Factorizing the time evolution operator

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Received 12 September 2006
Accepted for publication 14 November 2006
Published 12 January 2007
Online at stacks.iop.org/PhysScr/75/185

Abstract
There is a widespread belief in the quantum physical community, and textbooks used to teach quantum mechanics, that it is a difficult task to apply the time evolution operator \( e^{i\hat{H}/\hbar} \) on an initial wavefunction. Because the Hamiltonian operator is, generally, the sum of two operators, then it is not possible to apply the time evolution operator on an initial wavefunction for it implies using terms like \((\hat{a} + \hat{b})^n\). A possible solution is to factorize the time evolution operator and then apply successively the individual exponential operator on the initial wavefunction. However, the exponential operator does not directly factorize, i.e. \( e^{\hat{a} + \hat{b}} \neq e^{\hat{a}} e^{\hat{b}} \).

In this study we present a useful procedure for factorizing the time evolution operator when the argument of the exponential is a sum of two operators, which obey specific commutation relations. Then, we apply the exponential operator as an evolution operator for the case of elementary unidimensional potentials, like a particle subject to a constant force and a harmonic oscillator. Also, we discuss an apparent paradox concerning the time evolution operator and non-spreading wave packets addressed previously in the literature.

PACS numbers: 03.65.—w, 03.65.Ge

(Some figures in this article are in colour only in the electronic version.)

1. Introduction

As is well known, quantum mechanics is a successful theory. Although highly counterintuitive, using it we are able to explain the microscopic world. Also, quantum mechanics has discovered many natural processes that have culminated in practical technological applications, like the transistor and quantum cryptography. However, quantum mechanics is a difficult field of study for it takes many years to develop the necessary skills to understand its relevant concepts.

One of the hardest cognitive skills to develop is to understand the technique used to solve the fundamental equation of quantum mechanics, i.e. the Schrödinger equation. In fact, there are few cases where this equation has been analytically solved. One of the principal factors that impede the straightforward solution of the Schrödinger equation is that it involves unusual mathematical concepts, like operators

\[
\hat{H} = \hat{a} + \hat{b},
\]

where the Hamiltonian \( \hat{H} \) is an operator that has to be self-adjoint, and it is generally the sum of two or more operators, let us say

\[
\hat{a} \quad \text{and} \quad \hat{b}.
\]

In the literature, the most used technique to solve equation (1) is to find the eigenvalues and eigenfunctions of the time-independent Schrödinger equation

\[
\hat{H} \psi_n(x) = E_n \psi_n(x),
\]

where \( E_n \) and \( \psi_n(x) \) are, respectively, the eigenvalues and eigenfunctions of the Hamiltonian \( \hat{H} \) [1–4]. Then, the time-independent wavefunction is constructed taking the superposition of the eigenfunctions of the Hamiltonian

\[
\Psi(x, t) = \sum_{n=0}^{\infty} e^{-iE_n t/\hbar} c_n \psi_n(x),
\]

where \( c_n = \int \psi_n(x, 0) \psi_n(x, 0) \textrm{d}x \) is the scalar product between the initial state of the system and the eigenfunctions of the Hamiltonian. In this paper, we call this method the eigenstates method.

Another way for solving equation (1), if we consider a time-independent Hamiltonian, is to integrate equation (1) respect to time, to obtain [1]

\[
\Psi(x, t) = e^{-i/\hbar} \Psi(x, 0) = e^{\hat{a} + \hat{b}} \Psi(x, 0),
\]

Let, by way of example, we consider an elementary unidimensional potential like a particle subject to a constant force and a harmonic oscillator, then we have

\[
\hat{H} = \hat{a} + \hat{b}.
\]

A possible solution is to factorize the time evolution operator \( e^{i\hat{H}/\hbar} \) on an initial wavefunction. However, the exponential operator does not directly factorize, i.e. \( e^{\hat{a} + \hat{b}} \neq e^{\hat{a}} e^{\hat{b}} \).

In this study we present a useful procedure for factorizing the time evolution operator when the argument of the exponential is a sum of two operators, which obey specific commutation relations. Then, we apply the exponential operator as an evolution operator for the case of elementary unidimensional potentials, like a particle subject to a constant force and a harmonic oscillator. Also, we discuss an apparent paradox concerning the time evolution operator and non-spreading wave packets addressed previously in the literature.

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where \( \Psi(x, 0) \) is the initial wavevector, \( \hat{A} = -(i\hbar/\partial)\hat{a} \) and \( \hat{B} = -(i\hbar/\partial)\hat{b} \). In this paper, we call this method the evolution operator method.

Essentially, both ways for solving the Schrödinger equation are the same. This can be proved by expanding \( \Psi(x, 0) \) in terms of the eigenfunctions of the Hamiltonian, i.e. \( \Psi(x, 0) = \sum \epsilon_n \psi_n(x) \), and inserting it on the right-hand side of equation (5) to produce equation (4). An alternative way to solve the Schrödinger equation is the technique developed by Feynman, called the Feynman propagator method [5–7].

The trouble with equation (5) is that, in general, \( \hat{A} \) and \( \hat{B} \) do not commute. This makes it difficult to apply the time evolution operator to the initial state vector given in equation (5). In fact, the problem is how to make the expansion of a function of noncommuting operators like that in equation (5), i.e. \( e^{\hat{A} \hat{B}} = \sum_{n=0}^{\infty} (1/n!) (\hat{A} + \hat{B})^n \), in such a way that all the \( \hat{B} \) precede the \( \hat{A} \), or vice versa. This problem has been already studied by many authors, and some theorems have been proved to handle this expansion. For example, Kumar proved the following expansion for a function of noncommuting operators [8]

\[
f(\hat{A} + \hat{B}) = \sum_{n=0}^{\infty} \frac{1}{n!} C^n(\hat{A}, \hat{B}) f^{(n)}(\hat{A}),
\]

\( C^n(\hat{A}, \hat{B}) \) is a coefficient operator given in terms of \( \hat{B} \) and the commutator \([\hat{A}, \hat{B}]\) [8].

Also, Cohen has proved the following expansion theorem for the operators \( \hat{x} \) and \( \hat{p} \) [9]: given a function \( F(\hat{x}, \hat{p}) \) then

\[
F^n(\hat{x}, \hat{p}) = \sum_{n=0}^{\infty} \alpha_k u_k(\hat{x}) \int_{-\infty}^{\infty} u_k^*(\hat{x} + \theta) e^{i\hbar \theta \hat{p}} d\theta,
\]

where \( \alpha_k \) and \( u_k(\hat{x}) \) are the eigenvalue and eigenfunction of the eigenvalue problem \( F(\hat{x}, \hat{p})u_k(\hat{x}) = \alpha_k u_k(\hat{x}) \). In particular, the expansion for the function \( (\lambda \hat{x} + \hat{p})^n \) has been given as [9]

\[
(\lambda \hat{x} + \hat{p})^n = \sum_{k=0}^{[\lambda \hbar/2]} \sum_{s=0}^{n-2k} \frac{(-1)^s n!}{k!(n-2k)!} \left( \begin{array}{c} n-2k \\ s \end{array} \right) \lambda^{n-k-1} \hbar^{-2k-s} \hat{p}^s.
\]

In general, these expansion theorems have produced highly cumbersome expressions that are very difficult to apply.

One of the possible paths to avoid the expansion of functions of two noncommuting operators, in the case of exponential operators, is to factorize the argument of the exponential. This approach facilitates the application of the exponential operator because now, when the exponential operator is factorized, we have only to expand the exponential of a single operator, i.e. \( e^{\hat{A}} e^{\hat{B}} \), which is more simple. However, the factorization of exponential operators is not an easy task. To the best of our knowledge, the evolution operator method has been applied to unidimensional problems in four related papers [10–13].

The main goal of this paper is 2-fold, first we shall show a procedure to factorize the exponential operator and, secondly, we shall show how to apply the factorized exponential operator on an initial wavefunction. The method of factorization that we shall present in this paper has been used in quantum optics. Also, this method has been proposed as a possible tool to improve some misconceptions in the teaching of quantum mechanics [14]. Therefore, an important objective of this paper is to review this method in order that it becomes available for people outside these fields.

Although the three methods for solving the Schrödinger equation mentioned above have to give the same result, the evolution operator method is, in some ways, quite different to the eigenstates method and the Feynman propagator. For example, in the eigenstates method, we need to find the eigenfunctions of the Hamiltonian where the particle is placed; on the contrary, the evolution operator method does not give any information about the eigenfunctions of the Hamiltonian. Also, the Feynman propagator method needs to take into account all the possible paths that the particle can take from an initial wavefunction to a final one, which implies performing sophisticated integrations, and the evolution operator method does not require these possible paths. In some senses, the evolution operator method is more direct than the other two.

In summary, this paper addresses the problem of factorizing the exponential of a sum of operators, in order to be able to apply it as an evolution operator, when the operators obey certain commutation rules. To make the factorization, we use the tool of the differential equation method [15, 16], which requires that both sides of an equation satisfy the same first-order differential equation and the same initial condition.

For a review of these tools see the study of Wilcox [15] and Lutzky [17]. This method has been used successfully in the field of quantum optics [18–21]. We shall show that this method is useful and easy to apply in the unidimensional problems of quantum mechanics.

It is worthwhile mentioning that a similar, although different, approach has been used extensively. This method applies the approximation procedure developed by Suzuki [22–24] and is suitable to apply using computational algorithms [25]. In this case the exponential operator, called the Suzuki–Trotter decomposition, has to be applied (or calculated) as

\[
e^{(\hat{A} + \hat{B})t} = e^{p_1 \hat{A}} e^{p_2 \hat{B}} e^{p_3 \hat{A}} e^{p_4 \hat{B}} \cdots e^{p_m \hat{A}} + O(x^{m+1}),
\]

where the set of parameters \( p_1, p_2, \ldots, p_m \) are adjusted so that the correction term may be of the order of \( x^{m+1} \), for details see [24]. This approach is based on the Suzuki–Trotter formula

\[
e^{(\hat{A} + \hat{B})t} = \lim_{m \to \infty} (e^{\hat{A}t/m} e^{\hat{B}t/m})^m,
\]

and has a rigorous mathematical proof [26], see also [27]. The Suzuki–Trotter method has been used extensively in the field of statistical physics [28–30] and Monte Carlo simulations [25]. See also [31, 32].

This paper is organized as follows: in section 2, we will present the method and show how to apply it for factorizing an exponential operator. In section 3, we give a specific example when the operators obey certain commutation rules. In subsection 3.1 of this section, we apply the found factorization to the case when the particle is subjected to a constant force. In section 4, we present the factorization
of the exponential operator when its argument obeys more complex commutation rules; in subsection 4.1 of this section the factorization found is applied to the harmonic oscillator. In subsection 4.2 we derive another way to factorize the harmonic oscillator and we show that both factorizations give the same evolution function (in appendix A, we derive yet another way to factorize the harmonic oscillator). In section 5 we address a supposed limitation of the evolution operator method, we demonstrate that the limitation is because the initial wavefunction used to show the apparent paradox is outside of the domain of the hamiltonian operator.

2. The method

As the global purpose of this paper is pedagogical, in this section, we show how the method works. Our intention is that this method can be used for researchers of any field to find the evolution state from an initial wavefunction. In order to be explicit we separate the method in three steps and apply it to obtain the well known Baker–Campbell–Hausdorff formula

$$e^{(\hat{A}+\hat{B})\xi} = e^{\hat{A}\xi} e^{\hat{B}\xi},$$

(11)

when $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$ i.e. $[\hat{A}, \hat{B}] = \delta$, where $\delta$ is a constant. Notice that after we have solved this easy problem, we will progressively increase the difficulty of the commutation relation.

To make the factorization of the exponential of the sum of two operators, we proceed as follows.

(i) Firstly, we define an auxiliary function in terms of the exponential of the sum of two operators, and the proposed factorization with its commutator and an auxiliary parameter $\xi$

$$F(\xi) = e^{\hat{A}+\hat{B}\xi},$$

(12)

$$F(\xi) = e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi},$$

(13)

where $f_1(\xi)$, $f_2(\xi)$ and $f_3(\xi)$ are analytical functions of the parameter $\xi$.

Note that in equations (12) and (13), we are defining separately $F(\xi)$ as a function and its factorization. That is to say, if $e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi}$ is the factorization of $e^{(\hat{A}+\hat{B})\xi}$, then $F(\xi) = e^{(\hat{A}+\hat{B})\xi} = e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi}$.

(ii) Secondly, we differentiate equations (12) and (13) with respect to the parameter $\xi$ to obtain

$$\frac{dF(\xi)}{d\xi} = (\hat{A} + \hat{B}) F(\xi),$$

(14)

$$\frac{dF(\xi)}{d\xi} = [\hat{A}, \hat{B}] e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi} + e^{f_1(\xi)\hat{A}\xi} \frac{df_2(\xi)}{d\xi} e^{f_2(\xi)\hat{B}\xi} + e^{f_1(\xi)\hat{A}\xi} \frac{df_2(\xi)}{d\xi} \hat{B} e^{f_2(\xi)\hat{B}\xi}. $$

(15)

After that, we need to order the operators in equation (15), so that we can move the function $F(\xi)$ to the right, like in equation (14). In order to make the new arrangement, we use the fact that the operators are self-adjoints, i.e. $e^{\hat{A}} = (e^{\hat{A}})^* e^{\hat{A}}$, and the well known relation $e^{\alpha \hat{A}} e^{-\alpha \hat{A}} = e^{\gamma\hat{A}} + \frac{\gamma^2}{\pi^2} [\hat{A}, [\hat{A}, \hat{B}]] + \ldots$, see [16]. In this case

$$e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi} = \hat{A},$$

(16)

and

$$e^{f_3(\xi)\hat{A}\xi} \hat{B} e^{-f_3(\xi)\hat{B}\xi} = \hat{B} + \delta f_2(\xi),$$

(17)

where we have used the fact that $[\hat{A}, \hat{B}] = \delta$. If we substitute these relations into equation (15) we obtain

$$\frac{dF(\xi)}{d\xi} = \frac{df_1(\xi)}{d\xi} [\hat{A}, \hat{B}] e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi} + \frac{df_2(\xi)}{d\xi} \hat{A} e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi} + \frac{df_2(\xi)}{d\xi} e^{f_1(\xi)\hat{A}\xi} [\hat{B} + \delta f_2(\xi)] e^{f_2(\xi)\hat{B}\xi}. $$

(18)

Now, using $e^{f_1(\xi)\hat{A}\xi} \hat{B} e^{-f_1(\xi)\hat{A}\xi} = \hat{B}$ in equation (18) we obtain

$$\frac{dF(\xi)}{d\xi} = \frac{df_1(\xi)}{d\xi} [\hat{A}, \hat{B}] e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi} + \frac{df_2(\xi)}{d\xi} \hat{A} e^{f_1(\xi)\hat{A}\xi} e^{f_2(\xi)\hat{B}\xi} + \frac{df_2(\xi)}{d\xi} [\hat{B} + \delta f_2(\xi)] e^{f_2(\xi)\hat{B}\xi}. $$

(19)

That is, we successfully passed all the exponential to the right and we can write equation (19) as

$$\frac{dF(\xi)}{d\xi} = \left\{ \frac{df_1(\xi)}{d\xi} [\hat{A}, \hat{B}] + \frac{df_2(\xi)}{d\xi} \hat{A} + \frac{df_2(\xi)}{d\xi} \left[ \hat{B} + \delta f_2(\xi) \right] \right\} F(\xi).$$

(20)

That is, using equation (13) we arrive to the following result

$$\frac{dF(\xi)}{d\xi} = \left\{ \frac{df_1(\xi)}{d\xi} [\hat{A}, \hat{B}] + \frac{df_2(\xi)}{d\xi} \hat{A} + \frac{df_2(\xi)}{d\xi} \left[ \hat{B} + \delta f_2(\xi) \right] \right\} F(\xi).$$

(21)

(iii) Finally, as a third step, we must compare the coefficients of equations (14) and (21), from which a set of differential equations is obtained

$$\frac{df_2(\xi)}{d\xi} = 1, \quad \frac{df_3(\xi)}{d\xi} = 1, \quad \frac{\delta df_1(\xi)}{d\xi} + \delta \frac{df_3(\xi)}{d\xi} f_2(\xi) = 0.$$
subjected to the initial condition \( F(0) = 1 \), which implies \( f_1(0) = f_2(0) = f_3(0) = 0 \). In this case the solutions are
\[
f_2(\xi) = \xi, \quad f_3(\xi) = \xi, \quad f_1(\xi) = -\frac{1}{2}\xi^2.
\]
(23)

After substituting equation (23) into equation (13) we arrive at the following equation
\[
e^{\xi(\hat{A} + \hat{B})} = e^{-\xi^2(\hat{A}, \hat{B})/2} e^{\xi\hat{A}} e^{\xi\hat{B}}.
\]
(24)

Setting \( \xi = 1 \), we obtain the usual Baker–Campbell–Hausdorff formula.

The evolution operator method facilitates the application of the exponential operator, because now we have to handle only individual operator functions. The proposed factorization in equation (13) is one of the possibilities, we can also define \( F(\xi) \) as
\[
F(\xi) = e^{\xi(\hat{A} + \hat{B})} e^{\xi(\hat{A})} e^{\xi(\hat{B})},
\]
(25)
or make another arrange of the exponentials, as for example \( e^{\xi A} e^{\xi B} e^{\xi C} \). Notice that equation (25), in contrast to equation (13), does not use the commutator in the exponential functions. This arrangement could be used to treat specific problems, such as the harmonic oscillator.

In fact, when the method is exploited, this arrangement is a set of crafted directions, which gives a factorization of the evolution operator. In the majority of cases, a different arrangement will produce a different set of differential equations and, obviously, a different set of solutions. We give an explicit example of this fact in the case of the harmonic oscillator, see equations (50), (58) and (A.1). It is very important not to confuse the Baker–Campbell–Hausdorff formula with the method addressed here. Each one represents a different way to factorize exponential operators.

On the other hand, this method can be used to improve some misconceptions of quantum mechanics [14, 33, 34]. Next, we present the different cases that appear when the operators obey different commutation rules.

3. Case 1: \([\hat{A}, \hat{B}] = \hat{C}, \quad [\hat{A}, \hat{C}] = 0 \) and \([\hat{C}, \hat{B}] = -k\)

This section is organized as follows: firstly, we make the factorization of the exponential operator when the operators obey the commutation relations given by equation (26). Secondly, in subsection 3.1 we use the factorized exponential to solve the problem of a particle subjected to a constant force.

Therefore, we begin the factorization of exponential operators by analysing the case when
\[
[\hat{A}, \hat{B}] = \hat{C}, \quad [\hat{A}, \hat{C}] = 0, \quad \text{and} \quad [\hat{C}, \hat{B}] = -k,
\]
(26)

where \( \hat{A}, \hat{B} \) and \( \hat{C} \) are operators and \( k \) is a c-number (in general, we use the symbol ‘\(' to denote operators).

In the present case, we propose the factorization function as
\[
F(\xi) = e^{\xi(\hat{A} + \hat{B})} = e^{\xi\hat{A}} e^{\xi\hat{B}} e^{\xi\hat{C}} e^{-\xi^2/2}\hat{C}.
\]
(27)

By differentiating equation (27) with respect to \( \xi \) we obtain
\[
\frac{dF(\xi)}{d\xi} = (\hat{A} + \hat{B})F(\xi),
\]
(28)

and,
\[
\frac{df(\xi)}{d\xi} = \left[ \frac{df(\xi)}{d\xi} \hat{A} + \frac{df(\xi)}{d\xi} \hat{B} + \frac{df(\xi)}{d\xi} (\hat{C} + \frac{d\hat{C}}{d\xi} + k \hat{g}) \right] F(\xi),
\]
(29)

where we have applied the fact that
\[
e^{\xi\hat{A}} e^{-\xi\hat{A}} = \hat{B} + \xi[\hat{A}, \hat{B}] + \xi^2/2! [\hat{A}, [\hat{A}, \hat{B}]] + \ldots,
\]
(30)

and we have used the commutation relations of equation (26).

By equating the coefficients of equations (28) and (29), we obtain the following system of differential equations
\[
\frac{df(\xi)}{d\xi} = 1, \quad \frac{dg(\xi)}{d\xi} = 1,
\]
\[
\frac{dg(\xi)}{d\xi} f(\xi) + \frac{dh(\xi)}{d\xi} = 0,
\]
\[
kg(\xi) \frac{dh(\xi)}{d\xi} + \frac{dr(\xi)}{d\xi} = 0,
\]
(31)

subjected to the initial condition \( F(0) = 1 \), which implies
\[
f(0) = g(0) = h(0) = r(0) = 0.
\]
(32)

By solving equation (31) with the initial condition stated in equation (32), we finally obtain
\[
e^{\xi(\hat{A} + \hat{B})} = e^{(\xi^2/3)k} e^{\xi\hat{C}} e^{\xi\hat{B}} e^{-\xi^2/2}\hat{C}.
\]
(33)

Setting \( \xi = 1 \), we obtain the factorization we were looking for.

3.1. Application: a particle subject to a constant force

One application of the evolution operator method is when we study the time dependence of a quantum state. There have been some results in this approach when the operator is the energy of a free particle [10], or the energy of a particle subjected to a constant force, that is \( V(x) = -Fx \) [11]. In this subsection, we use the factorization found above to solve the problem of a particle subjected to a constant force, with the help of Blinder’s method [10]. Blinder’s method shows how to apply the evolution operator like an infinite sum for a free particle
\[
e^{-\frac{\hbar^2}{2m}} = \sum_{n=0}^{\infty} \left( \frac{i\hbar}{2m} \right)^n \frac{1}{n!} \left( \frac{\partial^2}{\partial x^2} \right)^n.
\]
(34)

For a free particle, the wavefunction at time \( t \) is obtained by operating with the evolution operator on the initial wavefunction. Taking as an initial wavefunction
\[
\Psi(x, 0) = \frac{1}{(\sigma \sqrt{\pi})^{1/2}} e^{-\frac{x^2}{2\sigma^2}},
\]
(35)

where \( \sigma \) is the width of the wave packet. Blinder’s method consists of the application of the identity [10]:
\[
\frac{1}{\sqrt{2\pi}} [z^{-1/2} \exp \{-x^2/2\sigma^2\}] = \frac{1}{2\pi} [z^{-1/2} \exp \{-x^2/4\sigma^2\}].
\]
This identity allows us to apply the evolution operator on initial wavefunctions, like Gaussian wave packets; for details see [10].
For a particle subject to a constant force, i.e. \( V(x) = -Fx \), the wavefunction at time \( t \) is given by

\[
\Psi(x, t) = \exp \left[ -\frac{i}{\hbar} \left( \frac{\hat{p}^2}{2m} - Fx \right) \right] \Psi(x, 0),
\]

(36)
defining \( \hat{A} = \frac{\hat{p}^2}{2m} \), \( \hat{B} = -Fx \), and using the commutation relations between \( \hat{p} \) and \( \hat{x} \) we can deduce the following commutation rules

\[
[\hat{A}, \hat{B}] = \frac{ihF}{m}, \quad [\hat{A}, \hat{C}] = 0, \quad \text{and} \quad [\hat{C}, \hat{B}] = -\frac{\hbar^2 F^2}{m},
\]

(37)
where \( \hat{C} = \hbar F \hat{p}/m \). If we identify \( k = \hbar^2 F^2/m \), then the commutation relations of equation (37) are similar to those of equation (26). Therefore, if we use equation (33), we can write equation (36) as

\[
\Psi(x, t) = \exp \left[ \frac{itF^2}{6hm} \right] \exp \left[ -\frac{it}{2m\hbar} \hat{p}^2 \right] \exp \left[ \frac{it F}{\hbar} \hat{x} \right] \times \exp \left[ \frac{it^2 F}{2m\hbar} \right] \Psi(x, 0).
\]

(38)

Using the theorem \( \exp[\xi \hat{A}] F(\hat{B}) \exp[-\xi \hat{A}] = F(\exp[\xi \hat{A}\hat{B}] \exp[-\xi \hat{A}] ) \) [16], we can rearrange equation (38) as follows

\[
\Psi(x, t) = \exp \left[ -\frac{iF^2 t^2}{6hm} \right] \exp \left[ \frac{iF}{\hbar} \hat{x} \right] \exp \left[ -\frac{it}{2m\hbar} \hat{p}^2 \right] \times \exp \left[ -\frac{it^2 F}{2m\hbar} \right] \Psi(x, 0).
\]

(39)

Taking as an initial state that of equation (35), we finally obtain

\[
\Psi(x, t) = \left( \frac{\alpha}{\sqrt{2\pi}} \right)^{-1/2} \left( 1 + (iht/2m\alpha^2) \right)^{-1} \exp \left[ \frac{itF}{\hbar} (x - (Ft^2/6m)) \right] \times \exp \left[ -\frac{(x - (Ft^2/2m))^2}{4(\alpha^2 + (iht/2m))} \right].
\]

(40)

Equations (39) and (40) are exactly the same as the equations obtained by Robinett [11].

4. Case 2: \([\hat{A}, \hat{B}] = \hat{C}, \quad [\hat{A}, \hat{C}] = 2\gamma \hat{A}\]
and \([\hat{B}, \hat{C}] = -2\gamma \hat{B}\)

In this case, we carry out the factorization of the exponential operator when the commutation rules are given by equation (41). Then, we will show in subsection 4.1 that these commutation relations are the same for the harmonic oscillator. On the other hand, in subsection 4.2 we show an alternative way of factorization for this problem, and show that the evolution given by the evolution operator is the same in both cases.

\[
[\hat{A}, \hat{B}] = \hat{C}, \quad [\hat{A}, \hat{C}] = 2\gamma \hat{A} \quad [\hat{B}, \hat{C}] = -2\gamma \hat{B}.
\]

(41)

In this case, using an arrangement similar to equation (25), we define the function as

\[
F(\xi) = e^{(\hat{A} + \hat{B})} e^{(\xi/\gamma) \hat{C}} e^{(\xi/\gamma) \hat{A}} e^{(\hbar \xi/\gamma) \hat{B}}.
\]

(42)

By differentiating equation (42) with respect to \( \xi \), we obtain

\[
\frac{dF(\xi)}{d\xi} = (\hat{A} + \hat{B}) F(\xi),
\]

(43)

and

\[
\frac{dF(\xi)}{d\xi} = \left\{ \left[ g(\xi) \frac{dh(\xi)}{d\xi} - f(\xi) \frac{dg(\xi)}{d\xi} \right] \hat{C} \left[ \frac{df(\xi)}{d\xi} + \gamma f^2(\xi) \frac{dg(\xi)}{d\xi} \right] + \frac{dh(\xi)}{d\xi} + \gamma f^2(\xi) g^2(\xi) \frac{dh(\xi)}{d\xi} \right\} \hat{B}.
\]

(44)

where we have applied the relation \( e^{\hat{A} \hat{B}} e^{-\xi \hat{A}} = \hat{B} + \xi [\hat{A}, \hat{B}] + \frac{\xi^2}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \ldots \).

By equating equations (43) and (44), we obtain the following system of differential equations

\[
\frac{dg(\xi)}{d\xi} + \gamma g^2(\xi) \frac{dh(\xi)}{d\xi} = 1,
\]

(45)

\[
\frac{df(\xi)}{d\xi} + \gamma f^2(\xi) \frac{dg(\xi)}{d\xi} + \frac{dh(\xi)}{d\xi} - 2f(\xi) g(\xi) \frac{dh(\xi)}{d\xi} = 1,
\]

\[
\frac{g(\xi)}{d\xi} - f(\xi) \frac{dg(\xi)}{d\xi} - \gamma g^2(\xi) f(\xi) \frac{dh(\xi)}{d\xi} = 0,
\]

subjected to the initial condition \( F(0) = 1 \), which means: \( g(0) = f(0) = h(0) = 0 \). By solving equation (45), with the initial conditions, we obtain the following solutions

\[
f(\xi) = h(\xi) = \frac{1}{\sqrt{\gamma}} \tan(\xi \sqrt{\gamma}/2),
\]

(46)

\[
g(\xi) = \frac{1}{\sqrt{\gamma}} \sin(\xi \sqrt{\gamma}).
\]

(47)

Setting \( \xi = 1 \), we obtain the factorization we were looking for, that is equation (42).

As was stated at the end of section 2, the factorization given in equation (42) is only one of many possibilities. Since the operators do not commute, various orderings on the right-hand side of equation (42) represent different substituting schemes as we will show in the following subsections and in the appendix. For example, we can propose a different arrangement \( F(\xi) = e^{f(\xi) \hat{A}} e^{f(\xi) \hat{B}} e^{f(\xi) \hat{A}} \), or include the commutator \( \hat{C} \): \( F(\xi) = e^{f(\xi) \hat{C}} e^{f(\xi) \hat{A}} e^{f(\xi) \hat{B}} \).
4.1. Application: the one-dimensional (1D) harmonic oscillator

One of the most important systems in quantum mechanics is the harmonic oscillator. It serves both to model many physical systems occurring in nature and to show the analytical solution of the Schrödinger equation. The Schrödinger equation for this system has been solved in two ways, firstly by analytically solving the eigenvalue equation and, secondly, by defining the creation and annihilation operators [1, 2]. Here, we solve this problem using the evolution operator method. This method allows us to find the evolution for the harmonic oscillator and avoids having to deal with the stationary states.

For the 1D harmonic oscillator the wavefunction at time \( t \) is given by

\[
\Psi(x, t) = \exp \left[ -\frac{i}{\hbar} \left( \hat{p}^2 + \frac{\hbar^2}{2m} x^2 \right) t \right] \Psi(x, 0). \tag{48}
\]

Defining \( \hat{A} = -(i\hbar m \omega^2/2h) \hat{x}^2, \hat{B} = -(i\hbar \hbar \omega) \hat{p}^2 \), and using the commutation relations between \( \hat{x} \) and \( \hat{p} \) we can deduce the following commutation rules

\[
[\hat{A}, \hat{B}] = \hat{C}, \quad [\hat{A}, \hat{C}] = -2\hbar^2 \hat{A} \quad \text{and} \quad [\hat{B}, \hat{C}] = 2\hbar^2 \hat{B}, \tag{49}
\]

where \( \hat{C} = i\hbar \omega^2/2h (\hat{p} \hat{x} + \hat{x} \hat{p}) \). If we identify \( \gamma = \hbar \omega^2 \), then these commutation relations correspond to those of equation (41). Therefore, using the factorization found in equation (42), equation (48) becomes

\[
\Psi(x, t) = e^{\mu(t) \hbar^2/2m} e^{-\frac{\hbar^2}{2m} x^2} e^{i\delta(t) x} \Psi(x, 0), \tag{50}
\]

where

\[
\mu(t) = \frac{i\hbar}{2m\omega} \tan (\omega t/2), \quad \delta(t) = \frac{im\omega}{2h} \sin (\omega t). \tag{51}
\]

The wavefunction at time \( t \) for the 1D harmonic oscillator is obtained by operating with the evolution operator, i.e. equation (50), on the initial wavefunction. Taking as an initial wavefunction

\[
\Psi(x, 0) = \frac{1}{(\sigma \sqrt{\pi})^{1/2}} e^{-\frac{x^2}{\sigma^2}},
\]

we finally obtain the state of the system at any time \( t \) as

\[
\Psi(x, t) = \frac{1}{(\sigma \sqrt{\pi})^{1/2}} \frac{1}{\sqrt{\cos (\omega t) + (2\hbar/m\omega) (1/4\sigma^2) \sin (\omega t)}} \times \exp \left[ \frac{(-im\omega/2\hbar \sin (\omega t) - (1/2\sigma^2) \times \sin^2 (\omega t/2) + (1/4\sigma^2) \cos (\omega t) + (2\hbar/m\omega) (1/4\sigma^2) \sin (\omega t))}{\cos (\omega t) + (2\hbar/m\omega) (1/4\sigma^2) \sin (\omega t)} \right] \Psi(x, 0). \tag{52}
\]

From equation (52), we can calculate the probability distribution function

\[
|\Psi(x, t)|^2 = \frac{1}{\cos (\omega t) + (2\hbar/m\omega) (1/4\sigma^2) \sin (\omega t)} \times \exp \left[ -\frac{\hbar^2}{2m} \left( \frac{1}{\cos (\omega t) + (2\hbar/m\omega) (1/4\sigma^2) \sin (\omega t)} \right)^{1/2} \right]. \tag{53}
\]

In the preceding case we have used the following trigonometric identities: \( 1 - 2\sin^2 (\omega t/2) = \cos (\omega t) \) and \( \sin (\omega t/2) = 2 \sin (\omega t/2) \cos (\omega t/2) \).

4.2. Another way to factorize the harmonic oscillator

In this subsection, we present another way to factorize the evolution operator the harmonic oscillator. Then, we apply the new factorization on an initial wavefunction.

In this case, we propose the factorization function as

\[
F(\xi) = e^{(A + i\hat{B})} = e^{f_1(\xi) \hat{A}} e^{f_2(\xi) \hat{B}} e^{f_3(\xi) \hat{A}}. \tag{54}
\]

Applying the method of factorization, we obtain the following set of differential equations

\[
\frac{df_1(\xi)}{d\xi} + \gamma f_2^2(\xi) \frac{df_2(\xi)}{d\xi} - 2\gamma f_1(\xi) f_2(\xi) \frac{df_3(\xi)}{d\xi} = 1, \quad \frac{df_2(\xi)}{d\xi} + \gamma f_1^2(\xi) \frac{df_1(\xi)}{d\xi} - 2\gamma f_1(\xi) f_2(\xi) \frac{df_3(\xi)}{d\xi} = 1, \quad f_1(\xi) \frac{df_2(\xi)}{d\xi} - f_2(\xi) \frac{df_1(\xi)}{d\xi} - \gamma f_1(\xi) f_2^2(\xi) \frac{df_3(\xi)}{d\xi} = 0 \tag{55}
\]

subjected to the initial condition \( F(0) = 1 \), which means: \( f_1(0) = f_2(0) = f_3(0) = 0 \). This set of differential equations is identical to that of equation (45). By solving equation (55), we obtain the following solutions

\[
f_1(\xi) = f_3(\xi) = \frac{1}{\sqrt{\gamma}} \tan (\xi \sqrt{\gamma}/2), \quad f_2(\xi) = \frac{1}{\sqrt{\gamma}} \sin (\xi \sqrt{\gamma}). \tag{56, 57}
\]

4.2.1. Application. Now, using the factorization given by equation (54) to solve the harmonic oscillator problem, we obtain the following evolution function

\[
\Psi(x, t) = e^{-\alpha(t) x^2} e^{\beta(t) x^2} e^{i\omega(t) x} \Psi(x, 0), \tag{58}
\]

where

\[
\alpha(t) = \frac{im\omega}{2\hbar} \tan (\omega t/2), \quad \beta(t) = \frac{i\hbar}{2m\omega} \sin (\omega t). \tag{59}
\]
wave function give the same result when they are applied to an initial factorization method and the solution is given by an ansatz.

which they presented a cautionary note about the usefulness of

by equation (35), i.e. equation (36). However, this work has not used the

Equation (60) is exactly the same as the wavefunction found in

subsection 4.1, i.e. equation (52). Therefore we can conclude

with one of the main points of this paper: the factorization could be made by different ways and all of them have to give the same result when they are applied to an initial wavefunction.

The evolution operator in equation (58) was also proved by Beauregard [35]. However, this work has not used the factorization method and the solution is given by an ansatz.

In figure 1, we have plotted the probability density given by equation (53), where we have set \( \sigma_0 = \sqrt{\hbar/m \omega} = 1 \) and \( x_0 = 1 \).

5. A note

Some time ago, Holstein and Swift [36] published a paper in which they presented a cautionary note about the usefulness of the evolution operator method for obtaining the wavefunction at any future time \( t \) from the one at \( t = 0 \). Notably, in this paper Holstein and Swift showed a particular case where the evolution operator method does not work, but if this case is analysed by the eigenstates method it works very well. That is to say, the results obtained with both methods do not coincide. Therefore, a contradiction between the evolution operator method and the eigenstates method arises. The goal in this section is to present a solution to this problem.

Firstly, we recall the arguments of [36]. In their argumentation, they considered a ‘free particle’ represented by a 1D wave packet described by the function

\[
\psi_H(x, 0) = \exp \left[-\frac{a^2}{(a^2 - x^2)}\right],
\]

for \( |x| < a = 0 \), for \( |x| \geq a \). (61)

They argued that \( \psi_H(x, 0) \) is a ‘good’ function because \( \psi_H(x, 0) \) and all its derivatives exist, are continuous for all \( x \), and vanish faster than any power as \( |x| \to \infty \). When they apply the evolution operator \( \exp (-\frac{i}{\hbar} H) \) to the function \( \psi_H(x, 0) \), they found that

\[
\sum_{n=0}^{\infty} \left( \frac{\hbar t}{2m} \right)^n (n!)^{-1} \left( \frac{d^2}{dx^2} \right)^n \psi_H(x, 0) = 0,
\]

when \( |x| > a \) since \( \psi_H(x, 0) \) and all its derivatives vanish for \( |x| > a \). From this result their conclusion was that the particle described by the function \( \psi_H(x, 0) \) is confined within the interval \(-a < x < a\) for all time. That is to say, the wave packet does not spread. However, if the problem is solved using the eigenstates method then the wave packet does spread, see [36].

In the next two subsections, we analyse this argument from two points of view. In subsection 5.1, we analyse it from the mathematical point of view. In subsection 5.2, we give a physical argument.

5.1. Mathematical view

Mathematically, the argument given by Holstein and Swift is well established. From the mathematical point of view, they correctly stated that the function is a well-behaved function. That is, because outside of the interval \( |x| \geq a \) it vanishes, this function does not have any singularity and, then, it is an analytical function. Therefore, the conclusion is that it is not possible to apply the series of \( e^{-iHt/\hbar} \) to the function \( \psi_H(x) \). In fact, there is a large set of such functions, i.e. \( C^\infty \), see [37].

From this conclusion, we can deduce that the evolution operator method fails when one applies it to \( \psi_H(x) \). This is a very subtle problem. As was stated in the previous paragraph, the function \( \psi_H(x) \) is a well-behaved function from the mathematical point of view. Therefore, it seems as if the evolution operator method fails when it is applied to an analytical function.

However, after careful analysis, the only thing that can be concluded is that the evolution operator method fails for a non analytical function. For example, the analysis of Klein concludes that the evolution operator method holds for \( \psi(x, 0) \) in a suitable dense subset, see section 4 of [37].

Another possible argument, stated in the following subsection, involves the differences between the Hermitian and self-adjoint operators [37] and the fact that the particle is free.

Before giving a possible argument, let us recall a similar function studied by Araujo et al [38]. Araujo et al exemplify with the function

\[
\psi(x, 0) = e^{\frac{i}{\hbar}(x-a)}(x-b), \quad \text{for} \quad a < x < b,
\]

\[
u_{ab} = 0, \quad \text{for} \quad 0 \leq x \leq a \quad \text{and} \quad x \geq b.
\]

(63)

For the entire interval, \(-\infty < x < \infty \), this function is very similar to the function of Holstein and Swift, \( \psi_H(x, 0) \). However, Araujo et al use the function (63) only to show that the Hamiltonian is not a self-adjoint operator [38].
5.2. Physical view

In this subsection, we will argue that the function used by Holstein and Swift is not a valid physical function in the case of the free particle. A crucial point is that unbounded operators cannot be defined on all functions of the Hilbert space [37, 38].

Firstly, let us recall the meaning of the wavefunction in quantum mechanics. In the first place, the wavefunction represents the physical state of a quantum system. That is to say, it represents a combination of the physical properties like energy, momentum, position, etcetera, that can be ascribed to the system. In the second place, \( |\psi(x,t)|^2 \) gives the probability that the particle could be found between \( x \) and \( dx \). Therefore, the wavefunction carries the whole information available for the system. For example, a confined particle is restricted to have certain eigenfunctions that belong to the domain of the Hamiltonian, and certain eigenfunctions that belong to the domain of the momentum operator [38–41], see also [42]. The most severe restriction is \( \int |\psi(x)|^2 \, dx < 0 \) in the entire interval.

Particularly, by definition, a particle is free when there is not any potential confining it, i.e. \( V(x) = 0 \). Therefore, there is no way that a particle knows that its state has to be zero outside certain interval, at least if there is not an infinite well where the particle is confined. That is, only in the case of a particle confined in an infinite well can we set the condition \( \psi(x,0) = 0 \) outside the well, and the physics changes from that associated with free particles to that associated with confined particles (for a different interpretation see [43]).

As a conclusion from the previous paragraph, we can state that physically the wavefunction \( \psi_H(x,0) \) (when it is defined in the entire interval \( -\infty \to +\infty \), where it has some singularities) is not valid for the free particle. In fact, the answer is related to the differences between Hermitian and self-adjoint operators. Mathematically, an operator consists of a prescription of operation together with a Hilbert space subset where the operator is defined [37–39, 41]. That is, the functions have to belong to the domain of the operator.

Let us explain, the difficulties come from the fact that in quantum mechanics the observable is represented by operators (in a Hilbert space) and the physical states are represented by vectors (wavefunctions). However, most textbooks define an operator as an action that changes a vector into another vector, and after that they define Hermitian operators as symmetric operators. However, there is not any mention of the domain of the operator and the differences between self-adjoint and Hermitian operators. Because of this weak definition there are many problems or ‘paradoxes’ in the calculations of physical properties, see the examples given in [38, 39, 41]. To handle these problems the concept of self-adjoint extension is reviewed in [38, 39, 41]. Also see [44].

Therefore, we advocate the recommendation of Klein [37], Araujo et al [38], Bonneau et al [39] and Gieres [41]: it is necessary to define always the domain of the operators. Then, it is necessary to state clearly that, as the cited authors have pointed out, unbounded operators cannot be defined on all vectors of the Hilbert space.

In conclusion, the main point in this subsection is that because the function \( \psi_H(x,0) \) is not square integrable in the interval \( -\infty < x < \infty \), then it does not belong to the domain of the Hamiltonian operator of the free particle.

6. Conclusion

From the work in this paper, we can conclude that the evolution operator method is an efficient method to calculate the evolution of a wavefunction. This method requires, at first instance, the factorization of exponential operators. The factorization allows us to apply the exponential operator individually. We have shown how this method works and applied it in elementary unidimensional cases.

As you may guess, all methods have their troubles and limitations. One trouble of the evolution operator method is that it is not always possible to find the factorization of the exponential operator. Another trouble with this method is that it is not always possible to group the evolving function in a single expression as we show in appendix A. However, this method is increasingly used by many authors. For example, we can recall the work of Balasubramanian [12] who discussed the time evolution operator method with time-dependent Hamiltonians. Also see [13].

Acknowledgments

We are grateful to Dr F A B Coutinho for his help and useful comments, it is important to point out that he does not agree with part of the content of section 5. Also, we are extremely grateful to Dr F M Cucchietti who brought to our attention both the work of M Suzuki and many useful references. We thank the referees for their suggestions. We would like to acknowledge support from Sistema Nacional de Investigadores (SNI).

Appendix A

Here, we show another way to factorize the harmonic oscillator. In this case, we define the function as

\[
F(\xi) = e^{i(\hat{A} + \hat{B})\xi} = e^{hi(\xi)C}e^{i(\xi)\hat{A}}e^{hi(\xi)\hat{B}}.
\]

(1.1)

Remember that \( \hat{C} = [\hat{A}, \hat{B}] \). By differentiating equation (1.1) with respect to \( \xi \), we obtain

\[
\frac{dF(\xi)}{d\xi} = (\hat{A} + \hat{B})F(\xi),
\]

(1.2)

and

\[
\frac{dF(\xi)}{d\xi} = \left[ \left( f \frac{d(\hat{g})}{d\xi} + \frac{dh}{d\xi} \right) \hat{C} + e^{2h(\xi)} \frac{dg}{d\xi} \right] \hat{B} + e^{-2h(\xi)} \left( f \frac{d(\hat{g})}{d\xi} + \frac{dh}{d\xi} \right) \hat{A} F(\xi).
\]

(1.3)

By equating equations (1.2) and (1.3), we obtain the following system of differential equations

\[
e^{-2h(\xi)} \left( f \frac{d(\hat{g})}{d\xi} + \frac{dh}{d\xi} \right) = 1, \quad e^{2h(\xi)} \frac{dg}{d\xi} = 1,
\]

(1.4)

\[
f \frac{d(\hat{g})}{d\xi} + \frac{dh}{d\xi} = 0,
\]

subjected to the initial condition

\[F(0) = 1.\]
By solving equation (A.4), with the initial condition, we obtain the following solutions

\[ f(\xi) = \frac{1}{\sqrt{\gamma}} \frac{\tanh (\xi \sqrt{\gamma})}{\sech^2 (-\xi \sqrt{\gamma})}, \quad (A.5) \]

\[ g(\xi) = \frac{1}{\sqrt{\gamma}} \tanh (\xi \sqrt{\gamma}), \quad (A.6) \]

\[ h(\xi) = \frac{1}{2\gamma} \ln[\sech^2 (\xi \sqrt{\gamma})], \quad (A.7) \]

and we obtain the factorization we were looking for.

A.1. Application

The trouble with the factorization given in equation (A.1) is that at some time we have to apply the exponential, which contains the operator \( C \), of the form

\[ e^{a_1 x^2} e^{i/4a^2}, \quad (A.8) \]

with \( a_1 \) a constant. The application of this exponential means applying \((xp)^{(a^2/\hbar)}\) which produces the following set of polynomials \( A_n(x) \) \((n = 0, 1, 2, \ldots)\),

\[
A_0 = 1, \\
A_1 = 2x^2, \\
A_2 = 4x^4 - 4x^2, \\
A_3 = 8x^6 - 24x^4 + 8x^2, \\
A_4 = 16x^8 - 96x^6 - 112x^4 + 16x^2. \quad (A.9)
\]

However, we were not able to find the generating function. Interestingly, after this study was finished, we received a private communication that other authors (working on a different problem) have found similar polynomials [45]. Now we are working together to find a solution to this problem.

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