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# Exponential 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.

## 1. Introduction

Exponential representations of the unitary time-displacement operator $U = U(t,0) = \exp(\Omega)$ have become increasingly popular following a much celebrated article by Magnus [1]. Usually $\Omega$ is expanded in a series, i.e. $U = \exp(\Sigma\,\Omega_n)$, 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 other.

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

$$\frac{\partial}{\partial t}U = \tilde{H}U \qquad \tilde{H} = H/\mathrm{i}\hbar \tag{1.1}$$

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 (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 $U = \Pi\ \exp(\Phi_n)$ (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] long ago in a paper devoted to the study of systems of differential equations. However, to the best of our knowledge, Fer's method was never employed to solve any physical problem. Sometimes Fer's paper 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, is also misleading since Wilcox's approach is in the spirit of

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perturbation theory, whereas Fer's original one was essentially non-perturbative. All this clearly shows that the Fer expansion is not sufficiently well known, and prompted us to re-examine its usefulness in physics.

Since Fer's paper is not readily accessible, we first outline his derivation in §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 §3 we discuss the Wilcox method and compare it with Fer's original one. This will make clear the different character of the two expansions. A simple procedure is then described by which the Wilcox approximants can be expressed in terms of Magnus operators. In §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

$$F_1(t) = \int_0^t \mathrm{d}t' \, \tilde{H}(t') \tag{2.1}$$

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

$$U(t) = \mathrm{e}^{F_1(t)} U_1(t) \qquad U_1(0) = I. \tag{2.2}$$

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

The problem now is to find the differential equation satisfied by $U_1$. Substituting (2.2) into (1.1), we have

$$\frac{\partial}{\partial t} U = \left( \frac{\partial}{\partial t} \mathrm{e}^{F_1} \right) U_1 + \mathrm{e}^{F_1} \frac{\partial}{\partial t} U_1 = \tilde{H} \mathrm{e}^{F_1} U_1. \tag{2.3}$$

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

$$\frac{\partial}{\partial t} \mathrm{e}^{F_1} = \mathrm{e}^{F_1} \int_0^1 \mathrm{d}\lambda \, \mathrm{e}^{-\lambda F_1} \dot{F}_1 \mathrm{e}^{\lambda F_1} \qquad \dot{F}_1 \equiv \frac{\partial}{\partial t} F_1 = \tilde{H} \tag{2.4}$$

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

$$\frac{\partial}{\partial t} U_1 = \tilde{H}^{(1)} U_1 \tag{2.5}$$

where

$$\tilde{H}^{(1)} = \mathrm{e}^{-F_1} \tilde{H} \mathrm{e}^{F_1} - \int_0^1 \mathrm{d}\lambda \, \mathrm{e}^{-\lambda F_1} \tilde{H} \mathrm{e}^{\lambda F_1}. \tag{2.6}$$

The above procedure can be repeated to yield a sequence of iterated Hamiltonians. After $n$ steps we find

$$U = \mathrm{e}^{F_1} \mathrm{e}^{F_2} \ldots \mathrm{e}^{F_n} U_n \tag{2.7}$$

with $U_n$ satisfying the equation

$$\frac{\partial}{\partial t} U_n = \tilde{H}^{(n)} U_n \qquad U_n(0) = I \tag{2.8}$$

where

$$\tilde{H}^{(n)} = \mathrm{e}^{-F_n} \tilde{H}^{(n-1)} \mathrm{e}^{F_n} - \int_0^1 \mathrm{d}\lambda\, \mathrm{e}^{-\lambda F_n} \tilde{H}^{(n-1)} \mathrm{e}^{\lambda F_n} \tag{2.9}$$

and

$$F_n = \int_0^t \mathrm{d}t' \tilde{H}^{(n-1)}(t') \qquad \tilde{H}^{(0)} = \tilde{H}. \tag{2.10}$$

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

$$\mathrm{e}^X Y \mathrm{e}^{-X} = \sum_{k=0}^{\infty} \frac{1}{k!} \{X^k, Y\} \tag{2.11}$$

where we have introduced the compact notation

$$\{X^k, Y\} = \underbrace{[X, [\ldots [X}_{k}, Y] \ldots]] \qquad \{X^0, Y\} = Y. \tag{2.12}$$

Substitution of (2.11) into (2.9) yields

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

Inspection of (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 (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 (2.7). Let us define the following upper bounds:

$$||\tilde{H}^{(n)}(t)|| \le k_n(t) \qquad ||F_n(t)|| \le K_n(t) \tag{2.14}$$

where

$$K_n(t) \equiv \int_0^t \mathrm{d}t'\, k_{n-1}(t')$$

and

$$||[F_{n+1}(t), \tilde{H}^{(n)}(t)]|| \le C_n(t). \tag{2.15}$$

Here $k_n$, $K_n$ 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 (2.7) converges for parameter values such that $\xi_1 < \xi$, where $\xi$ is the positive root of the equation $e^{\xi} = 1 + 2\xi$ ($\xi \simeq 1.256$).

Explicit convergence bounds were obtained by Fer in two cases:

(a) when nothing is known about the function $C_0$ in (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

$$\int_0^t \mathrm{d}t'\, C_0(t') \frac{e^{2dk_0 t'} - 1}{k_0 t'} < \xi. \tag{2.16}$$

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 (1.1) as an expansion parameter and to determine the successive factors in the product

$$U = e^{W_1} e^{W_2} e^{W_3} \ldots \tag{3.1}$$

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 [4]. It is noteworthy that the operators $W_n$ can be expressed in terms of Magnus operators $\Omega_k$, for which compact formulae and recursive procedures are available, see [5] and references therein. To this end we simply use the well known Baker–Campbell–Hausdorff formula

$$e^X e^Y = \exp(X + Y + \tfrac{1}{2}[X, Y] + \tfrac{1}{12}[X, [X, Y]] + \ldots) \tag{3.2}$$

to extract from the identity

$$e^{W_1} e^{W_2} e^{W_3} \ldots = e^{\Omega_1 + \Omega_2 + \Omega_3 + \ldots} \tag{3.3}$$

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

$$W_1 = \Omega_1 \qquad W_2 = \Omega_2 \qquad W_3 = \Omega_3 - \tfrac{1}{2}[\Omega_1, \Omega_2] \tag{3.4a}$$

$$W_4 = \Omega_4 - \tfrac{1}{2}[\Omega_1, \Omega_3] + \tfrac{1}{6}[\Omega_1, [\Omega_1, \Omega_2]] \qquad \text{etc.} \tag{3.4b}$$

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 (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, it is known that the Magnus expansion reduces to two terms ($\Omega = \Omega_1 + \Omega_2$) and provides the exact $U$ operator [6]. The Hamiltonian for this system is

$$H = \hbar\omega a^{+} a + f(t)(a^{+} + a) \qquad [a, a^{\dagger}] = 1 \tag{4.1}$$

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

$$H_{\mathrm{I}} = f(t)(\mathrm{e}^{\mathrm{i}\omega t} a^{+} + \mathrm{e}^{-\mathrm{i}\omega t} a). \tag{4.2}$$

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 (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 is

$$U_{\mathrm{I}} = \mathrm{e}^{\Omega_1 + \Omega_2} = \mathrm{e}^{W_1}\mathrm{e}^{W_2} = \mathrm{e}^{F_1}\mathrm{e}^{F_2} = \mathrm{e}^{-\mathrm{i}\beta}\mathrm{e}^{-\mathrm{i}\alpha a^{+} - \mathrm{i}\alpha^{*} a} \tag{4.3}$$

where

$$\alpha(t) = \frac{1}{\hbar}\int_0^t \mathrm{d}t_1\, f(t_1)\mathrm{e}^{i\omega t} \qquad \beta(t) = \frac{1}{\hbar^2}\int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1\, f(t_1)f(t_2)\sin[\omega(t_1 - t_2)]. \tag{4.4}$$

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

$$H = \tfrac{1}{2}\hbar\omega\sigma_z + f(t)\sigma_x \tag{4.5}$$

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

$$H_{\mathrm{I}} = f(t)(\sigma_x \cos\omega t - \sigma_y \sin\omega t). \tag{4.6}$$

The first-order Fer and Wilcox operators are given by (for brevity the I subscript is omitted hereafter)

$$F_1 = W_1 = \int_0^t \mathrm{d}t_1 \tilde{H}(t_1) \tag{4.7}$$

which readily yields

$$F_1 = W_1 = -\mathrm{i}\frac{\gamma}{\xi}[\sigma_x \sin\xi + \sigma_y(1 - \cos\xi)] \tag{4.8}$$

where $\gamma = V_0 t/\hbar$ and $\xi = \omega t$.

For the second-order Wilcox operator $W_2$ one has [4]

$$W_2 = \frac{1}{2}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \, [\tilde{H}(t_1), \tilde{H}(t_2)] \tag{4.9}$$

which leads to

$$W_2 = -\mathrm{i}\left(\frac{\gamma}{\xi}\right)^2 (\sin\xi - \xi)\,\sigma_z. \tag{4.10}$$

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

$$\mathrm{e}^A = \cos\alpha + \frac{\sin\alpha}{\alpha}A \qquad \alpha^2 = -\det A \qquad \operatorname{tr} A = 0 \tag{4.11}$$

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

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

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 $\sigma_z$). 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

$$P(t) = |\langle -|U_{\mathrm{I}}(t)|+\rangle|^2 \tag{4.13}$$

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: $U_{\mathrm{I}} \simeq \mathrm{e}^{F_1} = \mathrm{e}^{W_1}$, $U_{\mathrm{I}} \simeq \mathrm{e}^{F_1}\mathrm{e}^{F_2}$ and $U_{\mathrm{I}} \simeq \mathrm{e}^{W_1}\mathrm{e}^{W_2}$, and the results have been compared with the exact analytical solution

$$P(t) = \frac{4\gamma^2}{4\gamma^2 + \xi^2}\sin^2[(\gamma^2 + \xi^2/4)^{1/2}] \tag{4.14}$$

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

In figures 1 and 2 we show the transition probability $P$ as a function of $\xi$ for two different values of $\gamma$, while in figure 3 we have plotted $P$ against $\gamma$ for fixed $\xi$. 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

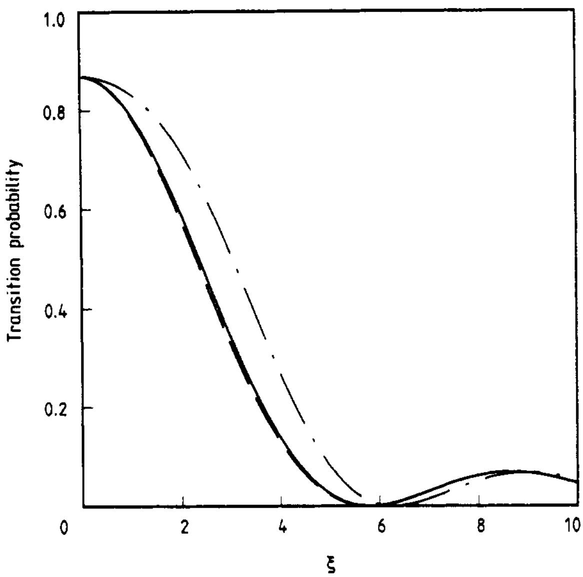


**Figure 1.** Transition probability in the two-level system as a function of $\xi$, for $\gamma = 1.2$, comparing the exact result of (4.12) (full curve); Fer's second-order result (broken curve); Wilcox's second-order result (chain curve).

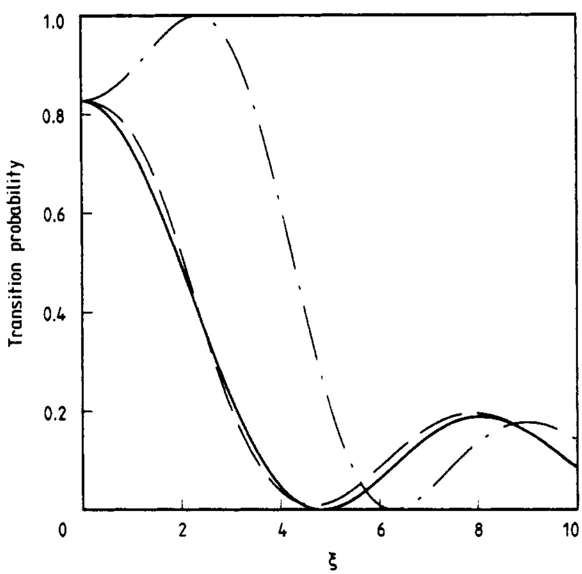


**Figure 2.** Transition probability in the two-level system as a function of $\xi$ for $\gamma = 2$. Lines are coded as in figure 1.

effort at each stage. This is clearly seen in 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 the methods of Fer and

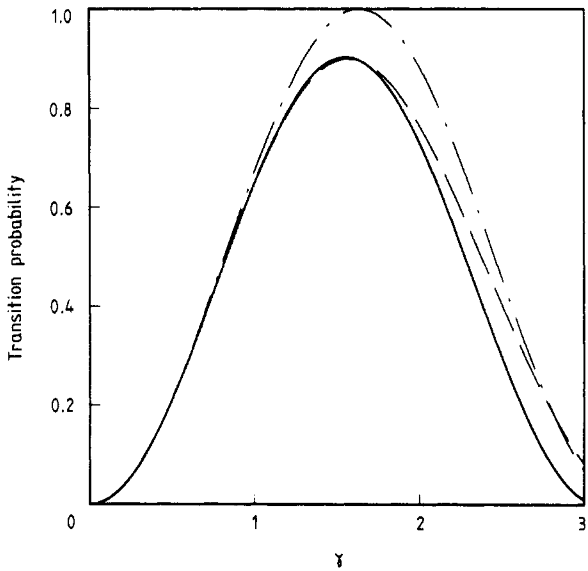


**Figure 3.** Transition probability in the two-level system as a function of $\gamma$ for $\xi = 1$. Lines are coded as in figure 1.

Wilcox perform 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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