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ON SUBDIAGONAL RATIONAL PADÉ APPROXIMATIONS AND THE BRENNER-THOMÉE APPROXIMATION THEOREM FOR OPERATOR SEMIGROUPS

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Abstract. The computational powers of Mathematica are used to prove polynomial identities that are essential to obtain growth estimates for subdiagonal rational Padé approximations of the exponential function and to obtain new estimates of the constants of the Brenner-Thomée Approximation Theorem of Semigroup Theory.

1. **Introduction.** The main result of this paper sharpens the estimate given in [13] regarding the size of the constant C_m in the following key result on the approximation of strongly continuous semigroups.

Theorem 1.1. *(Hersh-Kato, Brenner-Thomée). Let r_m be an $\mathscr{A}$-stable rational approximation scheme of the exponential of order m and $(A, D(A))$ be the generator of a strongly continuous semigroup $T(t)$ of type $(M, 0)$. Then there exists a constant C_m depending solely on r_m such that*

$$\left\| r_m\left(\frac{t}{n}A\right)^n x - T(t)x \right\| \leq MC_m t^{m+1} \frac{1}{n^m} \left\| A^{m+1}x \right\|$$

for $n \in \mathbb{N}, t \geq 0$, and $x \in D(A^{m+1})$. In particular, if $A^{m+1}x = 0$, then $r_m(tA)x = T(t)x$ for $t \geq 0$.

This result appeared first in a 1979 paper of Reuben Hersh and Tosio Kato in the SIAM Journal of Numerical Analysis [8] (for the more general Chernoff Product formula, see [6]). In the same issue, Philip Brenner and Vidar Thomée [3] weakened the regularity assumptions and showed the theorem as stated above. Also, in [3]

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error estimates were given for $\left\|r(\frac{t}{n}A)^n x - T(t)x\right\|$ for $x \in D(A^k)$, where $0 \leq k \leq m+1$. In 2007, this result was improved by Mihály Kovács [11] giving error estimates for $x \in \mathscr{F}$, where $\mathcal{F}$ are interpolation spaces between $D(A^{m+1})$ and X. In all these contributions, no estimates were provided for the constant C_m. This was done first in [4] and [13] for subdiagonal rational Padé-approximations r_m (where [4] applies some of the estimates given in Section 1 of this paper to show that, for all $x \in D(A^\alpha)$ $(\alpha > \frac{1}{2})$, $\lim_{m\to\infty} r_m(tA)x = T(t)x$ uniformly for t in compact intervals). The same estimates allow us to revisit and significantly improve the estimates concerning C_m that were given in [13]. In particular, we will show that for subdiagonal Padé approximations r_m with $m \geq 1$ the following estimate holds.

$$\left\|r_m\left(\frac{t}{n}A\right)^n x - T(t)x\right\| \leq M\frac{20^{1/4}\sqrt{\pi}}{m!}\frac{1}{n^{m-\frac{1}{2}}}\left(\frac{(m-1)!(m+1)!}{(2m+1)!}\right)^{\frac{1}{2}} t^{m+1}\left\|A^{m+1}x\right\|$$

for all $t \geq 0$, $n \in \mathbb{N}$, and $x \in D(A^{m+1})$.

To get started, let $r_m = \frac{P}{Q}$ be an $\mathscr{A}$-stable rational approximation to the exponential function of order $m \geq 1$; i.e., P and Q are polynomials with $p := deg(P) \leq deg(Q) =: q$, and

(i) $|r_m(z) - e^z| \leq C_m|z|^{m+1}$ for $|z|$ sufficiently small, and
(ii) $|r_m(z)| \leq 1$ for $\mathrm{Re}(z) \leq 0$.

It is a well-known result of Padé [14] that $m \leq p+q$ for all rational approximations to the exponential function. The rational approximations of maximal order $m = p+q$ are called *Padé* approximations. They are of the form $r_m = \frac{P}{Q}$, where

$$P(z) = \sum_{j=0}^{p} b[j,p]z^j, \text{ where } b[j,p] = \frac{(m-j)!p!}{m!j!(p-j)!}, \quad \text{and}$$

$$Q(z) = \sum_{j=0}^{q} a[j,q](-z)^j, \text{ where } a[j,q] = \frac{(m-j)!q!}{m!j!(q-j)!}.$$

Moreover, for every Padé approximation $r_m(z) = \frac{P(z)}{Q(z)}$ of the exponential of order $m = p+q$,

$$r_m(z) - e^z = \frac{(-1)^{q+1}}{Q(z)}\frac{1}{m!}z^{m+1}e^z\int_0^1 s^p(1-s)^q e^{-sz}ds \tag{1}$$

(see, for example, [15], Section 75 (Die Exponentialfunktion), or [17]). As shown in [5], Padé approximations are $\mathscr{A}$-stable if and only if $q-2 \leq p \leq q$. A rational Padé approximation $r(z) = \frac{P(z)}{Q(z)}$ is called subdiagonal if $p = q-1$. In particular, a subdiagonal Padé approximation is always $\mathscr{A}$-stable and of odd approximation order $m = 2q-1$.

2. **Estimates for subdiagonal rational Padé approximations of the exponential.**

In applications to operator semigroups and the inversion of the Laplace transform (see, for example [4], [13], [19]), the following identities and estimates are useful.

Proposition 1. *Let $r(z) = \frac{P(z)}{Q(z)}$ be a subdiagonal Padé approximation, then*

$$|Q(is)|^2 = Q(is) * Q(-is) = \sum_{j=0}^{q} d[2j,q]s^{2j}, \text{ and} \tag{2}$$

$$|P(is)|^2 = P(is) * P(-is) = \sum_{j=0}^{q-1} d[2j,q]s^{2j}, \tag{3}$$

where $d[0,q] = 1$, $d[2q,q] = (\frac{(q-1)!}{(2q-1)!})^2$, and

$$d[2j,q] = \frac{1}{2^j j!} \prod_{k=1}^{j} \frac{(q-k+1)}{(2q-k)(2q-2k+1)} \text{ if } 0 < j < q.$$

In particular,

(a) $\sup_{s\in\mathbb{R}} |r(is)| = r(0) = 1$.
(b) $\sup_{s\in\mathbb{R}} \frac{1}{|Q(is)|} = 1$.
(c) $\sup_{s\in\mathbb{R}} |\frac{s^q}{Q(is)}| = \frac{(2q-1)!}{(q-1)!} = \frac{m!}{p!}$.
(d) $\sup_{s\in\mathbb{R}} |\frac{s^n}{Q(is)}| \le \sqrt{\frac{1}{d[2n,q]}}$ *for all* $0 \le n \le q$.

Proof. Clearly,

$$|Q(is)|^2 = Q(is) * Q(-is) = \left(\sum_{j=0}(-1)^j i^j a[j,q]s^j\right) * \left(\sum_{j=0} i^j a[j,q]s^j\right)$$
$$= \sum_{n=0}^{2q} d[n,q]s^n,$$

where $d[n,q]$ is given by the Cauchy product

$$d[n,q] = \sum_{j=0}^{n}(-1)^j i^j a[j,q] * i^{n-j}a[n-j,q] = i^n \sum_{j=0}^{n}(-1)^j a[j,q] * a[n-j,q]$$

and where we set $a[j,q] := 0$ if $j > q$. It can be easily seen that $d[n,q] = 0$ if n is odd and it follows immediately that[1]

$$d[0,q] = a[0,q]^2 = 1 \quad \text{and} \quad d[2q,q] = a[q,q]^2 = \left(\frac{p!}{m!}\right)^2 = \left(\frac{(q-1)!}{(2q-1)!}\right)^2.$$

For $0 < j < q$ and $n = 2j$, the identity

$$d[n,q] = d[2j,q] = (-1)^j \sum_{k=0}^{2j}(-1)^k a[k,q] * a[2j-k,q]$$
$$= \frac{1}{2^j j!} \prod_{k=1}^{j} \frac{(q-k+1)}{(2q-k)(2q-2k+1)}$$

can be proven with the following Mathematica code.

```
a[j_, q_] := ((2q-1-j)!q!)/((2q-1)!j!(q-j)!);
```
[2]

[1] Other identities are $d[2,q] = \frac{q}{2m^2}$, $d[2q-2,q] = \left(\frac{q!}{m!}\right)^2$ and $d[2q-4,q] = \left(\frac{q!}{(m-1)!}\right)^2$.

[2] Notice that a[j,q] is well defined as long as $0 \le j < 2q$ and that Mathematica will evaluate a[j,q] to be zero if $q < j < 2q$ since in this case $1/(q-j)! = 0$.

```
d[n_, q_] :=(−1)^(n/2) Sum[(−1)^j a[j, q]a[n-j,q], {j, 0, n}];
Ans[n_, q_] := 1/((2^(n/2))(n/2)!) Product[(q-k+1)/((2*q-k)(2q-2k+1)), {k, 1, n/2}];
FullSimplify[d[2m, q] - Ans[2m, q]]
```

Since the answer is "0", the statement (2) is proved. The statement (3) holds because the following Mathematica code produces the answer "1".

```
b[j_, q_] := ((2q-1-j)!(q-1)!)/((2q-1)!j!(q-1-j)!);
e[n_, q_] :=(−1)^(n/2) Sum[(−1)^j b[j, q]b[n-j, q], {j, 0, n}];
Ans[n_, q_] := 1/((2^(n/2))(n/2)!) Product[(q-k+1)/((2*q-k)(2q-2k + 1)), {k, 1, n/2}];
FullSimplify[e[2m, q]/Ans[2m, q]]
```

It follows from (2) and (3) that

$$|Q(is)|^2 - |P(is)|^2 = d[2q,q]s^{2q} \geq 0$$

for all $s \in \mathbb{R}$. This proves statement (a).[3]

Since $d[0,q] = 1$ and $d[2j,q] \geq 0$ for all $j \in \mathbb{N}_0$, it follows from (2) that $\min_{s\in\mathbb{R}} |Q(is)| = 1$. Moreover, since

$$\frac{|Q(is)|^2}{s^{2n}} = \sum_{j=0}^{q} d[2j,q]s^{2j-2n} \geq d[2n,q],$$

it follows that

$$\left|\frac{s^n}{Q(is)}\right| \leq \frac{1}{\sqrt{d[2n,q]}}$$

for all $s \in \mathbb{R}$ and that $\sup_{s\in\mathbb{R}} |\frac{s^q}{Q(is)}| = d[2q,q]$. □

Proposition 2. *Let* $r(z) = \frac{P(z)}{Q(z)}$ *be a subdiagonal Padé approximation, then*

(a) $\frac{|Q'(is)|}{|Q(is)|} \leq 1$ *for all* $s \in \mathbb{R}$.
(b) $\frac{|P'(is)|}{|P(is)|} \leq 1$ *for all* $s \in \mathbb{R}$.
(c) $|r'(is)| \leq 2$ *for all* $s \in \mathbb{R}$.[4]

Proof. It follows from

$$Q'(z) = \sum_{j=1}^{q} a[j,q]j(-1)^j z^{j-1} = \sum_{j=0}^{q-1} \tilde{a}[j,q](-1)^{j+1}z^j,$$

where $\tilde{a}[j,q] = (j+1)a[j+1,q]$, that

$$\begin{aligned}|Q'(is)|^2 = Q'(is) * Q'(-is) &= \left(\sum_{j=0}(-1)^{j+1}i^j\tilde{a}[j,q]s^j\right) * \left(\sum_{j=0} -i^j\tilde{a}[j,q]s^j\right)\\ &= \sum_{n=0}^{2q-2} \tilde{d}[n,q]s^n,\end{aligned}$$

[3]Clearly, statement (a) is an immediate consequence from Ehle's work in [5]. However, compared to the Mathematica based proof given here, Ehle's proof is quite elaborate.

[4]In fact, the sharper estimate $\max_{s\in\mathbb{R}} |r'(is)| = 1$ holds. A Mathematica code that can be used to verify this estimate for any $q \geq 1$ is given in the remark below.

where

$$\tilde{d}[n,q] = \sum_{j=0}^{n} (-1)^j i^j \tilde{a}[j,q] * i^{n-j} \tilde{a}[n-j,q] = i^n \sum_{j=0}^{n} (-1)^j \tilde{a}[j,q] * \tilde{a}[n-j,q]$$

and where we set $\tilde{a}[j,q] := 0$ if $j > q-1$. It can be easily seen that $\tilde{d}[n,q] = 0$ if n is odd. For $0 \le j < q$ and $n = 2j$, the identity

$$\tilde{d}[n,q] = \tilde{d}[2j,q] = \frac{q(q-j)}{(2q-j-1)(2q-2j-1)} d[2j,q]$$

can be proven with the following Mathematica code.

```
aa[j_, q_] := ((2q - 2 - j)!q!)/((2q - 1)!(j)!(q - j - 1)!);
dd[n_, q_] := (-1)^(n/2)Sum[(-1)^j aa[j, q] aa[n - j, q], {j, 0, n}];
Ans[n_, q_] := 1/((2^(n/2))(n/2)!)
   Product[(q - k + 1)/((2*q - k)(2q - 2k + 1)), {k, 1, n/2}];
AAns[n_,q_] := (q*(q - n/2)/((2 q - n/2 - 1)*(2 q - n - 1)))*Ans[n, q];
FullSimplify[dd[2*r, x]/AAns[2*r, x]]
```

Now, $\frac{|Q'(is)|}{|Q(is)|} \le 1$ for all $s \in \mathbb{R}$ if and only

$$0 \le Q(is)Q(-is) - Q'(is)Q'(-is) = d[2q,q]s^{2q} + \sum_{j=0}^{q-1} \left(d[2j,q] - \tilde{d}[2j,q] \right) s^{2j}$$

for all $s \in \mathbb{R}$. However, the last statement holds since $d[2j,q] - \tilde{d}[2j,q] \ge 0$ for all $0 \le j \le q-1$. This proves statement (a). To prove (b), observe that

$$P(z) = \sum_{j=0}^{q-1} b[j,q] z^j, \text{ where } b[j,q] = \frac{(2q-1-j)!(q-1)!}{(2q-1)!j!(q-1-j)!} = \frac{q-j}{q} a[j,q]$$

for $0 \le j$. Then

$$\begin{aligned} |P(is)|^2 = P(is) * P(-is) &= \left(\sum_{j=0} i^j b[j,q] s^j \right) * \left(\sum_{j=0} (-1)^j i^j b[j,q] s^j \right) \\ &= \sum_{n=0}^{2q-2} e[n,q] s^n, \end{aligned}$$

where

$$e[n,q] = \sum_{j=0}^{n} i^j b[j,q] * i^{n-j} (-1)^{n-j} b[n-j,q] = (-i)^n \sum_{j=0}^{n} (-1)^j b[j,q] * b[n-j,q]$$

and where we set $b[j,q] := 0$ if $j > q-1$. It can be easily seen that $e[n,q] = 0$ if n is odd. For $0 \le j < q$ and $n = 2j$ the identity

$$e[n,q] = d[n,q]$$

can be proven with the following Mathematica code.

```
b[j_, q_] := ((q - j)/q)a[j, q];
e[n_, q_] := (-1)^(n/2)Sum[(-1)^j b[j, q] b[n - j, q], {j, 0, n}];
FullSimplify[d[2r, x]/Ans[2r, x]]
```

This shows that

$$|Q(is)|^2 - |P(is)|^2 = d[2q,q]s^{2q} = \left(\frac{(q-1)!}{(2q-1)!}\right)^2 s^{2q} \tag{4}$$

(see also Theorem 3.3 in [5]). It follows from

$$P'(z) = \sum_{j=1}^{q-1} b[j,q]jz^{j-1} = \sum_{j=0}^{q-2} \tilde{b}[j,q]z^j,$$

where $\tilde{b}[j,q] = (j+1)b[j+1,q]$, that

$$\begin{aligned}|P'(is)|^2 = P'(is) * P'(-is) &= \left(\sum_{j=0} i^j \tilde{b}[j,q]s^j\right) * \left(\sum_{j=0} (-i)^j \tilde{b}[j,q]s^j\right) \\ &= \sum_{n=0}^{2q-2} \tilde{e}[n,q]s^n,\end{aligned}$$

where

$$\tilde{e}[n,q] = \sum_{j=0}^{n} i^j \tilde{b}[j,q] * (-i)^{n-j} \tilde{b}[n-j,q] = (-i)^n \sum_{j=0}^{n} (-1)^j \tilde{b}[j,q] * \tilde{b}[n-j,q],$$

and where we set $\tilde{b}[j,q] := 0$ if $j > q-1$. It can be easily seen that $\tilde{e}[n,q] = 0$ if n is odd. For $0 \le j < q$ and $n = 2j$ the identity

$$\tilde{e}[n,q] = \tilde{e}[2j,q] = \frac{(q-1)(q-j-1)}{(2q-j-1)(2q-2j-1)} d[2j,q] = \frac{q-1}{q}\frac{q-j-1}{q-j}\tilde{d}[2j,q]$$

can be proven with the following Mathematica code.

```
bb[j_, q_] := (j + 1)b[j + 1, q];
ee[n_, q_] := (−1)^(n/2) Sum[(−1)^j bb[j, q] bb[n - j, q], {j, 0, n}];
EEAns[n_,q_] := ((q - 1)(q - n/2 - 1)/((2 q - n/2 - 1)(2 q - n - 1))) Ans[n, q];
FullSimplify[ee[2r, x]/EEAns[2r, x]]
```

It follows from (4) that

$$\begin{aligned}|P(is)|^2 - |P'(is)|^2 &= |Q(is)|^2 - d[2q,q]s^{2q} - |P'(is)|^2 \\ &= \sum_{j=0}^{2q-2} \left(d[2j,q] - \tilde{e}[2j,q]\right) s^{2j} \ge 0\end{aligned}$$

since

$$\begin{aligned}d[2j,q] - \tilde{e}[2j,q] &= \left(1 - \frac{(q-1)(q-j-1)}{(2q-j-1)(2q-2j-1)}\right) d[2j,q] \\ &= \frac{(3q-2j-2)(q-j)}{(2q-j-1)(2q-2j-1)} d[2j,q] \ge 0\end{aligned}$$

for all $0 \le j \le q-1$. This proves statement (b). Finally, statement (c) follows from

$$r'(z) = \frac{P'(z)Q(z) - P(z)Q'(z)}{Q(z)^2} = r(z)\left(\frac{P'(z)}{P(z)} - \frac{Q'(z)}{Q(z)}\right)$$

and the fact that $|r(z)| \le 1$ for $Re(z) \le 0$ ($\mathscr{A}$-stability). □

Remark 1. It follows from the above that $|r'(is)| \leq 1$ for all $s \in \mathbb{R}$ if

$$|Q(is)^2|^2 - |P'(is)Q(is) - P(is)Q'(is)|^2 = Q(is)^2Q(-is)^2 - (P'(is)Q(is) - P(is)Q'(is))(P'(-is)Q(-is) - P(-is)Q'(-is)) \geq 0.$$

For a given value of q (degree of Q), this can be proved by the following Mathematica code which uses the fact that $b[j,q] = \frac{q-j}{q} a[j,q]$.

```
a[j_,q_]:= Piecewise[{{(2 q - 1 - j)! q!/((2 q - 1)! j! (q - j)!), j ≤ q}}];
Q[z_, q_] := Sum[a[j, q]*(−z)^j, {j, 0, q}];
P[z_, q_] := Sum[((q - j)/q) a[j, q]*z^j, {j, 0, q - 1}];
QQ[z_, q_] := D[Q[z, q], z];
PP[z_, q_] := D[P[z, q], z];
HH[z_, q_] := PP[z, q]*Q[z, q] - P[z, q]*QQ[z, q];
GG[z_, q_] := Q[z,q]^2 ∗ Q[−z,q]^2];
HHH[s_, q_] := HH[z, q] . z → I*s;
GGG[s_, q_] := GG[z, q] . z → I*s;
UU[s_, q_] := HHH[s, q]*HHH[-s, q];
CCC[s_, q_] := [GGG[s, q] - UU[s, q];
Simplify[CCC[s, q]]
```

3. **The constant in the Brenner-Thomée theorem.** In this section we prove the following estimate for subdiagonal Padé approximations r_m and generators $(A, D(A))$ of strongly continuous semigroups $T(t)$ with $\|T(t)\| \leq M$ for all $t \geq 0$.

$$\left\| r\left(\frac{t}{n}A\right)^n x - T(t)x \right\| \leq M \frac{20^{1/4}\sqrt{\pi}}{m!} \frac{1}{n^{m-\frac{1}{2}}} \left(\frac{(m-1)!(m+1)!}{(2m+1)!}\right)^{\frac{1}{2}} t^{m+1} \|A^{m+1}x\| \tag{5}$$

for all $n \geq 1$, $t \geq 0$ and $x \in D(A^{m+1})$.

Proof. The first part of the proof follows exactly the proof given by Kovács [10] up to shortly after (13) below. For further reference, see also Kovács and Neubrander [12]; for the bi-continuous case, see Jara [9]. The new part of the proof starts with the Perron representation of rational Padé approximation in (14).

To begin, if $r = \frac{P}{Q}$ is a subdiagonal Padé approximation of the exponential, then all the distinct poles λ_i of r lie in the right half-plane. By using partial fractions,

$$r(z) = \frac{P(z)}{Q(z)} = \frac{b_1}{(\lambda_1 - z)} + \frac{b_2}{(\lambda_2 - z)} + \ldots + \frac{b_q}{(\lambda_q - z)}$$

for $Re(z) \leq 0$, where the λ_i are the roots of $Q(z)$ and

$$b_i := \frac{m!P(\lambda_i)}{p! \prod_{\substack{j=1 \\ j \neq i}}^{q} (\lambda_j - \lambda_i)}.$$

For $t > 0$, let H_t be the normalized Heaviside function defined on $[0, \infty)$ with $H_t(s) := 1$ if $s > t$, $H_t(t) := \frac{1}{2}$, and $H_t(s) := 0$ if $0 \leq s < t$. Moreover, let $H_0(0) := 0$ and $H_0(s) := 1$ for $s > 0$. The Laplace-Stieltjes transforms of the normalized Heaviside functions are

$$e^{zt} = \int_0^\infty e^{zs}\, dH_t(s)$$

for all $z \in \mathbb{C}$ with $Re(z) \le 0$ and all $t \ge 0$. Moreover, if $Re(z) \le 0$ and $Re(\lambda) > 0$,

$$\frac{1}{\lambda - z} = \int_0^\infty e^{zs} e^{-\lambda s}\, ds = \int_0^\infty e^{zs}\, d\alpha_\lambda(s),$$

where $\alpha_\lambda(s) := \frac{1}{\lambda}\left(1 - e^{-\lambda s}\right) = \int_0^s e^{-\lambda r}\, dr$ is a normalized function of bounded variation. (See Chapter I of [18] or Sections 1.9 − 1.10 of [2] for details on the Laplace-Stieltjes integral.) The space $NBV^0[0,\infty)$ of functions of bounded variation normalized at zero is a Banach algebra with multiplication defined by the Stieltjes convolution

$$(\alpha * \beta)(t) := \int_0^t \alpha(t-s)\, d\beta(s)$$

(see [10], p. 8). The Laplace-Stieltjes transform maps convolution onto multiplication. Thus,

$$\frac{1}{(\lambda - z)^j} = \int_0^\infty e^{zs}\, d\alpha_\lambda^{*j}(s)$$

where $s \to \alpha_\lambda^{*j}(s) := (\alpha_\lambda * \cdots * \alpha_\lambda)(s)$ is again in $NBV^0[0,\infty)$.

If r is a subdiagonal Padé approximation of the exponential, then there exists $\alpha \in NBV^0[0,\infty)$ such that $r(z) = \int_0^\infty e^{zs}\, d\alpha(s)$, where $\alpha(s) = \sum_{j=1}^q \alpha_{\lambda_i}(s)$. Then, for $Re(z) \le 0$, r and $r^{(n)}$ have the representations

$$r(z) = \int_0^\infty e^{zs}\, d\alpha(s) \text{ and } r^n(z) = \int_0^\infty e^{zs}\, d\alpha^{*n}(s).$$

It follows that $r\left(\frac{tz}{n}\right)^n = \int_0^\infty e^{zs}\, d\alpha_n(s)$, where $\alpha_n(s) := \alpha^{*n}(\frac{ns}{t})$ is in $NBV^0[0,\infty)$. This means that $\alpha_n - H_t$ is also in $NBV^0[0,\infty)$ and

$$r\left(\frac{tz}{n}\right)^n - e^{tz} = \int_0^\infty e^{zs}\, d[\alpha_n - H_t](s). \tag{6}$$

Consider

$$\mathscr{G}_0 := \{f | f(z) = \int_0^\infty e^{zs}\, d\alpha(s) \text{ if } Re(z) \le 0 \text{ for some } \alpha \in NBV^0[0,\infty)\}.$$

Then $\mathscr{G}_0$ is a Banach algebra with norm $\|f\|_0 := \|\alpha\|_{var} = V_\alpha(\infty)$. Furthermore, the Hille-Phillips functional calculus (see [10]) provides the framework and justification to replace $z \in \mathbb{C}$ with $Re(z) \le 0$ by a suitable operator A in (6). Suppose A is the generator of a bounded, strongly continuous semigroup and r is an $\mathscr{A}$-stable rational approximation of the exponential, then the Hille-Phillips functional calculus along with (6) implies that

$$r\left(\frac{t}{n}A\right)^n x - T(t)x = \int_0^\infty T(s)x\, d[\alpha_n - H_t](s).$$

Since $\alpha_n(0) - H_t(0) = \alpha_n(\infty) - H_t(\infty) = 0$, integration by parts yields

$$r\left(\frac{t}{n}A\right)^n x - T(t)x = -\int_0^\infty [\alpha_n - H_t](s)\, dT(s)x$$

for all $x \in X$. If $x \in D(A)$ then $s \to T(s)x$ is continuously differentiable with $\frac{d}{ds}T(s)x = T(s)Ax$. Therefore, for $x \in D(A)$,

$$r\left(\frac{t}{n}A\right)^n x - T(t)x = -\int_0^\infty [\alpha_n - H_t](s) T(s)Ax\, ds.$$

For $1 \leq k \leq m$ let $I_k[\alpha_n - H_t](s)$ denote the k-th antiderivative of $\alpha_n - H_t$; i.e.

$$I_k[\alpha_n - H_t](s) := \int_0^s \int_0^{s_k} \cdots \int_0^{s_2} [\alpha_n - H_t](s_1)\, ds_1\, ds_2 \cdots ds_k$$
$$= \int_0^s \frac{(s-r)^{k-1}}{(k-1)!} [\alpha_n - H_t](r)\, dr.$$

It can be shown that

$$I_k[\alpha_n - H_t](0) = I_k[\alpha_n - H_t](\infty) = 0$$

for $1 \leq k \leq m$ (see [10] or Lemma III.6 in [16]). Thus, for $1 \leq k \leq m$ and $x \in D(A^{k+1})$, k consecutive integrations by parts yield

$$r\left(\frac{t}{n}A\right)^n x - T(t)x = (-1)^{k+1} \int_0^\infty I_k[\alpha_n - H_t](s) T(s) A^{k+1} x\, ds. \tag{7}$$

As a consequence of (7), one obtains

$$\left\| r\left(\frac{t}{n}A\right)^n x - T(t)x \right\| = M \|A^{k+1}x\| \, \|I_k[\alpha_n - H_t]\|_{L^1(\mathbb{R}^+)} \tag{8}$$

for $t \geq 0$, $n \in \mathbb{N}$, and $x \in D(A^{k+1})$.

Our estimate of $\|I_k[\alpha_n - H_t]\|_{L^1(\mathbb{R}^+)}$ uses the following Fourier representation of $I_k[\alpha_n - H_t]$ (for details see [10], [12], or Lemma III.6, [16]). Namely,

$$I_k[\alpha_n - H_t](s) = \left(\frac{-1}{i}\right)^{k+1} \frac{1}{\sqrt{2\pi}} \mathscr{F}\left[\frac{r^n(i\frac{t}{n}(\cdot)) - e^{it(\cdot)}}{(\cdot)^{k+1}}\right](s) \tag{9}$$

for all $n \in \mathbb{N}$ and $s \in (0, \infty)$, where

$$\mathscr{F}[f](s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{-isv} f(v)\, dv.$$

It follows from (6) that

$$r\left(-\frac{t}{n}z\right)^n - e^{-tz} = \int_0^\infty e^{-zs}\, d[\alpha_n - H_t](s) \tag{10}$$

for $Re(z) \geq 0$, where $\alpha_n - H_t \in NBV^0[0, \infty)$. Recall that the complex inversion formula (see [18], Chapter II, Theorem 7.6a) states that if $\alpha \in NBV^0[0, \infty)$ and $f(z) = \int_0^\infty e^{-zs}\, d\alpha(s)$ converges for all $Re(z) > \sigma_c$, then for $c > \max[\sigma_c, 0]$,

$$\frac{1}{2\pi i} \lim_{R\to\infty} \int_{c-iR}^{c+iR} \frac{f(z)}{z} e^{zs}\, dz = \begin{cases} \alpha(s) & : n > 0 \\ \frac{\alpha(0+)}{2} & : s = 0 \\ 0 & : s < 0 \end{cases}.$$

It follows from (10) that

$$\alpha_n(s) - H_t(s) = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{c-iR}^{c+iR} \frac{r(-\frac{t}{n}z)^n - e^{-tz}}{z} e^{zs}\, dz.$$

Recall that a subdiagonal Padé approximation is always $\mathscr{A}$-stable (see [7], pp. 475-489, or [5]). Using the $\mathscr{A}$-stability of r as well as Cauchy's Theorem, it follows that

$$\begin{aligned}\alpha_n(s) - H_t(s) =& \frac{1}{2\pi i} \lim_{R\to\infty} \int_{-iR}^{iR} \frac{r(-\frac{t}{n}z)^n - e^{-zt}}{z} e^{zs}\, dz \\ =& i\frac{-1}{\sqrt{2\pi}} \mathscr{F}\left[\frac{r(i\frac{t}{n}(\cdot))^n - e^{it(\cdot)}}{(\cdot)}\right](s)\end{aligned} \tag{11}$$

(see [10] or [16] Lemma III.6 for details). With an induction argument, one can show that (11) implies (9). Thus,

$$\begin{aligned}\|I_m[\alpha_n - H_t]\|_{L^1(\mathbb{R}^+)} =& \frac{1}{\sqrt{2\pi}} \left\| \mathscr{F}\left[\frac{r(i\frac{t}{n}(\cdot))^n - e^{it(\cdot)}}{(\cdot)^{m+1}}\right]\right\|_{L^1(\mathbb{R}+)} \\ \leq& \frac{1}{\sqrt{2\pi}} \left\| \mathscr{F}\left[\frac{r(i\frac{t}{n}(\cdot))^n - e^{it(\cdot)}}{(\cdot)^{m+1}}\right]\right\|_{L^1(\mathbb{R})}.\end{aligned}$$

With two substitutions (see [10], [12], or [16] for details) one obtains

$$\|I_m[\alpha_n - H_t]\|_{L^1(\mathbb{R}^+)} \leq \frac{1}{\sqrt{2\pi}} \frac{1}{n^m} t^{m+1} \left\| \mathscr{F}\left[\frac{[e^{-in^{\frac{-1}{m+1}}(\cdot)} r(in^{\frac{-1}{m+1}}(\cdot))]^n - 1}{(\cdot)^{m+1}}\right]\right\|_{L^1(\mathbb{R})}.$$

Now define

$$h_n(s) := \frac{\left[e^{-in^{\frac{-1}{m+1}}s} r(in^{\frac{-1}{m+1}}s)\right]^n - 1}{s^{m+1}}$$

for $s \in \mathbb{R}$. Then

$$\|I_m[\alpha_n - H_t]\|_{L^1(\mathbb{R}^+)} \leq \frac{1}{\sqrt{2\pi}} \frac{1}{n^m} t^{m+1} \|\mathscr{F}[h_n]\|_{L^1(\mathbb{R})}. \tag{12}$$

Let $f \in L^2(\mathbb{R})$ and $g : s \to sf(s) \in L^2(\mathbb{R})$. Then, by Carlson's inequality, $f \in L^1(\mathbb{R})$ and

$$\|f\|_{L^1(\mathbb{R})} \leq \sqrt{\pi}\|f\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \|g\|_{L^2(\mathbb{R})}^{\frac{1}{2}}.$$

Now recall the following well-known property of the Fourier transform. If $g \in L^2(\mathbb{R})$ is absolutely continuous with $g' \in L^2(\mathbb{R})$, then

$$is\mathscr{F}[g](s) = \mathscr{F}[g'](s)$$

almost everywhere. Thus, if $f = \mathscr{F}[g] \in L^2(\mathbb{R})$ for some absolutely continuous $g \in L^2(\mathbb{R})$ with $g' \in L^2(\mathbb{R})$, then Carlson's inequality implies that

$$\|F(g)\|_1 \leq \sqrt{\pi}\|\mathscr{F}[g]\|_2^{\frac{1}{2}} \|\mathscr{F}[g']\|_2^{\frac{1}{2}}.$$

By Parseval's identity, $\|\mathscr{F}[g]\|_2 = \|g\|_2$ for $g \in L^2(\mathbb{R})$. This shows that

$$\|\mathscr{F}[g]\|_1 \leq \sqrt{\pi}\|g\|_2^{\frac{1}{2}} \|g'\|_2^{\frac{1}{2}}.$$

Using these properties and inequalities, it follows from (12) that

$$\|I_m[\alpha_n - H_t]\|_{L^1(\mathbb{R}^+)} \leq \frac{1}{\sqrt{2}} t^{m+1} \frac{1}{n^m} \|h_n\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \|h_n'\|_{L^2(\mathbb{R})}^{\frac{1}{2}}.$$

Now, returning to (8), it follows that

$$\left\| r\left(\frac{t}{n}A\right)^n x - T(t)x\right\| \leq M\|A^{m+1}x\| \frac{1}{\sqrt{2}} t^{m+1} \frac{1}{n^m} \|h_n\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \|h_n'\|_{L^2(\mathbb{R})}^{\frac{1}{2}}, \tag{13}$$

where

$$h_n(s) = \frac{[e^{-in^{\frac{-1}{m+1}}s} r(in^{\frac{-1}{m+1}}s)]^n - 1}{s^{m+1}} = \frac{[e^{-in^{\frac{-1}{m+1}}s} r(in^{\frac{-1}{m+1}}s)]^n - 1}{(in^{\frac{-1}{m+1}}s)^{m+1}} i^{m+1} \frac{1}{n}.$$

Defining $u(s) := n^{\frac{-1}{m+1}}s$, one has that

$$\begin{aligned} h_n(s) &= \frac{[e^{-ius} r(iu(s))]^n - 1}{[iu(s)]^{m+1}} i^{m+1} \frac{1}{n} \\ &= \frac{e^{iu(s)} r(iu(s)) - 1}{[iu(s)]^{m+1}} i^{m+1} \frac{1}{n} \sum_{j=0}^{n-1} e^{-iju(s)} r(iu(s))^j. \end{aligned}$$

By (1),

$$r(z) - e^z = \frac{(-1)^{q+1}}{Q(z)} \frac{1}{m!} z^{m+1} e^z \int_0^1 s^p (1-s)^q e^{-sz} \, ds, \tag{14}$$

where $z \in \mathbb{C}$, $z \neq \lambda_1, \ldots, \lambda_q$, and $p = q - 1$ (since r is subdiagonal). Thus,

$$\frac{e^{-z} r(z) - 1}{z^{m+1}} = \frac{(-1)^{q+1}}{Q(z)} \frac{1}{m!} \int_0^1 t^p (1-t)^q e^{-tz} \, dt,$$

and therefore

$$\begin{aligned} h_n(s) =& (-1)^{q+1} i^{m+1} \frac{1}{m!} \frac{1}{Q(iu(s))} \int_0^1 t^p (1-t)^q e^{-tiu(s)} \, dt \left[\frac{1}{n} \sum_{j=0}^{n-1} e^{-iju(s)} r(iu(s))^j \right] \\ =& g_n(s) \cdot f_n(s), \end{aligned} \tag{15}$$

where

$$\begin{aligned} g_n(s) &:= (-1)^{q+1} i^{m+1} \frac{1}{m!} \frac{1}{Q(iu(s))} \int_0^1 t^p (1-t)^q e^{-tiu(s)} \, dt \\ f_n(s) &:= \frac{1}{n} \sum_{j=0}^{n-1} e^{-iju(s)} r(iu(s))^j. \end{aligned}$$

Since r is $\mathscr{A}$-stable, $\sum_{j=0}^{n-1} e^{-iju(s)} r(iu(s))^j$ is bounded by n which implies that $|f_n(s)| \leq 1$ for all $s \in \mathbb{R}$. In order to estimate $g_n(s)$, recall from Proposition 1 that $\left|\frac{1}{Q(is)}\right| \leq 1$ for all $s \in \mathbb{R}$. Thus,

$$|g_n(s)| \leq \frac{1}{m!} \left| \int_0^1 t^p (1-t)^q e^{-tiu(s)} \, dt \right|.$$

Now

$$\int_0^1 t^p (1-t)^q e^{-tiu(s)} \, dt = \int_0^1 t^p (1-t)^q e^{-tin^{\frac{-1}{m+1}}s} \, dt,$$

and by substituting $\tau = n^{\frac{-1}{m+1}} t$, it follows that

$$\begin{aligned} \int_0^1 t^p (1-t)^q e^{-tin^{\frac{-1}{m+1}}s} \, dt =& n^{\frac{p+1}{m+1}} \int_0^{n^{\frac{-1}{m+1}}} \tau^p (1 - n^{\frac{1}{m+1}} \tau)^q e^{-i\tau s} \, d\tau \\ =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi_{n,m}(\tau) e^{i\tau s} \, d\tau, \end{aligned}$$

where

$$\Psi_{n,m}(\tau) := \sqrt{2\pi} n^{\frac{p+1}{m+1}} \begin{cases} \tau^p(1-n^{\frac{1}{m+1}}\tau)^q & : 0 \le \tau < n^{\frac{-1}{m+1}} \\ 0 & : \text{else} \end{cases}.$$

Then

$$\left\| \int_0^1 t^p(1-t)^q e^{-tiu(s)}\, dt \right\|_2 = \|\mathscr{F}(\Psi_{n,m}(t))\|_2 = \|\Psi_{n,m}\|_2$$

implies that

$$\left\| \int_0^1 t^p(1-t)^q e^{-tiu(s)}\, dt \right\|_2^2 = \|\mathscr{F}(\Psi_{n,m}(t))\|_2^2 = \|\Psi_{n,m}\|_2^2.$$

In order to estimate $\|\Psi_{n,m}\|_2^2$, the following representation of the Beta function is needed; see [1] Section 4.21. For $p, q > -1$ and $\Gamma(n+1) = n!$,

$$B(p+1, q+1) = \int_0^1 x^p(1-x)^q\, dx = \frac{\Gamma(p+1)\Gamma(q+1)}{\Gamma(p+q+2)}.$$

Then

$$\|\Psi_{n,m}\|_2^2 = \int_{-\infty}^{\infty} |\Psi_{n,m}(\tau)|^2\, d\tau = 2\pi n^{\frac{2(p+1)}{m+1}} \int_0^{n^{\frac{-1}{m+1}}} \tau^{2p}(1-n^{\frac{1}{m+1}}\tau)^{2q}\, d\tau.$$

Then, via the substitution $t = n^{\frac{1}{m+1}}\tau$,

$$\begin{aligned} 2\pi n^{\frac{2(p+1)}{m+1}} \int_0^{n^{\frac{-1}{m+1}}} \tau^{2p}(1-n^{\frac{1}{m+1}}\tau)^{2q}\, d\tau &= 2\pi n^{\frac{1}{m+1}} \int_0^1 t^{2p}(1-t)^{2q}\, dt \\ &= 2\pi n^{\frac{1}{m+1}} \frac{(2p)!(2q)!}{(2p+2q+1)!}. \end{aligned}$$

This implies that

$$\left\| \int_0^1 t^p(1-t)^q e^{-tiu(s)}\, dt \right\|_2^2 = 2\pi n^{\frac{1}{m+1}} \frac{(2p)!(2q)!}{(2p+2q+1)!}. \tag{16}$$

Returning to (15), it follows that $|h_n(s)| \le \frac{1}{m!} \left| \int_0^1 t^p(1-t)^q e^{-tiu(s)}\, dt \right|$. Therefore,

$$\begin{aligned} \|h_n\|_{L^2(\mathbb{R})}^2 \le \int_{-\infty}^{\infty} |g_n(s)|^2\, ds &\le \left(\frac{1}{m!}\right)^2 \left\| \int_0^1 t^p(1-t)^q e^{-tiu(s)}\, dt \right\|_2^2 \\ &= \left(\frac{1}{m!}\right)^2 \left[2\pi n^{\frac{1}{m+1}} \frac{(2p)!(2q)!}{(2p+2q+1)!} \right]. \end{aligned}$$

Hence,

$$\|h_n\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \le \|g_n\|_{L^2(\mathbb{R})}^{\frac{1}{2}} \le \frac{1}{\sqrt{m!}} \left[2\pi n^{\frac{1}{m+1}} \frac{(2p)!(2q)!}{(2p+2q+1)!} \right]^{\frac{1}{4}}. \tag{17}$$

Working towards an estimate for $\|h_n'\|_{L^2(\mathbb{R})}^{\frac{1}{2}}$, first recall that $h_n(s) = g_n(s) \cdot f_n(s)$ which implies $h_n'(s) = g_n'(s) f_n(s) + f_n'(s) g_n(s)$. Since $|a+b|^2 \le 2|a|^2 + 2|b|^2$, it follows that

$$\begin{aligned} \|h_n'\|_2^2 = \int_{-\infty}^{\infty} |h_n'(s)|^2\, ds &\le 2\int_{-\infty}^{\infty} |g_n'(s)|^2\, ds + 2\int_{-\infty}^{\infty} |f_n'(s) g_n(s)|^2\, ds \\ &= 2\|g_n'\|_2^2 + 2\|f_n' g_n\|_2^2. \end{aligned}$$

To estimate $\|g_n'\|_2$, notice that $g_n'(s)$ is given by

$$\frac{(-1)^{q+2} i^{m+2} n^{\frac{-1}{m+1}}}{m!} \frac{1}{Q(iu(s))} \left[\frac{Q'(iu(s))}{Q(iu(s))} \int_0^1 t^p (1-t)^q e^{-tiu(s)}\, dt + \int_0^1 t^{p+1} (1-t)^q e^{-tiu(s)}\, dt \right].$$

Recall from Propositions 1 and 2 that $\left|\frac{1}{Q(is)}\right| \leq 1$ and $\left|\frac{Q'(is)}{Q(is)}\right| \leq 1$ for all $s \in \mathbb{R}$. Using these facts and defining $c_1 := \left(\frac{n^{\frac{-1}{m+1}}}{m!}\right)^2$, it follows from (16) that

$$\begin{aligned}
\|g_n'\|_2^2 &\leq c_1 \int_{-\infty}^{\infty} \left| \int_0^1 t^p (1-t)^q e^{-tiu(s)}\, dt + \int_0^1 t^{p+1} (1-t)^q e^{-tiu(s)}\, dt \right|^2 ds \\
&\leq c_1 \int_{-\infty}^{\infty} \left[2 \left| \int_0^1 t^p (1-t)^q e^{-tiu(s)}\, dt \right|^2 + 2 \left| \int_0^1 t^{p+1} (1-t)^q e^{-tiu(s)}\, dt \right|^2 \right] ds \\
&\leq c_1 \left[2 \left(2\pi n^{\frac{1}{m+1}} \frac{(2p)!(2q)!}{(2p+2q+1)!} \right) + 2 \left(2\pi n^{\frac{1}{m+1}} \frac{(2p+2)!(2q)!}{(2p+2q+3)!} \right) \right].
\end{aligned}$$

Then,

$$\|g_n'\|_2^2 \leq \frac{4\pi}{(m!)^2} \frac{1}{n^{\frac{1}{m+1}}} \frac{(2p)!(2q)!}{(2p+2q+1)!} \left[1 + \frac{(2p+2)(2p+1)}{(2p+2q+3)(2p+2q+2)} \right].$$

To estimate $\|f_n' g_n\|_2^2$, recall that $f_n(s) = \frac{1}{n} \sum_{j=0}^{n-1} e^{-iju(s)} r(iu(s))^j$. This implies that

$$\begin{aligned}
f_n'(s) = &\frac{1}{n} \sum_{j=0}^{n-1} e^{-iju(s)} (-iju'(s)) r(iu(s))^j \\
&+ \frac{1}{n} \sum_{j=0}^{n-1} e^{-iju(s)} j r(iu(s))^{j-1} r'(iu(s)) iu'(s).
\end{aligned}$$

By Proposition 2, $|r'(iu(s))| \leq 2$ for all $s \in \mathbb{R}$. Thus,

$$|f_n'(s)| \leq \frac{3}{n} |u'(s)| \sum_{j=0}^{n-1} j = \frac{3}{n} n^{\frac{-1}{m+1}} \frac{(n-1)n}{2} = \frac{3}{2}(n-1) n^{\frac{-1}{m+1}}.$$

It follows from (16) that

$$\begin{aligned}
\|f_n' g_n\|_2^2 &\leq \left[\frac{3}{2}(n-1) n^{\frac{-1}{m+1}} \right]^2 \|g_n\|_2^2 \\
&\leq \left[\frac{3}{2}(n-1) n^{\frac{-1}{m+1}} \right]^2 \frac{1}{(m!)^2} 2\pi n^{\frac{1}{m+1}} \frac{(2p)!(2q)!}{(2p+2q+1)!}.
\end{aligned}$$

This means that

$$\begin{aligned}
\|h_n'\|_2^2 &\leq 2\|g_n'\|_2^2 + 2\|f_n' g_n\|_2^2 \\
&\leq \frac{8\pi}{(m!)^2} \frac{1}{n^{\frac{1}{m+1}}} \frac{(2p)!(2q)!}{(2p+2q+1)!} \left[1 + \frac{(2p+2)(2p+1)}{(2p+2q+3)(2p+2q+2)} \right]
\end{aligned}$$

$$+\frac{4\pi}{(m!)^2}\left[\frac{3}{2}(n-1)n^{\frac{-1}{m+1}}\right]^2 n^{\frac{1}{m+1}}\frac{(2p)!(2q)!}{(2p+2q+1)!}$$
$$\leq \frac{8\pi}{(m!)^2}\frac{(2p)!(2q)!}{(2p+2q+1)!}\frac{1}{n^{\frac{1}{m+1}}}\left[\left(1+\frac{(2p+2)(2p+1)}{(2p+2q+3)(2p+2q+2)}\right)\right.$$
$$\left.+\frac{3}{4}(n-1)^2\right].$$

Since $p=q-1$, we have that

$$1+\frac{(2p+2)(2p+1)}{(2p+2q+3)(2p+2q+2)}+\frac{3}{4}(n-1)^2 = 1+\frac{2q-1}{2(4q+1)}+\frac{3}{4}(n-1)^2 \leq \frac{5}{4}n^2.$$

It follows that

$$\|h_n'\|_2^2 \leq \frac{8\pi}{(m!)^2}\frac{(2p)!(2q)!}{(2p+2q+1)!}\frac{1}{n^{\frac{1}{m+1}}}\left[\frac{5}{4}n^2\right].$$

Recalling the estimate for $\|h_n\|_{L^2(\mathbb{R})}^{\frac{1}{2}}$ from (17), it follows that

$$\|h_n\|_2^{\frac{1}{2}}\|h_n'\|_2^{\frac{1}{2}} \leq \frac{1}{\sqrt{m!}}\left[2\pi n^{\frac{1}{m+1}}\frac{(2p)!(2q)!}{(2p+2q+1)!}\right]^{\frac{1}{4}}\cdot\frac{1}{\sqrt{m!}}\left[10\pi\frac{n^2}{n^{\frac{1}{m+1}}}\frac{(2p)!(2q)!}{(2p+2q+1)!}\right]^{\frac{1}{4}}$$
$$\leq \frac{20^{1/4}\sqrt{\pi}}{m!}n^{\frac{1}{2}}\left(\frac{(2p)!(2q)!}{(2p+2q+1)!}\right)^{\frac{1}{2}}$$
$$\leq \frac{20^{1/4}\sqrt{\pi}}{m!}n^{\frac{1}{2}}\left(\frac{(m-1)!(m+1)!}{(2m+1)!}\right)^{\frac{1}{2}}$$

since $m=p+q=2q-1=2p+1$. Thus, by (13),

$$\left\|r\left(\frac{t}{n}A\right)^n x - T(t)x\right\| \leq M\frac{2\sqrt{\pi}}{m!}\frac{1}{n^{m-\frac{1}{2}}}\left(\frac{(m-1)!(m+1)!}{(2m+1)!}\right)^{\frac{1}{2}} t^{m+1}\|A^{m+1}x\|.$$

This completes the proof of estimate (5). □

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