarity with Hamiltonian (19) cannot be shown for the state satisfying $\hat{x}\,|\psi\rangle = x_0\,|\psi\rangle$ when working on indefinite norm space.

♢ **Asymptotic states**: the case in which $t - t_0 = \infty$, as typically involved in the definition of the S-matrix.

2.2. How to Unitarize $\hat{U}$?

The main point of the last section was that unitarity is not a manifest property of $\hat{U}$ for a general choice of space, but rather a property that follows only under a certain restrictive assumptions. An advancement toward a manifestly unitary can be done by introducing the replacement

$$\hat{\mathcal{O}} \longrightarrow \sqrt{\hat{\mathcal{O}}^{\dagger-1}\,\hat{\mathcal{O}}^{-1}}\,\hat{\mathcal{O}}, \tag{21}$$

which leads to the proposed solution in (5). This decomposition is analogous to the polar decomposition, which always exists and is always unique [13]. By construction, the solution $\hat{\mathcal{P}}(t, t_0)$ manifestly preserves the exactness of unitarity at all orders and at all times,

$$\hat{\mathcal{P}}^\dagger(t, t_0)\,\hat{\mathcal{P}}(t, t_0) = \hat{U}^\dagger(t, t_0)\,\hat{U}^{\dagger-1}(t, t_0)\,\hat{U}^{-1}(t, t_0)\,\hat{U}(t, t_0) = \hat{\mathbf{1}}, \tag{22}$$

from which it is immediately apparent that $\hat{\mathcal{P}}^\dagger(t, t_0) = \hat{\mathcal{P}}^{-1}(t, t_0)$. The expression for the inverse of $\hat{U}$ can be uniquely determined by the condition $\hat{U}^{-1}(t, t_0)\,\hat{U}(t, t_0) = \hat{\mathbf{1}}$ so that[15],

$$\hat{U}^{-1}(t,t_0) = \hat{\mathbf{1}} + i\int_{t_0}^{t} dt'\,\hat{H}(t') - \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^2 + \int_{t_0}^{t} dt'\,\hat{H}(t')\int_{t_0}^{t'} dt''\,\hat{H}(t'') + \ldots \tag{23}$$

[14] Otherwise, by tracing both sides of the relation, an illogical result is obtained [7].

[15] Similarly, $\hat{U}^{\dagger-1}(t,t_0) = \hat{\mathbf{1}} - i\left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^\dagger - \left(\int_{t_0}^{t} dt'\,\hat{H}(t')\right)^{\dagger 2} + \left(\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,\hat{H}(t')\,\hat{H}(t'')\right)^\dagger + \ldots$.

By insertion back to (6) along with the Taylor expansion of the square root, the following result is obtained for the case of bounded self-adjoint Hamiltonian:

$$\hat{\mathcal{N}}(t,\, t_0) \;=\; \hat{\mathbf{1}} - \frac{1}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 + \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \{\hat{H}(t'),\, \hat{H}(t'')\} + \dots \tag{24}$$

Then, by using the definition (5), we find the expansion

$$\begin{aligned}&\hat{\mathcal{P}}(t,\, t_0)\\ &= \hat{\mathbf{1}} - i\int_{t_0}^{t} dt'\, \hat{H}(t') - \frac{1}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 - \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, [\hat{H}(t'),\, \hat{H}(t'')] + \dots\end{aligned} \tag{25}$$

However, generally the original terms must be kept in their full glory[16 17],

$$\begin{aligned}\hat{\mathcal{N}}(t,t_0) \;=\; &\hat{\mathbf{1}} + \frac{i}{2}\int_{t_0}^{t} dt'\, \hat{H}(t') - \frac{i}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^{\dagger} - \frac{3}{8}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 - \frac{3}{8}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^{\dagger 2}\\ &+ \frac{1}{4}\left|\int_{t_0}^{t} dt'\, \hat{H}(t')\right|^2 + \frac{1}{2}\int_{t_0}^{t} dt' \hat{H}(t') \int_{t_0}^{t'} dt'' \hat{H}(t'') + \frac{1}{2}\left(\int_{t_0}^{t} dt' \hat{H}(t') \int_{t_0}^{t'} dt'' \hat{H}(t'')\right)^{\dagger} + \dots\end{aligned} \tag{26}$$

from which we arrive at the manifestly unitary result,

$$\begin{aligned}\hat{\mathcal{P}}(t,t_0) \;=\; &\hat{\mathbf{1}} - \frac{i}{2}\int_{t_0}^{t} dt'\, \hat{H}(t') - \frac{i}{2}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^{\dagger} + \frac{1}{8}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^2 - \frac{3}{8}\left(\int_{t_0}^{t} dt'\, \hat{H}(t')\right)^{\dagger 2}\\ &- \frac{1}{4}\left|\int_{t_0}^{t} dt'\, \hat{H}(t')\right|^2 - \frac{1}{2}\int_{t_0}^{t} dt' \hat{H}(t') \int_{t_0}^{t'} dt'' \hat{H}(t'') + \frac{1}{2}\left(\int_{t_0}^{t} dt' \hat{H}(t') \int_{t_0}^{t'} dt'' \hat{H}(t'')\right)^{\dagger} + \dots\end{aligned} \tag{27}$$

As expected, expansions (26) and (27) are consistent with expressions (24) and (25) under the assumption of a bounded self-adjoint Hamiltonian.

2.3. *Classification of Quantum Evolution*

In this part we discuss the circumstances under which the solution $\hat{U}$ can no longer be considered a complete unitary description. This will be done by characterizing two types of Hamiltonians and spaces that typically play a role in problems of quantum physics.

2.3.1. The bounded self-adjoint evolution

In this part we would like to provide specific details under which conditions our new proposal will not matter and the equivalence $\hat{\mathcal{N}} = \hat{\mathbf{1}}$ will be sustained throughout the entire evolution. One of the fundamental postulate in quantum mechanics is that any measurable dynamical quantity is represented by a bounded self-adjoint operator. A crucial property of the Hamiltonians belonging to this category is spectrum that involves eigenvalues that belong to $\mathbb{R}$. As a simple example for a practical realization of such an operator it is possible to use a matrix of finite dimensions $\hat{H}(t) : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ with entries given by a finite valued and continuous functions[18]:

$$\hat{H}(t) \;=\; f_1\,\hat{\sigma}_1 + f_2\,\hat{\sigma}_2 + f_3\,\hat{\sigma}_3 \;=\; \begin{pmatrix} f_3 & f_1 - i f_2 \\ f_1 + i f_2 & -f_3 \end{pmatrix}, \tag{28}$$

[16] The approximation $\sqrt{1 + ix - x^2} \approx 1 + \frac{i}{2}x - \frac{3}{8}x^2$ is used.

[17] The notation $|\hat{A}| \equiv \sqrt{\hat{A}^\dagger \hat{A}}$ is introduced. Notice the difference with the definition of the norm: the outcome of $|\cdot|$ is another operator, while the operation $\|\cdot\|$ includes an additional tracing operation, and therefore, leaves us with just a number.

[18] More generally, such a choice of Hamiltonian can be expressed by using a complete orthonormal Hilbert space $\{|\phi_i\rangle\}$, $\hat{H}(t) = \sum_i E_i(t)\,|\phi_i\rangle\langle\phi_i| + \sum_{i,j} f_{ij}(t)\,|\phi_i\rangle\langle\phi_j|$, where $E_i(t) \in \mathbb{R}$, $f_{ij}(t) = f^*_{ji}(t)$ with $|E_i(t)|, |f_{ij}(t)| < \infty$ for any value of t.

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with $f_i = f_i(t) \in \mathbb{R}$ and $|f_i| < \infty$ where $i \in \{1,2,3\}$. In case that $\Delta t < \infty$ it can be shown that a bounded self-adjoint Hamiltonians implies that

$$\left\| \left(\hat{U}(t_2, t_0) - \hat{U}(t_1, t_0) \right) |\psi(t_0)\rangle \right\|_{\mathcal{H}_2} \leq \| 2\, |\psi(t_0)\rangle \|_{\mathcal{H}_1}, \tag{29}$$

for any $t_2, t_1 \in [t_0, t]$ and $|\psi(t_0)\rangle \in \mathcal{H}_1$. All that have been discussed in this part can be translated to the main property that characterize these Hamiltonians: the evolution dictated by $\hat{U}$ preserves the norm of the Hilbert space. Thus, for any given $|\psi(t_0)\rangle \in \mathcal{H}_1$ and action of $\hat{U}$ generates an isometric transformation,

$$\left\| \hat{U}(t, t_0)\, |\psi(t_0)\rangle \right\|_{\mathcal{H}_2} = \| |\psi(t_0)\rangle \|_{\mathcal{H}_1}. \tag{30}$$

For time-independent self-adjoint Hamiltonians, the boundness condition ensures the existence of the Taylor series expansion, and it is immediate to show that the construction (2) is indeed unitary:

$$\left(\exp\left[-i\Delta t\, \hat{H}\right]\right)^{\dagger} = \left(\hat{\mathbf{1}} + \sum_{n=1}^{\infty} \frac{(-i\Delta t\, \hat{H})^n}{n!}\right)^{\dagger} = \hat{\mathbf{1}} + \sum_{n=1}^{\infty} \frac{(i\Delta t\, \hat{H})^n}{n!} = \left(\exp\left[i\Delta t\, \hat{H}\right]\right)^{-1}, \tag{31}$$

Moreover, even if the Hamiltonian includes time dependence, as long as it is bounded self-adjoint the argument presented in Section 2 is valid and therefore construction (4) provides us with a unitary description as well. The reason for that is since the boundness requirement ensures the integrability of the expansion, as guaranteed by the Lebesgue's criterion for integrablility[19]. An alternative way to establish unitarity in this case relies on a simple well-known argument [21]. By multiplying Equation (3) by $\hat{U}^{\dagger}(t, t_0)$ on the left side, and multiplying the conjugate equation of motion by $\hat{U}(t, t_0)$ on the right side,

$$\begin{aligned} \hat{U}^{\dagger}(t, t_0)\, \frac{d\hat{U}(t, t_0)}{dt} &= -i\hat{U}^{\dagger}(t, t_0)\, \hat{H}(t)\, \hat{U}(t, t_0), \\ \frac{d\hat{U}^{\dagger}(t, t_0)}{dt}\, \hat{U}(t, t_0) &= i\hat{U}^{\dagger}(t, t_0)\, \hat{H}(t)\, \hat{U}(t, t_0). \end{aligned} \tag{32}$$

Adding the two equations in (32), one can make use of the Leibniz product rule,

$$\hat{U}^{\dagger}(t, t_0)\frac{d\hat{U}(t, t_0)}{dt} + \frac{d\hat{U}^{\dagger}(t, t_0)}{dt}\hat{U}(t, t_0) = \frac{d}{dt}\left(\hat{U}^{\dagger}(t, t_0)\, \hat{U}(t, t_0)\right) = 0. \tag{33}$$

Provided that the initial conditions holds, $\hat{U}^{\dagger}(t_0, t_0)\, \hat{U}(t_0, t_0) = \hat{\mathbf{1}}$, this is sufficient to ensure that unitarity is also preserved at all later times,

$$\hat{U}^{\dagger}(t, t_0)\, \hat{U}(t, t_0) = \hat{\mathbf{1}}. \tag{34}$$

However, it is important to realize that the argument above is crucially based on the operatorical equivalence $\hat{H}^{\dagger}(t) = \hat{H}(t)$ for any t, which implies the equivalence of domains,

$$\mathcal{D}(\hat{H}^{\dagger}(t)) = \mathcal{D}(\hat{H}(t)). \tag{35}$$

An additional property that can be shown for any intermediate time $t_1 \in [t_2, t_0]$ is that

$$\hat{U}(t_2, t_1)\, \hat{U}(t_1, t_0) = \hat{U}(t_2, t_0). \tag{36}$$

[19] Stating that if $f : \mathbb{R} \to \mathbb{R}$, then f is Riemann integrable if and only if f is bounded and the set of discontinuities of f has measure 0.

The property above, known as the Markovian property [22], is a characteristic of various stochastic processes. Its intuitive meaning is that the evolution associated with the operator $\hat{U}$ has 'no memory', or differently said, that the evolution from time t_1 to time t_2 depends only on the state of the system at time t_1, and not on the preceding part of the evolution. The generalization of the above is given by the Trotter formula [23],

$$\lim_{n\to\infty} \hat{U}(t_n, t_{n-1}) \cdots \hat{U}(t_2, t_1)\, \hat{U}(t_1, t_0) = \lim_{n\to\infty} \hat{U}(t_n, t_0). \tag{37}$$

2.3.2. The Unbounded Evolution

The capacity of the bounded Hamiltonian to describe the quantum phenomena is limited only for systems that evolve in a gradual (functional) way. However, there are plethora of quantum processes for which the condition mentioned in footnote 1 is not satisfied. The mathematical characterization of these type of Hamiltonians can be done in accordance with footnote 1. As demonstrated in example 4.3, it can be shown that up to indefinite terms in these cases the transformation generated by $\hat{U}$ changes the norm of the evolved state,

$$\left\|\hat{U}(t, t_0)\, |\psi(t_0)\rangle\right\|_{\mathcal{D}(\hat{H})} = \mathcal{Z}(t, t_0)\, \||\psi(t_0)\rangle\|_{\mathcal{Y}}\,. \tag{38}$$

The factor $\mathcal{Z}(t, t_0)$ is typically known as the WF normalization, the LSZ factor, or the field strength. The preservation of the norm is obtained after including the compensation via the action of $\hat{\mathcal{N}}$, so that

$$\left\|\hat{\mathcal{P}}(t, t_0)\, |\psi(t_0)\rangle\right\|_{\mathcal{D}(\hat{H})} = \||\psi(t_0)\rangle\|_{\mathcal{Y}}\,. \tag{39}$$

A simple example is the Dirac comb potential (see example in 4.3,) which involves periodic kicks [26],

$$H(t) = \sum_{n=-\infty}^{\infty} \delta(t - nT), \tag{40}$$

with $T \in \mathbb{R}$. In order to get an impression of the subtleties that arise when handling this case we can simply take $H(t) = \delta(t - T)$. Due to (A12), for such a choice the differentiation and integration are not commutative operations[20],

$$\frac{d}{dt}\left(\int_{t_0}^{t} dt'\, \hat{H}(t') \int_{t_0}^{t'} dt''\, \hat{H}(t'')\right) \nrightarrow \hat{H}(t) \int_{t_0}^{t} dt'\, \hat{H}(t'). \tag{41}$$

It is also clear that for this choice the validity of the Fubini theorem (14) for evolution intervals which contain the singular times T has no mathematical justification to be used,

$$\int_{t_0}^{t} dt'\, \delta(t' - T) \int_{t_0}^{t'} dt''\, \delta(t'' - T) \nrightarrow \int_{t_0}^{t} dt'\, \delta(t' - T) \int_{t'}^{t} dt''\, \delta(t'' - T)\,. \tag{42}$$

In addition, the additivity property (17) holds only as long as $t' \neq T$, but fails when reaching the singular moment $t' = T$ as required by the unitarity argument,

$$\int_{t_0}^{t'=T} dt'\, \delta(t' - T) + \int_{t'=T}^{t} dt'\, \delta(t' - T) \nrightarrow \int_{t_0}^{t} dt'\, \delta(t' - T). \tag{43}$$

Obviously, without these properties the unitarity argument presented in 2.1 cannot be established. At this point one might be tempted to replace the delta function with its corresponding smeared version

[20] The notation of a broken arrow $\nrightarrow$ signifies here an invalid transition

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in order to avoid these problems. However, this means that our approach is fundamentally incapable of handling singular objects as they really are. As long as $T \notin [t_0, t]$ is outside of the evolution interval, unitarity is trivially preserved,

$$U^\dagger(t,\, t_0)\, U(t,\, t_0)\Big|_{T\notin[t_0,t]} = 1. \tag{44}$$

But for evolution intervals such that $t_1 \in (t_0,\, t)$ this is no longer the case,

$$U^\dagger(t,\, t_0)\, U(t,\, t_0)\Big|_{T\in[t_0,t]} \neq 1, \tag{45}$$

which is the reason behind (38). Note that contrary to the bounded case, as in Equation (36), the unbounded Hamiltonians describe non-Markovian process, so there exists at least one values of $t_1 \in (t,\, t_0)$ such that $U(t_2,\, t_1)\, U(t_1,\, t_0) \neq U(t_2,\, t_0)$.

3. The Properties of the Pitaron

In this part we would like to discuss more about the characteristics of the new solution with regards to the initial conditions and its ability to solve the Schrödinger equation.

3.1. Satisfying the Initial Conditions

An immediate observation is that satisfaction of the initial conditions by $\hat{U}$ implies they are also satisfied by $\hat{\mathcal{P}}$. Generally speaking, bounded Hamiltonians allow to satisfy the initial conditions trivially, as in that case both $\hat{U}(t_0,\, t_0) = \hat{\mathbf{1}}$ and $\hat{\mathcal{N}}(t_0,\, t_0) = \hat{\mathbf{1}}$ by continuity. Tackling the case of unbounded Hamiltonians is slightly less straightforward, and for $\hat{U}$ one has to make a fair necessary assumption that the initial time does not coincide with the places in which the Hamiltonian becomes singular[21], so that,

$$\lim_{t\to t_0} \int_{t_0}^{t} dt'\hat{H}(t') \longrightarrow 0. \tag{46}$$

For $\hat{\mathcal{P}}$, the necessary condition for ensuring the initial condition is

$$\lim_{t\to t_0} \hat{U}(t,\, t_0) = \lim_{t\to t_0} \hat{U}^\dagger(t,\, t_0) \quad \longrightarrow \quad \lim_{t\to t_0} \hat{\mathcal{N}}(t,\, t_0) = \lim_{t\to t_0} \hat{U}^{-1}(t,\, t_0), \tag{47}$$

which implies,

$$\lim_{t\to t_0} \hat{\mathcal{P}}(t,\, t_0) = \lim_{t\to t_0} \hat{U}^{-1}(t,\, t_0)\, \hat{U}(t,\, t_0) = \hat{\mathbf{1}}. \tag{48}$$

3.2. Solving the Schrödinger Equation

In this part we provide mathematical proof for our claim that the solution provided in (5) solves the original Schrödinger Equation (3). Let us start first with performing the calculation under the assumption of an Hermitian Hamiltonian. By using the Leibniz's product rule, the time derivative of $\hat{\mathcal{P}}$ can be expressed as[22],

$$\frac{d\hat{\mathcal{P}}(t,\, t_0)}{dt} = \hat{\mathcal{N}}(t,\, t_0)\frac{d\hat{U}(t,\, t_0)}{dt} + \frac{d\hat{\mathcal{N}}(t,\, t_0)}{dt}\hat{U}(t,\, t_0). \tag{49}$$

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21 For example, the value of $\lim_{t\to t_0} \int_{t_0}^{t} dt\, f(t)\, \delta(t - t_0)$ is undefined.

22 Note that differentiation and conjugation are not commutative operations, $\frac{d}{dt}\hat{\mathcal{P}}^\dagger(t,\, t_0) \neq \left(\frac{d}{dt}\hat{\mathcal{P}}(t,\, t_0)\right)^\dagger$, with equivalence only when using a self-adjoint Hamiltonian.

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By taking the time derivative of Equations (9) and (24), one arrives at the following set of equations (a detailed computation of the time derivative of $\hat{\mathcal{N}}$ is provided in Appendix B): The regular Schrödinger-Liouville dynamics: let $\hat{H}(t)$ be a bounded Hermitian Hamiltonian, then

$$\frac{d\hat{\mathcal{U}}(t,t_0)}{dt} = -i\hat{H}(t)\,\hat{\mathcal{U}}(t,t_0), \qquad \frac{d\hat{\mathcal{N}}(t,t_0)}{dt} = -i\left[\hat{H}(t),\hat{\mathcal{N}}(t,t_0)\right]. \tag{50}$$

By plugging Equations (50) inside relation (49), we note that indeed the Schrödinger equation is satisfied[23],

$$\begin{aligned}\frac{d\hat{\mathcal{P}}(t,t_0)}{dt} &= \hat{\mathcal{N}}(t,t_0)\left(-i\hat{H}(t)\hat{\mathcal{U}}(t,t_0)\right)\\ &+\left(-i\left[\hat{H}(t),\hat{\mathcal{N}}(t,t_0)\right]\right)\hat{\mathcal{U}}(t,t_0) = -i\hat{H}(t)\hat{\mathcal{P}}(t,t_0).\end{aligned} \tag{51}$$

One recognizes that the resulting equation for $\hat{\mathcal{N}}(t,t_0)$ is, in fact, the quantum Liouville equation [33], known alternatively as von Neuman equation [34], ensuring the probability conservation in our phase-space, and more commonly written in the equivalent form,

$$\begin{aligned}\frac{d\hat{\mathcal{N}}^2(t,t_0)}{dt} &= -i\hat{\mathcal{N}}(t,t_0)\left[\hat{H}(t),\hat{\mathcal{N}}(t,t_0)\right] - i\left[\hat{H}(t),\hat{\mathcal{N}}(t,t_0)\right]\hat{\mathcal{N}}(t,t_0)\\ &= -i\left[\hat{H}(t),\hat{\mathcal{N}}^2(t,t_0)\right].\end{aligned} \tag{52}$$

The dynamics of the above Liouville equation can be shown to be trivial: the value of $\hat{\mathcal{N}}(t_0,t_0) = \hat{\mathbf{1}}$ will remain unchanged throughout the entire evolution. However, this will no longer be justified in the case where the Hamiltonian is unbounded, or alternatively – non-Hermitian. The Hamiltonians which are under consideration here can be decomposed as a sum of a self-adjoint and singular component[24]. This singular component is non-vanishing on a measure-0 set and exists as a generalized object (see example 4.2),

$$\hat{H}(t) = \hat{\mathcal{H}}(t) - i\hat{\mathcal{J}}(t). \tag{53}$$

The corresponding evolution equations are:

$$\begin{aligned}\frac{d\hat{\mathcal{U}}(t,t_0)}{dt} &= -i\left(\hat{\mathcal{H}}(t) - i\hat{\mathcal{J}}(t)\right)\hat{\mathcal{U}}(t,t_0),\\ \frac{d\hat{\mathcal{N}}(t,t_0)}{dt} &= -i\left[\hat{\mathcal{H}}(t),\hat{\mathcal{N}}(t,t_0)\right] + \hat{\mathcal{N}}(t,t_0)\,\hat{\mathcal{J}}(t).\end{aligned} \tag{54}$$

It is straightforward to verify that Equation (54) above indeed solve the time-dependent Schrödinger equation (3) by inserting them to (49),

$$\begin{aligned}\frac{d\hat{\mathcal{P}}(t,t_0)}{dt} &= \hat{\mathcal{N}}(t,t_0)\left(-i\left(\hat{\mathcal{H}}(t) - i\hat{\mathcal{J}}(t)\right)\hat{\mathcal{U}}(t,t_0)\right)\\ &+\left(-i\left[\hat{\mathcal{H}}(t),\hat{\mathcal{N}}(t,t_0)\right] + \hat{\mathcal{N}}(t,t_0)\,\hat{\mathcal{J}}(t)\right)\hat{\mathcal{U}}(t,t_0) = -i\hat{\mathcal{H}}(t)\,\hat{\mathcal{P}}(t,t_0).\end{aligned} \tag{55}$$

Not surprisingly, the RHS of the above equation no longer depends on the anti self-adjoint component, $i\hat{\mathcal{J}}(t)$. This should have been expected – unlike the case of $\hat{\mathcal{U}}$, the differential equation for $\hat{\mathcal{P}}$ does not predict the decay of the probabilistic wave-function with time, even in the presence of a complex

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[23] The simplification $\hat{\mathcal{N}}(t,t_0)\hat{H}(t) + \left[\hat{H}(t),\hat{\mathcal{N}}(t,t_0)\right] = \hat{H}(t)\hat{\mathcal{N}}(t,t_0)$ is used.

[24] In order for operators $\hat{\mathcal{H}}(t)$ and $\hat{\mathcal{J}}(t)$ to represent an eligible decomposition of a diagonalizible Hamiltonian, they need to share a common set of eigenvectors. In that case they are simultaneously diagonalizable, which implies the relations $\left[\hat{\mathcal{H}}(t),\hat{\mathcal{J}}(t)\right] = 0$.

Hamiltonian. In case that the component $\hat{\mathcal{H}}(t)$ is bounded and evaluated on a proper time interval, the time evolution operator based on (55) can be constructed analogously to (4),

$$\hat{\mathcal{P}}(t,\, t_0) \;=\; \hat{T}\exp\left[-i\int_{t_0}^{t} dt'\, \hat{\mathcal{H}}(t')\right]. \tag{56}$$

Note that according to the current approach, in situtions in which the Hamiltonian is Hermitian but not self-adjoint, the replacement $\hat{U} \to \hat{\mathcal{N}}\hat{U}$ should not have affected the corresponding differential equation, but in reality we see that it does.

4. Examples

In this part we demonstrate with simple examples how our proposed solution affects the description of quantum systems practically. We start with examples in quantum mechanics, involving a single particle subjected to complex Hamiltonian, unbounded Hamiltonian, then we move to study the case of quantum field theory. However, even without studying any particular case, one can observe that when using the Born approximation[25] [40]. Naturally, a necessity of multiplying $\hat{U}(t,\, t_0)$ with an additional operator to maintain unitarity is apparent. In fact, similar consideration will apply whenever truncating the expansion for $\hat{U}(t,\, t_0)$ at any odd power. Our intention here is to demonstrate situations that unitarity is absent when even order of approximation is involved.

4.1. The Free Particle

Generally, a particle subject to a time-independent Hamiltonian is given as a sum of its kinetic and potential energy,

$$\hat{H}(\hat{x},\hat{p}) \;=\; \frac{\hat{p}^2}{2m} \;+\; \hat{V}(\hat{x},\hat{p}). \tag{57}$$

A simple choice is to examine the case of $\hat{V}(\hat{x},\hat{p}) \;=\; 0$, with a setup such that $x \;\in\; [0,1]$. The corresponding Hilbert space is spanned via the complete set of momentum eigenstates such that their corresponding eigenvalues belong to the extended real numbers set $\overline{\mathbb{R}}$,

$$\overline{\mathbb{R}} \;=\; \mathbb{R} \cup \{-\infty,\, \infty\}. \tag{58}$$

The resulting differential equation for a particle with mass m is obtained via $\hat{p} \;=\; i\hbar\frac{d}{dx}$,

$$i\hbar\frac{d}{dt}\left|\psi(x,t)\right\rangle \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left|\psi(x,t)\right\rangle. \tag{59}$$

The kinetic part can be resolved by introducing $|\psi(x,t)\rangle \;=\; \exp\left[-i\Delta t\,\frac{\hat{p}^2}{2m}\right]|\psi(x,t_0)\rangle$, from which we infer the time evolution operator

$$\hat{U}(t,\, t_0) \;=\; \exp\left[-i\Delta t\,\frac{\hat{p}^2}{2m}\right]. \tag{60}$$

As previously mentioned, an operator $\hat{\mathcal{O}}$ on the Hilbert space $\mathcal{H}$ is called self-adjoint if it is operatorically identical to its adjoint, $\hat{\mathcal{O}}^\dagger \;=\; \hat{\mathcal{O}}$. The equivalence between two operators implies two conditions:

$$\langle\varphi|\,\hat{\mathcal{O}}^\dagger\,|\psi\rangle = \langle\varphi|\,\hat{\mathcal{O}}\,|\psi\rangle \qquad\qquad |\varphi\rangle\,,|\psi\rangle \in \mathcal{H}, \tag{61}$$

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[25] In that case only the leading order term dominates the expansion of $\hat{U}(t,\, t_0)$, $\left\|\int_{t_0}^{t} dt'\, \hat{H}(t')\right\| \gg \left\|\int_{t_0}^{t} dt'\, \hat{H}(t')\, \int_{t_0}^{t'} dt''\hat{H}(t'')\right\|$.

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and additionally the domains are identical, $\mathcal{D}(\hat{\mathcal{O}}^\dagger) = \mathcal{D}(\hat{\mathcal{O}})$.

The second condition holds automatically when $\hat{\mathcal{O}}$ is finite-dimensional operator, since in that case $\mathcal{D}(\hat{\mathcal{O}}) = \mathcal{H}$ for every non-singular linear operator on a finite-dimensional space. However, in the infinite-dimensional case the domain $\mathcal{D}(\hat{\mathcal{O}}^\dagger)$ may be a larger subspace than $\mathcal{D}(\hat{\mathcal{O}})$, so that $\mathcal{D}(\hat{\mathcal{O}}) \subseteq \mathcal{D}(\hat{\mathcal{O}}^\dagger)$. In that case the operator $\hat{\mathcal{O}}$ is called Hermitian. Thus, any self-adjoint operator is Hermitian, but an Hermitian operator is not necessarily self-adjoint [6]. Noticeably, for a bounded self-adjoint Hamiltonian the spectrum is real and the eigenvectors associated to different eigenvalues are mutually orthogonal. Moreover, all the eigenvectors are having a finite norm and together they form a complete Hilbert space [27]. These properties do not hold for operators which are only Hermitian [28]. As demonstrated in [7] for the momentum operator $\hat{p}$ of a particle living on a compact domain $L^2[0,1]$, the equivalence $\langle\varphi|\,\hat{p}^\dagger\,|\psi\rangle = \langle\varphi|\,\hat{p}\,|\psi\rangle$ holds for any $|\varphi\rangle\,, |\psi\rangle \in \mathcal{D}(\hat{p})$. This since for all $|\psi(x)\rangle \in \mathcal{D}(\hat{p})$,

$$\begin{aligned}&\int_0^1 dx\;\langle\varphi(x,t)|\,\hat{p}^\dagger\,|\psi(x,t)\rangle - \int_0^1 dx\;\langle\varphi(x,t)|\,\hat{p}\,|\psi(x,t)\rangle \\ &= \frac{\hbar}{i}\left(\langle\varphi(x=1,t))\,|\psi(x=1,t))\rangle - \langle\varphi(x=0,t))\,|\psi(x=0,t)\rangle\right) = 0\,.\end{aligned} \tag{62}$$

However, since the boundary conditions satisfied by $|\psi(x)\rangle \in \mathcal{D}(\hat{p})$ are already sufficient for annihilating the surface term,

$$\mathcal{D}(\hat{p}) \subset \mathcal{D}(\hat{p}^\dagger). \tag{63}$$

Thus, the operator $\hat{p}$ is Hermitian but not self-adjoint [8],

$$\hat{p}^\dagger \neq \hat{p}\,, \tag{64}$$

and the same conclusion remains true also at the level of the Hamiltonian. Thus, the corresponding time evolution operator (60), cannot be regarded as unitary, $\hat{U}^\dagger(t,\,t_0) \neq \hat{U}^{-1}(t,\,t_0)$. Our approach is also related with the well known problem that the solution in this case is non-normalizable. In the standard approach, the result for the WF is taken as

$$|\psi(x,t)\rangle = N\,e^{-i(kx-\omega t)}\,|\psi_0\rangle\,, \tag{65}$$

and one attempts to fix the overall pre-factor N via the normalization condition,

$$\int_{all\ space} \||\psi(x,t)\rangle\|^2\,dx = 1. \tag{66}$$

As long as the space is of finite size, based on the transitions

$$\left(e^{-i(kx-\omega t)}\right)^\dagger e^{-i(kx-\omega t)} = e^{i(kx-\omega t)}e^{-i(kx-\omega t)} = e^{i(kx-\omega t)-i(kx-\omega t)} = 1, \tag{67}$$

the condition (66) yields

$$|N| = \frac{1}{\sqrt{L}} \in \mathbb{R}. \tag{68}$$

However, if our intention is to use the complete unbounded space $\overline{\mathbb{R}}$, its cover has to be considered separately, as the case $kx - \omega t = \infty$ does not allow to apply the familiar simplification rules. Therefore, based on our logic the solution is given by

$$|\psi(x,t)\rangle = \mathcal{N}(t)\,e^{-i(kx-\omega t)}\,|\psi_0\rangle\,. \tag{69}$$

The result above includes an indefinite norm that cannot be further simplified,

$$\mathcal{N}(t) = \sqrt{\left(\int dy\ \left(e^{-i(ky-\omega t)}\right)^{\dagger} e^{-i(ky-\omega t)}\right)^{-1}}\,. \tag{70}$$

Another perspective can be found by working in momentum representation.

4.2. The Coulomb Potential

The inter-atomic and molecular potentials are known empirically to be described by inverse positive powers of the Euclidean norm, and therefore, cannot be defined everywhere [24][25]. Well known examples are the Coulomb, Yukawa, van der Waals, Lennard-Jones, and London potentials [26]. Here our interest is to provide a new perspective for analyzing the Coulomb force. Let us start with an explanation the current approach for dealing with this case, then discuss its drawback, and provide an alternative approach. This potential is expressed via

$$V(\hat{r}) = -\frac{\kappa}{\|\hat{r}\|}, \qquad \kappa > 0\,, \tag{71}$$

and full Hamiltonian, including the kinetic term, is given by

$$H(\hat{r},\hat{p}) = T(\hat{p}) + V(\hat{r}) = \frac{\hat{p}^2}{2m} - \frac{\kappa}{\|\hat{r}\|}\,. \tag{72}$$

For simplicity, in order to focus on the part that matters, let us assume that the kinetic term is sufficiently well behaved and the limit $m \to \infty$ is taken. In the current approach, an additional assumption that is unjustifiably introduced is that the problem can be adequately studied on the space $L^2(\mathbb{R})$. Under such an assumption contributions of measure-0 has no importance, and the singularity at the origin can be disregarded. Thus, it is sufficient to specify the potential only on a densely defined part of the space,

$$V(r) = \begin{cases} -\frac{\kappa}{r} & r \neq 0 \\ 0 & r = 0 \end{cases}\,. \tag{73}$$

As expected, the corresponding time evolution operator, Equation (2), based on representation (73) is unitary everywhere. However, expression (73) is an over simplification of the original singular potential and is incompatible with the classically correspondent case in which the source to be represented by a distribution. Suppose now that we no longer assume dealing with $L^2(\mathbb{R})$, and therefore our previous assumption that measure-0 contributions can be ignored is no longer justified. The first thing we have to do is to provide a meaning to the singularity in terms of familiar objects. This can be done by generalizing the framework, $\mathbb{R} \to \mathbb{C}$, so that $V(r) \to V(r,\epsilon) = \frac{1}{r-i\epsilon}$. Eventually, we can get back to the real line by taking vanishing imaginary component, $\epsilon \to 0$. A valuable relation in our case is the Sokhotski theorem,

$$V(r) = \lim_{\epsilon\to 0} V(r,\epsilon) = \lim_{\epsilon\to 0} \frac{1}{r-i\epsilon} = P.v.\left(\frac{1}{r}\right) + i\pi\delta(r). \tag{74}$$

Thus, in our approach the consistent representation of the Coulomb force is:

$$V(r) = \begin{cases} -\frac{\kappa}{r} & r \neq 0 \\ -i\pi\kappa\,\delta(r) & r = 0 \end{cases}\,. \tag{75}$$

The corresponding expression for the time evolution operator is

$$U(r,\Delta t)=\begin{cases}\exp\left[-\frac{i\kappa}{r}\Delta t\right] & r\neq 0\\ \exp\left[\kappa\pi\delta(r)\,\Delta t\right] & r=0\end{cases}, \tag{76}$$

Although the last result is unitary for any $r \neq 0$, our approach regard the case $r = 0$ as non-unitary,

$$\left(\exp\left[\kappa\pi\delta(r)\,\Delta t\right]\right)^{\dagger} \neq \left(\exp\left[\kappa\pi\delta(r)\,\Delta t\right]\right)^{-1}. \tag{77}$$

despite the fact that a rigorous proof is still not at hand. An important observation is that since the Taylor series expansion does not exist for generalized object, one cannot repeat the considerations of (31). Therefore, without getting into the details of how to define $\exp\left[\pi\delta(\hat{r})\,\Delta t\right]$, we can use the following formal structure as a unitary operator

$$\mathcal{P}(r,\Delta t) = \sqrt{\exp^{\dagger-1}\left[\kappa\pi\delta(r)\,\Delta t\right]\,\exp^{-1}\left[\kappa\pi\delta(r)\,\Delta t\right]}\,\exp\left[\kappa\pi\delta(r)\,\Delta t\right]. \tag{78}$$

The situation becomes more interesting when passing from potentials with only a single singular point to the case in which a measure-0 set of singularities is involved. An explicit example for such a potential is the Poschl-Teller potential (see Figure 2),

$$V(r) = \frac{V_0}{\cos^2 \alpha r}, \tag{79}$$

which after extracting the generalized part can be written

$$\lim_{\epsilon\to 0}\frac{V_0}{\cos^2\alpha r - i\epsilon} = P.v.\left(\frac{V_0}{\cos^2 \alpha r}\right) + i\pi\delta(\cos^2 \alpha r). \tag{80}$$

Showing us that unitarity is not maintained at the tunneling points. Without solving the singular dynamics, one has to specify itself only for a specific branch of the potential, and cannot realize the entire dynamics that includes the singular locations.

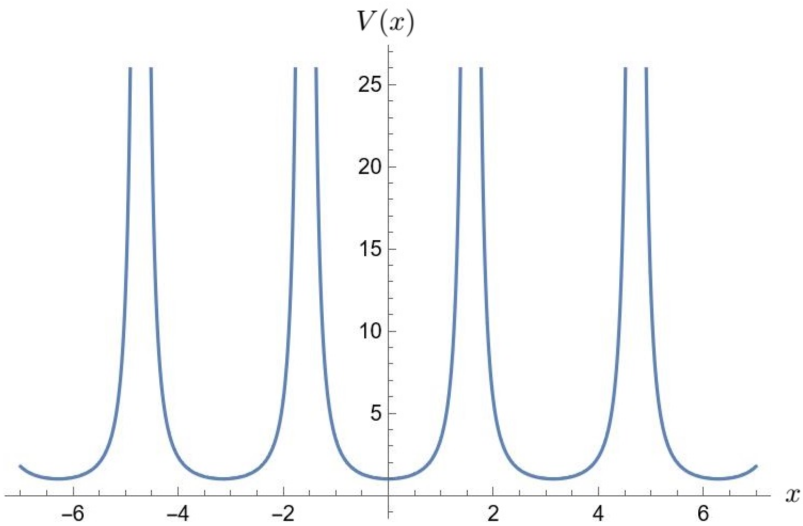

Figure 2. The Poschl-Teller potential with $V_0 = \alpha = 1$.

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4.3. The Dirac Comb Potential

One of the simplest examples in order to demonstrate the dynamics of a time-dependent unbounded (distributional) Hamiltonian is to use the Dirac comb potential (see Figure 3). The properties of this potential has already been previously briefly mentioned in Section 2.3.2.

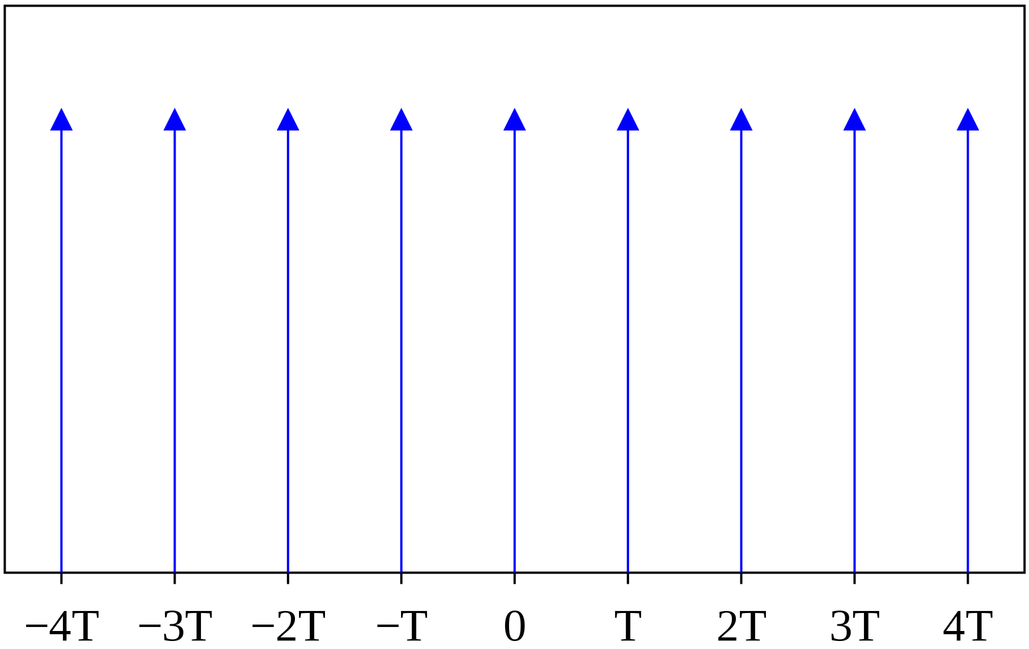

Figure 3. The Dirac comb.

For our purpose it will be sufficient to use a truncated version of the series,

$$V(t) = \sum_{i=1}^{n} V_i\,\delta(t - t_i), \tag{81}$$

where $V_i \in \mathbb{R}$ denotes an array of n values. Clearly, the unitarity argument presented in Section 2.1 is inadequate for the above choice of Hamiltonian due to the failure of additivity at the singular times t_i. Let us now examine the resulting expansion from the Dyson series. With the aid of the integration in Equation (A9), one finds the following expressions for Equations (9) and (24):

$$\begin{aligned} U(t,0) &= 1 - i\sum_{i=1}^{n} V_i\,\Theta(t-t_i) - \sum_{i=1}^{n} V_i^2 \int_0^t dt'\,\delta(t'-t_i)\,\Theta(t'-t_i) + \ldots \\ \mathcal{N}(t,0) &= 1 - \frac{1}{2}\left(\sum_{i=1}^{n} V_i\,\Theta(t-t_i)\right)^2 + \sum_{i=1}^{n} V_i^2 \int_0^t dt'\,\delta(t'-t_i)\,\Theta(t'-t_i) + \ldots \end{aligned} \tag{82}$$

As expected, based on the discussion in Appendix A, both the results for U and $\mathcal{N}$ above are ill-defined due to the last term (which cancels when taking their products.) Therefore, one can think of $\mathcal{N}$ as a regulator which replaces indefinite integrals involved in U by valid integrals describing the singular dynamics. In order to get an impression on how $\mathcal{N}$ evolves, it is useful to work with a truncated version of $\mathcal{N}$ which does not involve integration over products of distributions,

$$\mathcal{N}(t,0)|_{trunc.} \equiv 1 - \frac{1}{2}\left(\sum_{i=1}^{n} V_i\,\Theta(t-t_i)\right)^2 + \ldots \tag{83}$$

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A plot of the last expression is shown in Figure 4. We note that if $\mathcal{N}$ was differentiable like an ordinary function, then indeed $\frac{d\mathcal{N}}{dt} = 0$, however, $\mathcal{N}$ is non-differentiable. However, the construction defined by $\mathcal{P}(t, 0)$, as defined by Equation (27), involves the action of $\mathcal{N}(t, 0)$ on $U(t, 0)$ before the evaluation of the integrals. One arrives at a result which does not include ill-defined terms,

$$\mathcal{P}(t, 0) = \mathcal{N}(t, 0)\, U(t, 0) = 1 - i \sum_{i=1}^{n} V_i \Theta(t - t_i) - \frac{1}{2} \left(\sum_{i=1}^{n} V_i \Theta(t - t_i) \right)^2 + \dots \tag{84}$$

Although our formalism does not describe what happens at the isolated transition time t_1, this is not of any concern. Practically, the time that a perturbation is turned on is well separated from the time that a measurement is conducted.

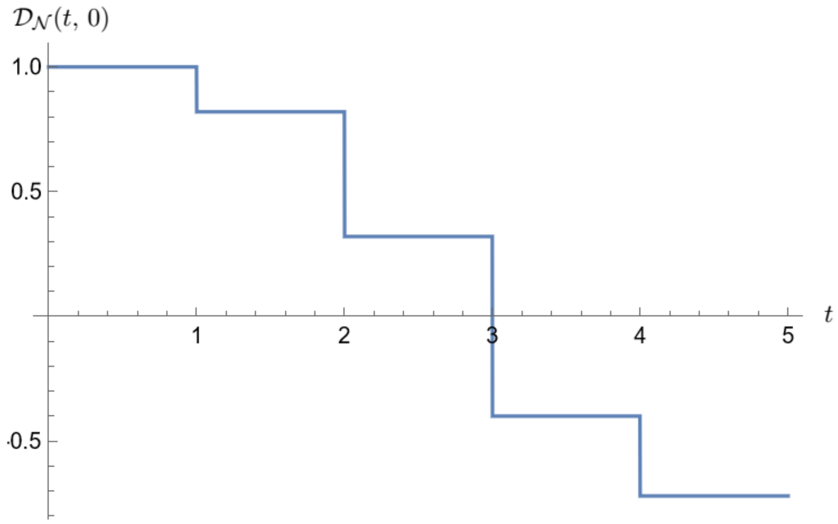

Figure 4. The value of the defined part of $\mathcal{N}(t, 0)$ for the Dirac comb Hamiltonian (81) with $n = 4$ and $V_i = \{0.6, 1, 1.2, 0.8\}$.

We would like to finish this part with a comment. It is tempting to think that the problem with products of distributions can be solved by replacing the Dirac delta function by a function with a finite width $\epsilon > 0$. This can be done by using either the nascent or Gaussian representation,

$$\delta(x) \to \frac{\epsilon}{\pi(x^2 + \epsilon^2)}, \qquad \delta(x) \to \frac{1}{2\sqrt{\pi\epsilon}} \exp\left(-\frac{x^2}{4\epsilon}\right). \tag{85}$$

By applying such a replacement one effectively replace an unbounded Hamiltonian with a bounded version, and the description of the system is given entirely by $U(t, 0)$. However, it is crucial to understand that this demands from us the introduction of an additional dimensionful parameter – the width. Of course, the replaced integrals exist only as long as the width is kept non-vanishing. While the introduction of dimensionful parameter can sometime be justified, a clear advantage is to have an approach that is compatible with the Hamiltonian already in its original form, expressed in terms of generalized objects.

5. Conclusions

In this part a summarized list of the consequences is provided for adopting (5) as the solution for the Schrödinger equation. These implications affect both the perturbative and the non-perturbative aspects.

- The currently widely used solution $\hat{U}$ should be regarded as a unitary everywhere operator only when working with a self-adjoint Hamiltonian on a Hilbert space (each state has a defined norm). On infinitely dimensional Hilbert spaces Hermiticity and self-adjoint are not equivalent properties, and Hermiticity is insufficient condition to guarantee a unitary evolution.

- ⊛ The Liouville part of the evolution is dormant for bounded Hamiltonians and become activated for unbounded Hamiltonians on a measure-0 set. It acts as a "probability conservation regulator," and produces a correction for the discontinuous evolution that is involved in the dynamics of $\hat{U}$.
- ⊛ For the proposed solution unitary is maintained manifestly, at all orders and at any given moment of the evolution, rather than asymptotically. The ordinary probabilistic interpretation is applicable even for unbounded Hamiltonians: the modulus of transitions amplitudes are always given by a defined expressions (up to regularization).
- ⊛ The dynamics of quantum systems with unbounded Hamiltonian is non-Markovian. The typical approach wrongly assumes that the space $L^2(\mathbb{R})$ is suitable to study these problems. However, a more faithful approach would be to assume no knowledge of space or "indefinite norm spaces" such as Krein space, such that a $\hat{\mathcal{N}}$ becomes non-trivial operator.
- ⊛ The solution provided will hopefully pave the way for a better understanding of various quantum systems in which unitarity is currently assumed to be broken. As such are systems with a non-Hermitian Hamiltonians, field theories on non-commutative spaces [46], field theories on factional dimensions [47], or open quantum systems [48].
- ⊛ The reason which has initiated this study and was not mentioned is scattering amplitudes for entangled states. In this setup, unlike that where fully on-shell states are involved, strangely the JIMWLK equation [45] is no longer applicable. That happens since the normalization of the WF via simple overall $\mathcal{Z}$ factor breaks down and a convolution is required. The analysis of the time evolution of entangled states is a key for experimental verification of our proposed idea.

Data Availability Statement: Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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Appendix A. Why May the Iterative Method Fail?

In this section we would like to discuss the Picard's method of successive approximations [14,15] in order to analyze the capacity of this approach to yield the solution for a differential evolution equation of first order. Our intention is to consider a differential equation of the type

$$\frac{dy}{dx} = f(x,y)\,, \tag{A1}$$

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subject to the initial condition $y(x_0) = y_0$. The key point of Picard's idea consist in replacing the original differential equation by a system of difference equations that approximate the evolution occurring in a small neighborhood of the domain[26] [16]. As demonstrated below, under certain assumptions, the resulting difference equation can reliably approximate the evolution on the whole domain. In that case, the resulting solution uniquely converges to the analytic solution of the original equation. Our intention is to provide an answer for the following fundamental question – what are the necessary conditions for the iterative method to be applicable? is the discretization limit always admissible?

Let us start by applying the method in the non-negative region $[0,\, x]$ with the simple choice of $f(x,y) = gy$ with $y_0 = 1$. The analytical solution corresponding to our choice can naturally be found by direct integration, $y(x) = e^{gx}$. Now let us reproduce the last solution via the iterative method. Our initial assumption is that the differential equation above allows to start a process of successive approximations by rewriting it in the integral form,

$$y_{n+1}(x) \;=\; y_0 + \int_0^x dx'\, f(x', y_n(x')). \tag{A2}$$

After a few iterations the following results are obtained:

$$\begin{aligned} y_1(x) \;&=\; 1 + g\int_0^x 1\, dx' = 1 + gx, \\ y_2(x) \;&=\; 1 + g\int_0^x (1+gx)\, dx' = 1 + gx + \frac{1}{2!}g^2x^2, \\ y_3(x) \;&=\; 1 + g\int_0^x (1 + gx + \frac{1}{2!}g^2x^2)\, dx' = 1 + x + \frac{1}{2!}g^2x^2 + \frac{1}{3!}g^3x^3, \end{aligned} \tag{A3}$$

from which we observe the series that is generated after n iterations,

$$y_n(x) \;=\; \sum_{i=0}^{n} \frac{g^n}{n!}x^n. \tag{A4}$$

As expected, the sequence $\{y_n(x)\}$ converges to the Taylor series for the exponent,

$$\lim_{n\to\infty} y_n(x) \;=\; e^{gx}\,, \tag{A5}$$

which indeed reproduced the expected result. This last equivalence was, in fact, guaranteed to us by the Picard–Lindelöf theorem [15]. As lengthy discussed in [17], the error at the nth step of the iterative procedure in the interval $x_0 - h < x < x_0 + h$ with $h \equiv \min\left(a,\, \frac{b}{M}\right)$, where $|x - x_0| \leq a$ and $|y(x) - y_0| \leq b$, is bounded by the inequality

$$|y_n(x) - y(x)| \;\leq\; \frac{MN^{n-1}}{n!}h^n, \tag{A6}$$

with the definitions $M \equiv \max_{(x,y)\in\mathcal{D}} |f(x,y)|$, $N \equiv \max_{(x,y)\in\mathcal{D}} \left|\frac{\partial f}{\partial y}\right|$. Clearly, in order for the solution obtained by iterative method to be considered valid, it must converge asymptotically to the analytic solution,

$$\lim_{n\to\infty} |y_n(x) - y(x)| \;=\; 0. \tag{A7}$$

---

[26] So that, (A1) is essentially replaced by solving the system $y_1 - y_0 \approx f(x,y_0)\,\Delta x$, $y_2 - y_1 \approx f(x,y_1)\,\Delta x$, $\ldots$, $y_{n+1} - y_n \approx f(x,y_n)\,\Delta x$, that leads to $y_{n+1} - y_0 \approx f(x,y_0)\,\Delta x + f(x, y_0 + f(x,y_0)\,\Delta x)\,\Delta x + \ldots$.

However, as we are about to see, the above theorem will fail to imply uniqueness when singularities are involved. For example, let us take a closer look on what happens when trying to solve a differential equation with RHS involving Dirac delta function [18],

$$\frac{df(x)}{dx} = \delta(x-a)\, f(x), \tag{A8}$$

subject to the initial condition $f(0) = 1$ with $a > 0$. The direct solution method leads to $f(x) = e^{\Theta(x-a)}$, where we have used the defining relation for the Heaveside theta function[27],

$$\int_0^x dx'\, \delta(x'-a) = \Theta(x-a). \tag{A9}$$

Now let us try to reproduce the last result by the iterative method. For that purpose we present the solution as

$$f(x) = 1 + \int_0^x dx'\, \delta(x'-a)\, f(x')\,, \tag{A10}$$

and then by substitution

$$f(x) = 1 + \int_0^x dx'\, \delta(x'-a) \left[1 + \int_0^{x'} dx''\, \delta(x''-a)\, f(x'')\right]. \tag{A11}$$

After performing the integration of the inner brackets by using (A9) it is clear that something goes wrong. One arrives at the badly defined result that involves integration over a product of two distributions [19],

$$\int_0^x dx'\, \delta(x'-a)\, \Theta(x'-a) \longrightarrow \texttt{Indefinite}. \tag{A12}$$

It is, therefore, clear that the iterative series (A11) will not converge to the expected result. We realize that in order for the iterative method to work, the integrand has to be well defined (measurable function) at each part of the domain. A more practical example, which allows to get a deeper understanding what happens when the conditions for Picard theorem fails, is given by the differential equation,

$$x\frac{dy}{dx} = A, \tag{A13}$$

which has an unbounded RHS when brought to the form of (A1). The solution is often taken as $y(x) = A \log|x| + C$, although a more general discontinuous solution can be found,

$$y = \begin{cases} A\log(x) + C & x > 0 \\ A\log(-x) + B & x < 0. \end{cases} \tag{A14}$$

In terms of distributions that can be expressed as $y(x) = A\, \log|x| + (B-C)\,\Theta(-x) + C$. Note that even thought the constant term changes in the passage between the two disjoint regions, this is still valid a solution. The discontinuous part, or alternatively, the singular dynamics at $x = 0$, is exactly the part in which the iterative procedure fails to provide a definitive answer. Thus, our main conclusion in this part is that singular differential equations[28] cannot be solved by a solution method that is based solely on the iterative method.

---

27 Generally, if the signs of a and x are unknown, $\int_0^x f(x')\,\delta(x'-a)\,dx' = f(a)\,(2\Theta(x)-1)\,\Theta(a-x\Theta(-x))\,\Theta(-a+x\Theta(x))$.

28 These are typically of the form $x^n \frac{d^m y}{dx^m} = 0$ with $n, m \in \mathbb{N}$. For example, as discussed in [20], if $m = 1$ the obtained result is given by $y(x) = c_1 + c_2\Theta(x) + c_3\delta(x) + c_4\delta'(x) + \ldots + c_{n+1}\delta^{(n-2)}(x)$ for which approximate expressions cannot be found.

Appendix B. The Dynamics of $\hat{\mathcal{N}}$

In this part we provide the proof for the second equation of (54). From the defining relation for the normalization operator, $\hat{\mathcal{U}}^{\dagger}(t, t_0)\,\hat{\mathcal{N}}^2(t, t_0)\,\hat{\mathcal{U}}(t, t_0) = \hat{\mathbf{1}}$. By applying the time derivative on the two side of this equation it follows that

$$\begin{aligned}&\hat{\mathcal{U}}^{\dagger}(t, t_0)\left(\hat{\mathcal{N}}(t, t_0)\frac{d\hat{\mathcal{N}}(t, t_0)}{dt} + \frac{d\hat{\mathcal{N}}(t, t_0)}{dt}\hat{\mathcal{N}}(t, t_0)\right)\hat{\mathcal{U}}(t, t_0)\\ &= -\frac{d\hat{\mathcal{U}}^{\dagger}(t, t_0)}{dt}\,\hat{\mathcal{N}}^2(t, t_0)\,\hat{\mathcal{U}}(t, t_0) - \hat{\mathcal{U}}^{\dagger}(t, t_0)\,\hat{\mathcal{N}}^2(t, t_0)\,\frac{d\hat{\mathcal{U}}(t, t_0)}{dt}.\end{aligned} \tag{A15}$$

After multiplication by $\hat{\mathcal{U}}^{\dagger-1}(t, t_0)$ from the right side and $\hat{\mathcal{U}}^{-1}(t, t_0)$ from the left side becomes

$$\begin{aligned}&\hat{\mathcal{N}}(t, t_0)\frac{d\hat{\mathcal{N}}(t, t_0)}{dt} + \frac{d\hat{\mathcal{N}}(t, t_0)}{dt}\hat{\mathcal{N}}(t, t_0)\\ &= -\hat{\mathcal{U}}^{\dagger-1}(t, t_0)\,\frac{d\hat{\mathcal{U}}^{\dagger}(t, t_0)}{dt}\,\hat{\mathcal{N}}^2(t, t_0) - \hat{\mathcal{N}}^2(t, t_0)\,\frac{d\hat{\mathcal{U}}(t, t_0)}{dt}\,\hat{\mathcal{U}}^{-1}(t, t_0),\end{aligned} \tag{A16}$$

which is a Sylvester type equation [35] for $\frac{d\hat{\mathcal{N}}(t, t_0)}{dt}$. In our case, due to positive definite property of $\hat{\mathcal{N}}$, this equation can be solved in a unique manner. In fact, this equation is not just a Sylvester equation, but more precisely the continuous time Lyapunov equation[29] [36]. As such, its solution is known to be given explicitly by the integral

$$\begin{aligned}\frac{d\hat{\mathcal{N}}(t, t_0)}{dt} &= -\int_0^{\infty} dy\, e^{-y\hat{\mathcal{N}}(t, t_0)}\\ \times&\left(\hat{\mathcal{U}}^{\dagger-1}(t, t_0)\,\frac{d\hat{\mathcal{U}}^{\dagger}(t, t_0)}{dt}\,\hat{\mathcal{N}}^2(t, t_0) + \hat{\mathcal{N}}^2(t, t_0)\,\frac{d\hat{\mathcal{U}}(t, t_0)}{dt}\,\hat{\mathcal{U}}^{-1}(t, t_0)\right)e^{-y\hat{\mathcal{N}}(t, t_0)}.\end{aligned} \tag{A17}$$

By plugging the dynamics of $\hat{\mathcal{U}}$ from Equation (54) in the above result we obtain

$$\begin{aligned}\frac{d\hat{\mathcal{N}}(t, t_0)}{dt} &= -\int_0^{\infty} dy\, e^{-y\hat{\mathcal{N}}(t, t_0)}\\ \times&\left(i\left(\hat{\mathcal{H}}(t) + i\hat{\mathcal{J}}(t)\right)\hat{\mathcal{N}}^2(t, t_0) - i\hat{\mathcal{N}}^2(t, t_0)\left(\hat{\mathcal{H}}(t) - i\hat{\mathcal{J}}(t)\right)\right)e^{-y\hat{\mathcal{N}}(t, t_0)},\end{aligned} \tag{A18}$$

which after simplifications[30] can equivalently written

$$\frac{d\hat{\mathcal{N}}(t, t_0)}{dt} = -\int_0^{\infty} dy\,\frac{d}{dy}\left[e^{-y\hat{\mathcal{N}}(t,t_0)}\left(-i\left[\hat{\mathcal{H}}(t), \hat{\mathcal{N}}(t,t_0)\right] + \hat{\mathcal{N}}(t, t_0)\,\hat{\mathcal{J}}(t)\right)e^{-y\hat{\mathcal{N}}(t,t_0)}\right]. \tag{A19}$$

Finally, an immediate integration[31] of the last result establishes the fact that $\hat{\mathcal{N}}(t, t_0)$ has a non-trivial dynamics that is given by the second equation that is written in (54).

---

[29] These are equtions of the type $\hat{\mathbf{A}}\hat{\mathbf{X}} + \hat{\mathbf{X}}\hat{\mathbf{A}}^{\dagger} + \hat{\mathbf{Q}} = 0$ where $\hat{\mathbf{Q}}$ is a self-adjoint operator.

[30] By using the identity $\left[\hat{\mathcal{H}}(t), \hat{\mathcal{N}}^2(t, t_0)\right] = \hat{\mathcal{N}}(t, t_0)\left[\hat{\mathcal{H}}(t), \hat{\mathcal{N}}(t, t_0)\right] + \left[\hat{\mathcal{H}}(t), \hat{\mathcal{N}}(t, t_0)\right]\hat{\mathcal{N}}(t, t_0)$ along with the observation that since the operator $\hat{\mathcal{N}}$ is fully expressible based on the operator $\hat{\mathcal{J}}$ they shares a common basis and domain, $\left[\hat{\mathcal{N}}(t, t_0), \hat{\mathcal{J}}(t)\right] = 0$.

[31] More explicitly, $\int_0^{\infty} dy \frac{d}{dy}\left[e^{-y\hat{\mathcal{N}}(t,t_0)}\hat{\mathcal{O}}(t, t_0)e^{-y\hat{\mathcal{N}}(t,t_0)}\right] = e^{-y\hat{\mathcal{N}}(t,t_0)}\hat{\mathcal{O}}(t, t_0)e^{-y\hat{\mathcal{N}}(t,t_0)}\Big|_0^{\infty} = -\hat{\mathcal{O}}(t, t_0)$.

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