EXPOENTIAL INFINITE PRODUCT REPRESENTATIONS
OF THE TIME-DISPLACEMENT OPERATOR

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Abstract

Fer's infinite product expansion is reconsidered and applied to the specific case of the
time-displacement operator in quantum mechanics. An alternative version of this expansion
due to Wilcox is also discussed and found to be quite different from the original one. In
general the latter is expected to possess better convergence properties.

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1. Introduction

Exponential representations of the unitary time-displacement operator $U = U(t, 0) = \exp(\Omega)$ have become increasingly popular in many different fields of quantum physics. Following Magnus [1] $\Omega$ is usually expanded in a series, i.e. $U = \exp(\sum \Omega_n)$, where $\Omega_n$ is of order $n$ with respect to the Hamiltonian. For this reason the Magnus method is sometimes called exponential perturbation theory. In contrast, much less attention has been paid to solutions in the form of infinite products of exponential operators. These are by no means equivalent to the previous form, because in general the operators $\Omega_n$ do not commute with each to other.

For a quantum system with Hamiltonian $H = H(t)$ the time-evolution operator $U$ satisfies the Schrödinger equation

$$\frac{\partial}{\partial t} U = \tilde{H} U, \quad (\tilde{H} = H/\hbar), \quad (1.1)$$

subject to the initial condition $U = I$ at $t = 0$, where $I$ is the unit operator. When $H$ does not depend on $t$ the solution of eq.(1.1) is simply $U = \exp(\tilde{H}t)$. If $\tilde{H}$ depends on $t$ explicitly then in general the convergence of the Magnus series is ensured only for sufficiently small values of $t$. The ansatz $U = \prod \exp(\Phi_n)$ (where $\Phi_n$ are operators to be determined) is an alternative to the Magnus expansion, also preserving the unitarity of the time-evolution operator. Such a solution was proposed by Fer [2] a long time ago in a paper devoted to the study of systems of differential equations. However, to the best of our knowledge,
is even misquoted as a reference for the Magnus expansion [3]. On the other hand Wilcox [4] associated Fer's name with an interesting alternative infinite product expansion which is indeed a continuous analogue of the Zassenhaus formula. This however also led to some confusion since his approach is in the spirit of perturbation theory, whereas Fer's original one was essentially nonperturbative. All this clearly shows that the Fer expansion is not sufficiently well known, and prompted us to reexamine its usefulness in physics.

Since Fer's paper is not readily accessible, we first outline his derivation in Sec.2 in a form better adapted to the specific needs of quantum mechanics. We also briefly recall two special convergence conditions obtained by Fer. In Sec.3 we discuss the Wilcox method and describe a simple procedure by which the Wilcox approximants can be expressed in terms of Magnus operators. This will make clear the different character of the two expansions. In Sec.4 we apply these expansions to two simple problems of physical interest.

2. The Fer method

When the Hamiltonian $\tilde{H}$ is constant in time, or when $\tilde{H}$ commutes with its time integral

$$F_1(t) = \int_0^t dt' \tilde{H}(t'), \quad (2.1)$$

the evolution operator is given exactly by $U = \exp(F_1)$. This led Fer to seek the solution of
eq.(1.1) in the factorized form

\[ U(t) = e^{F_1(t)} U_1(t), \quad U_1(0) = I. \]  \hspace{1cm} (2.2)

He also noticed that quite generally \( U_1 \) will be closer to unity than \( U \) for small \( t \).

The question now is to find the differential equation satisfied by \( U_1 \). Substituting eq.(2.2) into eq.(1.1) we have

\[ \frac{\partial}{\partial t} U = \left( \frac{\partial}{\partial t} e^{F_1} \right) U_1 + e^{F_1} \frac{\partial}{\partial t} U_1 = \tilde{H} e^{F_1} U_1. \]  \hspace{1cm} (2.3)

The derivative of the exponential operator can be expressed as [4]

\[ \frac{\partial}{\partial t} e^{F_1} = e^{F_1} \int_0^1 \, d\lambda e^{-\lambda F_1} \dot{F}_1 e^{\lambda F_1} + \dot{F}_1 = \frac{\partial}{\partial t} F_1 = \tilde{H}, \]  \hspace{1cm} (2.4)

so that from eq.(2.3) we readily arrive at the new Schrödinger equation

\[ \frac{\partial}{\partial t} U_1 = \tilde{H}^{(1)} U_1, \]  \hspace{1cm} (2.5)

where

\[ \tilde{H}^{(1)} = e^{-F_1} \tilde{H} e^{F_1} - \int_0^1 \, d\lambda \, e^{-\lambda F_1} \tilde{H} e^{\lambda F_1}. \]  \hspace{1cm} (2.6)

The above procedure can be repeated to yield a sequence of iterated Hamiltonians.

After \( n \) steps we find

\[ U = e^{F_1} e^{F_2} \ldots e^{F_n} U_n, \]  \hspace{1cm} (2.7)

with \( U_n \) satisfying the equation

\[ \frac{\partial}{\partial t} U_n = \tilde{H}^{(n)} U_n, \quad U_n(0) = I, \]  \hspace{1cm} (2.8)
where

\[
\tilde{H}^{(n)} = e^{-F_n} \tilde{H}^{(n-1)} e^{F_n} - \int_0^1 d\lambda \, e^{-\lambda F_n} \tilde{H}^{(n-1)} e^{\lambda F_n}, \quad (2.9)
\]

and

\[
F_n = \int_0^t dt' \tilde{H}^{(n-1)}(t'), \quad \tilde{H}^{(0)} = \tilde{H}. \quad (2.10)
\]

An alternative expression for \( \tilde{H}^{(n)} \) is obtained by using the well-known formula [4]

\[
e^{X}Y e^{-X} = \sum_{k=0}^{\infty} \frac{1}{k!} \{X^k, Y\}, \quad (2.11)
\]

where we have introduced the compact notation

\[
\{X^k, Y\} = [X, \ldots [X, Y] \ldots], \quad \{X^0, Y\} = Y. \quad (2.12)
\]

Substitution of eq.(2.11) into eq.(2.9) yields

\[
\tilde{H}^{(n)} = \sum_{k=1}^{\infty} \frac{(-1)^k}{(k+1)!} \{F_n^k, \tilde{H}^{(n-1)}\} = \frac{1}{2} [\tilde{H}^{(n-1)}, F_n] + \ldots, \quad (n = 1, 2, 3, \ldots). \quad (2.13)
\]

Inspection of eq.(2.13) reveals an interesting feature of the Fer expansion. Since \( \tilde{H} \sim 1/\hbar \) and \( F_n \) is of the same order as \( \tilde{H}^{(n-1)} \), one easily sees that \( \tilde{H}^{(n)} \) starts with a term of order \( 2^n \) (correspondingly the operator \( F_n \) contains terms of order \( 2^{n-1} \) and higher). This should greatly enhance the convergence of the product in eq.(2.7). Another promising possibility consists in using 'mixed' expansions. Thus one can leave Fer's scheme after a few steps, and apply perturbation theory, or the Magnus expansion, to the iterated Hamiltonian \( \tilde{H}^{(n)} \).
For completeness we give now without proof two results due to Fer relating to the convergence of the expansion in eq.\(2.7\). Let us define the following upper bounds:

\[
|\tilde{H}^{(n)}(t)| \leq k_n(t), \quad |F_n(t)| \leq K_n(t), \quad (K_n(t) \equiv \int_0^t dt' k_{n-1}(t')), \quad (2.14)
\]

\[
||[F_{n+1}(t), \tilde{H}^{(n)}(t)]|| \leq C_n(t), \quad (2.15)
\]

where \(k_n, K_n, \) and \(C_n\), are positive functions. Let \(\xi_n \equiv 2K_n d\), with \(d\) standing for the dimension of the matrices considered.

Fer was able to show that the expansion in eq.\(2.7\) converges for parameter values such that \(\xi_1 < \xi\), where \(\xi\) is the positive root of the equation \(e^\xi = 1 + 2\xi\) (\(\xi \approx 1.256\)).

Explicit convergence bounds have been obtained by Fer in two cases:

a) when nothing is known about the function \(C_0\) in eq.\(2.15\) and \(k_0\) is constant. Then one has \(2k_0 td < \xi\), which determines a neighbourhood where convergence is ensured.

b) when the function \(C_0(t)\) is known and \(k_0\) is constant. This leads eventually to

\[
\int_0^t dt' C_0(t') \frac{e^{2k_0 t'} - 1}{k_0 t'} < \xi. \quad (2.16)
\]

In practice such conditions however are not of great help, and numerical convergence tests should be conducted for each specific application.

3. The Fer-Wilcox expansion

A more tractable form of the Fer expansion has been devised by Wilcox [4] in analogy with the Magnus approach. The idea is to treat \(1/\hbar\) in eq.\(1.1\) as an expansion parameter
and to determine the successive factors in the product

$$U = e^{W_1}e^{W_2}e^{W_3}\ldots$$

(3.1)

by assuming that $W_n$ is exactly of order $(1/\hbar)^n$, i.e. of order $n$ with respect to the Hamiltonian. Hence, it is clear from the very beginning that the methods of Fer and Wilcox give rise indeed to completely different infinite product representations of the time-evolution operator $U$.

The explicit expressions of $W_1$, $W_2$ and $W_3$ are given in Ref.[4]. It is noteworthy that the operators $W_n$ can be expressed in terms of Magnus operators $\Omega_k$, for which compact formulas and recursive procedures are available [5]. To this end we simply use the well known Baker-Campell-Hausdorff formula

$$e^X e^Y = \exp(X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] + \ldots)$$

(3.2)

to extract from the identity

$$e^{W_1} e^{W_2} e^{W_3}\ldots = e^{\Omega_1 + \Omega_2 + \Omega_3 + \ldots},$$

(3.3)

terms of the same order in $1/\hbar$. After a straightforward calculation one finds

$$W_1 = \Omega_1, \quad W_2 = \Omega_2, \quad W_3 = \Omega_3 - \frac{1}{2}[\Omega_1,\Omega_2],$$

(3.4a)

$$W_4 = \Omega_4 - \frac{1}{2}[\Omega_1,\Omega_3] + \frac{1}{6}[\Omega_1,[\Omega_1,\Omega_2]], \quad \text{etc.}$$

(3.4b)
The main interest of the Wilcox formalism stems from the fact that it provides explicit expressions for the successive approximations to a solution represented as an infinite product of exponential operators. This offers a useful alternative to the Fer expansion whenever the computation of $F_n$ from eq.(2.10) is too cumbersome. We note in passing that to first order the three expansions yield the same result ($F_1 = W_1 = \Omega_1$).

4. Two examples

For the purpose of illustration we apply now the two infinite product expansions discussed above to two simple physical systems frequently encountered in the literature for which exact solutions are available: 1) the time-dependent forced harmonic oscillator and 2) a particle of spin $\frac{1}{2}$ in a constant magnetic field (double Stern-Gerlach experiment).

In the first case, the driven harmonic oscillator, the Magnus expansion reduces to two terms ($\Omega = \Omega_1 + \Omega_2$) and provides the exact $U$ operator [6]. The Hamiltonian for this system reads

$$H = \hbar \omega a^\dagger a + f(t)(a^\dagger + a), \quad [a, a^\dagger] = 1,$$

where $f(t)$ is an unspecified function of time and $a^\dagger, a$ are the usual raising and lowering operators. In the Dirac interaction picture we obtain

$$H_1 = f(t)(e^{i\omega t}a^\dagger + e^{-i\omega t}a).$$

Since the commutator $[a, a^\dagger]$ is a c-number Fer’s iterated Hamiltonians $H^{(n)}$ with $n > 1$.
vanish so that one has $F_n = 0$ for $n > 2$. The Wilcox operators $W_n$ with $n > 2$ in eq.(3.1) vanish for the same reason. Thus, in this particular case, the second-order approximation in either method leads to the exact solution of the Schrödinger equation. The final result reads

$$U_I = e^{\Omega_1 + \Omega_2} = e^{W_1} e^{W_2} = e^{F_1} e^{F_2} = e^{-i\beta} e^{-i\alpha \hat{a}^\dagger \hat{a}}, \quad (4.3)$$

where

$$\alpha(t) = \frac{1}{\hbar} \int_0^t dt_1 f(t_1) e^{i\omega t}, \quad \beta(t) = \frac{1}{\hbar^2} \int_0^t dt_2 \int_0^{t_2} dt_1 f(t_1) f(t_2) \sin \omega(t_1 - t_2). \quad (4.4)$$

The second example is a two-level system described by the Schrödinger equation (1.1) with Hamiltonian

$$E = \frac{1}{2} \hbar \omega \sigma_z + f(t) \sigma_x, \quad (4.5)$$

where $f(t) = 0$ for $t < 0$ and $f(t) = V_0$ for $t > 0$; $\hbar \omega$ is the energy difference between the two levels and $\sigma_x, \sigma_z$ are Pauli matrices. In the Dirac interaction picture we have

$$H_I = f(t)(\sigma_x \cos \omega t - \sigma_y \sin \omega t). \quad (4.6)$$

The first-order Fer and Wilcox operators are given by (for brevity the $l$-subscript is omitted in the sequel)

$$F_1 = W_1 = \int_0^t dt_1 \tilde{H}(t_1), \quad (4.7)$$

which readily yields

$$F_1 = W_1 = -i \frac{\gamma}{\xi} [\sigma_x \sin \xi + \sigma_y (1 - \cos \xi)], \quad (4.8)$$
where $\gamma = V_0 t / \hbar$ and $\xi = \omega t$.

For the second-order Wilcox operator $W_2$ one has \cite{4}

$$W_2 = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [\tilde{H}(t_1), \tilde{H}(t_2)], \quad (4.9)$$

which leads to

$$W_2 = -i \left( \frac{\gamma}{\xi} \right)^2 (\sin \xi - \xi) \sigma_x . \quad (4.10)$$

To proceed further with Fer's method we must calculate the modified Hamiltonian $\tilde{H}^{(1)}$ of eq.(2.6). This can be done analytically by using the known property

$$e^A = \cos \alpha + \frac{\sin \alpha}{\alpha} A, \quad \alpha^2 = -\det A \quad (\text{tr} A = 0), \quad (4.11)$$

valid for $2 \times 2$ matrices. After straightforward algebra one eventually obtains

$$\tilde{H}^{(1)} = \frac{1}{2\theta} \left( \frac{\sin^2 \theta}{\theta} - \sin 2\theta + \frac{1}{\theta} \left( \frac{\sin 2\theta}{\theta} - \cos 2\theta \right) F_1 \right) [F_1, \tilde{H}], \quad (4.12)$$

where $\theta = (2\gamma / \xi) \sin(\xi / 2)$ (notice that $\tilde{H}^{(1)}$ and therefore $F_2$ depend on $\sigma_x$ and $\sigma_y$, while $W_2$ is proportional to $\sigma_x$). Since it does not seem possible to derive an analytical expression for $F_2$, the corresponding matrix elements have been computed numerically.

The transition probability $P(t)$ from an initial state with spin up to a state with spin down (or vice versa) is given by

$$P(t) = | < -|U_I(t)| + > |^2 , \quad (4.13)$$
where $|\pm \rangle$ are eigenstates of the non-perturbed Hamiltonian $\frac{1}{2} \hbar \omega \sigma_z$, with eigenvalues $\pm \hbar \omega / 2$. This expression has been computed on assuming: $U_I \simeq e^{F_I} = e^{W_I}$, $U_I \simeq e^{F_I} e^{F_2}$ and $U_I \simeq e^{W_I} e^{W_2}$, and the results have been compared with the exact analytical solution

$$P(t) = \frac{4 \gamma^2}{4 \gamma^2 + \xi^2} \sin^2(\gamma^2 + \xi^2/4)^{1/2},$$

(4.14)

where we recall that $\xi = \omega t$.

In Figures 1 and 2 we show the transition probability $P$ as a function of $\xi$ (i.e. of time) for two different values of $\gamma$, while in Fig.3 we have plotted $P$ versus $\gamma$ for $\xi$ fixed. Notice that the second order in the Wilcox expansion does not contribute to the transition probability (this is similar to what happens in perturbation theory). On the other hand, Fer’s second-order approximation is in remarkable agreement with the exact result.

5. Conclusions

In this paper we have carried out a detailed comparison between Fer’s original method and a related one subsequently developed by Wilcox. These generate two distinct representations of the time-displacement operator $U$ as an infinite product of exponentials. Fer’s expansion appears to converge faster, but requires much more computational effort at each stage. This is clearly seen on the example of the two-level system for which the second-order Fer approximation works already quite well. In the Wilcox approach the even orders do not contribute to the transition probability in this case. On the other hand for the forced
harmonic oscillator, where the second order of the Magnus expansion is known to yield the exact solution, both Fer's and Wilcox's methods do the same.

Rather than being competitive the Fer, Wilcox, and Magnus expansions can be considered as complementary. The degree of performance of each depends on the nature of the particular physical problem under consideration.

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References


Figure Captions

Figure 1. Transition probability in the two-level system as a function of $\xi$ for $\gamma = 1.2$. Solid line: exact result (eq.(4.12)); dashed line: Fer's second order; dot-dashed line: Wilcox' second order.

Figure 2. Transition probability in the two-level system for $\gamma = 2$. Lines are coded as in Fig.1.

Figure 3. Transition probability in the two-level system for $\xi = 1$. Lines are coded as in Fig.1.