Quasi-Feynman formulas for the one-dimensional Schrödinger equation with a bounded smooth potential via the Remizov theorem

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Plan of the talk:

1. **Preliminaries**
   - Feynman formula — definition and example
   - Quasi-Feynman formula — definition
   - The Chernoff theorem
   - The Chernoff tangency
   - Remizov's approach for structuring conditions of the Chernoff theorem
   - Remizov's theorem
2. **Main result**
   - We solve the Cauchy problem for the Schrödinger equation $\psi_t'(t,x) = iaH\psi(t,x)$, where a is a non-zero real parameter
   - Constructing the operator $S(t)$ that is Chernoff tangent to H
   - The solution in a form of a quasi-Feynman formula
3. **Main steps of the proof**
   - Operator $S(t)$ is well-defined
   - Operator $S(t)$ is self-adjoint
   - Four conditions of the Chernoff tangency
   - Operator H is well-defined
   - Operator H is self-adjoint

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 — well known 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

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

with a smooth bounded potential V has the solution

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

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

At the right side here $x_n = x$.

Quasi-Feynman formula — 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.

The Chernoff theorem

Theorem (P. R. Chernoff, 1968)
Let $\mathcal{F}$ be a Banach space and $G : [0, \infty) \to \mathcal{L}(\mathcal{F}, \mathcal{F})$ — (strongly) continuous mapping such that $G(0) = I$ and $\|G(t)\| \leq e^{\omega t}$ for some $\omega \in [0, \infty)$ and for all $t \geq 0$. Let $\mathcal{D}$ be a linear subspace of $\mathrm{Dom}(G'(0))$ such that restriction of operator $G'(0)$ to $\mathcal{D}$ has a closure. Denote this closure as $(L, \mathrm{Dom}(L))$.
If $(L, \mathrm{Dom}(L))$ is a generator of a strongly continuous semigroup $(T_t)_{t\geq 0}$, then for all $t_0 > 0$ sequence of operators $\big((G(t/n))^n\big)_{n\in\mathbb{N}}$ converges to $(T_t)_{t\geq 0}$ while $n \to \infty$ in strong topology uniformly with respect to $t \in [0, t_0]$, i.e. $T_t = \lim\limits_{n\to\infty} (G(t/n))^n$.

The Chernoff tangency

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

Remizov's approach for structuring conditions of the Chernoff theorem

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

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

(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 $n\to\infty$) uniformly with respect to $t\in[0,t_0]$ for every fixed $t_0>0$.

Remizov's theorem

Theorem (I. D. Remizov, 2014) **Suppose** that a linear self-adjoint operator $H \colon \mathcal{F} \supset \mathrm{Dom}(H) \to \mathcal{F}$ 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 $f \in \mathcal{F}$

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

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, because $(S(|t/n|))^m$ is multiple integral operator with multiplicity m.

Part II: Main result

We solve the Cauchy problem for the Schrödinger equation

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 $L^2(\mathbb{R}, \mathbb{C})$

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

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

Constructing the operator $S(t)$ that is Chernoff tangent to operator H

Operator $S(t)$ suggested by A. S. Plyashechnik is constructed as a symmetric composition:

$$S(t) = F(t) \circ B(t) \circ F(t),$$

where $F(t)$ is a multiplication operator:

$$(F(t)f)(x) = e^{-\frac{t}{2}V(x)}f(x);$$

and $B(t)$ is an integral operator:

$$(B(t)f)(x) = \frac{1}{\sqrt{2\pi t}} \int\limits_{\mathbb{R}} e^{\frac{-(x-y)^2}{2t}} f(y)dy.$$

So when we prove some statement concerning operator $S(t)$, first we usually prove the same thing for $F(t)$ and $B(t)$ separately.

The solution in a form of a quasi-Feynman formula

Let's set $\mathcal{F} = L^2(\mathbb{R})$ and $\mathrm{Dom}(H) = W_2^2(\mathbb{R})$. As was constructed:

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

This family provides the following quasi-Feynman formula:

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

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

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

Part III: Main steps of the proof

Operator $S(t)$ is well-defined

What we prove: $\forall t \geq 0 \; \forall f \in L^2(\mathbb{R}): \; S(t)f \in L^2(\mathbb{R})$.
How we prove it:

1. $F(t)$ is bounded $\forall t \geq 0$, as it's the operator of multiplication by a bounded function, hence it is well-defined;
2. $B(t)$ is also bounded $\forall t \geq 0$, which appears form inequality

$$\int_{\mathbb{R}} \left| \frac{1}{\sqrt{2\pi t}} \int_{\mathbb{R}} e^{\frac{-(x-y)^2}{2t}} f(y) dy \right|^2 dx \leq \int_{\mathbb{R}} |f(x)|^2 dx < \infty$$

which also means that $||B(t)|| \leq 1$. We prove this inequality in several steps by using straightforward transformations, various integral estimations and Tonelli's theorem.

Operator $S(t)$ is self-adjoint

What we prove: $\forall t \geq 0$ operator $S(t)$ is self-adjoint.
How we prove it:

1. $F(t)$ is self-adjoint $\forall t \geq 0$, as it's the operator of multiplication by a real-valued function;
2. $B(t)$ being self-adjoint $\forall t \geq 0$ is shown by using straightforward transformations and Fubini's and Tonelli's theorems;
3. $S(t)$ is self-adjoint due to the symmetry of the composition:

$$\langle S(t)f, g\rangle = \langle F(t)\circ B(t)\circ F(t)f, g\rangle = \langle B(t)\circ F(t)f, F(t)g\rangle =$$

$$= \langle F(t)f, B(t)\circ F(t)g\rangle = \langle f, F(t)\circ B(t)\circ F(t)g\rangle = \langle f, S(t)g\rangle$$

Chernoff tangency: 1^{st} condition (CT1)

What we prove:
$\forall f \in L^2(\mathbb{R})$ function $t \longmapsto S(t)f$ is continuous in $[0, +\infty)$.
How we prove it:
in 4 steps we prove the following functions to be continuous:

1. function $t \longmapsto F(t)f$ in $[0, +\infty)$ with fixed $f \in L^2(\mathbb{R})$;
2. function $t \longmapsto B(t)f$ in $(0, +\infty)$ with fixed $f \in L^2(\mathbb{R})$;
3. function $t \longmapsto B(t)\varphi$ in $\{0\}$ with fixed $\varphi \in C_0^\infty(\mathbb{R})$
4. function $t \longmapsto B(t)f$ in $\{0\}$ with fixed $f \in L^2(\mathbb{R})$

Lebesgue's dominated convergence theorem is one of the main technical tool through all of the steps.

Chernoff tangency: 2^{nd} condition (CT2)

What we prove: $S(0) = I$.
How we prove it:
$F(0) = I$ by construction,
$B(0) = I$ by definition,
hence $S(0) = F(0) \circ B(0) \circ F(0) = I$.

Chernoff tangency: 3^{rd} condition (CT3)

What we prove: $\forall\varphi \in C_0^\infty(\mathbb{R}) : \ \exists \lim\limits_{t\to 0} \frac{S(t)\varphi-\varphi}{t} := S'(0).$

How we prove it:

we show that

$$(S(t)\varphi)(x) = \varphi(x) + t\underbrace{\left(\frac{1}{2}\varphi''(x) - V(x)\varphi(x)\right)}_{=(H\varphi)(x)} + A(t,x),$$

where $A(t,x) = o(t)$ in $L^2(\mathbb{R})$, by representing all of participating functions in form of Taylor polynomials. The result is obtained though tedious process of parentheses removing, calculating some of resulted integrals and estimating the others. Estimation is based on the fact that functions V and φ are bounded with their derivatives.

Chernoff tangency: 4^{th} condition (CT4)

What we prove:
Operator $(S'(0), C_0^\infty(\mathbb{R}))$ has a closure $(H, W_2^2(\mathbb{R}))$.
How we prove it:
In the proof of the condition CT3 we've shown that $S'(0) = H$, where $Hf = \frac{1}{2}f'' - Vf$.

1. First we show that operator $(H, C_0^\infty(\mathbb{R}))$ is symmetric and hence it has a closure.
2. Considering that operator $Lf := Vf$ is bounded (as it's a multiplication by a bounded function), we show that operator $\overline{(H, C_0^\infty(\mathbb{R}))}$ has the same domain as operator $\overline{(H_0, C_0^\infty(\mathbb{R}))}$, where $H_0 f = \frac{1}{2}f''$.
3. Finally we show that the domain of $\overline{(H_0, C_0^\infty(\mathbb{R}))}$ is $W_2^2(\mathbb{R})$, which proves the result.

Operator H is well-defined

What we prove: $\forall f \in W_2^2(\mathbb{R}): \;\; Hf \in L^2(\mathbb{R})$.
How we prove it:
we consider

$$\int\limits_{\mathbb{R}} \left| \frac{1}{2} f''(x) - V(x) f(x) \right|^2 dx \leq$$

$$\leq \underbrace{\frac{1}{4} \int\limits_{\mathbb{R}} |f''(x)|^2 dx}_{<\infty} + \underbrace{\int\limits_{\mathbb{R}} |V(x)|^2 |f(x)|^2 dx}_{\leq A^2 \int\limits_{\mathbb{R}} |f(x)|^2 dx < \infty} + \underbrace{\int\limits_{\mathbb{R}} |V(x) f(x) f''(x)| dx}_{A \int\limits_{\mathbb{R}} |f(x) f''(x)| dx < \infty} < \infty$$

since $|V(x)| < A$ and $|f \times g| \leq \frac{|f|^2 + |g|^2}{2}$.

Operator H is self-adjoint

What we prove: operator $(H, W_2^2(\mathbb{R}))$ is self-adjoint.
How we prove it:

1. We use a theorem (1.1, chapter 2) from the book "The Schrödinger Equation" by F.A.Berezin, M.A.Shubin (1983) which implies that $(H, C_0^\infty(\mathbb{R}))$ is *essentially* self-adjoint. That means that $\overline{(H, C_0^\infty(\mathbb{R}))} = \left(\overline{(H, C_0^\infty(\mathbb{R}))}\right)^*$.
2. Condition CT4 gives us that $\overline{(H, C_0^\infty(\mathbb{R}))} = (H, W_2^2(\mathbb{R}))$, therefore $(H, W_2^2(\mathbb{R}))$ is self-adjoint.

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