Quasi-Feynman formulas – a method of obtaining evolution operator for the Schrödinger equation

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Abstract

For a densely defined self-adjoint operator $\mathcal{H}$ in Hilbert space $\mathcal{F}$ the operator $\exp(-it\mathcal{H})$ is known to be an evolution operator for the Schrödinger equation $i\psi'_t = \mathcal{H}\psi$, i.e. if $\psi(0,x) = \psi_0(x)$ then $\psi(t,x) = (\exp(-it\mathcal{H})\psi_0)(x)$ for $x \in Q$. The space $\mathcal{F}$ here is the space of wave functions ψ defined on the configuration space Q of a quantum system, and $\mathcal{H}$ is the Hamiltonian of the system. In this paper the operator $\exp(-it\mathcal{H})$ for all real values of t is expressed in terms of the family of self-adjoint bounded operators $S(t), t \geq 0$ that is Chernoff-tangent to the operator $\mathcal{H}$. One can take $S(t) = \exp(t\mathcal{H})$, or use even more simple families S that are listed in the paper in the guidelines on applying the method. The main theorem is proven on the level of semigroups of bounded operators in $\mathcal{F}$ so it can be widely used due to it's generality.

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Schrödinger equation, heat equation, Chernoff theorem, (semi)group of operators, Stone theorem, Feynman formulas, quasi-Feynman formulas, Cauchy problem, PDE solutions representation, multiple integral
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1. Introduction

Feynman formula is a representation of a function (usually — a solution to the Cauchy problem for a partial differential equation (PDE)) in a form of the limit of a multiple integral where the multiplicity tends to infinity. In this article I introduce a more general concept:

Definition 1.1. Quasi-Feynman formula is a representation of a function in a form which includes multiple integrals of an infinitely increasing multiplicity.

The difference from a Feynman formula is that in a quasi-Feynman formula summation and other functions/operations may be used while in a Feynman formula only the limit of a multiple integral where the multiplicity tends to infinity is allowed.

The formula (2) and other formulas from the theorem 3.1 proven in this article are examples of quasi-Feynman formulas in the case when some important (and later discussed) family $(S(t))_{t\geq 0}$ consists of integral operators; formulas obtained give the exact solution to the Cauchy problem for the Schrödinger equation.

The Schrödinger equation is one of the main equations in quantum mechanics. The solution to the Cauchy problem for this equation $i\psi'_t(t,x) = \mathcal{H}\psi(t,x), \psi(0,x) = \psi_0(x)$ is known to be provided by the evolution operator $\exp(-it\mathcal{H})$ in the form $\psi(t,x) = (\exp(-it\mathcal{H})\psi_0)(x)$. From the point of view of functional analysis $\exp(-it\mathcal{H})$ is a one-dimensional (parametrized by $t \in \mathbb{R}$) group of unitary operators in Hilbert space. Both physicists and mathematicians study the properties of $\exp(-it\mathcal{H})$ from the middle of

XX century in different aspects, e.g. asymptotic behavior, estimates, related spatio-temporal structures, wave traveling, boundary conditions etc. Some of the recent papers related to the Cauchy problem solution study are [4, 34, 14, 17, 30, 26, 35, 36, 37].

In this paper I propose a method of obtaining the exact formulas that express $\exp(-it\mathcal{H})$ explicitly in terms of coefficients of the operator $\mathcal{H}$. The solution is obtained in the form of quasi-Feynman formula. Quasi-Feynman formulas are easier to obtain (compared with Feynman formulas) but they provide lengthier approximation expressions.

Having appeared first in the pioneering works by R. P. Feynman [2, 3] on the physical level of rigor, Feynman formulas were extremely useful for physicists in studying the Schrödinger equation. Later mathematicians developed a consistent theory of such formulas and still continue finding more and more applications of Feynman's idea to various PDEs. Note that since 1948 the evolution led us to a rather complicated terminology: now we have Feynman integral, Feynman (pseudo)measure, Feynman formulas and all these are different objects from the mathematical point of view, and different authors define all that in a different way.

In this paper I touch only Feynman formulas and following [13] use the term "Feynman formula" in the sense given above. The history of research into Feynman formulas and a sketch of results obtained up to 2009 one can find in [5], see also the overview [6] dedicated to Feynman formulas for a Schrödinger semigroup (2011). The most recent (but not complete) overview is [7] (2014, in Russian).

One of the ways of obtaining and proving Feynman formulas is to use a one-parameter strongly continuous semigroup of bounded linear operators (this means the same as C_0-semigroup, the definition will be provided below) as a solution-giving object, and the Chernoff theorem as the main technical tool to deal with the C_0-semigroup. Below I cite the full text of the Chernoff theorem and propose a way of structuring its conditions into blocks. This theorem says that to obtain an explicit formula for a C_0-semigroup it is enough to find a one-parameter family of bounded linear operators that is Chernoff-equivalent to the C_0-semigroup. So the task of solving the Cauchy problem for an evolutionary PDE is reformulated as the task of finding an appropriate family of operators. In all known examples families of integral operators are used, and the Chernoff theorem requires to compose them many times, this is how multiple integrals in Feynman formulas arise in this approach. After an example of such a way was presented [13] in 2002 by

O. G. Smolyanov, there were published about 25 papers using it by 2015.

The advances achieved employing this idea one can find in the papers by Ya. A. Butko (now Kinderknecht), M. S. Buzinov, V. A. Dubravina, A. V. Duryagin, A. S. Plyashechnik, V. Zh. Sakbaev, N. N. Shamarov, O. G. Smolyanov and in the references therein (the list of researchers provided is incomplete). Some of the relevant papers are [19, 29, 31, 32, 33, 8, 15, 16, 18] but this list is also incomplete.

In this paper I make the next step after the inventors of the Trotter product formula and the Chernoff product formula presenting the formula $R(t) = \exp[i(S(t) - I)]$ from which the quasi-Feynman formulas for $\exp(-it\mathcal{H})$ are derived. The method presented seems accessible to a broad audience, which includes specialists in functional analysis, quantum mechanics, quantum informatics and mathematical physics.

To help people in employing the method in this paper I put not only the proof of the main theorem (th. 3.1 below), but also an explanation of its emergence, guidelines for using it and simple model example of its application. In the end of the text one can find a short summary of what is done.

2. Preliminaries

In this section the essential background in C_0-(semi)group theory is provided. The reader may skip it or refer to textbooks [9, 10, 11]. However, I recommend to look it through to keep in mind what methods and definitions will be used in the main part of the paper.

Definition 2.1. Let $\mathcal{F}$ be a Banach space over the field $\mathbb{C}$. Let $\mathcal{L}(\mathcal{F})$ be a set of all bounded linear operators in $\mathcal{F}$. Suppose we have a mapping $V\colon [0, +\infty) \to \mathcal{L}(\mathcal{F})$, i.e. $V(t)$ is a bounded linear operator $V(t)\colon \mathcal{F} \to \mathcal{F}$ for each $t \geq 0$. The mapping V is called a C_0*-semigroup*, or *a strongly continuous one-parameter semigroup* if it satisfies the following conditions:

1) $V(0)$ is the identity operator I, i.e. $\forall \varphi \in \mathcal{F} : V(0)\varphi = \varphi$;

2) V maps the addition of numbers in $[0, +\infty)$ into the composition of operators in $\mathcal{L}(\mathcal{F})$, i.e. $\forall t \geq 0, \forall s \geq 0 : V(t + s) = V(t) \circ V(s)$, where for each $\varphi \in \mathcal{F}$ the notation $(A \circ B)(\varphi) = A(B(\varphi))$ is used;

3) V is continuous with respect to the strong operator topology in $\mathcal{L}(\mathcal{F})$, i.e. $\forall \varphi \in \mathcal{F}$ function $t \longmapsto V(t)\varphi$ is continuous as a mapping $[0, +\infty) \to \mathcal{F}$.

The definition of a C_0*-group* is obtained by the substitution of $[0, +\infty)$ by $\mathbb{R}$ in the paragraph above.

If $(V(t))_{t\geq 0}$ is a C_0-semigroup in Banach space $\mathcal{F}$, then the set

$$\left\{\varphi \in \mathcal{F} : \exists \lim_{t\to+0} \frac{V(t)\varphi - \varphi}{t}\right\} \overset{denote}{=} Dom(L)$$

is dense in $\mathcal{F}$. The operator L defined on the domain $Dom(L)$ by the equality

$$L\varphi = \lim_{t\to+0} \frac{V(t)\varphi - \varphi}{t}$$

is called an infinitesimal generator (or just generator to make it shorter) of the C_0-semigroup $(V(t))_{t\geq 0}$. The generator is a closed linear operator that defines the C_0-semigroup uniquely, and the notation $V(t) = e^{tL}$ is used. If L is a bounded operator and $Dom(L) = \mathcal{F}$ then e^{tL} is indeed the exponent defined by the power series $e^{tL} = \sum_{k=0}^{\infty} \frac{t^k L^k}{k!}$ converging with respect to the norm topology in $\mathcal{L}(\mathcal{F})$. In most interesting cases the generator is an unbounded differential operator such as Laplacian Δ.

One of the reasons for the popularity of C_0-semigroups is their connection with differential equations. Let us briefly explain the main idea of this connection not touching upon particular cases. If Q is a set, then the function $u\colon [0, +\infty) \times Q \to \mathbb{C}$, $u\colon (t, x) \longmapsto u(t, x)$ of two variables (t, x) can be considered as a function $u\colon t \longmapsto [x \longmapsto u(t, x)]$ of one variable t with values in the space of functions of the variable x. If $u(t, \cdot) \in \mathcal{F}$ then one can define $Lu(t, x) = (Lu(t, \cdot))(x)$. If there exists a C_0-semigroup $(e^{tL})_{t\geq 0}$ then the Cauchy problem

$$\begin{cases} u'_t(t, x) = Lu(t, x) \text{ for } t > 0, x \in Q \\ u(0, x) = u_0(x) \text{ for } x \in Q \end{cases}$$

has a unique (in sense of $\mathcal{F}$, where $u(t, \cdot) \in \mathcal{F}$ for every $t \geq 0$) solution $u(t, x) = (e^{tL}u_0)(x)$ depending on u_0 continuously. See [9, 10, 11] for the details or [19] for a particular example of employing this technique. Note that if there exists a strongly continuous group $(e^{tL})_{t\in\mathbb{R}}$ then in the Cauchy problem the equation $u'_t(t, x) = Lu(t, x)$ can be considered not only for $t > 0$, but for $t \in \mathbb{R}$, and the solution is provided by the same formula $u(t, x) = (e^{tL}u_0)(x)$. One should also keep in mind that $V(t)$ and V_t are widely used as synonyms in the papers and books on C_0-semigroups.

The following famous theorem is one of the basic facts in quantum mechanics because it implies the existence and uniqueness of the solution for the Cauchy problem for the Schrödinger equation.

Theorem 2.1. *(*M. H. Stone [20], 1932*) There is a one-to-one correspondence between the linear self-adjoint operators H in Hilbert space $\mathcal{F}$ and the unitary strongly continuous groups $(W(t))_{t\in\mathbb{R}}$ of linear bounded operators in $\mathcal{F}$. This correspondence is the following: iH is the generator of $(W(t))_{t\in\mathbb{R}}$, which is denoted as $W(t) = e^{itH}$.*

Corollary 2.1. If A is a linear self-adjoint operator in Hilbert space, then $\|e^{iA}\| = 1$.

Remark 2.1. Note that a linear self-adjoint operator in Hilbert space $\mathcal{F}$ by definition is closed and its domain is dense in $\mathcal{F}$.

The following Chernoff theorem allows to construct the C_0-semigroup in $\mathcal{F}$ having suitable family of linear bounded operators in $\mathcal{F}$. This family usually does not have a semigroup composition property but is pretty close to a C_0-semigroup in the sense described in the theorem below. For many C_0-semigroups such families G are known or have been constructed in the past 15 years, see [19, 29, 31, 32, 33, 8, 15, 16, 18].

Theorem 2.2. *(*P. R. Chernoff, 1968*; see [12] or theorem 10.7.21 in [21]) Let $\mathcal{F}$ be a Banach space, and $\mathcal{L}(\mathcal{F})$ be the space of all linear bounded operators in $\mathcal{F}$ endowed with the operator norm. Let $L\colon Dom(L) \to \mathcal{F}$ be a linear operator defined on $Dom(L) \subset \mathcal{F}$, and G be an $\mathcal{L}(\mathcal{F})$-valued function.*

***Suppose** that L and G satisfy:*

(E). There exists a C_0-semigroup $(e^{tL})_{t\geq 0}$ and its generator is $(L, Dom(L))$.

(CT1). The function G is defined on $[0, +\infty)$, takes values in $\mathcal{L}(\mathcal{F})$, and the mapping $t \longmapsto G(t)f$ is continuous for every vector $f \in \mathcal{F}$.

(CT2). $G(0) = I$.

(CT3). There exists a dense subspace $\mathcal{D} \subset \mathcal{F}$ such that for every $f \in \mathcal{D}$ there exists a limit $G'(0)f = \lim_{t\to 0}(G(t)f - f)/t$.

(CT4). The operator $(G'(0), \mathcal{D})$ has a closure $(L, Dom(L))$.

(N). There exists $\omega \in \mathbb{R}$ such that $\|G(t)\| \leq e^{\omega t}$ for all $t \geq 0$.

***Then** for every $f \in \mathcal{F}$ I have $(G(t/n))^n f \to e^{tL}f$ as $n \to \infty$, and the limit is uniform with respect to $t \in [0, t_0]$ for every fixed $t_0 > 0$.*

Definition 2.2. Let $\mathcal{F}$ and $\mathcal{L}(\mathcal{F})$ be as before. Let us call two $\mathcal{L}(\mathcal{F})$-valued mappings G_1 and G_2 defined both on $[0, +\infty)$ (respectively, both on $\mathbb{R}$) *Chernoff-equivalent* iff $G_1(0) = G_2(0) = I$ and for each $f \in \mathcal{F}$ and each $T > 0$

$$\lim_{n\to\infty} \sup_{\substack{t\,\in\,[0,T] \\ (resp.\ t\,\in\,[-T,T])}} \left\| \left(G_1\left(\frac{t}{n}\right)\right)^n f - \left(G_2\left(\frac{t}{n}\right)\right)^n f \right\| = 0.$$

Remark 2.2. There are several slightly different definitions of the Chernoff equivalence, I will just follow [18] not going into details. The only thing I need from this definition is that if G_1 and L satisfy all the conditions of the Chernoff theorem, then by the Chernoff theorem the mapping G_1 is Chernoff-equivalent to the mapping $G_2(t) = e^{tL}$. In other words, the limit of $(G_1(t/n))^n$ yields the C_0-(semi)group $(e^{tL})_{t\geq 0}$ as n tends to infinity.

Definition 2.3. Let us call a mapping G *Chernoff-tangent* to the operator L iff it satisfies the conditions (CT1)-(CT4) of the Chernoff theorem.

Remark 2.3. With these definitions the Chernoff-equivalence of G to $(e^{tL})_{t\geq 0}$ follows from: the existence (E) of the C_0-semigroup + Chernoff-tangency (CT) + the growth of the norm (N) bound.

Corollary 2.2. If $\mathcal{F}$ is a Banach space, and $A\colon \mathcal{F} \to \mathcal{F}$ is a linear bounded operator, then

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!} = \lim_{k\to\infty} \left(I + \frac{A}{k}\right)^k.$$

Proof. The operator A is the generator of the C_0-semigroup $\left(e^{tA}\right)_{t\geq 0}$ defined by the formula $e^{tA} = \sum_{k=0}^{\infty} \frac{t^k A^k}{k!}$, see [10] Chapter I, section 3: Uniformly continuous operator semigroups. Setting $L = A$, $\mathcal{D} = \mathcal{F}$, $G(t) = I + tA$ and $\omega = \|A\|$ in theorem 2.2 establishes the equality $e^{tA} = \lim_{n\to\infty} \left(I + \frac{tA}{n}\right)^n$. The proof is complete after setting $t = 1$.□

Remark 2.4. The condition (CT3) of the Chernoff theorem says that $G(t)f = f + tLf + o(t)$ for each $f \in \mathcal{D}$. It seems promising to claim for fixed $k \in \mathbb{N}$ that $G(t)f = f + tLf + o(t^k)$ and try to prove that this implies faster convergence $(G(t/n))^n f \to e^{tL} f$.

Remark 2.5. Also note that the (N) condition $\|G(t)\| \leq e^{\omega t}$ in practice of constructing Chernoff-equivalent families $(G(t))_{t\geq 0}$ is usually hard to obtain for $0 < t \ll 1$ and the case $t \gg 1$ is simple.

3. The Method

Remark 3.1. Usually the Schrödinger equation is written in the form $i\psi'_t = \mathcal{H}\psi$ where $\mathcal{H}$ is the Hamiltonian of the system studied. However, to apply the (semi)group theory it is more natural to write it in the form $\psi'_t = iH\psi$. I do not call the operator $H = -\mathcal{H}$ a Hamiltonian, but use the notation $\psi'_t = iH\psi$ for the Schrödinger equation. Even more, I write it in the form

$$\psi'_t = iaH\psi$$

for some real non-zero number a. This allows us to write the C_0-groups $(e^{itH})_{t\in\mathbb{R}}$ and $(e^{-itH})_{t\in\mathbb{R}}$ in one formula $(e^{iatH})_{t\in\mathbb{R}}$ just setting $a = 1$ or $a = -1$. One can also consider a as a small or large parameter for studying degenerate equations or applying perturbation theory.

Theorem 3.1. ***Suppose*** *that a linear self-adjoint operator $H: \mathcal{F} \supset Dom(H) \to \mathcal{F}$ in a complex Hilbert space $\mathcal{F}$ and a non-zero number $a \in \mathbb{R}$ are given. Suppose that the mapping S is Chernoff-tangent to H and $(S(t))^* = S(t)$ for each $t \geq 0$.*

Then *the following holds. First, the family $\left(e^{ia(S(t)-I)}\right)_{t\geq 0}$ is Chernoff-equivalent to the C_0-semigroup $(e^{iatH})_{t\geq 0}$ and for each fixed $t \geq 0$ and $f \in \mathcal{F}$ with respect to the norm in $\mathcal{F}$*

$$e^{iatH} f = \left(\lim_{n\to\infty} \left(e^{ia(S(t/n)-I)}\right)^n\right) f, \quad e^{iatH} f = \left(\lim_{n\to\infty} e^{ian(S(t/n)-I)}\right) f, \tag{1}$$

$$e^{iatH} f = \left(\lim_{n\to\infty} \lim_{k\to\infty} \sum_{m=0}^{k} \frac{i^m a^m n^m}{m!} (S(t/n) - I)^m\right) f, \tag{2}$$

$$e^{iatH} f = \left(\lim_{n\to\infty} \lim_{k\to\infty} \sum_{m=0}^{k} \sum_{q=0}^{m} \frac{(-1)^{m-q} i^m a^m n^m}{q!(m-q)!} (S(t/n))^q\right) f, \tag{3}$$

$$e^{iatH} f = \left(\lim_{n\to\infty} \lim_{k\to\infty} \left[\left(1 - \frac{ian}{k}\right) I + \frac{ian}{k} S(t/n)\right]^k\right) f, \tag{4}$$

$$e^{iatH} f = \left(\lim_{n\to\infty} \lim_{k\to\infty} \sum_{m=0}^{k} \frac{k!(k-ian)^{k-m}(ian)^m}{m!(k-m)!k^k} (S(t/n))^m\right) f, \tag{5}$$

$$e^{iatH}f = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{m=0}^{k}\sum_{q=0}^{k-m}\frac{(-1)^{k-m-q}k!\,(ian)^{k-q}}{m!q!(k-m-q)!k^{k-q}}(S(t/n))^m\right).f \qquad (6)$$

Second, the family $\left(e^{ia(S(|t|)-I)\mathrm{sign}(t)}\right)_{t\in\mathbb{R}}$ *is Chernoff-equivalent to the group* $(e^{iatH})_{t\in\mathbb{R}}$ *and for each fixed* $t\in\mathbb{R}$ *and* $f\in\mathcal{F}$ *with respect to the norm in* $\mathcal{F}$

$$e^{iatH}f = \left(\lim_{n\to\infty}\left(e^{ia(S(|t/n|)-I)\mathrm{sign}(t)}\right)^n\right)f,\ e^{iatH}f = \left(\lim_{n\to\infty}e^{ian(S(|t/n|)-I)\mathrm{sign}(t)}\right)f, \qquad (7)$$

$$e^{iatH}f = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{m=0}^{k}\frac{i^m a^m n^m(\mathrm{sign}(t))^m}{m!}(S(|t/n|)-I)^m\right)f, \qquad (8)$$

$$e^{iatH}f = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{m=0}^{k}\sum_{q=0}^{m}\frac{(-1)^{m-q}i^m a^m n^m(\mathrm{sign}(t))^m}{q!(m-q)!}(S(|t/n|))^q\right)f, \qquad (9)$$

$$e^{iatH}f = \left(\lim_{n\to\infty}\lim_{k\to\infty}\left[\left(1-\frac{ian\,\mathrm{sign}(t)}{k}\right)I+\frac{ian\,\mathrm{sign}(t)}{k}S(|t/n|)\right]^k\right)f, \qquad (10)$$

$$e^{iatH}f = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{q=0}^{k}\frac{k!(k-ian\,\mathrm{sign}(t))^{k-q}(ian\,\mathrm{sign}(t))^q}{q!(k-q)!k^k}(S(|t/n|))^q\right)f, \qquad (11)$$

$$e^{iatH}f = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{m=0}^{k}\sum_{q=0}^{k-m}\frac{(-1)^{k-m-q}k!\,(ian\,\mathrm{sign}(t))^{k-q}}{m!q!(k-m-q)!k^{k-q}}(S(|t/n|))^m\right)f, \qquad (12)$$

where $|x|$ *above stands for the absolute value of the number* x*.*

Proof. Let us check the conditions of the Chernoff theorem for the $\mathcal{L}(\mathcal{F})$-valued mapping $R(t) = \exp(ia(S(t) - I))$ and the operator iaH. For fixed $t > 0$ the operator $ia(S(t) - I)$ is linear and bounded (recall (CT1) for S), so the exponent $e^{ia(S(t)-I)}$ is well-defined by the power series and the operator $e^{ia(S(t)-I)}$ is linear and bounded. The continuity of $t \longmapsto R(t)$ in the strong operator topology follows from the continuity of $t \longmapsto S(t)$ in the strong operator topology and the continuity of the exponent in the norm topology. So (CT1) for R is completed. (CT2) for R follows from (CT2) for S: $R(0) = e^{ia(S(0)-I)} = e^{ia(I-I)} = e^0 = I$.

Let us prove (CT3) for R. Remember that (CT1) for S says that for every $f \in \mathcal{F}$ the function $K_f\colon [0, +\infty) \ni t \longmapsto S(t)f \in \mathcal{F}$ is continuous. So by the Weierstrass extreme value theorem the set $K_f([0, 1]) \subset \mathcal{F}$ is compact and hence bounded for each $f \in \mathcal{F}$. This means that for each $f \in \mathcal{F}$ there exists a number $C_f > 0$ such that $\|S(t)f\| \leq C_f$ for all $t \in [0, 1]$. Next, by the Banach-Steinhaus uniform boundedness principle the family of linear bounded operators $(S(t))_{t\in[0,1]}$ is bounded collectively, i.e. there exists a number $C > 0$ such that $\|S(t)\| < C$ for all $t \in [0, 1]$. Suppose that linear operator $A\colon \mathcal{F} \to \mathcal{F}$ is bounded. Then $e^A = I + A + A^2\frac{1}{2!} + A^3\frac{1}{3!} + \ldots = I + A + A^2 \sum_{n=0}^{\infty} \frac{A^n}{(n+2)!} \overset{denote}{=} I + A + A^2\Psi(A)$. One can see that

$$\|\Psi(A)\| = \left\| \sum_{n=0}^{\infty} \frac{A^n}{(n+2)!} \right\| \leq \sum_{n=0}^{\infty} \frac{\|A\|^n}{(n+2)!} \leq \sum_{n=0}^{\infty} \frac{\|A\|^n}{n!} = e^{\|A\|}.$$

Set $A = ia(S(t) - I)$. Then the estimates $\|A\| = \|ia(S(t) - I)\| \leq |a|(C + 1)$ and $\Psi(ia(S(t) - I)) \leq e^{|a|(C+1)}$ hold for all $t \in [0, 1]$. So for all $t \in (0, 1]$ I have

$$\frac{R(t)f - f}{t} = ia\frac{S(t)f - f}{t} - a^2\Psi\Big(ia(S(t) - I)\Big)\Big(S(t) - I\Big)\frac{S(t)f - f}{t}. \quad (13)$$

Suppose that $f \in \mathcal{D}$ is fixed. Due to (CT3) for S there exists a limit $\lim_{t\to 0} \frac{S(t)f-f}{t} = Hf$, so $\frac{S(t)f-f}{t} = Hf + o(1)$. In the right-hand side of (13) the last term for $t \in (0, 1]$ can be estimated as follows:

$$\left\| -a^2\Psi(ia(S(t) - I))\ (S(t) - I)\ \frac{S(t)f - f}{t} \right\| \leq$$

$$| - a^2| \cdot \|\Psi(ia(S(t) - I))\| \cdot \left\| (S(t) - I)\frac{S(t)f - f}{t} \right\| \leq$$

$$|a|^2 e^{|a|(C+1)}\|(S(t)-I)(Hf+o(1))\| \leq$$
$$|a|^2 e^{|a|(C+1)}\Big(\|(S(t)-I)(Hf)\| + \|(S(t)-I)(o(1))\|\Big).$$

If $t \to 0$ then $\|(S(t)-I)(Hf)\| \to 0$ by (CT1) and (CT2) for S. Also $\|(S(t)-I)(o(1))\| \to 0$ because $\|o(1)\| \to 0$ and for $t \in (0,1]$ I have the norm bound $\|S(t)-I\| \leq C+1$. So proceeding to the limit $t \to 0$ in (13) I obtain $\lim_{t\to 0} \frac{R(t)f-f}{t} = ia \lim_{t\to 0} \frac{S(t)f-f}{t} = iaHf$, which is (CT3) for R.

[(CT4) for S]=[$(H,\mathcal{D})$ has the closure $(H, Dom(H))$] $\Longleftrightarrow$ [$(iaH,\mathcal{D})$ has the closure $(iaH, Dom(H))$]=[(CT4) for R] because $Dom(H) = Dom(iaH)$.

By the Stone theorem the operator $(iaH, Dom(H))$ is the generator for the strongly continuous group $(e^{iatH})_{t\in\mathbb{R}}$ and of the strongly continuous semigroup $(e^{iatH})_{t\geq 0}$ in particular, so (E) for R also holds. (N) with $\omega = 0$ for R follows from the condition $(S(t))^* = S(t)$ and the corollary 2.1.

All the conditions of the Chernoff theorem for R are fulfilled, which proves the formulas (1). To obtain (2) and (4) recall corollary 2.2 which states for the bounded operator A the equalities $e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!} = \lim_{k\to\infty}(I + \frac{A}{k})^k$ and set $A = ian(S(t/n) - I)$. Applying the Newton binomial formula to (2) and (4), one obtains (3) and (5) respectively. Applying it to (5) provides (6).

To prove (7) – (12) substitute t by $-t$, a by $-a$ and apply the generation theorem for the groups from [10] at p.79. $\Box$

Remark 3.2. Note that all the limits in the theorem 3.1 are NOT formal signs. They exist in $\mathcal{F}$, and this is an important part of theorem's statement.

Remark 3.3. Note that in the theorem 3.1 $f \in \mathcal{F}$ is fixed. The theorem does not state the uniform convergence of the limits with respect to $f \in \mathcal{F}$ or with respect to f from some subset of $\mathcal{F}$. If $\mathcal{F}$ is a space of some functions $\mathcal{F} \ni f\colon Q \to \mathbb{C}$, $x \longmapsto f(x)$, then the theorem does not state the uniform convergence of the limits with respect to $x \in Q$.

Remark 3.4. If the operators $(S(t))_{t\geq 0}$ are integral operators, then the formulas obtained in the theorem above include both multiple integration (like Feynman formulas) and summation (not like Feynman formulas), this is why I propose to call them quasi-Feynman formulas. Such formulas give us one of the ways to solve the Cauchy problem for the equation $\psi'_t(t,x) = iaH\psi(t,x)$. Possibly it is better to call this equation the *general* Schrödinger equation for two reasons. First, I allow H to be more complicated than a second-order differential (with respect to the spatial coordinate x) operator. Second, I admit that x can range over more complicated spaces than $\mathbb{R}^3$.

Remark 3.5. The conditions $S(t) = (S(t))^*$ and $H = H^*$ in the theorem above are not independent because the Chernoff tangency implies that $S(t)f = f + tHf + o(t)$ as $t \to 0$ for each f from the core of H.

Remark 3.6. If S is Chernoff-tangent to H but $S(t) \neq (S(t))^*$ for some t, one can substitute $S(t)$ by $(S(t) + (S(t))^*)/2$.

Remark 3.7. As we do not need to control the norm growth (N) anymore, one can write a polynomial of $S(t)$ in the index of the exponent like $R(t) = \exp[i(a_0 I + a_1 S(t) + a_2 (S(t))^2 + \ldots + a_n (S(t))^n)]$ or calculate $S(t)$ in many points like $R(t) = \exp[i(a_0 I + a_1 S(g_1(t)) + \ldots + a_n S(g_n(t)))]$ for the given functions $g_j\colon \mathbb{R} \to \mathbb{R}$ and numbers $a_j \in \mathbb{R}$, or combine these approaches.

Remark 3.8. Yu. A. Komlev and D. V. Turaev have found the following application of the remarks 3.7 and 2.4. Let us consider $S(t) - I = \frac{S(t)-I}{t} t$ as a two-point finite difference approximation for $\frac{d}{dt} S(t)\big|_{t=0}$. Then, if I try e.g. a simple three-point approximation $\frac{d}{dt} S(t)\big|_{t=0} \approx \frac{1}{t}(-\frac{3}{2} I + 2S(t) - \frac{1}{2} S(2t))$ then the family $R(t) = e^{ia\left(-\frac{3}{2} I + 2S(t) - \frac{1}{2} S(2t)\right)}$ may give better Chernoff approximations to e^{iatH}, than $e^{ia(S(t)-I)}$. One can also ask what will happen if we take a d-point approximation and then consider $d \to \infty$.

Remark 3.9. For fixed t the $S(t)\colon f \longmapsto S(t)f$ is usually an integral operator over Gaussian measure. If one applies the finite difference approximation approach from remark 3.8 directly to the function f, i.e. under the sign of the integral, the we can get family $S(t)$ with $S(t)\big|_{t=0} = I$, $\frac{d}{dt} S(t)\big|_{t=0} = H$, $\frac{d^2}{dt^2} S(t)\big|_{t=0} = 0, \ldots, \frac{d^n}{dt^n} S(t)\big|_{t=0} = 0$ using fewer terms because the Gaussian measure is symmetric.

Remark 3.10. Theorem 3.1 will be more useful if one proves that (at least in the most important cases) the continued limit in (2), (4), (8), (10) exists as double limit, or at least that there exists a sequence (k_n) of integers on which the limit $\lim_{n\to\infty} \lim_{k\to\infty}$ can be substituted by the limit $\lim_{n\to\infty}$.

4. Why this Method Occurs Naturally

It is usually not easy to construct a family which is Chernoff-equivalent to $(e^{itH})_{t\geq 0}$ because the conditions of the Chernoff theorem obstruct each other in some sence when dealing with a Schrödinger equation. To see on a particular example what the difficulty is and how to overcome it refer to

[8]. In the case of the heat equation and the C_0-semigroup $(e^{tH})_{t\geq 0}$ the situation is usually more simple. So the initial idea (introduced in [24]) was to use the family $(S(t))_{t\geq 0}$ which is Chernoff-equivalent to the C_0-semigroup $(e^{tH})_{t\geq 0}$ for constructing the family $(R(t))_{t\geq 0}$ which is Chernoff-equivalent to the C_0-semigroup $(e^{itH})_{t\geq 0}$.

Start from separating the conditions of the Chernoff theorem for $(R(t))_{t\geq 0}$ into independent blocks: existence of the C_0-semigroup + Chernoff-tangency + growth of the norm bound. The first block is granted by the Stone theorem as H is self-adjoint. The second block is algebraic, so one can try to use algebraic operations to save identity at zero and add i to the derivative at zero. If we have an analytic function $r\colon \mathbb{C} \to \mathbb{C}$ with $r(0) = 1$ and $r'(0) = i$ then we can define $R(t) = r(S(t))$. And if we choose $r(z) = e^{i(z-1)}$ and claim that $S(t) = (S(t))^*$ then we can use the corollary 2.1 to obtain the third block. So we come to the formulas $R(t) = e^{i(S(t)-I)}$ and $e^{itH} = \lim_{n\to\infty}(R(t/n))^n$.

After all we see that in the proof we do not need the Chernoff-equivalence of the family $(S(t))_{t\geq 0}$ to the C_0-semigroup $(e^{tH})_{t\geq 0}$, we need only the Chernoff-tangency of $(S(t))_{t\geq 0}$ to the operator H. Indeed, the proof holds on even if the C_0-semigroup $(e^{tH})_{t\geq 0}$ does not exist and the norm of $S(t)$ grows at any rate with respect to the growth of t. So I have reduced the difficult task of constructing the family which is Chernoff-equivalent to $(e^{itH})_{t\geq 0}$ to a more simple task of constructing a family which is Chernoff-tangent to H. And the condition $S(t) = (S(t))^*$ that I require does not seem very restraining due to remarks 3.5 and 3.6.

Writing $e^{i(S(|t|)-I)\mathrm{sign}(t)}$ instead of $e^{i(S(t)-I)}$ arises as formal generalization step from the case $t \geq 0$ to the case $t \in \mathbb{R}$. Adding $a \neq 0$ to the formula helps to write the C_0-groups $(e^{itH})_{t\in\mathbb{R}}$ and $(e^{-itH})_{t\in\mathbb{R}}$ in one formula $(e^{iatH})_{t\in\mathbb{R}}$ just setting $a = 1$ or $a = -1$, also a may be used as a small or large parameter.

5. Guidelines on Applying the Method

As already mentioned, C_0-semigroups can be used to study so-called evolutionary equations, i.e. equations in the form $u'_t(t,x) = Lu(t,x)$. Bright examples of such equations are the heat equation $u'_t(t,x) = Hu(t,x)$ and the Schrödinger equation $\psi'_t(t,x) = iH\psi(t,x)$. Here $t \in [0,+\infty)$ is time, and the spatial variable x ranges over the set Q. In practice, Q is a configuration space of the system studied and is defined by the physical process that motivates a mathematical setting of the problem. For example, if we study the heat propagation in a ball $B \subset \mathbb{R}^3$, then $Q = B$.

Above I discussed a very general case as I dealed only with C_0-semigroups and C_0-groups not taking into account what space Q stays behind them. So the technique presented may be potentially employed in a case when Q is $\mathbb{R}^n$ or some subset of $\mathbb{R}^n$, $\mathbb{C}^n$ or some subset of $\mathbb{C}^n$, a linear (Hilbert, Banach, etc.) space or some subset of it, a lattice [34], a manifold of a finite or infinite dimension, a group, an algebra, a graph etc.

If one wants to do this, then $\mathcal{F}$ should be a complex Hilbert space of some functions $f: Q \to \mathbb{C}$. With the method presented we can study equations for such functions $\psi: [0, +\infty) \times Q \to \mathbb{C}$ that for every fixed moment of time $t \in [0, +\infty)$ the function $x \longmapsto \psi(t, x)$ belongs to $\mathcal{F}$, and the function $t \longmapsto \psi(t, \cdot)$ is continuous and differentiable as a mapping $[0, +\infty) \to \mathcal{F}$. The discussion above does not lean on the nature of the scalar product in $\mathcal{F}$. For example, it can originate from the fact that $\mathcal{F} = L^2(Q, \mu)$ for some measure μ in Q, or it can be based on some more complicated structures. As a very particular yet important case let us mention $Q = \mathbb{R}^3$ and $\mathcal{F} = L^2(\mathbb{R}^3)$ for the classical Schrödinger equation.

As for the operator H, we need it to be linear and self-adjoint (hence densely defined and closed). For example, $H = \Delta$ or $H = \Delta^2$ or $(H\psi)(x) = (\Delta\psi)(x) + V(x)\psi(x)$ or some other. We need the coefficients of H not to depend on t; nevertheless, they may depend on $x \in Q$.

Next, to construct a family $(S(t))_{t\geq 0}$ which is Chernoff-tangent to the operator H in $\mathcal{F} = L^2(Q, \mu)$ one can use the following identities. They depend on Q and I state them without some important details just to sketch the idea. Denote a Gaussian measure [27, 28] in Q with a correlation operator B as μ_B. Let $g: Q \to \mathbb{R}$ be a function bounded from zero and infinity plus some other properties, one can consider $g(x) \equiv \frac{1}{2}$ in this paragraph as a particular case. Let $V: Q \to \mathbb{R}$ be a function with $V(x) \leq 0$ and some other properties. Then the identities similar to $\int_Q f(x + y)\mu_{2tg(x)A}(dy) = f(x) + tg(x)\mathrm{trace}[Af''(x)] + o(t)$ and $e^{tV(x)}f(x) = f(x) + tV(x) + o(t)$ hold. If one denotes $(S(t)f)(x) = \int_Q f(x + y)\mu_{2tg(x)A}(dy)$ then $(S(t))_{t\geq 0}$ is Chernoff-tangent to $H = g(\cdot)\Delta$ as $(S(t)f)(x) = f(x) + tg(x)\Delta f(x) + o(t)$. If one denotes $(S(t)f)(x) = e^{tV(x)} \int_Q f(x+y)\mu_{2tg(x)A}(dy)$ then $(S(t))_{t\geq 0}$ is Chernoff-tangent to $H = g(\cdot)\Delta + V(\cdot)$ as $(S(t)f)(x) = f(x) + t[g(x)\Delta f(x) + V(x)f(x)] + o(t)$. See these and some other useful formulas in more details with precise mathematical statements in [19, 29, 31, 32, 33, 8, 15, 16, 18].

Final step. Suppose that all the conditions mentioned in this section above are satisfied. Suppose that we have constructed a family $(S(t))_{t\geq 0}$

which is Chernoff-tangent to H. Then the Cauchy problem in $\mathcal{F}$

$$\begin{cases} \psi'_t(t,x) = iaH\psi(t,x); \quad t \in \mathbb{R}, x \in Q \\ \psi(0,x) = \psi_0(x); \quad x \in Q \end{cases}$$

stated for arbitrary $\psi_0 \in \mathcal{F}$ and non-zero $a \in \mathbb{R}$ has the unique in sense of $\mathcal{F}$ solution $\psi(t,x) = \left(e^{iatH}\psi_0\right)(x)$ depending on ψ_0 continuously with respect to the norm in $\mathcal{F}$, where for every $t \in \mathbb{R}$ the operator e^{iatH} from the C_0-group $\left(e^{iatH}\right)_{t\in\mathbb{R}}$ in $\mathcal{F}$ is granted by the theorem 3.1. If $\psi_0 \in Dom(H)$ then the solution obtained is called a strong solution, and in the general case $\psi_0 \in \mathcal{F}$ it is called a mild solution, see [11] for the details.

6. Toy Model Example: the Method in Use

A. S. Plyashechnik proposed a simple model to show how the method works and what sort of formulas for the solution it provides. Suppose that non-zero number $a \in \mathbb{R}$ and a differentiable function $V \in C^1_b(\mathbb{R},\mathbb{R})$ bounded with its first derivative are given. Consider the Cauchy problem in $L^2(\mathbb{R}^1,\mathbb{C})$

$$\begin{cases} \frac{i}{a}\psi'_t(t,x) = -\frac{1}{2}\psi''_{xx}(t,x) + V(x)\psi(t,x); \quad t \in \mathbb{R}, x \in \mathbb{R} \\ \psi(0,x) = \psi_0(x); \quad x \in \mathbb{R} \end{cases} \tag{14}$$

Let us rewrite it in the form

$$\begin{cases} \psi'_t(t,x) = iaH\psi(t,x); \quad t \in \mathbb{R}, x \in \mathbb{R} \\ \psi(0,x) = \psi_0(x); \quad x \in \mathbb{R} \end{cases} \tag{15}$$

where H is an operator defined for $f \in W^2_2(\mathbb{R})$ by the formula

$$(Hf)(x) = \frac{1}{2}f''(x) - V(x)f(x).$$

Here $W^2_2(\mathbb{R}) \subset L^2(\mathbb{R})$ is the Sobolev class, i.e. the linear space of all the functions $f \in L^2(\mathbb{R})$ such that $f' \in L^2(\mathbb{R})$ and $f'' \in L^2(\mathbb{R})$ where f' and f'' are the distributional derivatives of f. So in theorem 3.1 one can set $\mathcal{F} = L^2(\mathbb{R})$ and $Dom(H) = W^2_2(\mathbb{R})$.

The operator $S(t)$ is constructed as follows. Define

$$(F_t f)(x) = \exp\left(-\frac{t}{2}V(x)\right) f(x)$$

and

$$(B_t f)(x) = \frac{1}{\sqrt{2\pi t}} \int_{\mathbb{R}} e^{\frac{-(x-y)^2}{2t}} f(y)dy = \frac{1}{\sqrt{2\pi t}} \int_{\mathbb{R}} e^{\frac{-y^2}{2t}} f(x+y)dy$$

for $t > 0$ and $B_0 f = f$. Then let us set $S(t) = F_t \circ B_t \circ F_t$, i.e.

$$(S(t)f)(x) = \frac{1}{\sqrt{2\pi t}} \int_{\mathbb{R}} \exp\left(-\frac{y^2}{2t} - \frac{t}{2}\Big[V(x) + V(x+y)\Big]\right) f(x+y)dy.$$

It is not very difficult to check that all the conditions of the theorem 3.1 are fulfilled. To do this one can take the set $C_0^\infty(\mathbb{R},\mathbb{R})$ of all infinitely differentiable functions $\mathbb{R} \to \mathbb{R}$ with compact support for $\mathcal{D}$ in the definition of the Chernoff tangency, and then perform the calculations that are similar to what is done in [25] in the proof of item 4 of theorem 4.1.

Now take one of the formulas stated in the theorem 3.1, say, formula (9):

$$e^{iatH} f = \left(\lim_{n\to\infty} \lim_{k\to\infty} \sum_{m=0}^{k} \sum_{q=0}^{m} \frac{(-1)^{m-q}(ian)^m(\mathrm{sign}(t))^m}{q!(m-q)!} (S(|t/n|))^q \right) f.$$

In our particular case it implies that the Cauchy problem (14) has defined for all $t \in \mathbb{R}$, the unique in $L^2(\mathbb{R})$ solution

$$\psi(t,x) = \lim_{n\to\infty} \lim_{k\to\infty} \sum_{m=0}^{k} \sum_{q=0}^{m} \frac{(-1)^{m-q}(ian)^m(\mathrm{sign}(t))^m}{q!(m-q)!} \left(\frac{n}{2\pi|t|}\right)^{q/2} \times$$

$$\underbrace{\int_{\mathbb{R}} \cdots \int_{\mathbb{R}}}_{q} \exp\left\{ \frac{|t|}{n} \left[-\frac{1}{2}V(x) - \sum_{p=1}^{q} V\left(x + \sum_{d=p}^{q} y_d\right)\right] - \frac{1}{2|t|} \sum_{r=1}^{q} y_r^2 \right\} \times$$

$$\psi_0\left(x + \sum_{j=1}^{q} y_j\right) \prod_{s=1}^{q} dy_s.$$

7. Summary

One of the ways to solve the Cauchy problem for an evolutionary partial differential equation (e.g. a heat equation and a Schrödinger equation) is to use a C_0-semigroup (or a C_0-group) as a solution-giving object, and the Chernoff theorem as the main technical tool to deal with the C_0-semigroup. The

Chernoff theorem says that to obtain an explicit formula for a C_0-semigroup it is enough to find a one-parameter family of linear bounded operators that is Chernoff-equivalent to the C_0-semigroup. It is known that constructing such Chernoff-equivalent families for a Schrödinger equation is much more difficult than doing the same for a heat equation. O.G.Smolyanov and members of his team in many cases have constructed Chernoff-equivalent families that provide the solution to the heat equation. With the method presented in this article this material can be used to solve the Schrödinger quation.

A C_0-group $(\exp(itH))_{t\in\mathbb{R}}$ with the infinitesimal generator iH exists for every linear self-adjoint H and provides the solution to the Cauchy problem for the Schrödinger equation $\psi'_t(t,x) = iH\psi(t,x)$. If $\psi(0,x) = \psi_0(x)$ for a given ψ_0 then $\psi(t,x) = (\exp(itH)\psi_0)(x)$. Usually $\mathcal{F}$ is the L^2 over the space that variable x belongs to, and H is the minus Laplacian plus multiplying by a potential function. In this article I study the general case when $\mathcal{F}$ may be some other Hilbert space and H may be some other linear self-adjoint operator in $\mathcal{F}$.

For this general setting of the problem I prove a short formula $R(t) = e^{i(S(t)-I)}$ to express explicitly a family R that is Chernoff-equivalent to the C_0-semigroup for a Schrödinger equation in the terms of the family S that is Chernoff-tangent to the operator from the heat equation. This formula leads to a new class of integral representations of the Cauchy problem solution – quasi-Feynman formulas. With the method presented the difficulty of solving the Cauchy problem for a Schrödinger equation reduces twice: we need to construct a less difficult (Chernoff-tangent) family to a less difficult (heat) equation. This technique deals with the semigroups and operator families only, so it works for a large class of Hamiltonians describing dynamics in a large class of configuration spaces. Quasi-Feynman formulas are easier to obtain but they provide lengthier approximation expressions (one simple example is shown in the article). Both Feynman formulas and quasi-Feynman formulas approximate Feynman path integrals because they are connected via the C_0-group.

The method presented opens several challenging questions – for example, it possibly may provide better approximations than Feynman formulas provide, but this needs to be clarified, see remarks 2.4 and 3.8 above.

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