Quasi-Feynman formulas for the Schrödinger group

What is it, how to obtain it, what are the benefits from it

Ivan D. Remizov[1]

[1]Bauman Moscow State Technical University

International Conference
Function Spaces and Function Approximation Theory
Dedicated to the 110th anniversary
of academician S.M. Nikolskii

May 25-29, 2015, Moscow

Plan of my talk about quasi-Feynman formulas:

1. **What is it**
   - Feynman formulas — definition
   - Feynman formulas — the toy model example
   - Quasi-Feynman formulas — definition
   - Quasi-Feynman formulas — the toy model example
2. **How to obtain it**
   - C_0−semigroups
   - C_0−groups
   - C_0-group solves the Cauchy problem for a Partial DE
   - The Stone theorem for the Schrödinger group
   - The Chernoff tangency
   - The Chernoff theorem
   - My theorem
   - Corollary: obtaining quasi-Feynman formulas
   - Toy model example revised

Plan of my talk about quasi-Feynman formulas:

3. **What are the benefits from it**
   - That's a new class of formulas that can be studied
   - Wide class of configuration spaces and Hamiltonians covered
   - Easier to obtain (compared with Feynman formulas)
     - 3.1 Do not need to control the norm growth anymore
     - 3.2 Many families that are already constructed for the Feynman formulas can be used to obtain quasi-Feynman formulas
   - Possibly faster convergence of approximations (compared with Feynman formulas)
4. **Discussion and criticism**
   - Quasi-Feynman formulas are really lengthy
   - The «curse of dimensionality» holds as in Feynman formulas
   - We need to count up to infinity twice or even more times
   - The connection with Feynman pseudomeasure and Feynman path integral is not so clear (compared with Feynman formulas)
5. **Acknowledgments**
6. **Questions**

Feynman formula — the definition

Definition (O.G.Smolyanov, 2002). **Feynman formula** is a representation of a function in a form of the **limit of a multiple integral** where the multiplicity tends to infinity.
Typical Feynman formula:

$$f(x) = \lim_{n\to\infty} \underbrace{\int_A \dots \int_A}_{n} [\text{Some expression}] dx_1 \dots dx_n$$

where A is a set with a measure, usually the configuration space or the phase space for some dynamical system.

Feynman formula — the toy model example

(R.P. Feynman 1942-48; Yu.L. Daleckii and H.F. Trotter 1960-61; E.Nelson 1964): the Cauchy problem for the Schrödinger equation

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

with a smooth bounded potential V has the solution

$$\psi(t,x) = \lim_{n\to\infty}\left(\frac{n}{2\pi i t}\right)^{n/2}\times$$

$$\times\underbrace{\int_{\mathbb{R}}\dots\int_{\mathbb{R}}}_{n}\exp\left(-i\sum_{j=1}^{n}\left[\frac{n(x_j-x_{j-1})^2}{2t}-\frac{t}{n}V(x_j)\right]\right)\psi_0(x_0)dx_0\dots dx_{n-1}.$$

Quasi-Feynman formula — the definition

Definition (I.D.Remizov, 2014; the word suggested by O.G.Smolyanov, 2015).

Quasi-Feynman formula is a representation of a function in a form which **includes multiple integrals** of an infinitely increasing multiplicity. Typical quasi-Feynman formula:

$$f(x) = [\mathrm{Expr\_1}] \underbrace{\int_A \dots \int_A}_{n} [\mathrm{Expr\_2}] dx_1 \dots dx_n [\mathrm{Expr\_3}]$$

where n grows to infinity, A is a set with a measure, and $[\mathrm{Expr\_k}]$ are some mathematical expressions. **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.

Quasi-Feynman formula — the toy model example

D.V.Grishin-I.D.Remizov-A.V.Smirnov, 2015: the Cauchy problem

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

with a smooth bounded potential V has the solution

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

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

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

C_0-semigroups

C_0-semigroup, or a strongly continuous one-parameter semigroup of linear bounded operators $(V(t))_{t\geq 0}$ in Banach space $\mathcal{F}$ is a mapping

$$V\colon [0,+\infty)\to L_b(\mathcal{F},\mathcal{F})$$

of the non-negative half-line into the space of all bounded linear operators on $\mathcal{F}$ which satisfies the following conditions
1) $\forall\varphi\in\mathcal{F}: V(0)\varphi=\varphi$,
2) $\forall t\geq 0, \forall s\geq 0: V(t+s)=V(t)\circ V(s)$,
3) $\forall\varphi\in\mathcal{F}$ function $t\longmapsto V(t)\varphi$ is continuous
as a mapping $[0,+\infty)\to\mathcal{F}$.

C_0-groups

C_0-group, or a strongly continuous one-parameter group of linear bounded operators $(V(t))_{t\geq 0}$ in Banach space $\mathcal{F}$ is a mapping

$$V\colon (-\infty, +\infty) \to L_b(\mathcal{F}, \mathcal{F})$$

of the real line into the space of all bounded linear operators on $\mathcal{F}$ which satisfies the following conditions

1) $\forall \varphi \in \mathcal{F} : V(0)\varphi = \varphi$,
2) $\forall t \in \mathbb{R}, \forall s \in \mathbb{R} : V(t+s) = V(t) \circ V(s)$,
3) $\forall \varphi \in \mathcal{F}$ function $t \longmapsto V(t)\varphi$ is continuous as a mapping $\mathbb{R} \to \mathcal{F}$.

C_0-group solves the Cauchy problem for a Partial DE

If M is a set, then the function $u\colon \mathbb{R}\times M\to\mathbb{C}$, $u\colon (t,x)\longmapsto u(t,x)$ 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-group $(e^{tL})_{t\in\mathbb{R}}$ in $\mathcal{F}$ then the Cauchy problem

$$\begin{cases} u_t'(t,x)=Lu(t,x) \text{ for } t\in\mathbb{R}, x\in M\\ u(0,x)=u_0(x) \text{ for } x\in M\end{cases}$$

has a unique (in sense of $\mathcal{F}$, where $u(t,\cdot)\in\mathcal{F}$ for every $t\in\mathbb{R}$) solution

$$u(t,x)=(e^{tL}u_0)(x)$$

depending on u_0 continuously.

The Stone theorem

Theorem (M. H. Stone, 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. If A is a linear self-adjoint operator in Hilbert space, then $\left\|e^{iA}\right\| = 1$.

The Chernoff tangency

Definition (I. D. Remizov, 2014) Let $\mathcal{F}$ be a Banach space, and $L_b(\mathcal{F},\mathcal{F})$ be the space of all linear bounded operators in $\mathcal{F}$ endowed with the operator norm. Let $L\colon \mathcal{F} \supset Dom(L) \to \mathcal{F}$ be a closed linear operator.

A function G is said to be **Chernoff-tangent** to L iff:

(CT1). G is defined on $[0,+\infty)$, takes values in $L_b(\mathcal{F},\mathcal{F})$ and $t \longmapsto G(t)f$ 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 $(L, Dom(L))$.

The Chernoff theorem

Theorem (P. R. Chernoff, 1968) Let $\mathcal{F}$ be a Banach space, and $L_b(\mathcal{F},\mathcal{F})$ be the space of all linear bounded operators in $\mathcal{F}$ endowed with the operator norm. Let $L\colon \mathcal{F} \supset Dom(L) \to \mathcal{F}$ be a linear operator.

Suppose there is a function G such that:

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

(CT1). G is defined on $[0,+\infty)$, takes values in $L_b(\mathcal{F},\mathcal{F})$ and $t \longmapsto G(t)f$ 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 $f \in \mathcal{F}$ we have $(G(t/n))^n f \to e^{tL} f$ as $n \to \infty$.

My theorem

Theorem (I. D. Remizov, 2014) **Suppose** that a linear self-adjoint operator $H\colon \mathcal{F} \supset Dom(H) \to \mathcal{F}$ 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 $t \geq 0$. Let us set

$$R(t) = \exp\left[ia(S(|t|) - I)\mathrm{sign}(t)\right]$$

defining the exponent by a series (it is possible because for each $t \in \mathbb{R}$ only linear bounded operators in $\mathcal{F}$ are present in the index of the exponent).
Then for all $t \in \mathbb{R}$ and all $f \in \mathbb{F}$

$$e^{iatH}f = \lim_{n\to\infty}\left(R\left(\frac{t}{n}\right)\right)^n f.$$

Corollary: obtaining quasi-Feynman formulas

For all $t \in \mathbb{R}$ and all $f \in \mathcal{F}$ one has $e^{iatH}f =$

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

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

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

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

Corollary: obtaining quasi-Feynman formulas

For all $t \in \mathbb{R}$ and all $f \in \mathcal{F}$ one has $e^{iatH} f =$

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

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

If $S(t)$ is an integral operator, then above we have quasi-Feynman formulas.

The toy model example revised

Suppose that non-zero number $a \in \mathbb{R}$ and a differentiable function $V \in C_b^1(\mathbb{R}, \mathbb{R})$ bounded with its first derivative are given. Consider the Cauchy problem in $L^2(\mathbb{R}^1, \mathbb{C})$

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

Let us rewrite it in the form

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

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 $f'' \in L^2(\mathbb{R})$.

The toy model example revised

One can set $\mathcal{F} = L^2(\mathbb{R})$ and $Dom(H) = W_2^2(\mathbb{R})$. Define

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

This family (suggested by A.S.Plyashechnik) provides

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

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

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

Some remarks

Remark. The conditions $S(t) = (S(t))^*$ and $H = H^*$ in my theorem 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. 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. One can try to study degenerate equations proceeding to $a \to 0$ or to $a \to \pm\infty$.

Some remarks: counting up to infinity twice

Remark. My theorem will be more useful if one proves that the continued limit in the quasi-Feynman formulas 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 $\lim_{n\to\infty}$.

Some remarks

Remark. As we do not need to control the norm growth (N) anymore, we can write a polynomial of $S(t)$ in the index of the exponent like

$$R(t) = \exp[i(a_0 I + a_1 S(t) + a_2 (S(t))^2 + \dots + a_n (S(t))^n)]$$

or calculate $S(t)$ in many points like

$$R(t) = \exp[i(a_0 I + a_1 S(f_1(t)) + \dots + a_n S(f_n(t)))]$$

for the given functions $f_j\colon \mathbb{R} \to \mathbb{R}$ and numbers $a_j \in \mathbb{R}$, or combine these approaches.

Some remarks

Remark. 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 $(G(t/n))^n f \to e^{tL} f$.

Some remarks

Remark. Yu. A. Komlev and D. V. Turaev have found the following application of the remarks above. 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 we try e.g. a simple three-point approximation

$$\frac{d}{dt}S(t)\Big|_{t=0} \approx \frac{1}{t}\left(-\frac{3}{2}I + 2S(t) - \frac{1}{2}S(2t)\right)$$

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 $d \to \infty$.

Acknowledgements

I thank my scientific advisor O. G. Smolyanov for his active kind criticism which helped me a lot on the way of finding better words and ideas.
I highly appreciate the impact of V. Zh. Sakbaev, N. N. Shamarov, D. V. Turaev and their continuous open hearted attention to the research and significant remarks which made the results obtained better.
I am thankful to D. V. Grishin, A. S. Plyashechnik, A. V. Smirnov for help with developing the example for the method presented.

This work has been supported by the Russian Scientific Foundation Grant 14-41-00044 in the Lobachevsky State University.

Thank you for your attention!

Proofs and more comments please see in the latest version of the preprint http://arxiv.org/abs/1409.8345

My email is ivremizov@yandex.ru