Splitting methods for the Schrödinger equation

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Abstract

The following text is a summary of the same-titled talk given within the frame of the seminar 'AKNUM: Seminar aus Numerik' at the Vienna University of Technology. We address time splitting methods for the Schrödinger equation. In particular, we concentrate on the Strang splitting and prove second order convergence in the case of a bounded potential and given bounds on the (iterated) commutators. In addition, we briefly describe the Split-Step Fourier method, which allows an efficient computation of the solution on an equispaced spatial grid.

1 Theoretical background

We consider the *time-dependent Schrödinger equation* (TDSE)

$$\mathrm{i}\hbar\dot{\psi} = -\frac{\hbar}{2m}\Delta\psi + V\psi, \tag{1}$$

where $\psi = \psi(x,t)$ is a wave function (state) with postulations

- $|\psi(.,t)|^2$ is a probability distribution for the particle position, i.e. $\int_\Omega |\psi(x,t)|^2\,\mathrm{d}x$ gives the probabilty that the particle is located in Ω,
- The initial state $\psi(x,t_0)$ determines later states (*Causality*),
- *Superposition*: linear combinations of states are again states.

For our mathematical considerations we consider the scaled version of (1), i.e. the scaling $x \leftarrow x\sqrt{2m/\hbar}$ leads to

Definition 1 (TDSE)**.**

$$\mathrm{i}\dot{\psi} = -\tfrac{1}{2}\Delta\psi + V\psi =: H\psi, \tag{2}$$

where V is a potential and H the Hamiltonian.

It is easily verified that the following quantities are preserved by the TDSE (2).

- **Energy is real:**

$$\langle H\psi,\psi\rangle \overset{H\ s.a.}{=} \langle\psi,H\psi\rangle = \overline{\langle H\psi,\psi\rangle} \tag{3}$$

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- **Conservation of norm:**

$$\frac{d}{dt}\|\psi\|^2 = -2Re(\mathrm{i}\underbrace{\langle H\psi,\psi\rangle}_{\in\mathbb{R}, cf.(3)}) = 0. \tag{4}$$

- **Conservation of energy:**

$$\frac{d}{dt}\langle H\psi,\psi\rangle = \langle H\psi,-\mathrm{i}H\psi\rangle + \langle -\mathrm{i}H\psi,H\psi\rangle = 0. \tag{5}$$

  This also holds for higher moments H^p.

In the following we briefly give an existence and uniqueness result for (2).
The formal solution to (2), i.e. $\dot{\psi}(t) = \mathrm{i}\frac{1}{2}\Delta\psi(t) - \mathrm{i}V\psi(t) = -\mathrm{i}H\psi(t),\ \psi(0) = \psi_0$ is written as

$$\psi(t) = e^{-\mathrm{i}tH}\psi_0. \tag{6}$$

The *notation* $e^{-\mathrm{i}tH}$ describes the flow of the differential equation and will be shown to be a **strongly continuous group of unitary operators**.
We therefore briefly recall some definitions.

Definition 2 (C_0-(semi)group)**.** *A one-parametric family $S(t)$, $t \in \mathbb{R}$ of linear operators on a Banach space X is a **group of operators on** X if*

1. $S(0) = I$,
2. $S(t+s) = S(t)S(s),\ s,t \in \mathbb{R}$.

*$S(t)$ is **strongly continuous** if*

$$\lim_{t\to 0} S(t)x = x, \tag{7}$$

for all $x \in X$, and called C_0-group.
The linear operator A definied by

$$Ax := \lim_{t\to 0}(S(t)x - x)/t \tag{8}$$

*on $D(A) := \{x \in X \mid Ax \text{ exists}\}$ is called **(infinitesimal) generator** of $S(t)$.*
*If the above holds for a family $S(t)_{t\geq 0}$ (with one-sided limits) we call it a C_0-**semigroup**.*

Within the the theory of C_0-(semi)groups the formal solution (6) can be shown to be indeed the unique solution to the TDSE (2).

Lemma 1. *[Solution of Cauchy problem] Let A be the generator of a C_0-semigroup $S(t)$ of operators on the Banach space X. Then we have*

$$S(t)x \in D(A) \ \text{ for } \ x \in D(A) \quad \text{and} \quad \frac{d}{dt}S(t)x = AS(t)x = S(t)Ax,\ t \geq 0. \tag{9}$$

Furthermore, the function $u : \mathbb{R}^+ \to X$, $t \mapsto S(t)x$ is the unique solution to the problem

$$\dot{u}(t) = Au(t),\ t \geq 0,\ u(0) = x. \tag{10}$$

Proof. See e.g. [1]. □

We recall some basic terms that occur in the following theorem. Let A be a densely defined operator on a Hilbert space $\mathbb{H}$.

Adjoint operator A^* of A: $\langle Ax, y\rangle = \langle x, A^*y\rangle$, $\forall x \in D(A), y \in D(A^*)$.

Self-adjoint operator on $\mathbb{H}$: $\quad A = A^*$.

Unitary operator on $\mathbb{H}$: $\quad AA^* = A^*A = I$.

Theorem 2. *[Stone 1930] Let $\mathbb{H}$ be a Hilbert space and $S(t)$, $t \in \mathbb{R}$ a one-parameter family of linear operators on $\mathbb{H}$.*

- *If $S(t)$ is C_0-group of unitary operators on $\mathbb{H}$, then there exists a unique self-adjoint operator A such that $S(t) = e^{-\mathrm{i}tA}$, i.e. $-\mathrm{i}A$ generates $S(t)$.*
- *Conversely, let A be a self-adjoint operator on $\mathbb{H}$. Then $S(t) := e^{-\mathrm{i}tA}$ is a C_0-group of unitary operators with generator $-\mathrm{i}A$.*

Proof. See e.g. [1]. □

Theorem 3. *[Laplace, self-adjoint] The operator $T = -\frac{1}{2}\Delta$ is self-adjoint on the Sobolev space $\mathbb{H} = \mathcal{H}^2 := \{u \in L^2 \mid$ weak derivatives up to order $2 \in L^2\}$.*[1]

Proof. See [5]. □

For a *Coulomb force potential* the corresponding Hamiltonian is self-adjoint in the Sobolev space $\mathcal{H}^2$.

Theorem 4 ($N-$electron Hamiltonian with Coulomb force potential)**.** *The $N-$electron Hamiltonian, i.e.*

$$H = \sum_{k=1}^{N}\Big(-\frac{1}{2}\Delta_k + \sum_{l\neq k}\frac{1}{|x_k - x_l|}\Big) \tag{11}$$

is self-adjoint on $\mathcal{H}^2$.

Proof. See Theorem 3, [3] and [6]. □

Hence, if the Hamiltonian H is self-adjoint in a suitable space, we imply from Stone's theorem Th. 2 that $S(t) := e^{-\mathrm{i}tH}$ is a C_0-group of unitary operators with generator $-\mathrm{i}H$. Finally, Lemma 1 shows that $S(t)\psi_0 = e^{-\mathrm{i}tH}\psi_0$ is the unique solution to the TDSE (2).

2 Time splitting methods

In the following we consider the initail value problem to (2) with the Hamiltonian $H = T + V$, i.e.

$$\mathrm{i}\dot{\psi} = H\psi,\ \psi(t_0) = \psi_0 \quad \text{with } H = T + V, \tag{12}$$

where T and V denote the kinetic energy operator and potential, respectively. We make the following notations:

- **Exact Solution:** $\psi(t_0 + h) = e^{-\mathrm{i}h(T+V)}\psi_0 \equiv \Phi(h)\psi_0$.

[1] weak derivative ∂u of u: $\langle \partial u, w\rangle = -\langle u, \partial w\rangle\ \forall w \in C_0^\infty$.

- **Numerical approximation:** $\widetilde{\psi}(t_0 + h) = \widetilde{\Phi}_{T+V}(h)\psi_0 \approx \psi(t_0 + h)$.
- **Exponential splitting:**

$$\psi(t_0 + h) \approx \widetilde{\Phi}_{T+V}(h)\psi_0 = \prod_{l=1}^{s} \Phi_V(b_l h)\Phi_T(a_l h)\psi_0 = \prod_{l=1}^{s} e^{-\mathrm{i}b_l hT} e^{-\mathrm{i}a_l hV}\psi_0. \tag{13}$$

Here, the operator product $\prod$ is defined 'downwards', i.e. $\prod_{l=1}^{s} L_l = L_s L_{s-1} \dots L_1$.
With $t_n := t_{n-1} + h, h \equiv \text{const.}$; ψ^n approximation at t_n, the *Lie-Trotter splitting* reads

$$\psi^{n+1} = e^{-\mathrm{i}hV} e^{-\mathrm{i}hT}\psi^n \quad \text{or} \ (T \rightleftharpoons V), \tag{14}$$

which is a first order method.
We will take a closer look at the so-called *Strang splitting* [Strang/Marchuk 1968], i.e.

$$\psi^{n+1} = e^{-\mathrm{i}h/2V} e^{-\mathrm{i}hT} e^{-\mathrm{i}h/2V}\psi^n \quad \text{or} \ (T \rightleftharpoons V), \tag{15}$$

where we will prove second-order convergence in the following section.
The Strang splitting has the following remarkable properties:

- **Unitary/Symplecticity:** If T and V are self-adjoint, operators $e^{-\mathrm{i}h/2V}$ and $e^{-\mathrm{i}hT}$ are unitary, i.e. norm and the symplectic two form $\omega(\zeta, \eta) = -2Im\,\langle\zeta, \eta\rangle$ is conserved.
- **Time-reversible:** Starting from ψ^{n+1} with (negative) time step $-h$ yields ψ^n.
- **Fourier collocation** can be applied.

2.1 Fourier collocation

We briefly consider the 1d TDSE with periodic boundary conditions in order to describe Fourier collocation as spatial discretization scheme [7]. In the next subsection we will combine this with the Strang splitting method. Let us assume the problem

$$\mathrm{i}\dot{\psi}(x, t) = -\tfrac{1}{2}\psi_{xx}(x, t) + V(x)\psi(x, t), \ x \in [-\pi, \pi], \quad \psi(-\pi, t) = \psi(\pi, t) \ \forall t \tag{16}$$

Spatial discretization and collocation: $x_j = \frac{2\pi j}{K}, j = -\frac{K}{2}, \dots, \frac{K}{2} - 1 =: I_K, K \in 2\mathbb{N}$,

$$\mathrm{i}\dot{\psi}(x_j, t) = -\tfrac{1}{2}\psi_{xx}(x_j, t) + V(x_j)\psi(x_j, t), \quad j \in I_K. \tag{17}$$

Discrete Fourier transform: ($\mathcal{F}_K v_k := \frac{1}{K}\sum_{k\in I_K} v_k e^{-\mathrm{i}kx}$ and $\mathcal{F}_K^{-1} v_k := \sum_{k\in I_K} v_k e^{\mathrm{i}kx}$.)

$$\psi \approx \psi(x_j, .)_{j\in I_K} =: \psi_K = \mathcal{F}_K^{-1} c_K, \ \text{where the } \textit{Fourier coefficients} \text{ are } \ c_K = \mathcal{F}_K \psi_K, \tag{18}$$

leads to

$$\mathrm{i}\dot{\psi}_K = \mathcal{F}_K^{-1} D_K \mathcal{F}_K \psi_K + V_K \psi_K, \tag{19}$$

where $D_K = \frac{1}{2}\mathrm{diag}(k^2)_{k\in I_K}$, $V_K = \mathrm{diag} V(x_k)_{k\in I_K}$ and $c_K = (c_k)_{k\in I_K}$, $\psi_K = \psi(x_j, .)_{j\in I_K}$.

2.2 Split-Step Fourier scheme

Combination of Fourier collocation and time splitting leads us to quasi-optimal method. We recall:
Time splitting:

$$\psi^{n+1} = e^{-\mathrm{i}h/2V} e^{-\mathrm{i}hT} e^{-\mathrm{i}h/2V} \psi^n. \tag{20}$$

Fourier collocation (spatial):

$$\mathrm{i}\dot{\psi}_K = \underbrace{\mathcal{F}_K^{-1} D_K \mathcal{F}_K}_{\equiv T_k} \psi_K + V_K \psi_K \tag{21}$$

leads to

$$\psi_K^{n+1} = e^{-\mathrm{i}h/2V_K} \mathcal{F}_K^{-1} e^{-\mathrm{i}hD_K} \mathcal{F}_K e^{-\mathrm{i}h/2V_K} \psi_K^n, \tag{22}$$

where *discrete Fourier transforms* $\mathcal{F}_K$ and $\mathcal{F}_K^{-1}$ are usually realized by *Fast Fourier transforms* (FFTs) [complexity: $K \log K$].

Remark.
- *There exists L^2 error bound for Fourier collocation (depends on spatial regularity of exact solution, i.e. $\partial_x^{s+2}\psi(.,t) \in L^2$, $s \geq 1$), see e.g. [4] and refs therein.*
- *Error bound for the Strang splitting will be proven in the following (also depends on the spatial regularity of ψ!).*

3 Error bound for the Strang Splitting

For *bounded* T and V, *Taylor expansion* of exponentials gives

$$\left\| e^{-\mathrm{i}h/2V} e^{-\mathrm{i}hT} e^{-\mathrm{i}h/2V} - e^{-\mathrm{i}h(T+V)} \right\| = O(h^3(\|T\| + \|V\|)^3). \tag{23}$$

Since $\|T\| \sim 1/\Delta x^2$ (discrete Laplace), this would lead to the *restriction* $h \ll \Delta x^2$. On the other hand, numerical experiments show that the error of *Strang splitting* is independed of Δx if the initial data are moderately bounded. Indeed, for smooth potential and initial data numerics show an error of $O(h^3)$ uniformly in Δx after one step, and $O(t_n h^2)$ uniformly in Δx at time $t_n := nh$. In the following we will prove this behaviour, cf. [2].
We will make the following assumptions:

- T and V are self-adjoint on the Hilbert space $\mathcal{H}$ and T is positive semi-definite.
- We require no bound for T.
- V is bounded, i.e.

$$\|V\varphi\| \leq \beta \|\varphi\| \quad \forall \varphi \in \mathcal{H}. \tag{24}$$

- Commutator bounds: ($[T, V] = TV - VT$)

$$\|[T, V]\varphi\| \leq c_1 \|\varphi\|_1 , \tag{25}$$

$$\|[T, [T, V]]\varphi\| \leq c_2 \|\varphi\|_2 , \tag{26}$$

$\forall \varphi \in D \subset \mathcal{H}$ dense and where $\|\varphi\|_p = \langle (T + I)^p \varphi, \varphi \rangle^{1/2}$ (usual Sobolev norm if $T = -\Delta$).

Remark. *If $T = -\Delta$ and $V(x)$ has bounded $1^{st}-$ to $4^{th}-$derivatives, then both commutator bounds are valid.*
If spatial descretization by the Fourier method is considered, then the constants c_1, c_2 are independent of Δx [2].

We will prove the following theorem.

Theorem 5 (Error Bound for Strang Splitting (Jahnke & Lubich, 2000))**.** *Under the above conditions, the error of the Strang splitting method at time $t_n = hn$ is bounded by*

$$\left\|\psi^n - \psi(t_n)\right\| \leq Ch^2 t_n \max_{0\leq\tau\leq t_n} \|\psi(\tau)\|_2 \,, \tag{27}$$

where C depends only on β and c_1, c_2.

The proof will be done by investigation of the **local error** and the **error propagation**, i.e.

$$\psi^n - \psi(t_n) = S^n\psi^0 - E^n\psi^0 \overset{\text{telescoping sum}}{=} \sum_{j=0}^{n-1} S^{n-j-1}(S-E)E^j\psi^0, \tag{28}$$

with $S = e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}$ and $E = e^{-\mathrm{i}h(T+V)}$.

We, therefore, only need a bound for the local error, i.e. the error after one step: $\|S\psi - E\psi\|$, which yields the result immediately by exploiting formula (28) and the unitarity of the C_0-semigroups.

Lemma 6. *[Local Error]*

(1) Under the conditions

$$\|V\varphi\| \leq \beta\,\|\varphi\| \quad \forall\varphi \in \mathcal{H}. \tag{29}$$

and

$$\|[T,V]\varphi\| \leq c_1\,\|\varphi\|_1 \quad \forall\varphi \in D_1 \subset \mathcal{H} \text{ dense}, \tag{30}$$

there holds

$$\left\|e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}\varphi - e^{-\mathrm{i}h(T+V)\varphi}\right\| \leq C_1h^2\,\|\varphi\|_1 \,, \tag{31}$$

where C_1 depends only on c_1 and β.

(2) Under the conditions in (1) and additionally

$$\|[T,[T,V]]\varphi\| \leq c_2\,\|\varphi\|_2 \quad \forall\varphi \in D_2 \subset \mathcal{H} \text{ dense}, \tag{32}$$

there holds

$$\left\|e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}\varphi - e^{-\mathrm{i}h(T+V)\varphi}\right\| \leq C_2h^3\,\|\varphi\|_2 \,, \tag{33}$$

where C_1 depends only on c_1, c_2 and β.

The main idea for the prove of Lemma 6 is as follows:
We employ the variation-of-constant formula for $e^{-\mathrm{i}h(T+V)}$ and Taylor expansion of $e^{-\mathrm{i}h/2V}$ in $e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}$. The latter one leads to the *trapezoidal rule* for the integral in the variation-of-constant formula. This allows us using *quadrature error bounds* (Peano kernel theorem) and *commutator bounds*.

We, therefore, give a brief introduction into *error analysis for quadrature rules*.

3.1 Error Analysis for quadrature rules

Suppose we have a *quadrature rule* (e.g. *Newton-Côtes formula*)

$$\int_a^b f(x)\,\mathrm{d}x \approx I(f) := \sum_{j=0}^{m} w_j f(x_j), \tag{34}$$

with distinct nodes $(x_j)_{j=0}^m \subset [a,b]$ and weights $(w_j)_{j=0}^m$.
We define the *quadrature error*:

$$E(f) := I(f) - \int_a^b f(x)\,\mathrm{d}x. \tag{35}$$

Assume that the quadrature rule I *integrates polynomials of degree n or less exactly*, i.e.

$$I(p) = \int_a^b p(x)\,\mathrm{d}x, \quad p \in \mathcal{P}_n, \tag{36}$$

and $f \in C^{n+1}[a,b]$.
Taylor expansion of the integrad leads to

$$f(x) = \underbrace{\sum_{k=0}^{n} \frac{1}{k!} f^{(k)}(a)(x-a)^k}_{=:p_n} + \underbrace{\frac{1}{n!}\int_a^x f^{(n+1)}(t)(x-t)^n\,\mathrm{d}t}_{=:r_n}. \tag{37}$$

Due to the fact that I is *exact of degree n*, we can write the error as

$$E(f) = E(r_n) = I(r_n) - \frac{1}{n!}\int_a^b \int_a^x f^{(n+1)}(t)(x-t)^n\,\mathrm{d}t\mathrm{d}x \tag{38}$$

$$\ldots = \frac{1}{n!}\int_a^b f^{(n+1)}(t)\underbrace{\Big(\sum_{j=0}^{m} w_j (x_j - t)_+^n - \int_a^b (x-t)_+^n\,\mathrm{d}x\Big)}_{=E\left((x-t)_+^n\right)=:K(t)}\,\mathrm{d}t, \tag{39}$$

with the *truncated power function* $(x-t)_+^n = \begin{cases} (x-t)^n, & t \le x \\ 0 & t > x \end{cases}$.

Theorem 7. *[Peano kernel theorem] Let $f \in C^{n+1}[a,b]$ and $I(f) = \sum_{j=0}^m w_j f(x_j)$ a quadrature rule that is exact of degree n. Then*

$$E(f) = \frac{1}{n!}\int_a^b f^{(n+1)}(t)K(t)dt, \tag{40}$$

with Peano kernel $K(t) = E\big((x-t)_+^n\big)$. □

Example (trapezoidal rule ($n = 1$) on $[0,h]$):

$$I_T(f) = \frac{h}{2}(f(h) + f(0)), \quad K(t) = \frac{1}{2}t(h-t).$$

$$E_T(f) = \frac{1}{2}\int_0^h f''(t)t(h-t)\,\mathrm{d}t = |t = \theta h|$$

$$= \frac{1}{2}h^3 \int_0^1 f''(\theta h)\theta(1-\theta)\,\mathrm{d}\theta \overset{\text{part. int.}}{=} -\frac{1}{2}h^2 \int_0^1 f'(\theta h)(1-2\theta)\,\mathrm{d}\theta. \tag{41}$$

3.2 Variation-of-constant formula

We start from the TDSE with $-\mathrm{i}V\varphi$ as inhomogeneity, i.e.

$$\dot{\psi} = -\mathrm{i}(T+V)\psi \;\rightarrow \dot{\psi} + \mathrm{i}T\psi = -\mathrm{i}V\psi \;\rightarrow e^{\mathrm{i}sT}(\dot{\psi} + \mathrm{i}T\psi) = -\mathrm{i}e^{\mathrm{i}sT}V\psi. \tag{42}$$

Writing the LHS as derivative (which is o.k. for C_0-groups), i.e.

$$e^{\mathrm{i}sT}(\dot{\psi} + \mathrm{i}T\psi) = \frac{\mathrm{d}}{\mathrm{d}s}(e^{\mathrm{i}sT}\psi) \stackrel{!}{=} -\mathrm{i}e^{\mathrm{i}sT}V\psi. \tag{43}$$

and integration over $[0,h]$ (which is o.k. for C_0-groups) and inserting the exact solution $\psi = e^{-\mathrm{i}t(T+V)}\varphi$ in the remaining integral yields

$$e^{-\mathrm{i}h(T+V)}\varphi = e^{-\mathrm{i}hT}\varphi - \mathrm{i}\int_0^h e^{-\mathrm{i}sT}Ve^{-\mathrm{i}(h-s)(T+V)}\varphi\,\mathrm{d}s. \tag{44}$$

3.3 Proof of Lemma 6

We start with proving the first bound, i.e.

$$\left\|e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}\varphi - e^{-\mathrm{i}h(T+V)\varphi}\right\| \leq C_1h^2\left\|\varphi\right\|_1. \tag{45}$$

We first apply two-times the variation-of-constants formula (44), which gives

$$e^{-\mathrm{i}h(T+V)}\varphi = e^{-\mathrm{i}hT}\varphi - \mathrm{i}\int_0^h e^{-\mathrm{i}sT}Ve^{-\mathrm{i}(h-s)(T+V)}\varphi\,\mathrm{d}s \tag{46}$$

$$= e^{-\mathrm{i}hT}\varphi - \mathrm{i}\int_0^h e^{-\mathrm{i}sT}Ve^{-\mathrm{i}(h-s)T}\varphi\,\mathrm{d}s + R_1\varphi, \tag{47}$$

where the remainder is

$$R_1 = -\int_0^h e^{-\mathrm{i}sT}V\int_0^{h-s} e^{-\mathrm{i}\sigma T}Ve^{-\mathrm{i}(h-s-\sigma)(T+V)}\,\mathrm{d}\sigma\,\mathrm{d}s, \tag{48}$$

which is bounded in the operator norm by $\|R_1\| \leq 1/2h^2\beta^2$. Here we used $\|V\varphi\| \leq \beta\|\varphi\|$ and the unitarity of the semigroups.

On the other hand, using the *exponential series* for $e^{-\mathrm{i}h/2V}$, i.e.

$$e^{-\mathrm{i}h/2V} = I - \mathrm{i}\tfrac{h}{2}V - \tfrac{h^2}{8}V^2 + O(h^3), \tag{49}$$

leads to

$$e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}\varphi = e^{-\mathrm{i}hT}\varphi - \mathrm{i}\tfrac{h}{2}(Ve^{-\mathrm{i}hT} + e^{-\mathrm{i}hT}V)\varphi + R_2\varphi, \tag{50}$$

with remainder

$$R_2 = -\tfrac{h^2}{8}(V^2e^{-\mathrm{i}hT} + 2Ve^{-\mathrm{i}hT}V + e^{-\mathrm{i}hT}V^2) + O(h^3), \tag{51}$$

which is again bounded in the operator norm by $\|R_2\| \leq 1/2h^2\beta^2$.

One observes:

$$-\mathrm{i}\int_0^h e^{-\mathrm{i}sT}Ve^{-\mathrm{i}(h-s)T}\varphi\,\mathrm{d}s \approx -\mathrm{i}\tfrac{h}{2}(Ve^{-\mathrm{i}hT} + e^{-\mathrm{i}hT}V)\varphi, \tag{52}$$

and, hence with $f(s) := -\mathrm{i}e^{-\mathrm{i}sT}Ve^{-\mathrm{i}(h-s)T}\varphi$, we have

$$\int_0^h f(s)\,\mathrm{d}s \overset{\text{trap. rule}}{\approx} \tfrac{h}{2}(f(0)+f(h)). \tag{53}$$

The error is of the form

$$e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}\varphi - e^{-\mathrm{i}h(T+V)} = r + d, \tag{54}$$

with $r = R_2\varphi - R_1\varphi$ ($\|r\| \le h^2\beta^2\,\|\varphi\| \le h^2\beta^2\,\|\varphi\|_1$) and by exploiting the *Peano kernel theorem* 7, we get

$$d \overset{\text{Peano kernel}}{=} -\frac{1}{2}h^2\int_0^1 f'(\theta h)(1-2\theta)\,\mathrm{d}\theta, \tag{55}$$

with $f'(s) = -e^{-\mathrm{i}sT}[T,V]e^{-\mathrm{i}(h-s)T}\varphi$.

Finally the bound on the commutator yields

$$\|r+d\| \le h^2\beta^2\,\|\varphi\|_1 + \frac{h^2}{2}c_1\,\|\varphi\|_1 = h^2C_1(\beta,c_1)\,\|\varphi\|_1\,, \tag{56}$$

which concludes the proof for (1). □

We next prove the second bound, i.e.

$$\left\|e^{-\mathrm{i}h/2V}e^{-\mathrm{i}hT}e^{-\mathrm{i}h/2V}\varphi - e^{-\mathrm{i}h(T+V)\varphi}\right\| \le C_2h^3\,\|\varphi\|_2\,. \tag{57}$$

We use the second Peano kernel form for the trapezoidal rule, i.e.

$$d \overset{\text{Peano kernel}}{=} \frac{1}{2}h^3\int_0^1 f''(\theta h)\theta(1-\theta)\,\mathrm{d}\theta, \tag{58}$$

with $f''(s) = \mathrm{i}e^{-\mathrm{i}sT}[T,[T,V]]e^{-\mathrm{i}(h-s)T}\varphi$.

The bound for iterated commutator immediately yields

$$\|d\| \le \tfrac{1}{12}h^3c_2\,\|\varphi\|_2\,. \tag{59}$$

It remains to derive a $O(h^3)$−bound for $r = R_2\varphi - R_1\varphi$.

In order to estimate $r = R_2\varphi - R_1\varphi$ we agian use the variation-of-constants formula for R_1 and expansion for R_2 up to order 3, i.e.

$$R_1 = -\int_0^h e^{-\mathrm{i}sT}V\int_0^{h-s} e^{-\mathrm{i}\sigma T}Ve^{-\mathrm{i}(h-s-\sigma)T}\,\mathrm{d}\sigma\,\mathrm{d}s + \widetilde{R}_1, \tag{60}$$

where $\left\|\widetilde{R}_1\right\| \le Ch^3\beta^3$ (similar as before), and

$$R_2 = -\tfrac{h^2}{8}(V^2e^{-\mathrm{i}hT} + 2Ve^{-\mathrm{i}hT}V + e^{-\mathrm{i}hT}V^2) + \widetilde{R}_2, \tag{61}$$

where also $\left\|\widetilde{R}_2\right\| \le Ch^3\beta^3$. We again get $r = \widetilde{r} + \widetilde{d}$, where

$$\widetilde{r} = (\widetilde{R}_2 - \widetilde{R}_1)\varphi, \tag{62}$$

which is bounded by $Ch^3\beta^3\,\|\varphi\|$, and $\widetilde{d}$ is again a quadrature error.

Indeed, by defining $g(s,\sigma) := -e^{-\mathrm{i}sT} V \int_0^{h-s} e^{-\mathrm{i}\sigma T} V e^{-\mathrm{i}(h-s-\sigma)T}$, one gets

$$\widetilde{d} = \tfrac{1}{8}h^2(g(0,0) + 2g(0,h) + g(h,0)) - \int_0^h \int_0^{h-s} g(s,\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s, \tag{63}$$

which is the *error of a quadrature formula* that integrates constants over the triangle $\Delta_h := \{(s,t) \in [0,h]^2 \mid 0 \le s+t \le h\}$ exactly.

Thus, the Peano kernel (for $n = 0$), i.e. $K(t_1,t_2) = E((s-t_1)_+ + (\sigma - t_2)_+)$ with max −value $\sim h$ and the integration area $\sim h^2$ yield the estimate

$$\left\|\widetilde{d}\right\| \le \max_{\Delta_h} (\,\|\partial_s g\| + \|\partial_\sigma g\|\,) \int_{\Delta_h} K(t_1,t_2) \le \widetilde{c}h^3 \max_{\Delta_h} (\,\|\partial_s g\| + \|\partial_\sigma g\|\,). \tag{64}$$

The derivatives of g can be estimated by the commutator bound, i.e.

$$\|\partial_s g\| \le (c_1(c_1+\beta) + \beta c_1)\,\|\varphi\|_1 \tag{65}$$

$$\|\partial_\sigma g\| \le \beta c_1\,\|\varphi\|_2\,, \tag{66}$$

and thus

$$\left\|\widetilde{d}\right\| \le Ch^3\,\|\varphi\|_1\,. \tag{67}$$

Together with the $O(h^3)$−bounds for d and $\widetilde{r}$, this gives

$$\|r + d\| \le h^3 C_2(\beta, c_1, c_2)\,\|\varphi\|_2\,, \tag{68}$$

which concludes the proof for bound (2). □

Remark. *Higher order methods can be derived by composition of a basic method, e.g.*
Basic method:

$$S(h) = e^{-\mathrm{i}h/2V} e^{-\mathrm{i}hT} e^{-\mathrm{i}h/2V}. \tag{69}$$

Composition:

$$\psi^{n+1} = S(\gamma_s h)\ldots S(\gamma_1 h)\,\psi^n, \tag{70}$$

where the coefficients $\gamma_j = \gamma_{s-j}$ are symmetrical and determined such that the order is $p > 2$, i.e.

$$S(\gamma_s h)\ldots S(\gamma_1 h) - e^{-\mathrm{i}h(T+V)} = O(h^{p+1}). \tag{71}$$

Order p error bounds were proven by Thalhammer [8] for p− fold repeated commutator bounds, $T = -\Delta$ and smooth potential.

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