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SHORT COMMUNICATIONS

Solution of the Schrödinger Equation with the Use of the Translation Operator

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Consider the Cauchy problem for the Schrödinger equation in the complex space $L_2(\mathbb{R}^1)$,

$$\begin{cases} \psi'_t(t,x) = \dfrac{1}{4} i\psi''_{xx}(t,x) - iV(x)\psi(t,x) = iH\psi(t,x), & t \in \mathbb{R}^1,\ x \in \mathbb{R}^1, \\ \psi(0,x) = \psi_0(x), & x \in \mathbb{R}^1. \end{cases} \tag{1}$$

The function V is assumed to be real-valued, bounded, and measurable. Then the self-adjoint operator H given by the formula $(Hf)(x) = (1/4)f''(x) - V(x)f(x)$ acts on $L_2(\mathbb{R}^1)$, and its domain $\mathrm{Dom}(H)$ is the Sobolev space $W(2,2)$ of functions in $L_2(\mathbb{R})$ whose first and second generalized (Sobolev) derivatives lie in $L_2(\mathbb{R})$.

This problem often serves as a model example in many situations and can be solved in many ways. That is why it is natural to use the problem to demonstrate a new technique for solving the Schrödinger equation, because there will be as few as possible unstudied details specific to the problem (in contrast to [1], [2]). We will use the standard technique of C_0 semigroups [3] and (implicitly) a somewhat less known Chernoff theorem [3]–[5]. The solution of the Cauchy problem is constructed in [6], [7], and other papers in the form of the limit of a multiple integral whose multiplicity tends to infinity. Feynman was the first to use similar formulas in 1948 at the physical level of rigor, and hence such expressions are referred to as Feynman formulas [8]–[10]. Theorem 1 and the notion of Chernoff tangency (see below for the precise statements), which were obtained in [11] in 2014, permit extending the class of approximation formulas to include quasi-Feynman formulas. Both Feynman and quasi-Feynman formulas contain integrals of arbitrarily large multiplicity.

In the present note, Theorem 1 is used to obtain a new type of formula. The novelty is that the translation operator is used instead of the integral operator, so that the solution formula for the Cauchy problem (1) does not contain integrals at all.

Definition 1 ([11]). Let $\mathcal{F}$ be a Banach space, and let $\mathscr{L}(\mathcal{F})$ be the space of linear bounded operators on $\mathcal{F}$. Given a function $G\colon [0,+\infty) \to \mathscr{L}(\mathcal{F})$ (or, which is the same, a family $(G(t))_{t\geq 0}$) and a closed linear operator $L\colon \mathrm{Dom}(L) \to \mathcal{F}$ with domain $\mathrm{Dom}(L) \subset \mathcal{F}$, one says that the function G is *Chernoff tangent* to the operator L if the following conditions hold:

(CT1) The function G is strongly continuous (that is, continuous in the strong operator topology on $\mathscr{L}(\mathcal{F})$); i.e., the function $t \mapsto G(t)f \in \mathcal{F}$ is continuous on $[0,+\infty)$ for each $f \in \mathcal{F}$.

(CT2) $G(0) = I$; i.e., $G(0)f = f$ for each $f \in \mathcal{F}$.

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(CT3) There exists a dense linear manifold $\mathcal{D} \subset \mathcal{F}$ such that, for each $f \in \mathcal{D}$, the limit

$$\lim_{t\to 0} \frac{G(t)f - f}{t},$$

denoted by $G'(0)f$, exists.

(CT4) The operator $(G'(0), \mathcal{D})$ is closable, and the closure is equal to $(L, \mathrm{Dom}(L))$.

Remark 1. The family $(G(t))_{t\geq 0}$ in the definition of Chernoff tangency is not required to be a semigroup. However, each C_0 semigroup is Chernoff tangent to its own generator.

Theorem 1 (a special case of what was proved in [11]). *Let $\mathcal{F}$ be a complex Hilbert space, and let $\mathrm{Dom}(H) \subset \mathcal{F}$ be a dense linear manifold. Assume that the operator $H\colon \mathrm{Dom}(H) \to \mathcal{F}$ is linear and self-adjoint. Let S be a function Chernoff tangent to H, and let $(S(t))^* = S(t)$ for each $t \geq 0$. Set $R(t) = \exp[i(S(t) - I)]$. (This is well defined, because the exponent contains linear bounded operators on $\mathcal{F}$ for each $t \geq 0$.)*

Then the function R is Chernoff equivalent to the semigroup $(e^{itH})_{t\geq 0}$, and the following relations hold for each $f \in \mathcal{F}$, where the limits are taken in the norm on $\mathcal{F}$:

$$e^{itH} f = \lim_{n\to\infty} \lim_{k\to\infty} \sum_{m=0}^{k} \sum_{q=0}^{m} \frac{(-1)^{m-q}(in)^m}{q!(m-q)!} \left(S\left(\frac{t}{n}\right)\right)^q f, \tag{2}$$

$$e^{itH} f = \lim_{n\to\infty} \lim_{k\to\infty} \sum_{q=0}^{k} \frac{k!(k-in)^{k-q}(in)^q}{q!(k-q)!k^k} \left(S\left(\frac{t}{n}\right)\right)^q f. \tag{3}$$

Theorem 2. *Let $V\colon \mathbb{R} \to \mathbb{R}$ be a bounded measurable function. For each $f \in L_2(\mathbb{R})$, each smooth compactly supported function $\varphi\colon \mathbb{R} \to \mathbb{R}$, and all $x \in \mathbb{R}$ and $t \geq 0$, set*

$$\begin{aligned} (S(t)f)(x) &= \frac{1}{4}[f(x+\sqrt{t}) + 2f(x) + f(x-\sqrt{t})] - \arctan[tV(x)]f(x), \\ (H\varphi)(x) &= \frac{1}{4}\varphi''(x) - V(x)\varphi(x). \end{aligned} \tag{4}$$

Then

1. *$\|S(t)\| \leq 1 + \pi/2$ for each $t \geq 0$.*
2. *$S(t) = S(t)^*$ for each $t \geq 0$.*
3. *S is Chernoff tangent to H.*

Proof. Set

$$(A(t)f)(x) = f(x+\sqrt{t}), \qquad (B(t)f)(x) = f(x-\sqrt{t}), \qquad (C(t)f)(x) = \arctan(tV(x))f(x).$$

Clearly, $\|A(t)\| = \|B(t)\| = 1$ and $\|C(t)\| \leq \pi/2$. Then

$$S(t) = \frac{1}{4}[A(t) + 2I + B(t)] - C(t), \tag{5}$$

and hence the estimate

$$\|S(t)\| = \left\| \frac{[A(t) + 2I + B(t)]}{4} - C(t) \right\| \leq \frac{(1+2+1)}{4} + \frac{\pi}{2} = 1 + \frac{\pi}{2}$$

is true for each $t \geq 0$. It follows from this estimate that $S(t) \in \mathscr{L}(L_2(\mathbb{R}))$; i.e.,

$$S\colon [0, +\infty) \to \mathscr{L}(L_2(\mathbb{R})),$$

which completes the proof of item 1.

To prove item 2, it suffices to note that $A(t)^* = B(t)$, $B(t)^* = A(t)$, $I^* = I$, and $C(t)^* = C(t)$.

Now let us verify that all four conditions for Chernoff tangency hold for S and H.

(CT1) Take an $f \in L_2(\mathbb{R})$. Let us separately prove the continuity of the mappings $t \mapsto A(t)f$, $t \mapsto B(t)f$, and $t \mapsto C(t)f$.

(i) Let $t_0 \geq 0$, $t_n \geq 0$, and $t_n \to t_0$. First, note that

$$\|A(t_0)f - A(t_n)f\|^2 = \int_{\mathbb{R}} (f(x+\sqrt{t_0}) - f(x+\sqrt{t_n}))^2\,dx = \int_{\mathbb{R}} (f(y) - f(y+\sqrt{t_n}-\sqrt{t_0}))^2\,dy,$$

and hence we can assume without loss in generality that $t_0 = 0$. Further, note that $A(0)f = f$. Let an $\varepsilon > 0$ be given. Find an N such that $\|f - A(t_n)f\| < \varepsilon$ for all $n > N$. The set D of all compactly supported uniformly continuous functions is dense in $L_2(\mathbb{R})$, and hence there exists a function $g \in D$ such that $\|f - g\| < \varepsilon/3$. Then

$$\|f - A(t_n)f\| \leq \|f - g\| + \|g - A(t_n)g\| + \|A(t_n)(f-g)\| < \frac{\varepsilon}{3} + \|g - A(t_n)g\| + 1 \cdot \frac{\varepsilon}{3}.$$

Let us show that $\|g - A(t_n)g\| \leq \varepsilon/3$ for sufficiently large n. Indeed, g is compactly supported; assume that it is zero everywhere outside some interval $[-M, M]$. Since g is uniformly continuous, it follows that there exists a $\delta > 0$ such that $|g(x_1) - g(x_2)| < \varepsilon(3\sqrt{2M})^{-1}$ for $|x_1 - x_2| < \delta$. Since $t_n \to 0$, we see that there exists an N such that, for $\sqrt{t_n} < \delta$ for all $n > N$. Then the estimate

$$\|g - A(t_n)g\| = \left(\int_{\mathbb{R}} |g(x) - g(x+\sqrt{t_n})|^2\,dx\right)^{1/2} \leq \left(\int_{-M}^{M} \left(\frac{\varepsilon}{3\sqrt{2M}}\right)^2 dx\right)^{1/2} = \frac{\varepsilon}{3}$$

holds for all $n > N$. Thus, the function $t \mapsto A(t)f$ is continuous.

(ii) The continuity of the function $t \mapsto B(t)f$ can be proved in a similar way.

(iii) The maximum (over $z \in \mathbb{R}$) absolute value of the derivative of the function $z \mapsto \arctan(z)$ is equal to unity, and so $|\arctan(z_1) - \arctan(z_2)| \leq |z_1 - z_2|$. Hence

$$\|C(t_0)f - C(t_n)f\| = \left(\int_{\mathbb{R}} |\arctan(t_0 V(x)) - \arctan(t_n V(x))|^2 |f(x)|^2\,dx\right)^{1/2} \leq |t_0 - t_n| \cdot \|Vf\|.$$

Thus, the function $t \mapsto C(t)f$ is continuous. It follows from (i), (ii), and (iii) that the function $t \mapsto S(t)f$ is continuous as well (as a linear combination of continuous functions), which completes the proof of (CT1).

(CT2) is obvious from the computation

$$S(0) = \frac{A(0) + 2I + B(0)}{4} - C(0) = \frac{I + 2I + I}{4} - 0 = I.$$

We will verify (CT3) by taking the set of all compactly supported infinitely smooth functions for $\mathcal{D}$. Let f be such a function. Then we can write Taylor's formula with Lagrange remainder,

$$f(x+\sqrt{t}) = f(x) + \sqrt{t}f'(x) + \frac{1}{2}f''(x)t + \frac{1}{6}f'''(\xi_1)t\sqrt{t}, \qquad \xi_1 \in [x, x+\sqrt{t}\,]$$

$$f(x-\sqrt{t}) = f(x) - \sqrt{t}f'(x) + \frac{1}{2}f''(x)t - \frac{1}{6}f'''(\xi_2)t\sqrt{t}, \qquad \xi_2 \in [x-\sqrt{t}, x]$$

$$\frac{f(x+\sqrt{t}) + 2f(x) + f(x-\sqrt{t})}{4} = f(x) + \frac{1}{4}f''(x)t + r(t,x),$$

where $r(t,x) = (1/6)f'''(\xi_1)t\sqrt{t} - (1/6)f'''(\xi_2)t\sqrt{t} = o(t)$ in $L_2(\mathbb{R})$. Indeed, let f be zero everywhere outside $[-M, M]$, and let $\sup_{x\in[-M,M]} |f'''(x)| = K$. Then

$$\|r(t,\,\cdot\,)\| \leq \frac{2}{6}t\sqrt{t}\left(\int_{-M}^{M} K^2\,dx\right)^{1/2} = \frac{K\sqrt{2M}}{3}t^{3/2} = o(t).$$

The first derivative of the function $z \mapsto \arctan(z)$ is equal to unity at zero, and the maximum (over $z \in \mathbb{R}$) absolute value of the second derivative is less than unity (more precisely, it is equal to $3\sqrt{3}/8$), and hence

$$\arctan(tV(x)) = 0 + tV(x) + h(t,x)t^2, \qquad |h(t,x)| < \frac{1}{2} < 1,$$
$$\arctan(tV(x))f(x) = tV(x)f(x) + h(t,x)f(x)t^2, \qquad \|h(t,\,\cdot\,)f\| \le \|f\|.$$

Recall that

$$(S(t)f)(x) = \frac{1}{4}[f(x+\sqrt{t}) + 2f(x) + f(x-\sqrt{t})] - \arctan(tV(x))f(x);$$

thus, for given $f \in D$, one has

$$S(t)f = f + \frac{1}{4}f''t - Vft + o(t) = (I + tH)f + o(t)$$

in $L_2(\mathbb{R})$.

(CT4) follows from the general theory of differential operators on $L_2(\mathbb{R})$. Here the set $\mathrm{Dom}(H)$ is the Sobolev space $W(2,2)$ of functions in $L_2(\mathbb{R})$ whose first and second derivatives lie in $L_2(\mathbb{R})$. □

Theorem 3. *For each $\psi_0 \in L_2(\mathbb{R})$, the Cauchy problem* (1) *has a unique solution in $L_2(\mathbb{R})$, which almost everywhere satisfies the relations*

$$\psi(t,x) = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{m=0}^{k}\sum_{q=0}^{m}\frac{(-1)^{m-q}(in)^m}{q!\,(m-q)!}\left(S\left(\frac{t}{n}\right)\right)^q\psi_0\right)(x), \tag{6}$$

$$\psi(t,x) = \left(\lim_{n\to\infty}\lim_{k\to\infty}\sum_{q=0}^{k}\frac{k!(k-in)^{k-q}(in)^q}{q!\,(k-q)!\,k^k}\left(S\left(\frac{t}{n}\right)\right)^q\psi_0\right)(x), \tag{7}$$

where the continuous linear operator $S(t)$ is defined in (4) *and $(S(t/n))^q$ is the qth power of a linear operator.*

Proof. It suffices to apply Theorems 1 and 2 and the standard assertion on the representability of the solution of the Cauchy problem (1) in the form

$$\psi(t,x) = (e^{itH}\psi_0)(x).$$

□

Remark 2. We have shown that the solution is given by a formula of a new type. It is neither a Feynman nor a quasi-Feynman formula; the formula is somewhat like a multiple weighted infinite sum of translations of the initial condition with respect to the space variable. It is of interest to verify whether these sums can be interpreted as Riemann integral sums.

Remark 3. The function arctan can be replaced by a different smooth function g that vanishes at zero and whose first derivative is nonzero at zero. Obviously, the solution formula for the Cauchy problem will then be different. The boundedness of g and its derivative simplifies the proof, but if we drop these conditions, then the proof remains valid with some modifications.

Remark 4. By appropriately choosing the coefficients of S, one can solve equations with derivatives of arbitrary even order in a similar way.

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