How to obtain $\exp(-itH)$ for arbitrary self-adjoint H if for each $t > 0$ you know $\exp(-tH)$ or $\exp(tH)$ or even less

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Answer to the question from the title. Consider Hilbert space $\mathcal{F}$ over the field $\mathbb{C}$ and (unbounded in interesting cases) densely defined self-adjoint operator H in $\mathcal{F}$. The main result of the talk is my formula

$$R(t) = \exp(ia(S(t) - I)) \tag{1}$$

where a is a non-zero real number and $(S(t))_{t\geq 0}$ is a family of self-adjoint bounded linear operators that is Chernoff-tangent to H. Omitting some minor details one can say that Chernoff-tangency means that

$$S(t)f = f + tHf + o(t) \text{ as } t \to +0 \tag{2}$$

for all f from $D \subset \mathcal{F}$ where D is a core of H. Then thanks to the Chernoff theorem [1] we have the following approximations that hold in the strong operator topology

$$\exp(aitH) = \lim_{n\to\infty} R(t/n)^n = \lim_{n\to\infty} \exp(ian(S(t/n) - I)) \tag{3}$$

where in the exponent there is a bounded linear operator $ian(S(t/n) - I)$ so exponent is well-defined by a power series $\exp(ian(S(t/n) - I)) = \sum_{k=0}^{\infty} \frac{(ian)^k}{k!}(S(t/n) - I)^k$. This approach was introduced in [2] with exact definitions, full proofs and comments.

For example, if $\exp(tH)$ exists and you have any explicit formula for it then you can set $a = -1$ and $S(t) = \exp(tH)$ will be Chernoff-tangent to H, so in the strong operator topology we obtain the limit expression

$$\exp(-itH) = \lim_{n\to\infty} \exp\left(-in\left(e^{\frac{t}{n}H} - I\right)\right). \tag{4}$$

Similarly, if $\exp(-tH)$ exists and you have any explicit formula for it then you can set $a = 1$ and $S(t) = \exp(-tH)$ will be Chernoff-tangent to $-H$, so in the strong operator topology we obtain the limit expression

$$\exp(-itH) = \lim_{n\to\infty} \exp\left(in\left(e^{-\frac{t}{n}H} - I\right)\right). \tag{5}$$

If e.g. $H = \Delta$ is the Laplacian then formula (4) means that we solve the heat equation $u'_t = \Delta u$ obtaining solution $u(t) = e^{t\Delta}u_0$, then mix this solution with the imaginary unit i via formula (1) and obtain the solution of the Schrödinger equation $i\psi'_t = \Delta\psi$ given by $\psi(t) = e^{-it\Delta}u_0$ where $e^{-it\Delta}$ is given by (4). This example is elementary but the formula (1) is universal and it works for all self-adjoint operators H, which can contain derivatives of arbitrary high order and variable coefficients.

What to do if $\exp(tH)$ and $\exp(-tH)$ are both not known. This situation is more difficult, but still formula (1) is helpful. The way is to find such $S(t)$ that $S(t)^* = S(t)$ and $S(t)f = f + tHf + o(t)$ or $S(t)f = f - tHf + o(t)$ as $t \to +0$ and apply formula (3). Construction of such $S(t)$ is much more simpler than constructing $\exp(tH)$ or $\exp(-tH)$ because S does not need to hold the composition property: it is ok when $S(t_1 + t_2) \neq S(t_1)S(t_2)$. Moreover, if $S_1(t)f = f + tH_1 f + o(t)$ and $S_2(t)f = f + tH_2 f + o(t)$ then $S_1(t) + S_2(t) - I$ is self-adjoint and

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Chernoff-tangent to $H_1 + H_2$. This gives a lot of freedom and allows to find representations for sulutions of rather complicated Schrödinger equations. As far as I know now (4 April 2021) this approach was used at least by V.Zh.Sakbaev, M.S.Businov, D.V.Grishin&A.V.Smirnov and can be found in the overview [1] by Ya.A.Butko. You are welcome to use it also. The only problem is that representations for $\exp(-itH)$ provided by (3) are rather lengthy.

Example 1. Solution to one-dimensional Schrödinger equation with derivatives of arbitrary high order and variable coefficients.

Theorem 1. (see in [3] with full proof) 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 $(\mathcal{H}, D(\mathcal{H}))$ — 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:

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

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

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

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

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 for each initial condition $\psi_0 \in L_2(\mathbb{R})$ the Cauchy problem

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

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 $F_0(t), \ldots, F_K(t)$ are defined above in conditions of the theorem for all $t \geq 0$ (hence $F_0(t/n), \ldots, F_K(t/n)$ 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 $\sum_{k=0}^{K} F_k(t/n)$.

Example 2. Solution to multi-dimensional Schrödinger equation with Laplacian and measurable locally square integrable potential.

Theorem 2. (see in [3] with full proof) Suppose that function $V\colon \mathbb{R}^d \to \mathbb{R}$ belongs to the space $L_2^{loc}(\mathbb{R}^d)$, i.e. V is measurable and $\int_{\|x\|\leq R} V(x)^2 dx < \infty$ for each $R > 0$, where $\|x\| = (x_1^2 + \cdots + x_d^2)^{1/2}$. Suppose that $a \in \mathbb{R}, a \neq 0$. Suppose that function $w\colon \mathbb{R} \to \mathbb{R}$ is bounded, continuous, differentiable at zero and $w(0) = 0$, $w'(0) = 1$; for example, one can take $w(x) = \sin(x)$, $w(x) = \arctan(x)$, $w(x) = \tanh(x) = (e^x - e^{-x})/(e^x + e^{-x})$ etc. Suppose that for each $j = 1, \ldots, d$ constant vector $e_j \in \mathbb{R}^d$ has 1 at position j and has 0 at other $d-1$ positions. For each function $f \in L_2(\mathbb{R}^d)$, each smooth function $\varphi\colon \mathbb{R}^d \to \mathbb{C}$ and each $x \in \mathbb{R}$, $t \geq 0$ define

$$(W(t)f)(x) = \frac{1}{2d}\sum_{j=1}^{d}\left[f\left(x + \sqrt{d}\sqrt{t}e_j\right) + f\left(x - \sqrt{d}\sqrt{t}e_j\right) - 2f(x)\right] + w(-tV(x))f(x), \quad (6)$$

$$(H\varphi)(x) = \frac{1}{2}\Delta\varphi(x) - V(x)\varphi(x).$$

Suppose also that at least one of these two conditions is satisfied:

A) if we use the symbol $C_0^\infty(\mathbb{R}^d)$ for the set of all infinitely smooth functions $\mathbb{R}^d \to \mathbb{R}$ with compact support then the closure of the operator $(H, C_0^\infty(\mathbb{R}^d))$ is a self-adjoint operator in $L_2(\mathbb{R}^d)$;

B) $V(x) \geq 0$ for all $x \in \mathbb{R}^d$.

Consider Cauchy problem for Schrödinger equation

$$\begin{cases} \psi_t'(t,x) = iaH\psi(t,x), & t \in \mathbb{R}^1, x \in \mathbb{R}^d, \\ \psi(0,x) = \psi_0(x), & x \in \mathbb{R}^d. \end{cases} \quad (7)$$

where the Hamiltonian is equal to $-aH$.

THEN for each $t \geq 0$ and $\psi_0 \in L_2(\mathbb{R}^d)$ Cauchy problem (7) have the unique (in $L_2(\mathbb{R}^d)$) solution $\psi(t,x) = \left(e^{iatH}\psi_0\right)(x)$, that continuously, with respect to norm in $L_2(\mathbb{R}^d)$, depends (for fixed t) on ψ_0. For almost all $x \in \mathbb{R}^d$ and all $t \geq 0$ this solution satisfies the formula

$$\psi(t,x) = \left(\lim_{n\to+\infty}\lim_{j\to+\infty}\sum_{k=0}^{j}\frac{(ian)^k}{k!}W(t/n)^k\psi_0\right)(x),$$

where $W(t/n)$ is obtained by substitution of t with t/n in (6), and $W(t/n)^k$ is a composition of k copies of linear bounded operator $W(t/n)$.

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References

[1] Ya. A. Butko. The Method of Chernoff Approximation. // In book: Semigroups of Operators - Theory and Applications — Springer International Publishing, 2020.

[2] I. D. Remizov. Quasi-Feynman formulas — a method of obtaining the evolution operator for the Schrödinger equation. // Journal of Functional Analysis, 270:12 (2016), 4540-4557

[3] I. D. Remizov. Formulas that represent Cauchy problem solution for momentum and position Schroödinger equation. // Potential Analysis, 52 (2020), 339-370