Approximations to solutions of Schrödinger equation with Hamiltonian that includes variable coefficients and derivatives of arbitrary high order

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In the talk I will explain the idea of the proof of the following theorem, which was published in Potential Analysis journal in 2020, see [1,2]. The theorem provides formulas for approximations for Cauchy problem solution for the Schrödinger equation with a very general Hamiltonian. The solution-giving formula is presented in the item 7) of the theorem.

Theorem 1. Fix arbitrary $K \in \mathbb{N}$. Suppose that for $k = 0, 1, \ldots, K$ functions $a_k \colon \mathbb{R} \to \mathbb{R}$ are given. Suppose that for each $k = 1, \ldots, K$ function a_k belongs to space $C_b^{2k}(\mathbb{R})$ of all bounded functions $\mathbb{R} \to \mathbb{R}$ with bounded derivatives up to $(2k)$-th order. Suppose that function $a_0 \colon \mathbb{R} \to \mathbb{R}$ is measurable and belongs to space $L_2^{loc}(\mathbb{R})$, i.e. $\int_{-R}^{R} |a_0(x)|^2 dx < \infty$ for each real number $R > 0$. Define

$$(\mathcal{H}\varphi)(x) = a_0(x)\varphi(x) + \sum_{k=1}^{K} \frac{d^k}{dx^k}\left(a_k(x)\frac{d^k}{dx^k}\varphi(x)\right)$$

for each φ from the space $C_0^\infty(\mathbb{R})$ of all functions $\varphi \colon \mathbb{R} \to \mathbb{R}$ wich are bounded together with their derivatives of all orders and have compact support (are zero outside of some closed interval). We also use the following condition for coefficients a_k, $k = 0, 1, \ldots, K$: operator $\mathcal{H}$ defined on $C_0^\infty(\mathbb{R})$ is essentially self-adjoint in $L_2(\mathbb{R})$, i.e. the operator $(\mathcal{H}, C_0^\infty(\mathbb{R}))$ is closable and its closure — let us denote it as $(\mathcal{H}, Dom(\mathcal{H}))$ — is a self-adjoint operator.

Suppose that function $w \colon \mathbb{R} \to \mathbb{R}$ is continuous, bounded, differentiable at zero and $w(0) = 0$, $w'(0) = 1$ (examples include: $w(x) = \arctan(x)$, $w(x) = \sin(x)$, $w(x) = \tanh(x) = (e^x - e^{-x})/(e^x + e^{-x})$, etc). For each $t \geq 0$, $k = 1, 2, \ldots, K$, each $x \in \mathbb{R}$, and each $f \in L_2(\mathbb{R})$ define:

$$(B_{a_k} f)(x) = a_k(x) f(x),$$

$$(A(t)f)(x) = f(x + t), \quad (A(t)^* f)(x) = f(x - t),$$

$$F_k(t) = \left(A(t^{1/2k}) - I\right)^k B_{a_k} \left(I - A(t^{1/2k})^*\right)^k, \quad F_0(t)f(x) = w(ta_0(x))f(x),$$

$$F(t) = \sum_{k=0}^{K} F_k(t), \quad S(t) = I + F(t) = I + \sum_{k=0}^{K} F_k(t), \tag{1}$$

where I is the identity operator ($If = f$), and expression such as Z^k means the composition $ZZ \ldots Z$ of k copies of linear bounded operator Z.

Then the following holds:

1) For each $t \geq 0$ operators $A(t)$, $A(t)^*$, B_{a_k} for $k = 1, 2, \ldots, K$, $F_k(t)$ for $k = 0, 1, \ldots, K$ and $F(t)$, $S(t)$ are linear bounded operators in $L_2(\mathbb{R})$, and their norms are bounded by a constant that does not depend on t

2) S is Chernoff-tangent to $\mathcal{H}$

3) $S(t) = S(t)^*$ for each $t \geq 0$

4) For each $t \geq 0$ operator $R(t) = \exp[-iF(t)]$ is a well-defined linear operator in $L_2(\mathbb{R})$

5) There exists a C_0-group $\left(e^{-it\mathcal{H}}\right)_{t\in\mathbb{R}}$ of linear boounded unitary operators in $L_2(\mathbb{R})$

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6) R is Chernoff-equivalent to $\left(e^{-it\mathcal{H}}\right)_{t\in\mathbb{R}}$, and the following formulas hold for each $f \in L_2(\mathbb{R})$ and $t \geq 0$, where limits exist with respect to norm in $L_2(\mathbb{R})$:

$$e^{-it\mathcal{H}} = \lim_{n\to\infty} R(t/n)^n = \lim_{n\to\infty} \exp\left[-inF(t/n)\right] = \lim_{n\to\infty} \exp\left[-in\sum_{k=0}^{K} F_k(t/n)\right],$$

$$e^{-it\mathcal{H}} = \lim_{n\to\infty}\lim_{j\to+\infty}\sum_{q=0}^{j}\frac{(-in)^q}{q!}\left(\sum_{k=0}^{K}F_k(t/n)\right)^q.$$

7) For each initial condition $\psi_0 \in L_2(\mathbb{R})$ the Cauchy problem (1) can be written in the form

$$\begin{cases} \psi_t'(t) = -i\mathcal{H}\psi(t), \\ \psi(0) = \psi_0, \end{cases}$$

and has a unique (in sense of $L_2(\mathbb{R})$) solution $\psi(t)$ that depends on ψ_0 continuously with respect to norm in $L_2(\mathbb{R})$, and for all $t \geq 0$ and almoust all $x \in \mathbb{R}$ can be expressed in the form

$$\psi(t,x) = \left(e^{-it\mathcal{H}}\psi_0\right)(x) = \left(\lim_{n\to\infty}\lim_{j\to+\infty}\sum_{q=0}^{j}\frac{(-in)^q}{q!}\left(\sum_{k=0}^{K}F_k(t/n)\right)^q\psi_0\right)(x).$$

Here linear bounded operators $F_0(t),\dots,F_K(t)$ are defined above in conditions of the theorem for all $t \geq 0$ (hence $F_0(t/n),\dots,F_K(t/n)$ are defined for all $t \geq 0$ and all $n \in \mathbb{N}$), and the power q in $\left(\sum_{k=0}^{K}F_k(t/n)\right)^q$ stands for a composition of q copies of linear bounded operator $\sum_{k=0}^{K}F_k(t/n)$.

References

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