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ERROR BOUNDS FOR EXPONENTIAL OPERATOR SPLITTINGS *

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Abstract.

Error bounds for the Strang splitting in the presence of unbounded operators are derived in a general setting and are applied to evolutionary Schrödinger equations and their pseudo-spectral space discretization.

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1 Introduction.

In partial differential equations of quantum mechanics and many other areas, a widely used approach to numerically solving the linear initial value problem

$$u' = (A+B)u, \quad u(0) = u_0, \tag{1.1}$$

is the symmetric operator splitting, known as Strang splitting (after [11]) or symmetric Trotter splitting,

$$u_{n+1} = e^{\frac{1}{2}\tau B} e^{\tau A} e^{\frac{1}{2}\tau B} u_n, \tag{1.2}$$

which determines recursively approximations u_n to $u(n\tau)$. Convergence of this approximation is known under very weak conditions from the Trotter product formula [12], which gives, however, no estimate for the speed of convergence. For bounded A and B, second-order error bounds follow easily by using the exponential series, but they depend on the norms of A and B. The question of error bounds in the case of unbounded A and/or B has recently received attention in various settings; see [1]–[10] and further references therein.

In the present paper we derive error bounds based on commutator bounds. Our results are apparently the first results showing second-order convergence in the case of an unbounded operator, under rather mild or even no regularity conditions on the initial data. The proof is rather simple but uses arguments

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different from those in the literature. A basic observation is that the principal error terms are just quadrature errors. In Section 2 we derive the error bounds in an abstract framework. Theorem 2.1 is concerned with A generating a strongly continuous semigroup and with bounded B. The estimates in Theorem 2.1 require higher regularity of the initial data. Theorem 2.2 deals with A generating an analytic semigroup and with bounded B. It gives a second-order error bound in the operator norm. Theorem 2.3 gives an error bound of order 3/2 in the operator norm in a situation where both A and B are unbounded, but $B(-A)^{-1/2}$ is bounded. In Section 3 the abstract error bounds are applied to a Schrödinger equation and its pseudo-spectral semi-discretization. Their asymptotic sharpness is illustrated by numerical experiments.

2 General error bounds.

In this section we consider the error of the Strang splitting for the abstract evolution equation (1.1) on a Banach space X with norm and induced operator norm denoted by $\|\cdot\|$. We assume that A is the generator of a strongly continuous semigroup e^{tA} on X, and B is a bounded linear operator on X. Possibly after a rescaling $u(t) \to e^{(\lambda+\mu)t}u(t)$ with associated shifts $A \to A + \lambda I$, $B \to B + \mu I$ and the choice of a suitable equivalent norm on X, we may assume

$$\|e^{tA}\| \leq 1, \qquad \|e^{tB}\| \leq 1, \qquad \|e^{t(A+B)}\| \leq 1 \quad (t \geq 0),$$

and the fractional power operators $(-A)^\gamma$ are well-defined for arbitrary positive γ, with $\|v\| \leq \|(-A)^\gamma v\|$ for all v. The phrase "for all v" means here and in the following: for all v in an appropriate dense domain, in the present case the domain of $(-A)^\gamma$. We may equally assume $\|v\| \leq \|(A+B)v\|$ for all v. These assumptions are made throughout this section, except for the boundedness of B, which is replaced by bounds of $B(-A)^{-1/2}$ in Theorem 2.3.

Our main assumptions concern the commutator $[A, B] = AB - BA$ and the repeated commutator $[A, [A, B]] = A^2B - 2ABA + BA^2$. We assume that there are non-negative α or β with

$$\|\,[A, B]\,v\| \leq c_1\,\|(-A)^\alpha v\| \qquad \text{for all } v, \tag{2.1}$$

$$\|\,[A, [A, B]]\,v\| \leq c_2\,\|(-A)^\beta v\| \qquad \text{for all } v. \tag{2.2}$$

Under these conditions, the following bounds hold for the local error of the Strang splitting for (1.1).

THEOREM 2.1. (a) *Under condition* (2.1) *with* $\alpha \geq 0$,

$$\left\|e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B}v - e^{\tau(A+B)}v\right\| \leq C_1\,\tau^2\,\|(-A)^\alpha v\| \tag{2.3}$$

for all v. *Here* C_1 *depends only on* c_1 *and* $\|B\|$.

(b) *Under conditions* (2.1) *and* (2.2) *with* $\beta \geq 1 \geq \alpha$,

$$\left\|e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B}v - e^{\tau(A+B)}v\right\| \leq C_2\,\tau^3\,\|(-A)^\beta v\| \tag{2.4}$$

for all v. Here C_2 depends only on c_1, c_2 and $\|B\|$.

PROOF. (a) We start from the variation-of-constants formula

$$e^{\tau(A+B)}v = e^{\tau A}v + \int_0^\tau e^{sA}Be^{(\tau-s)(A+B)}v\,ds.$$

Expressing the last term under the integral once more by the same formula yields

$$e^{\tau(A+B)}v = e^{\tau A}v + \int_0^\tau e^{sA}Be^{(\tau-s)A}v\,ds + R_1v,$$

where

$$R_1 = \int_0^\tau e^{sA}B\int_0^{\tau-s} e^{\sigma A}Be^{(\tau-s-\sigma)(A+B)}\,d\sigma\,ds,$$

which is bounded by $\|R_1\| \le \frac{1}{2}\tau^2\|B\|^2$. On the other hand, using the exponential series for $e^{\frac{1}{2}\tau B}$ leads to

$$e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B}v = e^{\tau A}v + \tfrac{1}{2}\tau\big(Be^{\tau A} + e^{\tau A}B\big) + R_2v,$$

where $\|R_2\| \le \frac{1}{2}\tau^2\|B\|^2$. Consequently, the error is of the form

$$e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B}v - e^{\tau(A+B)}v = d + r, \tag{2.5}$$

where $r = R_2v - R_1v$ and, with $f(s) = e^{sA}Be^{(\tau-s)A}v$,

$$\begin{aligned} d &= \tfrac{1}{2}\tau\big(f(0) + f(\tau)\big) - \int_0^\tau f(s)\,ds \\ &= -\tau^2\int_0^1 (\tfrac{1}{2} - \theta)\,f'(\theta\tau)\,d\theta = \tfrac{1}{2}\tau^3\int_0^1 \theta(1-\theta)f''(\theta\tau)\,d\theta \end{aligned} \tag{2.6}$$

is the error of the trapezoidal rule, written in first- and second-order Peano form. Since $f'(s) = e^{sA}[A,B]e^{(\tau-s)A}v$, condition (2.1) yields the error bound (2.3).

(b) For the error bound (2.4), we use $f''(s) = e^{sA}[A,[A,B]]e^{(\tau-s)A}v$ and condition (2.2) to bound

$$\|d\| \le \tfrac{1}{12}\,c_2\tau^3\,\|(-A)^\beta v\|. \tag{2.7}$$

It remains to study $r = R_2v - R_1v$. We have

$$R_1 = \int_0^\tau e^{sA}B\int_0^{\tau-s} e^{\sigma A}Be^{(\tau-s-\sigma)A}\,d\sigma\,ds + \widetilde{R}_1$$

with $\|\widetilde{R}_1\| \le C\tau^3\|B\|^3$, and

$$R_2 = \tfrac{1}{8}\,\tau^2\,\left(B^2e^{\tau A} + 2Be^{\tau A}B + e^{\tau A}B^2\right) + \widetilde{R}_2$$

with $\|\widetilde{R}_2\| \le C\tau^3 \|B\|^3$. We thus obtain

$$r = \widetilde{d} + \widetilde{r}, \tag{2.8}$$

where $\widetilde{r} = \widetilde{R}_2 v - \widetilde{R}_1 v$ is bounded by $\|\widetilde{r}\| \le C\tau^3\, \|B\|^3\, \|v\|$ and, with $g(s,\sigma) = e^{sA} B e^{\sigma A} B e^{(\tau-s-\sigma)A} v$,

$$\widetilde{d} = \tfrac{1}{8}\,\tau^2 \bigl(g(0,0) + 2g(0,\tau) + g(\tau,0)\bigr) - \int_0^\tau \int_0^{\tau-s} g(s,\sigma)\, d\sigma\, ds$$

is the error of a quadrature formula that integrates constant functions exactly. Hence,

$$\|\widetilde{d}\| \le \widetilde{c}\,\tau^3 \left(\max \left\| \frac{\partial g}{\partial s} \right\| + \max \left\| \frac{\partial g}{\partial \sigma} \right\| \right),$$

where the maxima are taken over the triangle $0 \le s \le \tau$, $0 \le \sigma \le \tau - s$. Since

$$\frac{\partial g}{\partial s}(s,\sigma) = e^{sA}[A,B] e^{\sigma A} B e^{(\tau-s-\sigma)A} v + e^{sA} B e^{\sigma A} [A,B] e^{(\tau-s-\sigma)A} v,$$

we obtain, using (2.1) with $\alpha = 1$,

$$\left\| \frac{\partial g}{\partial s} \right\| \le c_1\,(c_1 + \|B\|)\, \|Av\| + \|B\|\, c_1\, \|Av\|.$$

Similarly, $\|\partial g/\partial \sigma\| \le \|B\|\, c_1\, \|Av\|$, so that finally

$$\|\widetilde{d}\| \le C\tau^3\, \|Av\|.$$

Together with the above bounds for $\widetilde{r}$ and d this yields the error bound (2.4). $\square$

REMARK. In Theorem 2.1 (b), the condition $\beta \ge 1 \ge \alpha$ can be replaced by $\beta \ge \alpha$ and $\|\,[(-A)^\alpha, B]\, v\| \le c_1\, \|(-A)^\beta v\|$ for all v.

The local error bounds (2.3) and (2.4) together with the formula

$$u_n - u(n\tau) = S^n u_0 - T^n u_0 = \sum_{j=0}^{n-1} S^{n-j-1} (S-T)\, T^j u_0, \tag{2.9}$$

with $S = e^{\frac{1}{2}\tau B} e^{\tau A} e^{\frac{1}{2}\tau B}$ and $T = e^{\tau(A+B)}$, immediately yield the following global error bounds for the Strang splitting (1.2) at $t = n\tau$ $(n \ge 0)$:

$$\|u_n - u(t)\| \le \tau \cdot C_1\, t \max_{0\le s\le t} \|(-A)^\alpha u(s)\|, \tag{2.10}$$

$$\|u_n - u(t)\| \le \tau^2 \cdot C_2\, t \max_{0\le s\le t} \|(-A)^\beta u(s)\| \tag{2.11}$$

in cases (a) and (b) of Theorem 2.1, respectively. If A generates an analytic semigroup, then stronger estimates hold which require only bounds of the norm $\|u_0\|$ of the initial data. In that case we have the operator bounds

$$\|Ae^{tA}\| \le \kappa/t, \qquad \|(A+B)e^{t(A+B)}\| \le \kappa/t \quad (t > 0). \tag{2.12}$$

THEOREM 2.2. *Assume that A generates an analytic semigroup. Under conditions* (2.1) *and* (2.2) *with $\alpha \le \beta = 1$, the error of the Strang splitting is bounded by*

$$\|u_n - u(n\tau)\| \le C\,\tau^2 \log n\,\|u_0\| \qquad (n \ge 2). \tag{2.13}$$

The constant C depends only on c_1, c_2, $\|B\|$ and κ of (2.12).

PROOF. The proof proceeds by estimating the terms in (2.9). By Theorem 2.1 with $\beta = 1$ and by (2.12), the following bounds hold for $j \ge 1$:

$$\begin{aligned} &\|(S-T)\,T^j u_0\| \le C_2\tau^3 \left\|Ae^{j\tau(A+B)}u_0\right\| \\ (2.14)\qquad &\le C_2\tau^3 \left\|(A+B)e^{j\tau(A+B)}u_0\right\| + C_2\tau^3\|B\|\cdot\left\|e^{j\tau(A+B)}u_0\right\| \\ &\le C_2\tau^3\,(1+\|B\|)\left\|(A+B)e^{j\tau(A+B)}u_0\right\| \le C_2(1+\|B\|)\,\frac{\kappa\tau^2}{j}\,\|u_0\|. \end{aligned}$$

The term for $j = 0$ is estimated using the arguments in the proof of Theorem 2.1 together with (2.12). This gives in particular (for $v = u_0$)

$$\|d\| \le \tfrac{1}{2}\tau^3 \int_0^1 \theta(1-\theta)\,c_2\left\|Ae^{(1-\theta)\tau A}u_0\right\| d\theta \le \tfrac{1}{4}\tau^2\,c_2\kappa\,\|u_0\|,$$

so that

$$\left\|e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B}u_0 - e^{\tau(A+B)}u_0\right\| \le C\tau^2\|u_0\|. \tag{2.15}$$

The bounds (2.14) and (2.15) inserted into (2.9) yield the result. □

The boundedness of B is not essential for the arguments in the proofs of Theorems 2.1 and 2.2. It does not enter into the estimate for d, and r can be estimated also under weaker assumptions on B. As an example we consider a situation that applies to convection-diffusion equations with smooth coefficients. We assume

$$\begin{aligned} \|(-A)^{(k-1)/2}Bv\| &\le K\,\|(-A)^{k/2}v\|, &&\text{for all } v, \\ \|(-A)^{k/2}e^{tB}v\| &\le M\,\|(-A)^{k/2}v\|, && k = 0,1,2,3. \end{aligned} \tag{2.16}$$

THEOREM 2.3. *Assume that A generates an analytic semigroup. Under condition* (2.16) *and the commutator bounds* (2.1) *and* (2.2) *with $\alpha = 1$ and $\beta = \frac{3}{2}$, the error of the Strang splitting is bounded by*

$$\|u_n - u(n\tau)\| \le C\tau^{3/2}\,\|u_0\| \quad (n \ge 1). \tag{2.17}$$

The constant C depends only on c_1, c_2, K, M, and on κ_γ with $\gamma = \frac{1}{2}, 1, \frac{3}{2}$ in (2.18) *below.*

PROOF. The proof follows the lines of the previous proofs. As in the proof of Theorem 2.1 and of (2.15), and via a careful estimation of the remainder terms using (2.16) and the bounds

$$\|(-A)^\gamma e^{tA}\| \le \kappa_\gamma t^{-\gamma}, \qquad \|(-A)^\gamma e^{t(A+B)}\| \le \kappa_\gamma t^{-\gamma} \quad (t > 0) \tag{2.18}$$

for $\gamma > 0$ (used with $\gamma = \frac{1}{2}, 1, \frac{3}{2}$), one obtains the local error bounds

$$\|e^{\frac{1}{2}\tau B} e^{\tau A} e^{\frac{1}{2}\tau B} v - e^{\tau(A+B)} v\| \le \begin{cases} C\tau^3 \, \|(-A)^{3/2} v\|, \\ C\tau^{3/2} \, \|v\|. \end{cases} \tag{2.19}$$

The result then follows as in the proof of Theorem 2.2, using (2.18) with $\gamma = \frac{3}{2}$. □

3 Application to a Schrödinger equation and its semi-discretization.

We consider the Schrödinger equation

$$i \frac{\partial u}{\partial t} = -\Delta u + Vu \tag{3.1}$$

and its parabolic counterpart, the imaginary-time Schrödinger equation

$$\frac{\partial u}{\partial t} = \Delta u - Vu \tag{3.2}$$

with the Laplacian Δ on $(-\pi, \pi)^m$ and a smooth potential $V : \mathbf{R}^m \to \mathbf{R}$ that is 2π-periodic in every coordinate direction. We impose periodic boundary conditions and the initial condition $u(x, 0) = u_0(x)$.

When considered as evolution equations on $L^2((-\pi, \pi)^m)$, the equations (3.1) and (3.2) fit into the framework of Theorems 2.1 and 2.2, respectively. The commutator bounds (2.1) and (2.2) are satisfied with $\alpha = \frac{1}{2}$ and $\beta = 1$, because the commutator of the Laplacian and a multiplication operator is a first-order differential operator, and the commutator of the Laplacian and a first-order differential operator is a second-order differential operator. In the following we show that Theorems 2.1 and 2.2 apply also to the spatial semi-discretization of (3.1) and (3.2), uniformly in the discretization parameter. For notational simplicity only, we discuss this for the one-dimensional case.

A standard space discretization of these equations is given by the pseudo-spectral method. Here, a trigonometric polynomial

$$U(x, t) = \sum_{k=-N}^{N-1} e^{ikx} \, \widehat{u}_k(t)$$

is determined such that, in the case of (3.1),

$$i \frac{\partial U}{\partial t}(x_\ell, t) = -\frac{\partial^2 U}{\partial x^2}(x_\ell, t) + V(x_\ell) U(x_\ell, t) \quad (t > 0), \quad U(x_\ell, 0) = u_0(x_\ell)$$

is satisfied at the mesh-points $x_\ell = \ell\pi/N$ with $\ell = -N, \ldots, N-1$. Setting $\widehat{U}(t) = (\widehat{u}_k(t))$ $(k = -N, \ldots, N-1)$ the vector of Fourier coefficients, this is equivalent to solving

$$i\widehat{U}' = -D^2 \widehat{U} + W \widehat{U} \quad (t > 0), \qquad \widehat{U}(0) = \widehat{U}^0, \tag{3.3}$$

where $D = \operatorname{diag}(ik)$ $(k = -N, \dots, N-1)$, $W = F_{2N} \operatorname{diag}\big(V(x_\ell)\big) F_{2N}^{-1}$ with F_{2N} the $2N$-dimensional discrete Fourier transform, and $\widehat{U}^0 = F_{2N}\big(u_0(x_\ell)\big)$. With the Strang splitting over a time step τ, this differential system is solved approximately by computing recursively $\widehat{U}^n = (\widehat{u}_k^n)$ $(k = -N, \dots, N-1)$ via

$$\widehat{U}^{n+1} = e^{-\frac{i}{2}\tau W} e^{i\tau D^2} e^{-\frac{i}{2}\tau W} \widehat{U}^n, \tag{3.4}$$

where the action of $e^{-\frac{i}{2}\tau W} = F_{2N} \operatorname{diag}\big(e^{-\frac{i}{2}\tau V(x_\ell)}\big) F_{2N}^{-1}$ is inexpensive to compute. Then, $U(x, n\tau)$ is approximated by

$$U^n(x) = \sum_{k=-N}^{N-1} e^{ikx}\, \widehat{u}_k^n. \tag{3.5}$$

The discrete equation corresponding to (3.2) is

$$\widehat{U}' = D^2 \widehat{U} - W\widehat{U} \quad (t > 0), \qquad \widehat{U}(0) = \widehat{U}^0, \tag{3.6}$$

for which the splitting reads

$$\widehat{U}^{n+1} = e^{-\frac{1}{2}\tau W} e^{\tau D^2} e^{-\frac{1}{2}\tau W} \widehat{U}^n. \tag{3.7}$$

In the following, $\|\cdot\|$ denotes the Euclidean norm on $\mathbf{R}^{2N}$ and the induced matrix norm, and $(\cdot,\cdot)$ is the Euclidean scalar product. Parseval's formula yields the norm identities

$$\begin{aligned} &\|U(\cdot,t)\|_{L^2} = \|\widehat{U}(t)\|, \\ &\|U(\cdot,t)\|_{H^1} = \big(\widehat{U}(t), (-D^2+I)\widehat{U}(t)\big)^{1/2} = \|(-D^2+I)^{1/2}\widehat{U}(t)\|, \\ &\|U(\cdot,t)\|_{H^2} = \|(-D^2+I)\widehat{U}(t)\|, \end{aligned} \tag{3.8}$$

where H^1 and H^2 refer to the first- and second-order Sobolev norms.

The following lemma establishes the commutator bounds (2.1) and (2.2) with $\alpha = \frac{1}{2}$ and $\beta = 1$, uniformly in N.

LEMMA 3.1. *For a C^5-smooth potential V, the commutator bounds*

$$\begin{aligned} \|\,[-D^2+I, W]\, v\| &\le c_1 \,\|(-D^2+I)^{1/2} v\|, \\ \|\,[-D^2+I, [-D^2+I, W]]\, v\| &\le c_2 \,\|(-D^2+I) v\| \end{aligned}$$

hold with constants c_1, c_2 independent of N and $v \in \mathbf{R}^{2N}$.

PROOF. W is the circulant matrix

$$W = \big(\widehat{w}_{k-l}\big)_{k,l=-N}^{N-1}, \qquad \text{where } \widehat{w}_j = \sum_{m=-\infty}^{\infty} \widehat{v}_{j+2mN}$$

with $\widehat{v}_j$ the Fourier coefficients of V. Hence,

$$[-D^2+I, W] = [-D^2, W] = \Big((k^2 - l^2)\widehat{w}_{k-l}\Big).$$

This matrix is split as $L+M+R$, where L contains only the entries for $k-l \geq N$, M those for $|k-l| < N$, and R those for $k-l \leq -N$. To bound M, we write

$$k^2 - l^2 = (k-l)^2 + 2(k-l)l$$

and split $M = M_2 - 2iM_1D$, where M_2 has entries $(k-l)^2\widehat{w}_{k-l}$ and M_1 has entries $(k-l)\widehat{w}_{k-l}$. We have

$$\sum_{j=-N}^{N-1} j^2|\widehat{w}_j| \leq \sum_{j=-\infty}^{\infty} j^2|\widehat{v}_j|,$$

which is a finite bound if V is C^3. Hence, the absolute row and column sums of M_2 and M_1 are bounded independently of N, and consequently also their matrix norms induced by the Euclidean norm. It follows that for $v \in \mathbf{R}^{2N}$

$$\|Mv\| \leq \|M_2\| \cdot \|v\| + 2\,\|M_1\| \cdot \|Dv\| \leq C\,\|(-D^2+I)^{1/2}v\|.$$

With $k^2 - l^2 = (k+l)^2 - 2(k+l)l$, similar arguments yield also

$$\|Lv\| + \|Rv\| \leq C\,\|(-D^2+I)^{1/2}v\|$$

with the same constant C. This proves the bound for $\|\,[-D^2+I, W]\,v\|$. Using

$$[-D^2+I, [-D^2+I, W]] = \big((k^2-l^2)^2\widehat{w}_{k-l}\big),$$

the second commutator bound is obtained in the same way. □

With these commutator bounds, Theorem 2.1 yields the following error bounds for the Strang splitting (3.4), (3.5) for Equation (3.1).

THEOREM 3.2. *For a C^5-smooth potential V, the error of the Strang splitting* (3.4), (3.5) *in the pseudo-spectral discretization of the Schrödinger equation* (3.1) *is bounded by*

$$\|U^n - U(\cdot, n\tau)\|_{L^2} \leq C\tau\,\|U^0\|_{H^1}, \tag{3.9}$$

$$\|U^n - U(\cdot, n\tau)\|_{L^2} \leq C\tau^2\,\|U^0\|_{H^2}. \tag{3.10}$$

The constants C are independent of the discretization parameter N, of n and τ with $n\tau$ in a bounded interval, and of the initial data U^0.

PROOF. Combining Lemma 3.1, Theorem 2.1, and the norm identities (3.8), we obtain the local error bounds

$$\|U^1 - U(\cdot, \tau)\|_{L^2} \leq C_1\tau^2\,\|U^0\|_{H^1},$$
$$\|U^1 - U(\cdot, \tau)\|_{L^2} \leq C_2\tau^3\,\|U^0\|_{H^2}.$$

The result then follows from formula (2.9) with the roles of S and T interchanged, and from the observation that

$$\|U^n\|_{H^1} \leq (1+cn\tau)\,\|U^0\|_{H^1}, \qquad \|U^n\|_{H^2} \leq (1+cn\tau)^2\,\|U^0\|_{H^2}$$

for all n. □

Theorem 2.2 yields the following error bound for the parabolic case.

THEOREM 3.3. *For a C^5-smooth non-negative potential V, the error of the Strang splitting* (3.7), (3.5) *in the pseudo-spectral discretization of the imaginary-time Schrödinger equation* (3.2) *is bounded by*

$$\|U^n - U(\cdot, n\tau)\|_{L^2} \le C\tau^2 \log n \, \|U^0\|_{L^2}.$$

The constant C is independent of N, n, τ, and U^0.

Let us illustrate these results by numerical experiments. We take $V(x) = 1 - \cos x$, $N = 256$, and choose a random vector $\widehat{v} \in \mathbf{R}^{2N}$ scaled to Euclidean norm 1. We define two initial values $\widehat{U}^0_{(1)}$ and $\widehat{U}^0_{(2)}$ as $(-D^2+1)^{-1/2}\widehat{v}$ and $(-D^2+1)^{-1}\widehat{v}$ scaled to Euclidean norm 1. They contain the Fourier coefficients of functions with $\|U^0_{(1)}\|_{H^1} \approx 14$ and $\|U^0_{(1)}\|_{H^2} \approx 2100$, and $\|U^0_{(2)}\|_{H^2} \approx 20$.

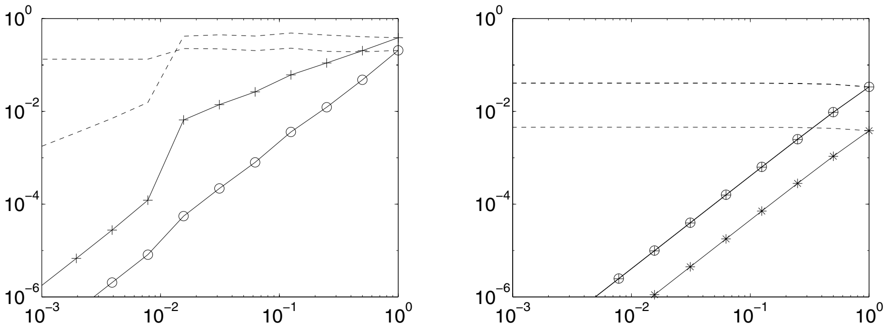

Figure 3.1: Error versus step size; smooth potential.

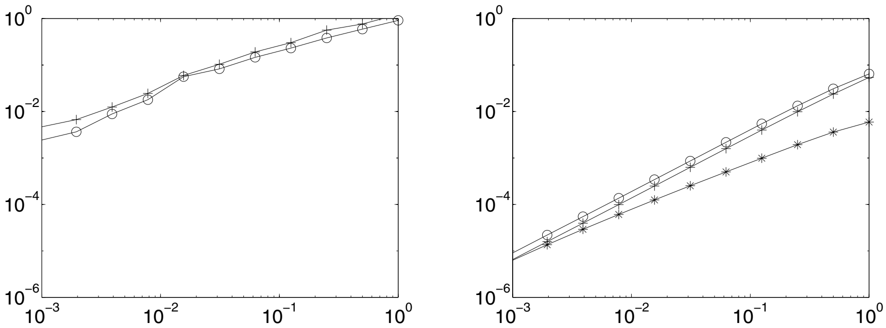

Figure 3.2: Error versus step size; nonsmooth potential.

The left-hand figure of Figure 3.1 shows the norms $\|\widehat{U}^n - \widehat{U}(t)\|$ at $t = n\tau = 1$ of the errors of the Strang splitting (3.4) versus the step size τ. The two error curves correspond to the two initial values $\widehat{U}^0_{(1)}, \widehat{U}^0_{(2)}$. The dashed lines indicate the errors divided by τ and τ^2, respectively. For step sizes larger than 10^{-2}, they are almost constant, in perfect agreement with Theorem 3.2. Only for smaller step sizes the convergence order becomes 2 also for the less regular initial data.

The right-hand figure gives the analogous error curves for the parabolic case (3.7), for initial data $\widehat{v}, \widehat{U}^0_{(1)}, \widehat{U}^0_{(2)}$, which all give second-order convergence, as predicted by Theorem 3.3. The dashed lines indicate the errors divided by τ^2. The least regular initial value $\widehat{v}$ even gives the best (absolute) accuracy, due to the strong smoothing in the parabolic case. The relative errors $\|\widehat{U}^n - \widehat{U}(1)\| / \|\widehat{U}(1)\|$ are almost identical for the three initial data, starting with a relative error of 0.1 for $\tau = 1$.

Figure 3.2 illustrates the role of the smoothness of the potential V in the error bounds. It shows the errors corresponding to the above data, but now for the discontinuous 2π-periodic extension of $V(x) = x + \pi$ for $x \in (-\pi, \pi)$. Compared with Figure 3.1, the observed convergence is slower for both equations (3.1) and (3.2).

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