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CONVERGENCE RATES FOR THE TROTTER-KATO SPLITTING

SIMON BECKER*, NIKLAS GALKE†, ROBERT SALZMANN‡, AND LAURITZ VAN LUIJK§

ABSTRACT. We study convergence rates of the Trotter-Kato splitting

$$e^{A+L} = \lim_{n \rightarrow \infty} \left(e^{L/n} e^{A/n} \right)^n$$

in the strong operator topology. In the first part, we use complex interpolation theory to treat generators L and A of contraction semigroups on Banach spaces, with L relatively A -bounded. In the second part, we study unitary dynamics on Hilbert spaces and develop a new technique based on the concept of energy constraints. Our results provide a complete picture of the convergence rates for the Trotter splitting for all common types of Schrödinger and Dirac operators, including singular, confining and magnetic vector potentials, as well as molecular many-body Hamiltonians in dimension $d = 3$. Using the Brezis-Mironescu inequality, we derive convergence rates for the Schrödinger operator with $V(x) = \pm|x|^{-a}$ potential. In each case, our conditions are fully explicit.

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1. INTRODUCTION

We derive explicit convergence rates for the Trotter-Kato splitting formula, which, under suitable assumptions on A and L , states that

$$e^{A+L} = \lim_{n \rightarrow \infty} \left(e^{L/n} e^{A/n} \right)^n \quad (1.1)$$

in the strong operator topology. Originally developed by Lie for matrices, it has been extended to operators by Trotter [T59], Chernoff [C68], and Kato [K78]. Nelson [N64] clarified the connection between the splitting formula to Feynman's path integral for the Schrödinger dynamics. The formula is also of key importance in numerical applications [Paz83, S94, JL00, Sec. 3.6], where the Trotter formula is also often referred to as Strang splitting, as it, for example, allows the separation of differential from multiplication operators in applications in quantum mechanics. For applications, convergence rates are important as they give a promise on the quality of the approximation. However, uniform convergence rates, i.e., convergence rates in operator norm, are typically not feasible since the Trotter product formula simply does not converge uniformly in general [I03, Sec. 4]. This motivates the study of convergence rates in the strong operator topology. That is, for a vector x , we are interested in the speed of convergence

$$\| (e^{L/n} e^{A/n})^n x - e^{A+L} x \| \rightarrow 0. \quad (1.2)$$

While a convergence rate of $\mathcal{O}(n^{-1})$ is guaranteed in finite dimensions, or more generally for bounded generators, this does not hold in general: It was shown in [B+23a] that the splitting of the Coulomb Hamiltonian $H = -\Delta - |x|^{-1}$, describing the hydrogen atom, converges with $\mathcal{O}(n^{-1/4})$ on (eigenstates in) s-orbitals, $\mathcal{O}(n^{-3/4})$ on p-orbitals and with $\mathcal{O}(n^{-1})$ on d- and higher orbitals. Their technique of establishing strong convergence

rates is restricted to the Hilbert space setting and to eigenvectors of $A + L$. In this article, we relax these restrictions by proving strong convergence rates on sufficiently regular vectors also in the Banach space setting, recovering, in particular, a form of $\mathcal{O}(n^{-1/4})$ convergence for the ground state of the hydrogen atom.

Our article features two directions. In the first part of the article, Section 2, our guiding principle is to develop a theory to obtain convergence rates under the assumption that L is “small” compared to A . We gauge the smallness using a relative boundedness condition of the operators. In this case, the appropriate notion of regularity is captured using special interpolation spaces defined through A , which are called *Favard spaces* and which we can characterize explicitly in many relevant cases. For Schrödinger operators, for instance, in terms of standard Sobolev spaces. We demand that L does not decrease this form of regularity by too much, i.e., when applied to a vector of high regularity, the output should remain regular, though possibly to a lesser extent. After establishing $\mathcal{O}(n^{-1})$ -convergence rates for (1.2) for sufficiently regular vectors x and for suitable L , we prove $\mathcal{O}(n^{-\delta})$ -convergence rates with $0 < \delta < 1$ on less regular vectors and for very general, but still relatively A -bounded L . The guiding motive for this first part of the article is to understand the convergence rates of the Trotter-splitting of Schrödinger operators with singular potentials. For instance, we find for the three-dimensional Coulomb potential

$$\left\| \left(e^{-it|x|^{-1}/n} e^{-it\Delta/n} \right)^n \psi - e^{it(-\Delta - |x|^{-1})} \psi \right\| \lesssim n^{-1/4+\varepsilon} \|\psi\|_{H^2(\mathbb{R}^3)} \quad (1.3)$$

for any fixed $\varepsilon > 0$ (cp. Corollary 2.22). Numerical evidence from [B+23a] suggests that, on the ground state, the true convergence rate is indeed $n^{-1/4}$. Thus, we expect our estimate to be essentially tight. Proving an analytical lower bound, however, remains an open problem.

In the second part of the article, in Section 3, the guiding motive is to understand Schrödinger operators with confining or trapping potentials. In this case, the kinetic energy and potential energy are not in any sense small with respect to one another. A standard example of such an operator is the quantum harmonic oscillator. To treat the Trotter splitting of such operators, we develop a new approach based on the concept of *energy constraints* [W17, S18, S20, vL24]. This approach differs from the first one due to the different nature of the perturbation. As a prototypical example of the results obtained with this approach, we mention the following convergence rate

$$\left\| \left(e^{-i\frac{t}{n}\Delta} e^{i\frac{t}{n}x^2} \right)^n \psi - e^{it(-\Delta+x^2)} \psi \right\| \leq \frac{6t^2}{n} \left\| (-\Delta + x^2) \psi \right\| \quad (1.4)$$

for the Trotter splitting of the harmonic oscillator on $L^2(\mathbb{R})$ (cp. Theorem 3.15).

Taken together, the two approaches yield a fairly complete understanding of Trotter convergence rates for closed quantum systems. The general nature of the first approach allows us to apply it to a much larger class of dynamical systems beyond just closed

quantum systems. We outline this in the first few sections of the article. The approach outlined in the second part of the article is limited to unitary dynamics on Hilbert spaces.

1.1. Techniques. Both approaches for providing convergence rates for the Trotter-Kato product formula (1.1) in Sections 2 and 3 follow similar proof techniques but diverge at certain points as we explain in the following:

Step 1: Key commutator bound. In both Sections 2 and 3, the first step of bounding the Trotter error is to use a telescoping sum argument, which gives for x of sufficient regularity

$$\|(e^{L/n}e^{A/n})^n x - e^{A+L}x\| \leq \sup_{s,\tau \in [0,1]} \|[L, e^{sA/n}]x_\tau\|. \quad (1.5)$$

Here, we can either have that x_τ is the original element x evolved by the joined dynamics, i.e. $x_\tau := e^{\tau(A+L)}x$, or by the product dynamics, i.e. $x_\tau := (e^{L/n}e^{A/n})^{\lfloor \tau n \rfloor}x$. We call this the *key commutator bound*, which can be found in Lemma 2.1 or by combining Lemma 3.6 and the relevant steps in the proof of Theorem 3.5.

Step 2: Stability of regularity. Next, we need to ensure that the evolved element x_τ has comparable regularity as the initial x . The way we quantify regularity depends on the context: In Section 2, we are in the regime in which A is the dominant generator as L is relatively bounded with A -bound < 1 . Hence, in this case, it is sensible to focus on notions of regularity defined through the generator A . In particular for that we consider the Favard spaces $F_\gamma(A)$ which for $\gamma \in [0, 1]$ are exactly given by elements x such that $\|(e^{tA} - I)x\| = \mathcal{O}(t^\gamma)$. Hence, higher values of γ correspond to higher regularity of the element x . For $x \in F_\gamma(A)$ the relative boundedness assumptions on L employed gives, by the stability result on Favard spaces Lemma 2.6, that also $x_\tau \in F_\gamma(A)$ where we chose $x_\tau = e^{\tau(A+L)}x$ in the above.

On the other hand, in Section 3, the role of A and L is symmetric. The right notion of regularity is given by the *energy* of a vector x as measured by a positive self-adjoint operator G , the ‘reference Hamiltonian’. We are free to choose this reference Hamiltonian as long as the dynamics generated A and L are energy-limited with respect to G in the sense of [vL24]. This ensures that x_τ above is of comparable regularity as the initial element x .

Step 3: Bounding the key commutator. As the final step, we need to estimate the key commutator, which appears on the right-hand side of (1.5). In Section 2 we write

$$[L, e^{sA/n}]x_\tau = L(e^{sA/n} - I)x_\tau - (e^{sA/n} - I)Lx_\tau \quad (1.6)$$

and bound each term individually. For the first term, we assume that the singularity of L is controlled when the operator is restricted to elements of sufficient regularity. More, precisely we assume that L is bounded on the Favard space $F_\alpha(A)$ for some

$0 \leq \alpha < \gamma$ from which we see that the first term decays as $\mathcal{O}(n^{-(\gamma-\alpha)})$. For the second term we assume that L does not decrease the regularity of $x_\tau \in F_\gamma(A)$ by too much. In particular if we still have $Lx_\tau \in F_\beta(A)$ for some $0 < \beta \leq \gamma$ the second term in (1.6) decays as $\mathcal{O}(n^{-\beta})$. Both assumptions on how L interacts with the notion of regularity dictated by A can explicitly be verified for many interesting examples, e.g., Schrödinger operators with Coulomb-type potentials and molecular Hamiltonians as shown at the end of Section 2.5.1.

In Section 3, we choose a different approach to bound the right-hand side of (1.5) by using

$$\|[L, e^{sA/n}]x_\tau\| \leq \frac{s}{n} \sup_{u \in [0, s]} \|[L, A]x_{\tau, u}\|, \quad (1.7)$$

where $x_{\tau, u} := e^{uA/n}x_\tau$. Under the above assumption of energy limitedness and given that the commutator $[L, A]$ is bounded with respect to $G^{1/2}$, the norm appearing on the right-hand side of (1.7) is indeed finite and we find that the Trotter error decays as $\mathcal{O}(n^{-1})$.

1.2. Related works. Our article outlines an approach to obtain initial state-dependent convergence rates for such splittings. Trotter schemes with applications to quantum mechanics have been improved in various directions, for example, for bosonic systems [M24], lattice systems [BL22], and in the context of the quantum Zeno effect [EI05, MW19, BDS21, MR23]. Our approach is different in the sense that we try to provide a framework that covers a wide range of, in some sense, singular splittings that are not covered by most results in the literature. While little about convergence rates beyond standard cases seems to be known in the quantum setting, a more elaborate theory is available for strictly dissipative dynamics; see [NSZ18, NSZ18b, NSZ19] and references therein. A strength of our approach is that it unites several types of dynamics under one umbrella approach. Finally, many works such as [M24] also consider generalizations of the Trotter Formula and applications to non-autonomous systems [NSZ20]. An overview of the current state of results can also be found in [ZNI24]. While our method also allows for such generalizations, we decided to focus on the most basic setting and will consider such applications in future work. State-dependent error bounds for quantum systems have been discussed in [AFL21, B+23b, B+23a, B+24, vL+24, vL24]. In particular, [B+23b, B+23a] prove state-dependent convergence for the Trotter product for more restrictive sets of vectors than what we are able to treat in this article. The idea of applying energy constraints to obtain state-dependent convergence rates was used before in the context of Lie group representations and so-called quantum speed limits [BD20, B+21, vL+24].

1.3. Outline of the article. In the first part of the article, we study the case of generators A and L where L is relatively A bounded with A -bound < 1 .

- In Section 2.1, we state in Theorem 2.2 a vanilla convergence result with $\mathcal{O}(n^{-1})$ Trotter convergence rate under fairly general assumptions on L and A .
- In Section 2.2, we introduce Favard spaces and discuss some of their properties. These interpolation spaces capture the propagation of regularity of data under the time evolution of contraction semigroups.
- In Section 2.3, we embed with our Theorem 2.7 the result of the previous section into the broader framework of Favard spaces and convergence rates.
- In Section 2.4 we apply the framework of Section 2.2 to the Trotter product of generators of contraction semigroups. We start with so-called positive generators, in which case one can easily define fractional powers and obtain Corollary 2.13 on the convergence of the Trotter product.
- In Section 2.5, we discuss applications for self-adjoint A .
- In Section 2.5.1, we turn to unitary dynamics, which covers the realm of Schrödinger dynamics in quantum mechanics. We provide an extensive discussion of the Trotter splitting for molecular Hamiltonians with Coulomb singularity, cf. Theorem 2.23.

In Section 3, we use a recently-developed framework of energy constraints to obtain general convergence rates in Theorem 3.5 and Corollary 3.9, which we illustrate in the subsequent Subsections:

- In Section 3.1, we apply Theorem 3.5 to show a $\mathcal{O}(n^{-1})$ convergence for all Schrödinger operators whose potentials have bounded second derivative.
- In Section 3.2, we apply the findings of Section 3.1 to the harmonic oscillator to obtain the convergence rate in (1.4).
- In Section 3.3, we discuss applications to Dirac operators, such as magnetic Dirac operators.

In Section 4, we illustrate our findings with some numerical experiments.

Notation. We denote the identity operator by I , write $a \lesssim b$ and $a = \mathcal{O}(b)$ to indicate that there is a constant $C > 0$ such that $a \leq Cb$ and furthermore $a \sim b$ if $a \lesssim b$ and $b \lesssim a$. We denote the resolvent set by $\rho(A)$ and its complement, the spectrum, by $\text{Spec}(A)$. The space of bounded operators between Banach spaces X and Y is denoted $B(X, Y)$ and the corresponding operator norm of a linear operator $T : X \rightarrow Y$ is denoted by $\|T\|_{X \rightarrow Y} := \sup_{\|x\|_X \leq 1} \|Tx\|_Y$. We use the so-called Japanese bracket notation $\langle \xi \rangle := (1 + |\xi|^2)^{1/2}$ for vectors $\xi \in \mathbb{R}^n$.

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2. TROTTER CONVERGENCE UNDER RELATIVE BOUNDEDNESS

In this section, we obtain convergence rates for the Trotter-Kato product formula (1.1) under the assumption that one of the generators, say L , is relatively bounded by the other: We say L is *relatively A -bounded* if $D(A) \subseteq D(L)$ and there exist $a, b \geq 0$ such that for all $x \in D(A)$ we have

$$\|Lx\| \leq a\|Ax\| + b\|x\|. \tag{2.1}$$

We call the infimum over all a for which there is a $b \geq 0$ such that the above inequality holds the *A -bound* of L .

For the remainder of this section, we consider situations in which L is relatively A -bounded with A -bound < 1 . The first consequence of this assumption is that for L and A being generators of C_0 contraction semigroups¹, also $A + L$ with domain $D(A + L) = D(A)$ defines a C_0 contraction semigroup [EN00, Thm. 2.7]. The joint dynamics $e^{t(A+L)}$ therefore leaves $D(A)$ invariant. As A is closed [EN00, Thm. 1.4], $D(A)$ becomes a Banach space when equipped with the graph norm $\|x\|_{D(A)} = \|x\| + \|Ax\|$ and $e^{t(A+L)} : D(A) \rightarrow D(A)$ is a bounded operator by the closed graph theorem. The latter can be seen explicitly by noting that since the A -bound of L is strictly smaller than 1, the graph norms of A and $A + L$ are equivalent: In fact, for $x \in D(A)$, we have

$$\|Ax\| \leq \|(A + L)x\| + \|Lx\| \leq \|(A + L)x\| + a\|Ax\| + b\|x\|$$

and hence

$$\|Ax\| \leq \frac{1}{1 - a} \left(\|(A + L)x\| + b\|x\| \right)$$

and furthermore

$$\|(A + L)x\| \leq \|Ax\| + \|Lx\| \leq (1 + a) \|Ax\| + b\|x\|$$

¹We call a C_0 semigroup $(T_t)_{t \geq 0}$ a contraction semigroup if all maps T_t are contractions, i.e., $\|T_t\| \leq 1$.

which gives $\|x\|_{D(A)} \sim \|x\|_{D(A+L)}$.²

In this regime, obtaining convergence rates in the Trotter-Kato formula reduces to studying the commutator $[L, e^{sA/n}]$, which from now on we shall refer to as the *key commutator*. This is the content of the following lemma:

Lemma 2.1 (Key commutator bound). *Let X be a Banach space and L and A be generators of strongly continuous contraction semigroups on X such that L is relatively A -bounded, with A -bound < 1 . Then for all $n \in \mathbb{N}$, $t \geq 0$ and $x \in D(A)$ we have*

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) x \right\| \leq t \sup_{s, \tau \in [0, t]} \left\| [L, e^{sA/n}] e^{\tau(A+L)} x \right\|.$$

Proof of Lemma 2.1. By the semigroup property, it is easy to check that we can write the operator difference of interest as a telescoping sum, i.e.

$$(e^{tL/n} e^{tA/n})^n - e^{t(A+L)} = \sum_{j=0}^{n-1} (e^{tL/n} e^{tA/n})^j (e^{tL/n} e^{tA/n} - e^{t(A+L)/n}) e^{t(n-j-1)(A+L)/n}.$$

Therefore, we see for $x \in D(A)$ using that $e^{tA/n}$ and $e^{tL/n}$ are contractions

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) x \right\| \leq \sum_{j=0}^{n-1} \left\| (e^{tL/n} e^{tA/n} - e^{t(A+L)/n}) e^{t(n-j-1)(A+L)/n} x \right\|.$$

Now, using that by the relative boundedness assumption $D(A+L) = D(A)$, we can write for all $y \in D(A) \subseteq D(L)$ ³

$$\begin{aligned} (e^{tL/n} e^{tA/n} - e^{t(A+L)/n}) y &= \int_0^1 \frac{d}{ds} (e^{stL/n} e^{stA/n} e^{(1-s)t(A+L)/n}) y ds \\ &= \frac{t}{n} \int_0^1 (e^{stL/n} L e^{stA/n} e^{(1-s)t(A+L)/n} - e^{stL/n} e^{stA/n} L e^{(1-s)t(A+L)/n}) y ds \\ &= \frac{t}{n} \int_0^1 e^{stL/n} [L, e^{stA/n}] e^{(1-s)t(A+L)/n} y ds. \end{aligned} \quad (2.2)$$

Plugging this into the telescopic sum, we find

$$\begin{aligned} \left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) x \right\| &\leq \frac{t}{n} \sum_{j=0}^{n-1} \left\| \int_0^1 e^{stL/n} [L, e^{stA/n}] e^{(n-j-s)t(A+L)/n} x ds \right\| \\ &\leq t \sup_{s, \tau \in [0, t]} \left\| [L, e^{sA/n}] e^{\tau(A+L)} x \right\|. \end{aligned}$$

□

²To conclude the boundedness of $e^{t(A+L)} : D(A) \rightarrow D(A)$ use $\|e^{t(A+L)} x\|_{D(A)} \lesssim \|e^{t(A+L)} x\|_{D(A+L)}$ together with $\|(A+L)e^{t(A+L)} x\| = \|e^{t(A+L)}(A+L)x\| \leq \|(A+L)x\| \lesssim \|x\|_{D(A)}$ where we used that $e^{t(A+L)}$ is a contraction.

³Note that the integral in (2.2) is well-defined as a Bochner integral as the integrand is continuous, which is true by L being relatively A -bounded and the graph norms of A and $A+L$ being equivalent.

2.1. Elementary $\mathcal{O}(n^{-1})$ scaling for regular L . In this section, we provide a first simple derivation of convergence rates for the Trotter product formula using the key commutator bound established in Lemma 2.1. We aim for a point-wise estimate with the Trotter product being applied to a fixed Banach space element of sufficient regularity, say $x \in D(A^2)$. Then, for generators L , which do not decrease this regularity by too much (with the precise meaning given in the following), we derive a $\mathcal{O}(n^{-1})$ convergence rate of the Trotter product.

Denoting the semigroup generated by A by $T_t = e^{tA}$ and furthermore $x_\tau := e^{\tau(A+L)}x$, we observe that we can decompose the key commutator in Lemma 2.1 as

$$[L, T_{s/n}]x_\tau = L(T_{s/n} - I)x_\tau - (T_{s/n} - I)Lx_\tau. \quad (2.3)$$

To estimate both terms on the right-hand side, we use here that for $y \in D(A)$, we have

$$\|(T_{s/n} - I)y\| = \frac{s}{n} \left\| \int_0^1 T_{s/n} A y \, dr \right\| \leq \frac{s}{n} \|Ay\|. \quad (2.4)$$

Hence, the first term in (2.3) can easily be estimated under the additional assumption that the joined dynamics $e^{\tau(A+L)}$ leaves $D(A^2)$ invariant and therefore

$$x_\tau \in D(A^2). \quad (2.5)$$

In this case using that L is relatively A -bounded as (2.1), we see

$$\|L(T_{s/n} - I)x_\tau\| \leq a\|A(T_{s/n} - I)x_\tau\| + b\|(T_{s/n} - I)x_\tau\| \leq \frac{s}{n} (a\|A^2x_\tau\| + b\|Ax_\tau\|).$$

Furthermore, the second term on the right-hand side of (2.3) can also be estimated, assuming that

$$Lx_\tau \in D(A), \quad (2.6)$$

in which case we have

$$\|(T_{s/n} - I)Lx_\tau\| \leq \frac{s}{n} \|ALx_\tau\|.$$

Both assumption (2.5) and (2.6) are fulfilled if L satisfies $LD(A^2) \subseteq D(A)$ and furthermore

$$\|ALy\| \leq a'\|A^2y\| + b'\|y\| \quad (2.7)$$

for some $0 \leq a' < 1$ and $b' \geq 0$ and all $y \in D(A^2)$. In fact (2.7) together with [P18, Lem. IV.3] gives that $D((A+L)^2) = D(A^2)$ and therefore that the restriction $e^{\tau(A+L)}|_{D(A^2)} : D(A^2) \rightarrow D(A^2)$ defines a well-defined, bounded operator from which we can conclude that $x_\tau \in D(A^2)$ and $Lx_\tau \in D(A)$ using $x \in D(A^2)$. Combining all of the above, we arrive at the following result, which we can think of as a straightforward operator theoretic generalization of the $\mathcal{O}(n^{-1})$ convergence rate for matrices.

Theorem 2.2 (Perturbative $\mathcal{O}(n^{-1})$ -Trotter). *Let X be a Banach space and $(L, D(L))$ and $(A, D(A))$ with $D(A) \subseteq D(L)$ generators of contraction semigroups. Assume there exist $0 \leq a < 1$ and $b \geq 0$ such that*

$$\|Lx\| \leq a\|Ax\| + b\|x\| \quad (2.8)$$

for all $x \in D(A)$. Moreover, assume that $LD(A^2) \subseteq D(A)$ and that there exist $0 \leq a' < 1$ and $b' \geq 0$ such that

$$\|ALx\| \leq a'\|A^2x\| + b'\|x\| \quad (2.9)$$

for all $x \in D(A^2)$. Then for all $n \in \mathbb{N}$, $t \geq 0$ and $x \in D(A^2)$ we have

$$\left\| \left(e^{tL/n} e^{tA/n} \right)^n - e^{t(A+L)} \right\| x \left\| \leq \frac{t^2}{n} (c_2\|A^2x\| + c_1\|Ax\| + c_0\|x\|) \quad (2.10)$$

for some $c_i \geq 0$ depending only on a, b, a' and b' . If we can choose $b = 0$, then $c_1 = 0$. If additionally $b' = 0$ then also $c_0 = 0$.

A formal proof of this result in which the constants c_0, c_1, c_2 are expressed in terms of a, b, a', b' can be found in Appendix A.

In many circumstances, the requirements of Theorem 2.2 are too strong for many practically relevant generators A and L . In particular, as we see below, the assumption $LD(A^2) \subseteq D(A)$ is not satisfied in the case of Schrödinger operators with singular potentials, e.g., $X = L^2(\mathbb{R}^3)$, $A = -i\Delta$ and multiplication operator $L = iV$ corresponding to the potential $V(x) = \pm|x|^{-1}$. To also be able to treat these cases, we extend the argument of Theorem 2.2 using milder regularity assumptions. For that, we use the so-called *Favard spaces* of A , which are interpolation spaces between the underlying Banach space X and the domains $D(A^k)$ for $k \in \mathbb{N}$. It turns out those provide a more nuanced regularity analysis compared to the setting of Theorem 2.2 leading to convergence rates of the Trotter product given by fractional powers of n^{-1} .

In the next section, we review the theory of Sobolev towers and Favard spaces of generators of C_0 contraction semigroups. After that, in Section 2.3, we provide an extension of Theorem 2.2 involving Favard spaces (see Theorem 2.7).

2.2. Sobolev towers and Favard spaces. For A being the generator of a strongly continuous contraction semigroup on some Banach space X the corresponding Sobolev tower is defined as follows: For $k \in \mathbb{N}_0$ consider the space $D(A^k)$, where $D(A^0) = X$, equipped with the graph norms $\|x\|_{D(A^k)} = \|x\| + \|A^kx\|$. The graph norm is equivalent to the sum of all $\|A^l x\|$ for $l \leq k$ [P18, Lem. II.10], i.e.

$$\|x\|_{D(A^k)} \lesssim \sum_{l=0}^k \|A^l x\| \lesssim \|x\|_{D(A^k)}. \quad (2.11)$$

Since A^k is a closed operator [P18, Lemma II.8, Lemma II.9], $D(A^k)$ is a Banach space. Furthermore, for $(T_t)_{t \geq 0}$ being the strongly continuous contraction semigroup generated by A , we have that the restrictions $T_t|_{D(A^k)}$ define strongly continuous semigroups with generator given by the restriction $A|_{D(A^{k+1})}$.

Inspired by the fact that A satisfies $\sup_{\lambda > 0} \|\lambda(\lambda - A)^{-1}\| < \infty$ [EN00, Thm. 3.5], we can define complex interpolation spaces between the different levels of the Sobolev tower: For that, let $\alpha \in (0, \infty)$ and furthermore $r_\alpha \in (0, 1]$ and $k_\alpha \in \mathbb{N}_0$ be the unique numbers such that $\alpha = r_\alpha + k_\alpha$. One then obtains complex interpolation spaces $(D(A^{k_\alpha}), D(A^{k_\alpha+1}))_{r_\alpha, \infty}$, commonly referred to as *Favard spaces*, of the form [L09, Prop. 3.1]

$$F_\alpha \equiv F_\alpha(A) \equiv F_\alpha(A; X) := \left\{ x \in D(A^{k_\alpha}); |x|_{F_\alpha} := \sup_{\lambda > 0} \|\lambda^{r_\alpha} A(\lambda - A)^{-1}x\|_{D(A^{k_\alpha})} < \infty \right\}.$$

Here, for later convenience, we introduced the notation $F_\alpha(A; X)$ explicitly denoting the Banach space X from which the Favard spaces are constructed. These spaces naturally become Banach spaces when equipped with an interpolation norm that is equivalent to $\|x\|_{F_\alpha} := \|x\|_{D(A^{k_\alpha})} + |x|_{F_\alpha}$. In particular, for $\alpha \in (0, 1]$, the Favard spaces F_α are interpolation spaces between the Banach space X and the domain $D(A)$. Furthermore, for $\alpha \geq 1$ the Favard space F_α can equivalently be understood as a Favard space of order $r_\alpha \in (0, 1]$ but with $D(A^{k_\alpha})$ as the underlying Banach space instead of X , i.e.

$$F_\alpha(A; X) = F_{r_\alpha}(A; D(A^{k_\alpha})). \quad (2.12)$$

Example 2.3. We consider the heat semigroup on $X = C_b(\mathbb{R}^d)$, see [BF19]. Its generator $A = \Delta$ has a domain $D(\Delta) = C_b^2(\mathbb{R}^d)$ for $d = 1$, while for $d \geq 2$ the domain is given by

$$D(\Delta) = \{f \in C_b(\mathbb{R}^d) \cap W^{2,p}(\mathbb{R}^d), \text{ for all } p \in [1, \infty) \text{ and } \Delta f \in C_b(\mathbb{R}^d)\}.$$

Then for $\alpha \in (0, 1) \setminus \{1/2\}$ the Favard spaces are the Hölder spaces

$$F_\alpha = C_b^{2\alpha}(\mathbb{R}^d)$$

of bounded continuous functions that are 2α Hölder continuous and for $\alpha = 1/2$

$$F_{1/2} = \left\{ f \in C_b(\mathbb{R}^d); \sup_{x,y} \frac{|f(x) + f(y) - 2f((x+y)/2)|}{|x-y|} < \infty \right\}.$$

Remark 2.4. One can define Sobolev towers and Favard spaces more generally for operators A only assuming $(0, \infty) \subseteq \rho(A)$ and $\sup_{\lambda > 0} \|\lambda(\lambda - A)^{-1}\| \leq C$ for some $C > 0$. Under this assumption, all statements in this section remain true apart from (2.17) below and the ones explicitly involving the semigroup T_t . Note that in the special case $C = 1$ and A being densely defined, A is immediately closed since $\rho(A) \neq \emptyset$ and hence this assumption is equivalent to A being the generator of a strongly continuous contraction semigroup [EN00, Thm. 3.5].

Note that for all $k \in \mathbb{N}_0$ and $k < \alpha \leq \beta \leq k + 1$ we have $D(A^{k+1}) \subseteq F_{k+1} \subseteq F_\beta \subseteq F_\alpha \subseteq D(A^k)$. Furthermore, for all $0 < \alpha \leq \beta$ and $x \in F_\beta$ we have the upper bound⁴

$$\|x\|_{F_\alpha} \lesssim \|x\|_{F_\beta}. \quad (2.13)$$

The importance of these spaces is in their relationship to the asymptotic behavior of associated semigroups. Indeed, we have the equivalent characterization [L09, Prop. 5.7]

$$F_\alpha = \left\{ x \in D(A^{k_\alpha}); \sup_{t>0} \|t^{-r_\alpha}(T_t x - x)\|_{D(A^{k_\alpha})} < \infty \right\}. \quad (2.14)$$

In particular, for $x \in F_\alpha$ we have

$$\|T_t x - x\|_{D(A^{k_\alpha})} = \mathcal{O}(\|x\|_{F_\alpha} t^{r_\alpha}). \quad (2.15)$$

In this context, it is useful to note that the Favard norm $\|x\|_{F_\alpha}$ is equivalent to

$$\|x\|_{D(A^{k_\alpha})} + \sup_{t>0} \|t^{-r_\alpha}(T_t - I)x\|_{D(A^{k_\alpha})}. \quad (2.16)$$

Furthermore, in the special case of analytic semigroups, the Favard spaces are equivalently described by the elements $x \in X$ for which the $\|x\|_{F_\alpha}$ equivalent norm

$$\|x\|_{D(A^{k_\alpha})} + \sup_{t \in (0,1)} t^{1-r_\alpha} \|AT_t x\|_{D(A^{k_\alpha})}$$

is finite.

The following lemma generalises (2.15) from the norms on X and $D(A^k)$ to the Favard norms.

Lemma 2.5. *Let A be the generator of a strongly continuous contraction semigroup $(T_t)_{t \geq 0}$ and $\alpha, \gamma \in (0, \infty)$ such that $\alpha \leq \gamma$. Then, for $\gamma' = \min\{\gamma - \alpha, 1\}$*

$$\|T_t - I\|_{F_\gamma \rightarrow F_\alpha} = \mathcal{O}\left(t^{\gamma'}\right).$$

Proof. For the proof, we use that

$$\|T_t - I\|_{F_\gamma \rightarrow F_\alpha} \lesssim \|T_t - I\|_{F_\gamma \rightarrow D(A^{k_\alpha})} + \sup_{s>0} \|s^{-r_\alpha}(T_s - I)(T_t - I)\|_{F_\gamma \rightarrow D(A^{k_\alpha})}. \quad (2.17)$$

First consider the case $\gamma - \alpha < 1$. In that case $k_\alpha = k_\gamma$ and hence $\gamma - \alpha = r_\gamma - r_\alpha \geq 0$. To bound the second term in (2.17) we use

$$\begin{aligned} & \sup_{s>0} \|s^{-r_\alpha}(T_s - I)(T_t - I)\|_{F_\gamma \rightarrow D(A^{k_\alpha})} \\ & \lesssim \sup_{0 < s \leq t} s^{r_\gamma - r_\alpha} \|T_t - I\|_{D(A^{k_\alpha})} + t^{r_\gamma} \sup_{s>t} s^{-r_\alpha} \|T_s - I\|_{D(A^{k_\alpha})} \leq 4t^{r_\gamma - r_\alpha}, \end{aligned}$$

⁴To see this, we use the fact that $\|x\|_{F_\alpha}$ is equivalent to the norm in (2.16). Consider then first the case $r_\beta \geq r_\alpha$. In that case, we have $\sup_{t>0} \|t^{-r_\alpha}(T_t - I)x\|_{D(A^{k_\alpha})} \leq \sup_{0 < t \leq 1} \|t^{-r_\beta}(T_t - I)x\|_{D(A^{k_\alpha})} + 2\|x\|_{D(A^{k_\alpha})} \lesssim \|x\|_{F_\beta}$ where we used (2.11) to bound $\|x\|_{D(A^{k_\alpha})} \lesssim \|x\|_{D(A^{k_\beta})}$. If on the other hand $r_\beta < r_\alpha$ then $k_\beta \geq k_\alpha + 1$ and the bound follows by $\sup_{0 < t \leq 1} \|t^{-r_\alpha}(T_t - I)x\|_{D(A^{k_\alpha})} \lesssim \sup_{0 < t \leq 1} \|t^{1-r_\alpha}x\|_{D(A^{k_\alpha+1})} \leq \|x\|_{D(A^{k_\beta})}$.

where for the last inequality we have used that $(T_t)_{t \geq 0}$ restricted to $D(A^{k_\alpha})$ defines a contraction semigroup. As for the first term in (2.17) we have $\|T_t - I\|_{F_\gamma \rightarrow D(A^{k_\alpha})} \lesssim t^{r_\gamma} = \mathcal{O}(t^{\gamma-\alpha})$ for $t \rightarrow 0$ immediately from definition, we have shown $\|T_t - I\|_{F_\gamma \rightarrow F_\alpha} = \mathcal{O}(t^{\gamma-\alpha})$.

Next we consider the case $\gamma - \alpha \geq 1$. For that note that for all $x \in D(A^{k_\alpha+1}) \subseteq F_\gamma$ we have

$$\|(T_t - I)x\|_{D(A^{k_\alpha})} = \left\| \int_0^t T_s A x \, ds \right\|_{D(A^{k_\alpha})} \leq t \|Ax\|_{D(A^{k_\alpha})} \lesssim t \|x\|_{D(A^{k_\alpha+1})}, \quad (2.18)$$

where for the second inequality, we have used (2.11). Using this and focusing on the second part in (2.17) we see

$$\begin{aligned} & \sup_{s>0} \|s^{-r_\alpha}(T_s - I)(T_t - I)\|_{F_\gamma \rightarrow D(A^{k_\alpha})} \\ & \lesssim t \sup_{s>0} \|s^{-r_\alpha}(T_s - I)\|_{F_\gamma \rightarrow D(A^{k_\alpha+1})} \lesssim t \sup_{s>0} \|s^{-r_\alpha}(T_s - I)\|_{F_{\alpha+1} \rightarrow D(A^{k_\alpha+1})} \lesssim t, \end{aligned}$$

where we used $F_\gamma \subseteq F_{\alpha+1}$ together with (2.13). For the first term in (2.17) we can use (2.18) directly which gives $\|T_t - I\|_{F_\gamma \rightarrow D(A^{k_\alpha})} \lesssim t$. Combining both yields $\|T_t - I\|_{F_\gamma \rightarrow F_\alpha} \lesssim t$ and finishes the proof. \square

Finally, we recall a basic but useful property of Favard spaces that shows that they are stable under relatively bounded perturbations.

Lemma 2.6 (Stability of Favard spaces). *Let A_0 and A be generators of strongly continuous contraction semigroups. Let $B = A - A_0$ be relatively A_0 bounded with A_0 -bound given by $a \geq 0$. Then $F_\alpha(A_0) \subset F_\alpha(A)$ for all $\alpha \in (0, 1]$ and in particular if $a < 1$ then $F_\alpha(A_0) = F_\alpha(A)$.*

Proof. It suffices to show the inclusion $F_\alpha(A_0) \subset F_\alpha(A)$, since for $a < 1$, we also have for some $b > 0$

$$\|A_0 x\| \leq \|Ax\| + \|Bx\| \leq \|Ax\| + a\|A_0 x\| + b\|x\|$$

and thus

$$\|Bx\| \leq a\|A_0 x\| + b\|x\| \leq \frac{a}{1-a}\|Ax\| + \frac{b}{1-a}\|x\|.$$

This implies $F_\alpha(A) \subset F_\alpha(A_0)$ by the first part.

Since A and A_0 generate strongly continuous contraction semigroups, we have $(0, \infty) \subset \rho(A_0), \rho(A)$ and $\sup_{\lambda>0} \|\lambda(\lambda - A_0)^{-1}\|, \sup_{\lambda>0} \|\lambda(\lambda - A)^{-1}\| \leq 1$. We observe that we have the simple estimate

$$\|A(\lambda - A)^{-1}x\| \leq \|x\| + \|\lambda(\lambda - A)^{-1}x\| \leq 2\|x\|.$$

This is enough to conclude that for fixed $\delta > 0$

$$\sup_{\lambda \in (0, \delta)} \|\lambda^\alpha A(\lambda - A)^{-1}x\| \leq 2\delta^\alpha \|x\|. \quad (2.19)$$

On the other hand, using the resolvent identity

$$\|A(\lambda - A)^{-1}x\| \leq \|A(\lambda - A_0)^{-1}x\| + \|A(\lambda - A)^{-1}B(\lambda - A_0)^{-1}x\|. \quad (2.20)$$

For the first term on the right-hand side of (2.20), relative boundedness yields

$$\|A(\lambda - A_0)^{-1}x\| \leq (1 + a)\|A_0(\lambda - A_0)^{-1}x\| + b\|(\lambda - A_0)^{-1}x\|.$$

For the second term on the right-hand side of (2.20), we find

$$\begin{aligned} \|A(\lambda - A)^{-1}B(\lambda - A_0)^{-1}x\| &\leq \|A(\lambda - A)^{-1}\| \|B(\lambda - A_0)^{-1}x\| \\ &\leq \left(1 + \|\lambda(\lambda - A)^{-1}\|\right) \|B(\lambda - A_0)^{-1}x\| \\ &\leq 2\|B(\lambda - A_0)^{-1}x\| \end{aligned}$$

Using A_0 -boundedness of B we find for the last expression in the previous line

$$\|B(\lambda - A_0)^{-1}x\| \leq a\|A_0(\lambda - A_0)^{-1}x\| + c\|(\lambda - A_0)^{-1}x\|.$$

For $\lambda > \delta$, we have

$$\|\lambda^\alpha(\lambda - A_0)^{-1}x\| \leq \frac{\|x\|}{\delta^{1-\alpha}}.$$

Thus, we have shown

$$\sup_{\lambda > \delta} \|\lambda^\alpha A(\lambda - A)^{-1}x\| \lesssim \sup_{\lambda > \delta} \|\lambda^\alpha A_0(\lambda - A_0)^{-1}x\| + \|x\|$$

which together with (2.19) implies the claim. \square

2.3. Trotter convergence on Favard spaces. In this section, we use the theory of Favard spaces outlined in Section 2.2 to extend Theorem 2.2 by interpolating initial data regularity $D(A^2)$ all the way down to X . In particular, we consider the case $x \in F_\gamma$ for some $0 < \gamma < 2$ and F_γ denoting the corresponding Favard space of A .

For that, we follow a similar argument as the one outlined in Section 2.1: The starting point of the derivation is again the key commutator bound obtained in Lemma 2.1 using the fact that we can decompose

$$[L, T_{s/n}]x_\tau = L(T_{s/n} - I)x_\tau - (T_{s/n} - I)Lx_\tau, \quad (2.21)$$

with $T_{s/n} = e^{sA/n}$ and $x_\tau = e^{\tau(A+L)}x$. Here, instead of relying on the naive estimate (2.4) we employ the refined version provided in Lemma 2.5:

For the first term on the right-hand side of (2.21) we assume that $F_\alpha \subseteq D(L)$ for some $\alpha < \min\{1, \gamma\}$ or in other words, by the closed graph theorem, that the restriction $L|_{F_\alpha} : F_\alpha \rightarrow X$ is bounded. This assumption, in particular, implies that L

is infinitesimally A -bounded [EN00, Lem. 2.13] and hence functions analogously to the relative boundedness assumption (2.8) in Theorem 2.2. Assuming furthermore that the joined dynamics $e^{\tau(A+L)}$ leaves the Favard space F_γ invariant which implies that

$$x_\tau \in F_\gamma. \quad (2.22)$$

This property together with Lemma 2.5 imply that

$$\|L(T_{s/n} - I)x_\tau\| \leq \|L\|_{F_\alpha \rightarrow X} \|(T_{s/n} - I)x_\tau\|_{F_\alpha} = \mathcal{O}_{\|L\|_{F_\alpha \rightarrow X} \|x_\tau\|_{F_\gamma}} \left(\left(\frac{s}{n} \right)^{\gamma'} \right). \quad (2.23)$$

with $\gamma' = \min\{1, \gamma - \alpha\}$.

The second term on the right-hand side of (2.21) can easily be estimated once we additionally assume

$$Lx_\tau \in F_\beta \quad (2.24)$$

for some $\beta \leq \gamma$ in which case we have

$$\|(T_{s/n} - I)Lx_\tau\| = \mathcal{O}_{\|Lx_\tau\|_{F_\beta}} \left(\left(\frac{s}{n} \right)^\beta \right). \quad (2.25)$$

As seen in the proof of Theorem 2.7 below, the invariance of F_γ under $e^{\tau(A+L)}$ and hence (2.22) as well as (2.24) both follow when assuming that $LF_\gamma \subseteq F_\beta$ with $k_\gamma < \beta \leq \gamma$, where $k_\gamma \in \{0, 1\}$ is such that $\gamma - k_\gamma \in (0, 1]$. In the case $k_\gamma = 1$, this assumption implies that L is also infinitesimally A -bounded on the graph space $D(A)$ and can hence be seen as the analog of (2.9) in Theorem 2.2.

We are now ready to state and formally prove our main theorem of this section in the following:

Theorem 2.7. *Let X be a Banach space and $(L, D(L))$ and $(A, D(A))$ be generators of strongly continuous contraction semigroups. Moreover, assume that the Favard spaces of A satisfy $F_\alpha \subseteq D(L)$ and $LF_\gamma \subseteq F_\beta$ for some positive numbers $\alpha < \min\{1, \gamma\}$ and $k_\gamma < \beta \leq \gamma < 2$, where $k_\gamma \in \{0, 1\}$ is such that $\gamma - k_\gamma \in (0, 1]$. Then for all $n \in \mathbb{N}$ and $t \geq 0$ we have*

$$\left\| (e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right\|_{F_\gamma \rightarrow X} = \mathcal{O} \left(\frac{t^{1+\delta}}{n^\delta} \right), \quad (2.26)$$

where $\delta = \min\{1, \beta, \gamma - \alpha\}$.

Remark 2.8. *In the special case $\gamma = 1$, using that $D(A) \subseteq F_1$, the same argument as for Theorem 2.7 gives under the condition that $F_\alpha \subseteq D(L)$ and $LD(A) \subseteq F_\beta$ for some $0 < \alpha, \beta < 1$ that*

$$\left\| (e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right\|_{D(A) \rightarrow X} = \mathcal{O} \left(\frac{t^{1+\delta}}{n^\delta} \right),$$

where $\delta = \min\{\beta, 1 - \alpha\}$.

Remark 2.9. *Theorem 2.2 can be seen as an extreme point of the above Theorem 2.7 extending it to the case $\gamma = 2$ and $\beta = \alpha = 1$. In this case the Favard spaces F_2 and F_1 are replaced by $D(A^2)$ and $D(A)$ respectively. Furthermore, relative A -boundedness of L with bound strictly smaller than 1 with respect to the norm on X and the graph norm on $D(A)$, i.e., (2.8) and (2.9), needs to be assumed additionally.*

Proof of Theorem 2.7. Since the map $L : F_\alpha \rightarrow X$, is well defined and closed (as $L : D(L) \rightarrow X$ is closed) we see by the closed graph theorem that it is also bounded and furthermore, using $\alpha < 1$, that L is infinitesimally A -bounded with respect to the norm on X [EN00, Lem. 2.13], i.e., for all $\varepsilon > 0$ and $x \in D(A)$ we have

$$\|Lx\| \leq \varepsilon \|Ax\| + b_\varepsilon \|x\| \quad (2.27)$$

for some $b_\varepsilon \geq 0$.

We want to repeat this argument to show that L is also infinitesimally A -bounded with respect to the graph norm on $D(A^{k_\gamma})$. In the case $k_\gamma = 0$ we have already done this (2.27), so we focus on $k_\gamma = 1$: From $LF_\gamma \subseteq F_\beta$ and the closed graph theorem we get that $L : F_\gamma \rightarrow F_\beta$ is bounded. Using $k_\gamma < \beta$ and hence $F_\beta \subseteq D(A^{k_\gamma})$, this in particular implies boundedness of $L : F_\gamma \rightarrow D(A^{k_\gamma})$. Furthermore, using $\gamma < k_\gamma + 1$ and [EN00, Lem. 2.13] on the Banach space $D(A^{k_\gamma})$, we see that L is infinitesimally A -bounded with respect to the graph norm, i.e., for all $\varepsilon > 0$ and $x \in D(A^{k_\gamma+1}) \subseteq F_\gamma \subseteq D(L)$ we have

$$\|Lx\|_{D(A^{k_\gamma})} \leq \varepsilon \|Ax\|_{D(A^{k_\gamma})} + c_\varepsilon \|x\|_{D(A^{k_\gamma})} \quad (2.28)$$

for some $c_\varepsilon \geq 0$.

Since $(L, D(L))$ generates a strongly continuous contraction semigroup and is hence dissipative, we can use (2.27) and [EN00, Theorem 2.7] which gives that $(A+L, D(A))$ generates a strongly continuous contraction semigroup as well. Furthermore, again from (2.27) we see that the graph norms of $A+L$ and A are equivalent. This shows that the restriction $e^{t(A+L)}|_{D(A)}$ defines a strongly continuous semigroup on the graph space $D(A)$, which satisfies $\|e^{t(A+L)}\|_{D(A)} \lesssim \|e^{t(A+L)}\|_{D(A+L)} \leq 1$ for all $t \geq 0$. Its generator is given by $A+L$ restricted on $D((A+L)^2)$.⁵ By [EN00, Theorem 3.8], it has the set of positive numbers in its resolvent set and satisfies $\sup_{\lambda > 0} \|\lambda(\lambda - A + L)^{-1}\|_{D(A)} \lesssim 1$.

We can hence employ the stability result of Favard spaces, Lemma 2.6⁶ on $D(A^{k_\gamma})$ as underlying Banach space together with (2.28), which gives $F_\gamma(A+L) = F_\gamma(A)$. Furthermore, we have that $e^{t(A+L)}$ is bounded uniformly over $t \geq 0$ with respect to

⁵In the case of $k_\gamma = 1$ we even have $D((A+L)^2) = D(A^2)$ which follows using (2.27) and (2.28) and [P18, Lem. IV.3].

⁶Note, that Lemma 2.6, is applicable in this context as $F_\gamma(A)$ and $F_\gamma(A+L)$ can be seen as Favard spaces of order $r_\gamma \in (0, 1]$ but with underlying Banach space being $D(A^{k_\gamma})$ instead of X .

the Favard norm of $F_\gamma \equiv F_\gamma(A)$ using the closed graph theorem for the operator $e^{t(A+L)} : F_\gamma \rightarrow F_\gamma$.

The key commutator bound in Lemma 2.1 gives for all $x \in D(A)$

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) x \right\| \leq t \sup_{s, \tau \in [0, t]} \left\| [L, e^{sA/n}] e^{\tau(A+L)} x \right\|. \quad (2.29)$$

In fact, since $L : F_\alpha \rightarrow X$ is bounded and furthermore $F_\gamma \subseteq \overline{D(A)}^{\|\cdot\|_{F_\alpha}}$, which holds by $\gamma < \alpha$ and [EN00, Prop. 5.14., Theo. 5.15], we get (2.29) for all $x \in F_\gamma$. Using this and the above we see

$$\begin{aligned} \left\| (e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right\|_{F_\gamma \rightarrow X} &\leq t \sup_{s, \tau \in [0, t]} \left\| [L, e^{sA/n}] e^{\tau(A+L)} \right\|_{F_\gamma \rightarrow X} \\ &\lesssim t \sup_{s \in [0, t]} \left\| [L, e^{sA/n}] \right\|_{F_\gamma \rightarrow X} \leq t \sup_{s \in [0, t]} \left\| L (e^{sA/n} - I) \right\|_{F_\gamma \rightarrow X} + t \sup_{s \in [0, t]} \left\| (e^{sA/n} - I) L \right\|_{F_\gamma \rightarrow X}. \end{aligned} \quad (2.30)$$

For the first term in (2.30) we can use Lemma 2.5 together with the fact that $L : F_\alpha \rightarrow X$ is bounded which gives

$$\sup_{s \in [0, t]} \left\| L (e^{sA/n} - I) \right\|_{F_\gamma \rightarrow X} \lesssim \sup_{s \in [0, t]} \left\| e^{sA/n} - I \right\|_{F_\gamma \rightarrow F_\alpha} = \mathcal{O} \left(\left(\frac{t}{n} \right)^{\gamma'} \right)$$

where $\gamma' = \min\{1, \gamma - \alpha\}$. To finish the proof we use the boundedness of $L : F_\gamma \rightarrow F_\beta$ to bound the second term in (2.30) as

$$\sup_{s \in [0, t]} \left\| (e^{sA/n} - I) L \right\|_{F_\gamma \rightarrow X} \lesssim \sup_{s \in [0, t]} \left\| e^{sA/n} - I \right\|_{F_\beta \rightarrow X} = \mathcal{O} \left(\left(\frac{t}{n} \right)^{\beta'} \right),$$

where $\beta' = \min\{1, \beta\}$. □

In the following subsections, we apply the result of Theorem 2.7 for special cases of generators for which we have good control over the corresponding Favard spaces. The first case, in Section 2.4, considers $-A$ to be a positive operator on some Banach space X . In the second case, in Section 2.5, we consider X to be a Hilbert space and A either self-adjoint with $-A$ being positive semidefinite or A being anti self-adjoint (i.e., iA self-adjoint) and hence A being the generator of a unitary group. In all of these cases, we see that the Favard spaces of A are closely linked to the domains of the fractional powers of A (or, more precisely, of $|A|$). This leads us to formulate the abstract result of Theorem 2.7 for these special cases in a more concrete way in Corollaries 2.13, 2.14, 2.18, 2.21 respectively.

2.4. Strictly dissipative dynamics. Positive operators on general Banach spaces are defined as follows:

Definition 2.10 (Positive operator). *A closed operator B is called positive on a Banach space X if $(-\infty, 0] \subseteq \rho(B)$ and $\|(\lambda - B)^{-1}\| = \mathcal{O}((1 - \lambda)^{-1})$ for $\lambda \in (-\infty, 0]$.*

Remark 2.11. *If B is a self-adjoint operator on a Hilbert space, then positivity in the usual sense, i.e., $\inf_{x \in D(B); \|x\|=1} \langle Bx, x \rangle > 0$ is equivalent to positivity as in the above definition.*

The relevance of this definition for us is by the following simple observation.

Lemma 2.12. *Let A be a generator of a strongly continuous contraction semigroup, then $-A$ is positive if $0 \in \rho(A)$.*

Proof. Since $0 \in \rho(A)$, we have for some $\varepsilon > 0$ by openness of the resolvent set and continuity of the resolvent in λ that $[-\varepsilon, \varepsilon] \subseteq \rho(A)$ and

$$\|(\lambda + A)^{-1}\| = \mathcal{O}(1) \text{ for } |\lambda| \leq \varepsilon.$$

Furthermore, we have by [EN00, Thm. 3.5], the bound $\|\lambda(\lambda - A)^{-1}\| \leq 1$ for $\lambda > 0$ for generators of contraction semigroups. Combining both, we see

$$\|(\lambda + A)^{-1}\| = \mathcal{O}((1 - \lambda)^{-1}) \text{ for } \lambda \in (-\infty, 0].$$

□

If one assumes that $-A$ is positive, one can define $A^{-\alpha}$ for $\alpha > 0$, and the operator is given by the explicit formula [EN00, Corr. 5.28]

$$A^{-\alpha} = \frac{1 - e^{-2\pi i \alpha}}{2\pi i} \int_0^\infty s^{-\alpha} (s - A)^{-1} ds \text{ for } \alpha \in (0, 1).$$

The operator A^α is then defined as the inverse of $A^{-\alpha}$ with $D(A^\alpha) = \text{ran}(A^{-\alpha})$. For $\alpha < \beta$, we also have $D(A^\beta) \subseteq F_\beta \subseteq D(A^\alpha)$, where the first inclusion can be found in [L09, Prop. 4.7] and the proof of the second inclusion follows from [EN00, Prop. 5.33]⁷

$$\|x\| + \|A^\alpha x\| \lesssim \|x\|_{F_\beta} \lesssim \|x\| + \|A^\beta x\|. \quad (2.31)$$

Using this, we can immediately deduce the following result from Theorem 2.7:

Corollary 2.13. *Let X be a Banach space and L and A be generators of strongly continuous contraction semigroups on X with $0 \in \rho(A)$, $D(A^\alpha) \subseteq D(L)$, and $LD(A) \subseteq D(A^\beta)$ for some $\alpha, \beta \in (0, 1)$. Then, for fixed $\varepsilon > 0$, the Trotter-Kato product satisfies*

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) \right\|_{D(A) \rightarrow X} = \mathcal{O}_\varepsilon \left(\frac{t^{1+\delta}}{n^\delta} \right),$$

where $\delta = \min\{\beta, 1 - \alpha - \varepsilon\}$.

⁷The proof assumes a negative growth bound of the semigroup since the book only defines Favard spaces in this context. However, a careful inspection of the proof shows that it applies to our setting, as well.

Proof. By (2.31) we have that $LD(A) \subseteq D(A^\beta) \subseteq F_\beta$. Furthermore, since $D(A^\alpha) \subseteq D(L)$ we have, again by (2.31) that for any $\varepsilon > 0$ fixed also $F_{\alpha+\varepsilon} \subseteq D(L)$. Hence, the conditions of Theorem 2.7 or Remark 2.8 are fulfilled which finishes the proof. \square

Assuming X to be a Hilbert space, see [L09, Corr. 4.30], we have equality $D(A^\beta) = F_\beta$. This way, we get rid of the $\varepsilon > 0$ dependence in Theorem 2.13 and one finds

Corollary 2.14. *Let X be a Hilbert space and L and A be generators of strongly continuous contraction semigroups on X with $0 \in \rho(A)$, $D(A^\alpha) \subset D(L)$, and $LD(A) \subset D(A^\beta)$ for some $\alpha, \beta \in (0, 1)$. Then, the Trotter-Kato product satisfies*

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) \right\|_{D(A) \rightarrow X} = \mathcal{O} \left(\frac{t^{1+\delta}}{n^\delta} \right)$$

where $\delta = \min\{\beta, 1 - \alpha\}$.

Our framework in the above theorem allows, for example, for A to be the Dirichlet-Laplacian on a sufficiently nice bounded domain $\Omega \subset \mathbb{R}^n$, since $0 \notin \text{Spec}(\Delta_{H^2(\Omega) \cap H_0^1(\Omega)})$. However, it does not allow us to study, for instance, basic operators such as $A = \Delta$ on \mathbb{R}^n . We will take care of this in the next two subsections.

2.5. Self-adjoint and anti self-adjoint generators on Hilbert spaces. In the case of self-adjoint or anti self-adjoint A , one can use the spectral theorem to easily characterize the Favard spaces. This is the content of the following Lemma:

Lemma 2.15. *Let $-A$ be self-adjoint and positive semi-definite on a Hilbert space X , then in the sense of the functional calculus for all $\alpha > 0$*

$$F_\alpha(A) = D(|A|^\alpha)$$

and the Favard norm is equivalent to the graph norm of $|A|^\alpha$.

Let K be self-adjoint, then for all $\alpha > 0$

$$F_\alpha(iK) = D(|K|^\alpha)$$

and the corresponding Favard norm is equivalent to the graph norm of $|K|^\alpha$.

Remark 2.16. *The specific form of the Favard spaces presented in Lemma 2.15 enables us to provide stronger connections between different levels of the Sobolev tower: Let $-A$ be self-adjoint and positive semidefinite. Then for all $\alpha > 0$ the graph space $D(|A|^\alpha)$ naturally becomes a Hilbert space when equipped with the scalar product $\langle x, y \rangle_\alpha := \langle |A|^\alpha x, |A|^\alpha y \rangle + \langle x, y \rangle$. It is easy to verify that the restriction $-A' := -A|_{D(|A|^{\alpha+1})}$ defines again a self-adjoint, positive semi-definite operator on $D(|A|^\alpha)$ with fractional powers $|A'|^\beta$ being defined on the domain $D(|A'|^\beta) = D(|A|^{\alpha+\beta})$. Hence, using Lemma 2.15, we see that the Favard spaces of A' satisfy*

$$F_\beta(A'; D(|A|^\alpha)) = D(|A|^{\alpha+\beta}) = F_{\alpha+\beta}(A; X), \quad (2.32)$$

which can be seen as a refined version of (2.12).

Let now L be closed and such that $F_\alpha(A; X) \subseteq D(L)$ and $LF_\gamma(A; X) \subseteq F_\beta(A; X)$ for some positive numbers $\alpha < 1$ and $\gamma - 1 < \beta \leq \gamma < 2$. Using (2.32) instead of (2.12), we can argue similarly as in the proof of Theorem 2.7 but replacing $D(A^{k_\gamma})$ with $D(|A|^\beta)$ in the case $\gamma \geq 1$ that $e^{t(A+L)} : F_\gamma(A; X) \rightarrow F_\gamma(A; X)$ is a well-defined bounded operator. This enables us in Corollary 2.18 to lift the restriction $\beta > k_\gamma$ needed in Theorem 2.7 and allow for all $\beta \geq \gamma - 1$. The same argument can also be employed for anti self-adjoint generators, i.e., $A = iK$ for K being self-adjoint, giving the same extended range on the parameter β in Corollary 2.21.

Proof of Lemma 2.15. Let $r \in (0, 1)$ and $m \in \mathbb{N}$. Using the functional calculus, we find with $E_{|A|}$ being the spectral measure of $|A| = -A$

$$\|\lambda^r A^m (\lambda - A)^{-1} x\|^2 = \int_0^\infty \lambda^{2r} \frac{t^{2m}}{(\lambda + t)^2} d\langle E_{|A|}(t)x, x \rangle.$$

The right-hand side is maximized for $\lambda = \frac{r}{1-r}t$ which shows that

$$\begin{aligned} \sup_{\lambda > 0} \|\lambda^r A^m (\lambda - A)^{-1} x\|^2 &= \left(\frac{r}{1-r} \right)^{2r} \int_0^\infty \frac{t^{2(m+r)}}{t^2 \left(1 + \frac{r}{1-r}\right)^2} d\langle E_{|A|}(t)x, x \rangle \\ &= r^{2r} (1-r)^{2-2r} \int_0^\infty t^{2(r+m-1)} d\langle E_{|A|}(t)x, x \rangle \\ &\sim \| |A|^{r+m-1} x \|^2. \end{aligned}$$

Noting that the maximising λ is independent of m , this shows in particular for all $\alpha > 0$, with $r_\alpha \in (0, 1)$ and $k_\alpha \in \mathbb{N}_0$, the unique numbers such that $\alpha = r_\alpha + k_\alpha$, that

$$\sup_{\lambda > 0} \|\lambda^{r_\alpha} A (\lambda - A)^{-1} x\|_{D(A^{k_\alpha})} \sim \| |A|^{r_\alpha} x \| + \| |A|^{\alpha} x \|$$

Noting that $\| |A|^{r_\alpha} x \| \leq \|x\| + \| |A|^{\alpha} x \|$, this gives by definition of the Favard norm $\|x\|_{F_\alpha(A)} \sim \|x\|_{D(|A|^\alpha)}$.

For the second part of the Lemma, using again the functional calculus for $r \in (0, 1)$ and $m \in \mathbb{N}$

$$\|\lambda^r K^m (\lambda - iK)^{-1} x\|^2 = \int_{-\infty}^\infty \lambda^{2r} \frac{t^{2m}}{\lambda^2 + t^2} d\langle E_K(t)x, x \rangle$$

The right-hand side is maximized for $\lambda = \frac{\sqrt{r}}{\sqrt{1-r}}t$ which shows that

$$\begin{aligned} \sup_{\lambda > 0} \|\lambda^r K^m (\lambda - iK)^{-1} x\|^2 &= \left(\frac{r}{1-r} \right)^r \int_{-\infty}^\infty \frac{t^{2(m+r)}}{\frac{r}{1-r}t^2 + t^2} d\langle E_K(t)x, x \rangle \\ &= r^r (1-r)^{1-r} \int_{-\infty}^\infty t^{2(r+m-1)} d\langle E_K(t)x, x \rangle \\ &\sim \| |K|^{r+m-1} x \|^2. \end{aligned}$$

Following the same argument as above this shows $\|x\|_{F_\alpha(iK)} \sim \|x\|_{D(|K|^\alpha)}$. \square

The two results presented in Lemma 2.15 can be unified in the following way: For normal operators N , defining contraction semigroups, we define commuting self-adjoint operators [S12, Prop. 5.30] $\operatorname{Re}(N) := \overline{(N + N^*)}/2$ and $\operatorname{Im}(N) := \overline{(N - N^*)}/(2i)$ such that $N = \operatorname{Re}(N) + i\operatorname{Im}(N)$. For N to generate a contraction semigroup, we demand that $\operatorname{Re}(N) \leq 0$. Then, we recall that $T_t = e^{tN} := e^{t\operatorname{Re}(N)}e^{it\operatorname{Im}(N)} = e^{it\operatorname{Im}(N)}e^{t\operatorname{Re}(N)}$. We then have the following generalization of Lemma 2.15, which we prove in the appendix.

Proposition 2.17. *Let N be a normal operator on a Hilbert space with $\operatorname{Re}(N) \leq 0$ as above, then for $\alpha \in (0, 1)$*

$$D(|N|^\alpha) = F_\alpha(\operatorname{Re}(N)) \cap F_\alpha(\operatorname{Im}(N)) = F_\alpha(N).$$

Using this characterization of the Favard spaces, we obtain the following Corollary 2.18 from Theorem 2.7 and Remark 2.16. It can be seen as the analogue of Corollary 2.14 without the requirement that $0 \in \rho(A)$.

Corollary 2.18. *Let X be a Hilbert space and L and A be generators of strongly continuous contraction semigroups on X with $-A$ self-adjoint and positive semidefinite. Moreover assume that $D(|A|^\alpha) \subseteq D(L)$, and $LD(|A|^\gamma) \subseteq D(|A|^\beta)$ for some positive numbers $\alpha < \min\{1, \gamma\}$ and $\gamma - 1 < \beta \leq \gamma < 2$. Then for all $n \in \mathbb{N}$ and $t \geq 0$ the Trotter-Kato product satisfies*

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) \right\|_{D(|A|^\gamma) \rightarrow X} = \mathcal{O} \left(\frac{t^{1+\delta}}{n^\delta} \right), \quad (2.33)$$

where $\delta = \min\{1, \beta, \gamma - \alpha\}$.

2.5.1. *Unitary dynamics and singular potentials.* In this section, we use the characterisation of the Favard spaces in Lemma 2.15 to formulate the result of Theorem 2.7 in the case of unitary dynamics on a Hilbert space. Hence, we shall now assume that X is a Hilbert space and that $A = iK$, with K being self-adjoint.

Example 2.19 (Schrödinger operators). *For the case of $K = -\Delta \geq 0$ on $X = L^2(\mathbb{R}^d)$, which is self-adjoint on the domain $D(K) = H^2(\mathbb{R}^d)$, Lemma 2.15 gives that the Favard spaces $F_\alpha \equiv F_\alpha(iK)$ are precisely given by the Sobolev spaces $H^{2\alpha}(\mathbb{R}^d)$ for all $\alpha > 0$*

Example 2.20 (Dirac operators). *Let $d = 2$ for simplicity, then the two-dimensional Dirac operator reads in terms of Pauli matrices σ_i*

$$K = \sum_{i=1}^2 \sigma_i D_{x_i} + \sigma_3 m.$$

By the standard Foldy-Wouthuysen transform, the operator K is unitarily equivalent to

$$\operatorname{diag}(\sqrt{(-\Delta) + m^2}, -\sqrt{(-\Delta) + m^2}).$$

From this it follows that $F_\alpha \equiv F_\alpha(iK) = H^\alpha(\mathbb{R}^2; \mathbb{C}^2)$.

Using Lemma 2.15 we obtain the following corollary from Theorem 2.7 and Remark 2.16 for the case of $A = iK$ and $L = iH$ for some self-adjoint operators K and H :

Corollary 2.21. *Let X be a Hilbert space and H and K be self-adjoint. Moreover assume that $D(|K|^\alpha) \subseteq D(H)$, and $HD(|K|^\gamma) \subseteq D(|K|^\beta)$ for some positive numbers $\alpha < \min\{1, \gamma\}$ and $\gamma - 1 < \beta \leq \gamma < 2$. Then for all $n \in \mathbb{N}$ and $t \in \mathbb{R}$ the Trotter-Kato product satisfies*

$$\left\| \left(e^{itH/n} e^{itK/n} \right)^n - e^{it(H+K)} \right\|_{D(|K|^\gamma) \rightarrow X} = \mathcal{O} \left(\frac{|t|^{1+\delta}}{n^\delta} \right), \quad (2.34)$$

where $\delta = \min\{1, \beta, \gamma - \alpha\}$.

Application to singular potentials. In the following we apply Corollary 2.21 for the case of $X = L^2(\mathbb{R}^d)$, multiplication operator $H = V$ with singular potential $V(x) = |x|^{-a}$,⁸ for some $a > 0$, $K = -\Delta \geq 0$. Here, from Lemma 2.15 and Example 2.19, we have that $F_\alpha(iK) = D(K^\alpha) = H^{2\alpha}(\mathbb{R}^d)$ for all $\alpha > 0$.

The relative boundedness condition in Corollary 2.21, i.e., the condition $H^{2\alpha}(\mathbb{R}^d) \subseteq D(V)$ for some suitable $\alpha \in (0, 1)$, can be obtained as follows: Assume that the potential satisfies $V = V_1 + V_2 \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ for some $p \geq 1$. Then we have for $1/2 = 1/p + 1/q$

$$\|V\varphi\|_2 \leq \|V_1\|_p \|\varphi\|_q + \|V_2\|_\infty \|\varphi\|_2. \quad (2.35)$$

By the Sobolev embedding, we have $H^k(\mathbb{R}^d) \subseteq L^q(\mathbb{R}^d)$ for parameters

$$\frac{1}{2} - \frac{k}{d} = \frac{1}{q}$$

and hence we can choose $k = \frac{d(q-2)}{2q}$ and $\alpha = \frac{d(q-2)}{4q}$. For the special case of $p = 2$ and $q = \infty$, we find $\alpha = \frac{d}{4}$. For the potential $V(x) = |x|^{-a}$, we can choose $p = 2$ as long as $a < d/2$, in which case we have shown that $H^{d/2}(\mathbb{R}^d) \subseteq D(V)$.

To verify the second condition in Corollary 2.21 for singular potentials, i.e., $VD((-\Delta)^\gamma) \subseteq D((-\Delta)^\beta)$ for some suitable $k_\gamma < \beta \leq \gamma < 2$, we can invoke the Brezis-Mironescu inequality [BM01, Corr.4] which states that for $s \in (1, \infty)$ and $\beta = \frac{s-1}{2}$

$$\|(-\Delta)^\beta(fg)\|_2 \lesssim \|f\|_\infty \|g\|_{H^{s-1}} + \|g\|_{2s} \|f\|_{H^s}^{1-1/s} \|f\|_\infty^{1/s}. \quad (2.36)$$

We use this for $g = V_1$ being the singular part of the potential $V(x) = |x|^{-a}$ as the remainder can be chosen to be smooth and hence trivially satisfies the desired condition. In order for $V(x) = |x|^{-a}$ to be in $L_{\text{loc}}^{2s}(\mathbb{R}^d)$ (and hence $V_1 \in L^{2s}(\mathbb{R}^d)$) we

⁸Note that the assumptions on H in Corollary 2.21 are independent of the sign of H . Hence, all arguments here also work for the attractive singular potentials $V(x) = -|x|^{-a}$.

require that $a < \frac{d}{2s}$. Thus, as above $a < \frac{d}{2}$ is necessary for this condition to apply. More generally, for this choice of potential $V \in H_{\text{loc}}^{s-1}(\mathbb{R}^d)$ if and only if $a < \frac{d}{2} - (s-1)$. With this choice and furthermore $f = \varphi \in H^{2\gamma}(\mathbb{R}^d) = D((-\Delta)^\gamma)$, we find from (2.36) for $\gamma \geq \frac{d}{4}$, and hence by Sobolev embedding $\varphi \in L^\infty(\mathbb{R}^d)$, and $s \leq 2\gamma$

$$\|(-\Delta)^\beta(V_1\varphi)\|_2 \lesssim \|\varphi\|_\infty \|V_1\|_{H^{s-1}} + \|V_1\|_{2s} \|\varphi\|_{H^s}^{1-1/s} \|\varphi\|_\infty^{1/s}. \quad (2.37)$$

Hence, collecting all constraints on s and using $\beta = \frac{s-1}{2}$, we see $VD((-\Delta)^\gamma) \subseteq D((-\Delta)^\beta)$ for all $\beta < \min\{\frac{d-2a}{4a}, \frac{d-2a}{4}, \gamma - \frac{1}{2}\}$

For the case $a = 1, d = 3$, i.e., for the Coulomb potential, and furthermore $\gamma = 1$, we can therefore choose any $\beta < 1/4$. Thus, Corollary 2.21 gives in the Coulomb case $V(x) = \pm|x|^{-1}$ a Trotter convergence as

$$\left\| \left((e^{itV/n} e^{-it\Delta/n})^n - e^{it(-\Delta+V)} \right) \right\|_{H^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)} = \mathcal{O}(n^{-1/4+\varepsilon}).$$

for all $t \in \mathbb{R}$ and $\varepsilon > 0$ fixed. More generally, the above derivations give the following:

Corollary 2.22. *Let $V(x) = \pm|x|^{-a}$ with $0 < a < d/2$ and $\gamma \in (0, 2)$. Then the Trotter formula converges as*

$$\left\| \left((e^{itV/n} e^{-it\Delta/n})^n - e^{it(-\Delta+V)} \right) \right\|_{H^{2\gamma}(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)} = \mathcal{O}(n^{d/4-\gamma} + n^{-\beta} + n^{-1})$$

for all $\gamma - 1 < \beta < \min\{\frac{d-2a}{4a}, \frac{d-2a}{4}, \gamma - \frac{1}{2}\}$.

Molecular Hamiltonians. We consider a molecule with N electrons of mass m_e and charge $-e$. In addition, we have M nuclei of masses m_j and charges $Z_j e$ for $j = 1, \dots, M$ described by the many-body Schrödinger operator

$$H = -\sum_{j=1}^N \frac{\Delta_{x_j}}{2m_e} - \sum_{j=1}^M \frac{\Delta_{y_j}}{2m_j} + V(x, y)$$

where

$$V(x, y) = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} - \sum_{i,j} \frac{e^2 Z_j}{|x_i - y_j|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|y_i - y_j|}. \quad (2.38)$$

In the many-body setting, we can repeat the steps leading to the result of Corollary 2.22 by working with (Sobolev-)Bochner spaces instead of standard Sobolev spaces.

To streamline the notation we shall no longer discriminate between x and y variables and just consider $x \in \mathbb{R}^{3(N+M)}$.

We shall allow for Trotter splittings

$$A := i\Delta - iV_1 \text{ and } L := -iV_2 \quad (2.39)$$

where V_1 and V_2 is any choice of summands in (2.38) such that $V = V_1 + V_2$. This includes, of course, the Trotter splitting into kinetic and potential energy, but also

allows us to consider the kinetic energy together with the nucleus-nucleus and nucleus-electron interaction, separated from the electron-electron interaction. We have this freedom since combining Lemma 2.6 with Lemma 2.15, we see that the Favard spaces $F_\alpha(A)$ are precisely the Sobolev spaces $H^{2\alpha}(\mathbb{R}^{N+M})$ for all $\alpha \in (0, 1)$ and are independent of V_1 , since V_1 is relatively $-\Delta$ bounded.

We shall show that:

Theorem 2.23. *For the Trotter-splitting (2.39), there is for any $\varepsilon > 0$ a constant $C_{\varepsilon, N, M}$ such that*

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) \right\|_{H^2(\mathbb{R}^{3(N+M)}) \rightarrow L^2(\mathbb{R}^{3(N+M)})} \leq C_{\varepsilon, N, M} n^{-1/4+\varepsilon}.$$

Proof. The potential V consists of linear combinations of Coulomb potentials $V_{\text{sp}}(x_i - x_j)$ in terms of the single particle Coulomb potential

$$V_{\text{sp}}(x) := |x|^{-1} \text{ for } x \in \mathbb{R}^3 \setminus \{0\}.$$

We start by proving the $V_{\text{sp}} : H^{3/2}(\mathbb{R}^{3(N+M)}) \rightarrow L^2(\mathbb{R}^{3(N+M)})$ boundedness. Let $\varphi \in H^2(\mathbb{R}^{3(N+M)})$, we have the natural identification of the multi-variable L^2 as a single particle L^2 Bochner space

$$\|V_{\text{sp}}\varphi\|_{L^2(\mathbb{R}^{3(N+M)})} = \|V_{\text{sp}}\varphi\|_{L^2(\mathbb{R}^3; X)},$$

where we defined $X := L^2(\mathbb{R}^{3(N+M-1)})$. We also notice that $\varphi \in H^2(\mathbb{R}^3; X)$ which follows easily using the Fourier representation of the Sobolev space and the simple inequality $\langle \xi_1 \rangle \leq \langle (\xi_1, \dots, \xi_{3(N+M)}) \rangle$. This allows us to repeat the estimate in (2.35) in the Bochner space and we obtain using the same composition of $V_{\text{sp}} = V_{\text{sp},1} + V_{\text{sp},2} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ as in the subsection before

$$\begin{aligned} \|V_{\text{sp}}\varphi\|_{L^2(\mathbb{R}^3; X)} &\leq \|V_{\text{sp},1}\|_{L^2(\mathbb{R}^3)} \|\varphi\|_{L^\infty(\mathbb{R}^3; X)} + \|V_{\text{sp},2}\|_{L^\infty(\mathbb{R}^3)} \|\varphi\|_{L^2(\mathbb{R}^3; X)} \\ &\lesssim \|V_{\text{sp},1}\|_{L^2(\mathbb{R}^3)} \|\varphi\|_{H^{3/2}(\mathbb{R}^3; X)} + \|V_{\text{sp},2}\|_{L^\infty(\mathbb{R}^3)} \|\varphi\|_{L^2(\mathbb{R}^3; X)} \\ &\lesssim \|V_{\text{sp},1}\|_{L^2(\mathbb{R}^3)} \|\varphi\|_{H^{3/2}(\mathbb{R}^{3(N+M)})} + \|V_{\text{sp},2}\|_{L^\infty(\mathbb{R}^3)} \|\varphi\|_{L^2(\mathbb{R}^3; X)} \\ &\lesssim (\|V_{\text{sp},1}\|_{L^2(\mathbb{R}^3)} + \|V_{\text{sp},2}\|_{L^\infty(\mathbb{R}^3)}) \|\varphi\|_{H^{3/2}(\mathbb{R}^{3(N+M)})}. \end{aligned} \tag{2.40}$$

Next, we show that $V_{\text{sp}} : H^2(\mathbb{R}^{3(N+M)}) \rightarrow H^{s-1}(\mathbb{R}^{3(N+M)})$ where $s < 3/2$. It suffices to consider the singular part of the potential $V_{\text{sp},1}$.

Using Peetre's inequality, which implies that for $t \geq 0$

$$\langle (\xi_1, \dots, \xi_m, \xi_{m+1}, \dots, \xi_n) \rangle^t \leq 2^t \langle (\xi_1, \dots, \xi_m) \rangle^t \langle (\xi_{m+1}, \dots, \xi_n) \rangle^t,$$

we have for $Y := H^{s-1}(\mathbb{R}^{3(N+M-1)})$ and $s < 3/2$ together with the Brezis-Mironescu inequality that

$$\begin{aligned} \|V_{\text{sp},1}\varphi\|_{H^{s-1}(\mathbb{R}^{3(N+M)})} &\lesssim \|V_{\text{sp},1}\varphi\|_{H^{s-1}(\mathbb{R}^3;Y)} \\ &\lesssim \|\varphi\|_{H^{3/2}(\mathbb{R}^3;Y)} \|V_{\text{sp},1}\|_{H^{s-1}(\mathbb{R}^3)} + \|V_{\text{sp},1}\|_{L^{2s}(\mathbb{R}^3)} \|\varphi\|_{H^s(\mathbb{R}^3;Y)}^{1-1/s} \|\varphi\|_{H^{3/2}(\mathbb{R}^3;Y)}^{1/s} \\ &\lesssim \|\varphi\|_{H^2(\mathbb{R}^{3(N+M)})} (\|V_{\text{sp},1}\|_{H^{s-1}(\mathbb{R}^3)} + \|V_{\text{sp},1}\|_{L^{2s}(\mathbb{R}^3)}), \end{aligned} \quad (2.41)$$

where we used in the last line that for $\alpha, \beta \geq 0$

$$\langle (\xi_1, \dots, \xi_m) \rangle^\alpha \langle (\xi_{m+1}, \dots, \xi_n) \rangle^\beta \leq \langle (\xi_1, \dots, \xi_m, \xi_{m+1}, \dots, \xi_n) \rangle^{\alpha+\beta}.$$

This extends the estimate (2.37) of the previous section to the many-particle Hilbert space.

It remains to argue that we can lift the bounds (2.40) and (2.41) to the two-body interactions appearing in the many-body Hamiltonian, instead of the single particle interaction V_{sp} . To see this, notice that the two-particle interaction $W(x_1, x_2) := \sqrt{2}V_{\text{sp}}(x_1 - x_2)$ – without loss of generality, we consider now the first two particles – is given by $W(x) := (V \circ U)(x)$, where we introduced the unitary map

$$U(x) := 2^{-1/2}(x_1 - x_2, x_1 + x_2, x_3, \dots, x_{N+M}).$$

Using the Fourier representation of the Sobolev spaces, we find that the Sobolev norms are invariant under composition by a unitary map

$$\begin{aligned} \|\langle -\Delta \rangle^\beta (s \circ U)\|_{L^2(\mathbb{R}^{3(N+M)})} &= \|\hat{s} \circ U\|_{L^2(\mathbb{R}^{3(N+M)}; \langle \xi \rangle^{2\beta} d\xi)} \\ &= \|\hat{s}\|_{L^2(\mathbb{R}^{3(N+M)}; \langle \xi \rangle^{2\beta} d\xi)} \\ &= \|\langle -\Delta \rangle^\beta s\|_{L^2(\mathbb{R}^{3(N+M)})}. \end{aligned}$$

This property allows us to lift bounds (2.40) and (2.41) to

$$\begin{aligned} \|W\varphi\|_{L^2(\mathbb{R}^3;X)} &= \|(V_{\text{sp}} \cdot (\varphi \circ U^*)) \circ U\|_{L^2(\mathbb{R}^3;X)} = \|(V_{\text{sp}} \cdot (\varphi \circ U^*))\|_{L^2(\mathbb{R}^3;X)} \\ &\lesssim (\|V_{\text{sp},1}\|_{L^2(\mathbb{R}^3)} + \|V_{\text{sp},2}\|_{L^\infty(\mathbb{R}^3)}) \|\varphi \circ U^*\|_{H^{3/2}(\mathbb{R}^{3(N+M)})} \\ &\lesssim (\|V_{\text{sp},1}\|_{L^2(\mathbb{R}^3)} + \|V_{\text{sp},2}\|_{L^\infty(\mathbb{R}^3)}) \|\varphi\|_{H^{3/2}(\mathbb{R}^{3(N+M)})} \end{aligned} \quad (2.42)$$

and

$$\begin{aligned} \|W_1\varphi\|_{H^{s-1}(\mathbb{R}^{3(N+M)})} &= \|(V_{\text{sp},1} \cdot (\varphi \circ U^*)) \circ U\|_{H^{s-1}(\mathbb{R}^{3(N+M)})} = \|V_{\text{sp},1} \cdot (\varphi \circ U^*)\|_{H^{s-1}(\mathbb{R}^{3(N+M)})} \\ &\lesssim \|\varphi \circ U^*\|_{H^2(\mathbb{R}^{3(N+M)})} (\|V_{\text{sp},1}\|_{H^{s-1}(\mathbb{R}^3)} + \|V_{\text{sp},1}\|_{L^{2s}(\mathbb{R}^3)}) \\ &\lesssim \|\varphi\|_{H^2(\mathbb{R}^{3(N+M)})} (\|V_{\text{sp},1}\|_{H^{s-1}(\mathbb{R}^3)} + \|V_{\text{sp},1}\|_{L^{2s}(\mathbb{R}^3)}). \end{aligned} \quad (2.43)$$

The identities (2.42) and (2.43) complete the proof, and the result follows from Theorem 2.7 and the characterization of Favard spaces in terms of Sobolev spaces as explained before the statement of the result. \square

In summary, we have shown that for very general input states, we can get arbitrarily close to the $\mathcal{O}(n^{-1/4})$ rate that was observed for the ground state of the single-particle Coulomb Hamiltonian in [B+23a], even for many-body Coulomb Hamiltonians.

3. CONVERGENCE RATES FOR ENERGY-LIMITED UNITARY DYNAMICS

In this section, we present a method for obtaining convergence rates inspired directly by quantum theory. Unlike the previous section, which focused on possibly singular but small perturbations, this approach is motivated to study regular but large perturbations tailored towards applications in quantum mechanics. Our approach is based on the “operator E -norm” introduced by Shirokov [S20] and the notion of “energy-limited dynamics” introduced in [vL24].

We fix a separable Hilbert space \mathcal{H} and a positive self-adjoint operator with $\inf \text{Spec } G = 0$. We may think about \mathcal{H} as the Hilbert space describing a quantum system and of G as an energy-observable (a reference Hamiltonian) for this system. For vectors $\psi \in \mathcal{H}$, the *energy-expectation value* $\mathbf{E}(\psi)$ is given by

$$\mathbf{E}(\psi) := \|G^{1/2}\psi\|^2 \quad (3.1)$$

if $\psi \in D(G^{1/2})$ and by $\mathbf{E}(\psi) := \infty$ otherwise.

In the following, we use the language of Sobolev towers, which we introduced in Subsection 2.2 and will briefly recall for the reader’s convenience the setting they are used in this section. For $n \in \mathbb{N}$, we set $\mathcal{H}_n = D(G^{n/2})$ which is a Hilbert space in the graph inner product $\langle \psi, \phi \rangle_n = \langle \psi, \phi \rangle + \langle G^{n/2}\psi, G^{n/2}\phi \rangle$. Note that \mathcal{H}_1 is precisely the space of finite-energy vectors because

$$\mathbf{E}(\psi) = \|\psi\|_1^2 - \|\psi\|^2. \quad (3.2)$$

For negative n , \mathcal{H}_n is defined as the completion of \mathcal{H} with respect to the inner product $\langle \psi, \phi \rangle_n = \langle \psi, (1 + G^n)\phi \rangle$. We have continuous embeddings

$$\dots \supset \mathcal{H}_{-1} \supset \mathcal{H} \supset \mathcal{H}_1 \supset \dots \quad (3.3)$$

The dual space of \mathcal{H}_n is naturally identified with \mathcal{H}_{-n} . Thus, the adjoint A^* of a bounded operator $A \in B(\mathcal{H}_n, \mathcal{H}_m)$ is naturally a bounded operator $A^* : \mathcal{H}_{-m} \rightarrow \mathcal{H}_{-n}$. An operator $A \in B(\mathcal{H}_n, \mathcal{H}_{-n})$ is called hermitian if $A = A^*$ [RS75, p. 192]. Note that relatively $G^{1/2}$ -bounded operators on $D(G^{1/2})$ are precisely the elements of $B(\mathcal{H}_1, \mathcal{H})$. Similarly, hermitian quadratic forms a on \mathcal{H} with form domain $Q(a) = \mathcal{H}_1$ for which $M > 0$ exists such that $\pm a \leq M(G + 1)$, i.e.,

$$\pm a(\psi, \psi) \leq M\|\psi\|_1^2, \quad \psi \in \mathcal{H}_1, \quad (3.4)$$

may be regarded as hermitian operators $A \in B(\mathcal{H}_1, \mathcal{H}_{-1})$ via the equation

$$a(\psi, \phi) = \langle \phi, A\psi \rangle_{-1}, \quad \psi, \phi \in \mathcal{H}_1. \quad (3.5)$$

Following [S20], the operator E -norm is defined as:

Definition 3.1 (E -norm, Shirokov [S20]). *The operator E -norm $\|\cdot\|_E^G$ is defined on the space $B(\mathcal{H}_1, \mathcal{H})$ of $G^{1/2}$ -bounded operators for $E > 0$ by*

$$\|A\|_E^G = \sup \{ \|A\psi\|; \|\psi\| \leq 1, \mathbf{E}(\psi) \leq E \}. \quad (3.6)$$

We remark that the optimization may be restricted to a core \mathcal{D} of $G^{1/2}$, i.e., a $\|\cdot\|_1$ -dense subspace $\mathcal{D} \subset \mathcal{H}_1$, [vL24]. It is shown in [S20] that the operator E -norm is equivalent to the operator norm in $B(\mathcal{H}_1, \mathcal{H})$. In particular, operator E -norms at different energy constraints $E > 0$ are equivalent. In fact, Shirokov showed [S20]:

$$\|\cdot\|_E^G \leq \|\cdot\|_{E'}^G \leq \sqrt{\frac{E'}{E}} \|\cdot\|_E^G, \quad E' \geq E > 0. \quad (3.7)$$

Since we are typically interested in upper bounds on the operator E -norm, the following equivalent definition via a minimization (see [vL24, Prop. 2.19]) will be useful:

$$\|A\|_E^G = \min \{ \sqrt{\lambda E + E_0} : \lambda, E_0 \geq 0, A^*A \leq \lambda G + E_0 \}. \quad (3.8)$$

The operator inequality in (3.8) is in the sense of quadratic forms on $\mathcal{H}_1 = D(G^{1/2})$. The reason that we are interested in the operator E -norm is that convergence in E -norm implies strong convergence.⁹ For instance, consider self-adjoint operators A and B on \mathcal{H} such that $A + B$ is essentially self-adjoint, then the Trotter product converges by [T59, K78], and convergence rates in E -norm

$$\|(e^{itA/n} e^{itB/n})^n - e^{it(A+B)}\|_E^G \leq \varepsilon(t, n, E) \quad (3.9)$$

immediately yield state-dependent convergence rates: If $\psi \in \mathcal{H}_1$ is a unit vector, then

$$\|(e^{itA/n} e^{itB/n})^n \psi - e^{it(A+B)} \psi\| \leq \varepsilon(t, n, \mathbf{E}(\psi)). \quad (3.10)$$

To prove such convergence rates for Trotter products in the operator E -norm, we need the dynamics to respect the energy scale determined by G . For this, we follow [vL24]. The maximal output energy given an energy-constraint $E > 0$ is described by [W17]

$$f_U(E) := \sup \{ \mathbf{E}(U\psi); \|\psi\| \leq 1, \mathbf{E}(\psi) \leq E \}, \quad E > 0. \quad (3.11)$$

The function f_U is a concave nondecreasing function $\mathbb{R}^+ \rightarrow [0, \infty]$. It is connected to the operator E -norm via

$$f_U(E) = \left(\|G^{1/2}U\|_E^G \right)^2. \quad (3.12)$$

Unitary operators for which f_U is finite are called energy-limited [W17, vL24, S19]. Thus, a unitary U is energy-limited if and only if it restricts to an operator $B(\mathcal{H}_1, \mathcal{H}_1)$.

⁹In fact, Shirokov showed that the operator E -norm induces the strong operator topology on bounded subsets of $B(\mathcal{H})$ if the reference Hamiltonian has compact resolvent [S20].

Definition 3.2 (Energy-limited dynamics [vL24]). *A unitary one-parameter group $U(t)$ is energy-limited if there exist ‘stability constants’ $\omega, E_0 \geq 0$ such that*

$$f_{U(t)}(E) \leq e^{\omega|t|}(E + E_0) - E_0, \quad t \in \mathbb{R}, \quad E > 0. \quad (3.13)$$

A collection of unitary one-parameter groups $U_j(t)$, $j \in I$, is jointly energy-limited if there exist joint stability constants ω, E_0 such that (3.13) holds for all $U_j(t)$.

Note that the right-hand side of (3.13) is a semigroup of affine functions of E for times $t > 0$. Energy-limitedness guarantees that the energy expectation value $E(t) := \mathbf{E}(U(t)\psi)$ depends continuously on t for vectors $\psi \in \mathcal{H}_1$. In fact, it guarantees the continuity bound [vL24]

$$|E(t+s) - E(s)| \leq \omega|t|(E(s) + E_0\|\psi\|^2) + \mathcal{O}(|t|^2). \quad (3.14)$$

It is easy to see that every f Energy-limited unitary one-parameter groups are fully characterized by the following structure theorem:

Theorem 3.3 ([vL24, Thm. 3.7]). *Let H be a self-adjoint operator and let $U(t) = e^{-itH}$. Let $\omega, E_0 \geq 0$. Then $U(t)$ is energy-limited with stability constants ω, E_0 if and only if*

- (i) \mathcal{H}_1 is invariant under $U(t)$ and the restriction $U_0(t) := U(t) \upharpoonright \mathcal{H}_1$ is a strongly continuous one-parameter group of bounded operators on \mathcal{H}_1 .
- (ii) The inequality $\pm i[G, H] \leq \omega(G + E_0)$ holds in the sense that

$$|\langle G^{1/2}\psi, G^{1/2}H\psi \rangle - \langle G^{1/2}H\psi, G^{1/2}\psi \rangle| \leq \omega(\|G^{1/2}\psi\|^2 + E_0\|\psi\|^2) \quad (3.15)$$

for all $\psi \in \mathcal{H}_1 \cap D(H)$ such that $H\psi \in \mathcal{H}_1$.

These necessary and sufficient conditions for energy-limitedness are rather hard to check in practice. The following result of Fröhlich [F77] (cp. [vL24, Thm. 3.8]) gives sufficient conditions for energy-limitedness that are much easier to check. Recall that an operator H is G -bounded if and only if H is in $B(\mathcal{H}_2, \mathcal{H})$.

Theorem 3.4 (Fröhlich [F77]). *Let $G_0 \geq 0$ be a positive self-adjoint operator with $\inf \text{Spec } G_0 = 0$ and set $G = (G_0 + E_0)^2 - E_0^2$. Let H be a G_0 -bounded self-adjoint operator with unitary group $U(t) = e^{itH}$ and let \mathcal{D} be a core for G_0 . Let $\omega, \nu \geq 0$ and $E_0 > 0$.*

- (i) *If the operator inequality $\pm i[H, G_0] \leq \omega(G_0 + E_0)$ holds for some $\omega, E_0 > 0$ in the sense of quadratic forms on \mathcal{D} , i.e.,*

$$|\langle H\psi, G_0\psi \rangle - \langle G_0\psi, H\psi \rangle| \leq \langle \psi, \omega(G_0 + E_0)\psi \rangle, \quad \psi \in \mathcal{D}, \quad (3.16)$$

then $U(t)$ is energy-limited with stability constants ω, E_0 with respect to G_0 .

(ii) If $-[H, G_0]^2 \leq \nu^2(G_0 + E_0)^2$ holds in the sense that¹⁰

$$\|[H, G_0]\psi\| \leq \nu\|(G_0 + E_0)\psi\|, \quad \psi \in \mathcal{H}_2, \quad (3.17)$$

then $U(t)$ is energy-limited with respect to the reference Hamiltonian G and has stability constants $2\nu, E_0^2$ with respect to G .

Proof. The result follows from Fröhlich's work [F77] applied to $N = G_0 + E_0$ (Nelson's assumption $N \geq 1$ can be relaxed to $N \geq c1$ for some $c > 0$ without causing any trouble in his proofs). Unfortunately, this result is stated with several additional assumptions that are not used in the proof (as he remarks in [F77, Rem. 1]). To obtain item (i), we apply [vL24, Thm. B.1], which is proved by adapting Fröhlich's argument, to the operators $N = G + E_0$ and $A = \pm iH$ yields item (i) under the assumptions stated above. We now come to item (ii). By [F77, Lem. A.1 and Rem. 1] (again applied to $N = G + E_0$ and $A = iH$), it holds that $\|NU(t)\psi\|^2 \leq e^{2\nu t}\|N\psi\|^2$ which proves the claim. \square

Readers familiar with Nelson's commutator theorem [RS75, Thm. X.37] may recognize that the assumption of self-adjointness is redundant: If \mathcal{D} is a core for G , every symmetric G -bounded operator H satisfying (3.16) on \mathcal{D} is essentially self-adjoint and satisfies the same inequality on $\mathcal{D} = \mathcal{H}_2$.

We now come to the main theorem of this section, which proves convergence rates for the Trotter product of energy-limited unitary groups in the operator E -norm.

Theorem 3.5. *Let A and B be self-adjoint operators generating energy-limited unitary one-parameter groups and let ω, E_0 be joint stability constants. Let \mathcal{D} be a core for $G^{1/2}$ such that*

$$(t, s) \mapsto e^{itA}e^{isB}\psi, \quad \text{and} \quad (t, s) \mapsto e^{itB}e^{isA}\psi \quad (3.18)$$

are both in $C^2(\mathbb{R}^2, \mathcal{H})$ for all $\psi \in \mathcal{D}$. If the commutator $[A, B] : \mathcal{D} \rightarrow \mathcal{H}$ is $G^{1/2}$ -bounded, then $A + B$ is essentially self-adjoint on \mathcal{D} and

$$\|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G \leq \frac{t^2}{2n} \|[A, B]\|_{f_{2t}(E)}^G \quad (3.19)$$

for all $n \in \mathbb{N}$, where $f_t(E) = E + (e^{\omega t} - 1)(E + E_0)$.

We remark that the C^2 assumption in Theorem 3.5 ensures that the commutator $[A, B]$ makes sense as an operator on the core \mathcal{D} . Furthermore, as seen in Step 2 in the proof of Theorem 3.5, essential self-adjointness of $A + B$ on \mathcal{D} is a direct consequence of the convergence of the Trotter product. This is in sharp contrast to the setup in Section 2 in which the fact that the sum of the generators is again a generator of

¹⁰The left-hand side of (3.17) is defined as the supremum over $|\langle H\phi, G_0\psi \rangle - \langle G_0\phi, H\psi \rangle|$ where ϕ ranges over all unit vectors in \mathcal{H}_2 .

a strongly continuous contraction semigroup or even unitary group followed already directly from the employed relative boundedness assumptions.

Recall that an operator K on a Hilbert space generates a contraction semigroup if and only if it is maximally dissipative, i.e., K is dissipative and admits no (proper) dissipative extension [ACE23].

Lemma 3.6. *Let A, B be self-adjoint operators generating energy-limited unitary dynamics with joint stability constants ω, E_0 . Let iC be a maximally dissipative operator. Then*

$$\|(e^{itA/n}e^{itB/n})^n - e^{itC}\|_E^G \leq n\|e^{itA/n}e^{itB/n} - e^{itC/n}\|_{f_{2t-2t/n}(E)}^G, \quad (3.20)$$

where $f_t(E) = e^{\omega t}E + (e^{\omega t} - 1)E_0$ and $t > 0$. If C is self-adjoint and e^{itC} is energy-preserving, i.e., commutes with G for all $t \in \mathbb{R}$, we have

$$\|(e^{itA/n}e^{itB/n})^n - e^{itC}\|_E^G \leq n\|e^{itA/n}e^{itB/n} - e^{itC/n}\|_E^G. \quad (3.21)$$

Proof. Set $V(t) = e^{itA}e^{itB}$. Then $f_{V(t)}(E) \leq f_{2t}(E)$ and

$$\begin{aligned} \|V(t/n)^n - e^{itC}\|_E^G &= \left\| \sum_{j=1}^n e^{i(t(j-1)/n)C} (V(t/n) - e^{itC/n}) V(t/n)^{n-j} \right\|_E^G \\ &\leq \sum_{j=1}^n \|(V(t/n) - e^{itC/n}) V(t/n)^{n-j}\|_E^G \\ &\leq \sum_{j=1}^n \|V(t/n) - e^{itC/n}\|_{f_{2t \frac{n-j}{n}}(E)}^G \\ &\leq n\|V(t/n) - e^{itC/n}\|_{f_{2t-2t/n}(E)}^G, \end{aligned}$$

where we used the semigroup property of f_t and that $f_t(E)$ is monotone in t . The second claim follows similarly by sorting the dynamics generated by C in the first equation to the right instead of the left. \square

Lemma 3.7. *Under the assumptions of Theorem 3.5, we have*

$$\|e^{-itA}Be^{itA} - B\|_E^G \leq t\|[A, B]\|_{f_t(E)}^G. \quad (3.22)$$

Proof. Let ψ, ϕ be unit vectors in \mathcal{D} and let $\langle \psi, G\psi \rangle \leq E$. Then

$$\begin{aligned} \langle \phi, (e^{-itA}Be^{itA} - B)\psi \rangle &= \int_0^t \frac{d}{ds} \langle e^{isA}\phi, Be^{isA}\psi \rangle ds \\ &= \int_0^t \langle Ae^{isA}\phi, Be^{isA}\psi \rangle - \langle e^{isA}\phi, BAe^{isA}\psi \rangle ds \\ &= \int_0^t \langle e^{isA}\phi, [A, B]e^{isA}\psi \rangle ds \end{aligned}$$

Optimizing over unit vectors $\phi, \psi \in \mathcal{D}$ with $\langle \psi, G\psi \rangle \leq E$, we get

$$\|e^{-itA}Be^{itA} - B\|_E^G \leq \int_0^t \|[A, B]\|_{f_s(E)}^G ds \leq t\|[A, B]\|_{f_t(E)}^G.$$

□

We need the following Lemma on dissipative extensions of symmetric operators (see [ACE23, Thm. 2.5]):

Lemma 3.8. *Let T be a symmetric operator on a separable Hilbert space \mathcal{H} . Let $S \supset T$ be an extension such that iS is dissipative, i.e., an extension such that $\text{Im}\langle \psi, S\psi \rangle \leq 0$, $\psi \in D(S)$, then it follows that*

$$T \subset S \subset T^* \quad \text{and} \quad T \subset S^* \subset T^*. \quad (3.23)$$

Using Lemmas 3.6 – 3.8, we can prove Theorem 3.5:

Proof of Theorem 3.5. As stated in the theorem, we set $f_t(E) = e^{\omega t}(E + E_0) - E_0$. Note that $f_{e^{itA}}(E), f_{e^{itB}}(E) \leq f_{|t|}(E)$.

Step 1. In the first step, we establish the desired bound (3.19) for $t > 0$ and a maximally dissipative, i.e., contraction-generating, extension iC of the skew-symmetric operator $i(A + B)$. It follows that $-iC^*$ generates a contraction semigroup as well, and, by Lemma 3.8, that C^* is also an extension of $A + B$. We start with Lemma 3.6, which gives

$$\|(e^{itA/n}e^{itB/n})^n - e^{itC}\|_E^G \leq n\|e^{itA/n}e^{itB/n} - e^{itC/n}\|_{f_{2t-2t/n}(E)}^G. \quad (3.24)$$

To estimate the right-hand side, we pick unit vectors and $\phi, \psi \in \mathcal{D}$ with $\langle \psi, G\psi \rangle \leq E$. We have

$$\begin{aligned} \langle \phi, (e^{itA}e^{itB} - e^{itC})\psi \rangle &= \langle e^{-itC^*}\phi, \psi \rangle - \langle \phi, e^{itA}e^{itB}\psi \rangle \\ &= \int_0^t \frac{d}{ds} \langle e^{-isC^*}\phi, e^{isA}e^{isB}\psi \rangle ds \\ &= \int_0^t \left(\langle -iC^*e^{-isC^*}\phi, e^{isA}e^{isB}\psi \rangle - \langle e^{-isC^*}\phi, e^{isA}(A+B)e^{-isB}\psi \rangle \right) ds \\ &= \int_0^t \left(\langle -ie^{-isC^*}\phi, Ce^{isA}e^{isB}\psi \rangle - \langle e^{-isC^*}\phi, e^{isA}(A+B)e^{-isB}\psi \rangle \right) ds \\ &= i \int_0^t \langle e^{-isC^*}\phi, ((A+B)e^{isA} - e^{isA}(A+B))e^{isB}\psi \rangle ds \\ &= i \int_0^t \langle e^{-isC^*}\phi, [B, e^{isA}]e^{isB}\psi \rangle ds, \end{aligned}$$

where we used that $\phi \in D(C^*)$ and that C equals $A + B$ on $e^{isA}e^{isB}\mathcal{D} \subset D(A + B)$. Using that e^{-isC^*} is a contraction, we get

$$|\langle \phi, (e^{itA}e^{itB} - e^{itC})\psi \rangle| \leq \int_0^t \|[B, e^{isA}]e^{isB}\psi\| ds. \quad (3.25)$$

Optimizing over ϕ and replacing t by t/n , gives

$$\|(e^{itA/n}e^{itB/n} - e^{itC/n})\psi\| \leq \int_0^{t/n} \|[B, e^{isA}]e^{isB}\psi\| ds \leq \int_0^{t/n} \|[B, e^{isA}]\|_{f_s(E)}^G ds.$$

Since $\|[B, e^{itA}]\|_E^G = \|e^{-itA}Be^{itA} - B\|_E^G$, we can apply Lemma 3.7 to obtain

$$\begin{aligned} \|(e^{itA/n}e^{itB/n} - e^{itC/n})\psi\| &= \int_0^{t/n} s\|[A, B]\|_{f_{2s}(E)}^G ds \\ &\leq \frac{t^2}{2n^2} \|[A, B]\|_{f_{2t/n}(E)}^G. \end{aligned} \quad (3.26)$$

Optimizing over ψ and inserting this estimate into (3.24), yields

$$\|(e^{itA/n}e^{itB/n})^n - e^{itC}\|_E^G \leq \frac{t^2}{2n} \|[A, B]\|_{f_{2t}(E)}^G. \quad (3.27)$$

Step 2. Since the commutator is $G^{1/2}$ -bounded by assumption, the right-hand side of (3.27) is finite and goes to zero as $n \rightarrow \infty$. This implies that the Trotter product converges strongly for $t > 0$ to the dynamics generated by a contraction-generating extension $i(A + B)|_{\mathcal{D}}$. Since this holds for all contraction-generating extensions of $i(A + B)|_{\mathcal{D}}$, it follows that $i(A + B)|_{\mathcal{D}}$ has a unique contraction-generating extension. This extension generates an isometry semigroup because strong limits of unitaries are isometries, and, hence, C is a symmetric operator. Thus, one of the defect indices of $(A + B)|_{\mathcal{D}}$ is zero. If we apply the same arguments (including step one) with A and B replaced by their negatives, we learn that the same holds for $-i(A + B)|_{\mathcal{D}}$. Thus, $(A + B)|_{\mathcal{D}}$ is essentially self-adjoint since both defect indices are zero. We conclude that (3.27) holds with $C = \overline{(A + B)}$ for $t \in \mathbb{R}$. \square

Using the variational principle (3.8) or the estimate (3.7), we can further bound the right-hand side of (3.19)

Corollary 3.9. *Under the assumptions of Theorem 3.5, the convergence rate of the Trotter product is bounded by*

$$\|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G \leq \frac{t^2}{2n} \|[A, B]\|_E^G \cdot \sqrt{1 + (e^{2\omega t} - 1)(1 + \frac{E_0}{E})} \quad (3.28)$$

Furthermore, if $M, E_1 \geq 0$ are such that $-[A, B]^2 \leq M(G + E_0)$ holds in the sense

$$\|[A, B]\psi\|^2 \leq M^2(\|G^{1/2}\psi\|^2 + E_1\|\psi\|^2), \quad \psi \in \mathcal{D}, \quad (3.29)$$

then

$$\|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G \leq \frac{t^2}{2n} M \sqrt{e^{2\omega t}(E + E_0) + E_1 - E_0}. \quad (3.30)$$

In particular, when we choose $E_1 = E_0$ the bound (3.30) takes the simple form

$$\|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G \leq \frac{t^2}{2n} M e^{\omega t} \sqrt{E + E_0}. \quad (3.31)$$

In cases where the joint dynamics is energy-preserving, i.e., commutes with the reference Hamiltonian, the exponential behaviour in the time parameter can be tamed:

Corollary 3.10. *Let A, B be self-adjoint operators satisfying the assumptions of Theorem 3.5 and let $\omega, E_0, f_t(E)$ be as in that theorem. Assume that $\overline{A+B}$ has energy-preserving dynamics with respect to G . Then*

$$\|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G \leq \frac{t^2}{2n} \|[A, B]\|_{f_{2t/n}(E)}^G \quad (3.32)$$

In particular, if $M > 0$ is such that $-[A, B]^2 \leq M(G + E_0)$ in the sense of (3.29), then

$$\|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G \leq \frac{t^2}{2n} M e^{\omega t/n} \sqrt{E + E_0}. \quad (3.33)$$

Proof. This follows from Lemma 3.6 and (3.26):

$$\begin{aligned} \|(e^{itA/n}e^{itB/n})^n - e^{i\overline{(A+B)}}\|_E^G &\leq n \|(e^{itA/n}e^{itB/n})^n - e^{it\overline{(A+B)}/n}\|_E^G \\ &\leq \frac{t^2}{2n} \|[A, B]\|_{f_{2t/n}(E)}^G. \end{aligned}$$

□

In Section 4, we will see numerically that these bounds correctly predict the actual convergence rates of the infinite-dimensional problem.

3.1. Application to Schrödinger operators. In this section, we consider Schrödinger operators $-\Delta + V(x)$ with potentials V whose second derivatives are bounded. Additionally, we need polynomial boundedness:

We write P and Q for the momentum and position operators $P\psi(x) = -i\psi'(x)$ and $Q\psi(x) = x\psi(x)$ defined on their natural domains. Note that the Schrödinger operator $-\Delta + V(x)$ equals $P^2 + V(Q)$. Throughout this section, we write $N = P^2 + Q^2$ for the harmonic oscillator.

Lemma 3.11. *Let $V \in C^4(\mathbb{R}, \mathbb{R})$ with V and its first 4 derivatives being polynomially bounded. Then for Schwartz function $\psi \in \mathcal{S}(\mathbb{R})$ we have that the maps*

$$(t, s) \mapsto e^{itP^2} e^{isV(Q)} \psi \quad \text{and} \quad (t, s) \mapsto e^{itV(Q)} e^{isP^2} \psi \quad (3.34)$$

are in $C^2(\mathbb{R}^2, \mathcal{H})$. In particular, the commutator $[V(Q), P^2]$ is well-defined on $\mathcal{S}(\mathbb{R})$.

Proof. We shall prove the claim for $G(t, s) := e^{itP^2} e^{isV(Q)} \psi$, the other ordering follows from analogous arguments. We first recall that, since $e^{isV(Q)} \psi \in D(P^2) = H^2(\mathbb{R})$, we can differentiate in t to find

$$\partial_t G(t, s) = i e^{itP^2} P^2 (e^{isV(Q)} \psi).$$

Since by assumption $P^2(e^{isV(Q)} \psi) \in D(P^2)$ as well, we can apply the same argument again to find that

$$\partial_t^2 G(t, s) = -e^{itP^2} P^4 (e^{isV(Q)} \psi).$$

We can explicitly compute the derivative $(iP)^2(e^{isV(Q)} \psi)$ to see that $\partial_t^2 G(t, s)$ is continuous in (t, s) . Finally, since

$$F(s) := P^2(e^{isV(x)} \psi(x)) = e^{isV(x)} (2is\psi'(x)V'(x) + \psi''(x) + s\psi(x)(iV''(x) - sV'(x)^2))$$

is differentiable in s with

$$\begin{aligned} F'(s) &= iV(x)e^{isV(x)} (2is\psi'(x)V'(x) + \psi''(x) + s\psi(x)(iV''(x) - sV'(x)^2)) \\ &\quad + ie^{isV(x)} (2V'(x)\psi'(x) + \psi(x)(V''(x) + 2isV'(x)^2)) \end{aligned}$$

by Lebesgue's differentiation theorem. This implies that $\lim_{h \rightarrow 0} \frac{\|F(s+h) - F(s) - hF'(s)\|_{L^2}}{h} = 0$. Continuity of e^{itP^2} thus allows us to interchange limits and conclude that

$$\partial_s \partial_t G(t, s) = \lim_{h \rightarrow 0} e^{itP^2} \frac{F(h+s) - F(s)}{h} = e^{itP^2} F'(s) = -e^{itP^2} P^2 (e^{isV(x)} V(x) \psi)(x)$$

exists. The continuity of the derivative $\partial_s \partial_t G(t, s)$ then just follows from the (strong) continuity of the semigroup e^{itP^2} and the continuity of the expression of $F'(s)$ in s .

The continuity of the semigroups (e^{itP^2}) , as above, and since $\psi \in D(V(Q)^k)$ for $k \geq 0$, implies that

$$\partial_s^k G(t, s) = e^{itP^2} e^{isV(x)} (iV(x))^k \psi.$$

By strong continuity of the two groups, this also implies that $(t, s) \mapsto \partial_s^k G(t, s)$ is continuous.

Finally, since $e^{isV(x)} (iV(x)) \psi \in D(P^2)$, we have

$$\partial_t \partial_s G(t, s) = -e^{itP^2} P^2 e^{isV(x)} V(x) \psi(x)$$

and by working out the derivative $P^2 e^{isV(x)} V(x) \psi(x)$ and using the strong continuity of the semigroups, we find that $(t, s) \mapsto \partial_t \partial_s G(t, s)$ is continuous which implies the claim. \square

Since we assume V'' is uniformly bounded, we can bound¹¹

$$|V'(x)| \leq (|V'(0)| + \|V''\|_{L^\infty})(1+x^2)^{1/2} \quad (3.35)$$

and, hence, $|V(x)| \lesssim 1+x^2$. In particular, this implies that $V(Q)$ is relatively bounded with respect to $N = P^2 + Q^2$.

Lemma 3.12. *Let V satisfy the assumption of Lemma 3.11. Then the commutator $[V(Q), P^2]$ is relatively bounded with respect to N . The energy-constrained operator norm with respect to the reference Hamiltonian $G = N^2 - 1$ is bounded by*

$$\|[V(Q), P^2]\|_E^G \leq \nu \sqrt{E+1} \quad (3.36)$$

where $\nu = 5\|V''\|_{L^\infty} + 4|V'(0)|$.

Proof. First note that

$$-i[V(Q), P^2] = PV'(Q) + V'(Q)P = 2V'(Q)P - iV''(Q).$$

Since $V'' \in L^\infty$, we only have to show that $V'(Q)P$ is N -bounded. Let $w = \|V''\|_{L^\infty} + |V'(0)|$ such that $|V'(x)|^2 \leq w^2(1+x^2)$, cf. (3.35). Then $V'(Q)^2 \leq w^2(1+Q^2)$ and, hence,

$$\|V'(Q)P\psi\|^2 \leq w^2\|(1+Q^2)^{1/2}P\psi\|^2 = w^2(\|QP\psi\|^2 + \|P\psi\|^2)$$

for $\psi \in D(N)$. This reduces the problem to showing that QP is N -bounded, which follows from the canonical commutation relations ($[Q, P] = i$):

$$\begin{aligned} 2PQ^2P &= PQPQ + PQ[Q, P] + QPQP + [P, Q]QP \\ &= PQPQ + QPQP + i(PQ - QP) \\ &= P^2Q^2 + P[Q, P]Q + Q^2P^2 + Q[P, Q]P + i(PQ - QP) \\ &= P^2Q^2 + Q^2P^2 + 2i(PQ - QP) \\ &\leq (P^2 + Q^2)^2 + 2 = N^2 + 2 \leq 3N^2, \end{aligned}$$

¹¹Let f be Lipschitz continuous (e.g. V' above). Then it has a weak derivative $f' \in L^\infty$. Let $a = |f(0)|$ and $M = \|f'\|_{L^\infty}$ be the optimal Lipschitz constant. Then noting that $|x| \leq (1+x^2)/2$ we have

$$f(x)^2 = (f(x) - f(0) + f(0))^2 \leq M^2x^2 + 2aM|x| + a^2 \leq M(M+a)x^2 + a(M+a) \leq w^2(1+x^2)$$

where $w = M + a$.

where we used that $N \geq 1$. Putting everything together, we get

$$\begin{aligned}
\|[V(Q), P^2]\psi\| &\leq \|V''\|_{L^\infty} \|\psi\| + 2\|V'(Q)P\psi\| \\
&\leq \|V''\|_{L^\infty} \|\psi\| + 2w(\|QP\psi\|^2 + \|P\psi\|^2)^{1/2} \\
&\leq \|V''\|_{L^\infty} \|\psi\| + 2w\left(\frac{3}{2}\|N\psi\|^2 + \|N\psi\|^2\right)^{1/2} \\
&= \|V''\|_{L^\infty} \|\psi\| + \sqrt{10}w\|N\psi\| = \nu\|N\psi\| \\
&= \nu\|(G_0 + 1)\psi\| = \nu\|(G + 1)^{1/2}\psi\|
\end{aligned} \tag{3.37}$$

where (with $\sqrt{10} < 4$)

$$\nu = 4w + \|V''\|_{L^\infty} = 4|V'(0)| + 5\|V''\|_{L^\infty}.$$

Finally, eq. (3.36) follows from eq. (3.8). \square

Lemma 3.13. *Let V satisfy the assumption of Lemma 3.11. Take $G = N^2 - 1$ as the reference Hamiltonian.*

- (1) *The unitary one-parameter group e^{itP^2} is energy-limited with stability constants $20, 1$*
- (2) *The unitary one-parameter group $e^{itV(Q)}$ is energy-limited with stability constants $2\nu, 1$ where ν is as in Lemma 3.12.*

In particular, $\gamma, 1$ are joint stability constants with $\gamma = \max\{2\nu, 20\}$.

Proof. We prove both items by applying the second part of Theorem 3.4 with reference Hamiltonian $G_0 = N - 1$. We start with the second statement. Clearly both $V(Q)$ and P^2 are N -bounded. By eq. (3.37), the inequality

$$-[V(Q), N]^2 = -[V(Q), P^2]^2 \leq \nu(G + 1) = \nu(G_0 + 1)^2 \tag{3.38}$$

holds in the sense of quadratic forms. Thus, Theorem 3.4 implies that $e^{itV(Q)}$ is energy-limited with stability constants $2\nu, 1$ with respect to $(G_0 + 1)^2 - 1 = G = N^2 + 1$.

The statement for e^{itP^2} follows from this. Since $[P^2, N] = [P^2, Q^2]$ is of above form with $V(x) = -x^2$, we have $|V'(0)| = 0$, $\|V''\|_{L^\infty} = 2$ and thus, cf. (3.36),

$$-[P^2, N]^2 \leq ((4 + 1) \cdot 2)N^2 = 10(G + 1). \tag{3.39}$$

Therefore, P^2 is energy-limited with stability constants $20, 1$ with respect to G , and the claim follows. \square

Theorem 3.14. *Let $V \in C^4(\mathbb{R}, \mathbb{R})$ have bounded second derivative and assume that $V^{(3)}$ and $V^{(4)}$ are polynomially bounded. Then $H = P^2 + V(Q)$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R})$. Set $\nu = 5\|V''\|_{L^\infty} + 4|V'(0)|$ and $\gamma = \max\{2\nu, 20\}$.*

Then

$$\|(e^{-itP^2/n} e^{tV/n})^n \psi - e^{-itH} \psi\| \leq \frac{t^2}{2n} \nu e^{\gamma t} \|N\psi\| \tag{3.40}$$

for all $\psi \in D(N)$.

Proof. We apply Corollary 3.9 with $A = P^2$, $B = V(Q)$ and $\mathcal{D} = \mathfrak{S}(\mathbb{R})$. Energy-limitedness of e^{itP^2} and $e^{itV(Q)}$ with the claimed stability constants is proved in Lemma 3.13. $G^{1/2}$ -boundedness of the commutator $[A, B] = [V(Q), P^2]$ is proved in Lemma 3.12, and the C^2 condition is proved in Lemma 3.11. Then, (3.29) holds with $M = \nu$ and $E_0 = 1$. Therefore, we get (cp. (3.31))

$$\|(e^{-itP^2/n} e^{tV/n})^n - e^{-itH}\|_E^G \leq \frac{t^2}{2n} \nu e^{\gamma t} \sqrt{E+1}. \quad (3.41)$$

If $\psi \in D(N)$ is a unit vector, the left-hand side of (3.40) is bounded by the operator E -norm $\|(e^{-itP^2/n} e^{tV/n})^n - e^{-itH}\|_E^G$ with $E = \mathbf{E}(\psi) = \|N\psi\|^2 - 1$. Thus, (3.40) follows from (3.41). \square

3.2. Explicit example: Trotter splitting for the Harmonic oscillator. Let us specialize to the Harmonic oscillator. In this case, the joint dynamics is energy-preserving relative to the reference Hamiltonian $G = N^2 - 1$. Making use of Corollary 3.10, we get:

Theorem 3.15. *Let $\psi \in D(N)$. Then*

$$\|(e^{itP^2/n} e^{itQ^2/n})^n \psi - e^{itN} \psi\| \leq 6 \frac{t^2 \|N\psi\|}{n} \quad (3.42)$$

for all $n \geq 55t$.

We will see numerically in Section 4 that this bound correctly predicts the actual convergence rates.

Proof. By Lemma 3.13, the dynamics of P^2 and Q^2 have joint stability constants 20, 1. Corollary 3.10 gives

$$\|(e^{itP^2/n} e^{itQ^2/n})^n - e^{itN}\|_E^G \leq \frac{t^2}{2n} \|[P^2, Q^2]\|_{e^{20t/n}(E+1)-1}^{N^2-1}.$$

By Lemma 3.12, we have

$$\|[P^2, Q^2]\|_E^{N^2-1} \leq 10\sqrt{E+1}.$$

Taken together, these imply

$$\|(e^{itP^2/n} e^{itQ^2/n})^n - e^{itN}\|_E^G \leq \frac{t^2}{2n} 10 e^{10t/n} \sqrt{E+1}$$

Since $10t/n \leq \log(6/5)$ guarantees $5e^{10t/n} \leq 6$ and since $10/\log(6/5) \leq 55$ the claim follows. \square

3.3. Application to magnetic Dirac operators. We consider the free Dirac operator in 2 and 3 dimensions, which takes the abstract form, for $D_{x_i} := \frac{1}{i} \frac{\partial}{\partial x_i}$,

$$H_{\text{free}} = \begin{pmatrix} mc^2 & cD^* \\ cD & -mc^2 \end{pmatrix} \in \mathbb{C}^{2(n-1) \times 2(n-1)},$$

with Pauli matrices σ_i

$$D = \begin{cases} \sum_{i=1}^3 \sigma_i D_{x_i} & \text{if } n = 3, \\ D_{x_1} + iD_{x_2} & \text{if } n = 2, \end{cases} \quad \text{with } D \in \mathbb{C}^{(n-1) \times (n-1)},$$

see [Th92] for a general introduction to Dirac operators. One then has:

Lemma 3.16. *Let $V \in C^2(\mathbb{R}^n, \mathbb{C}^{2(n-1) \times 2(n-1)})$ hermitian for $n \in \{2, 3\}$ with V and its first 2 derivatives being polynomially bounded. If $\psi \in \mathcal{S}(\mathbb{R}^n; \mathbb{C}^{2(n-1)})$, then the maps*

$$(t, s) \mapsto e^{itH_{\text{free}}} e^{isV(Q)} \psi \quad \text{and} \quad (t, s) \mapsto e^{itV(Q)} e^{isH_{\text{free}}} \psi \quad (3.43)$$

are in $C^2(\mathbb{R}^2, \mathcal{H})$, where $\mathcal{H} = L^2(\mathbb{R}^n; \mathbb{C}^{2(n-1) \times 2(n-1)})$.

We omit its proof as it is very similar to Lemma 3.11. It follows from [Th92, Thm. 4.3] that the Dirac operator $H_{\text{free}} + V$ with V as in Lemma 3.16 is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^n; \mathbb{C}^{2(n-1)})$.

Magnetic Dirac operators.

Unlike potential perturbations that we considered for Schrödinger operators, we may also consider quantum systems incorporating a magnetic field.

For Dirac operators, magnetic fields are incorporated as follows: In three dimensions, the magnetic vector potential $A \in C^\infty(\mathbb{R}^3; \mathbb{R}^3)$ gives a magnetic field $\mathbf{B} = \text{curl}(A)$, whereas in two dimensions, the magnetic field strength just reduces to a scalar field $B = \partial_{x_1} A_2 - \partial_{x_2} A_1$.

The magnetic Dirac operator then takes the abstract form

$$H = \begin{pmatrix} mc^2 & cD^* \\ cD & -mc^2 \end{pmatrix},$$

with

$$D = \begin{cases} \sum_{i=1}^3 \sigma_i (D_{x_i} - A_i) & \text{if } n = 3, \\ (D_{x_1} - A_1) + i(D_{x_2} - A_2) & \text{if } n = 2 \end{cases}$$

and $D_{x_1} = -i\partial_{x_1}$. The Pauli operator is then, for $\sigma = (\sigma_1, \sigma_2, \sigma_3)$, defined by

$$H_P = D^* D = (-i\nabla - A)^2 - \begin{cases} \sigma \cdot \mathbf{B} & \text{if } n = 3, \\ B & \text{if } n = 2. \end{cases} \quad (3.44)$$

Homogeneous magnetic fields. For illustration purposes, we shall now consider a homogeneous magnetic field in two dimensions, i.e., $\mathbf{B} = (0, 0, B_0)$ and $B_0 > 0$. We can

then choose the unbounded(!) magnetic potential $A(x) = \frac{B_0}{2}(-x_2, x_1, 0)$ that yields the constant magnetic field and observe that

$$[D, D^*] = 2B_0. \quad (3.45)$$

From this, we can deduce that

$$\text{Spec}(H_P) = 2\mathbb{N}_0 B_0$$

such that $G := H_P$ is a positive self-adjoint operator with $\inf \text{Spec } G = 0$. We also notice that

$$D = 2D_{\bar{z}} - \frac{iB_0}{2}z \text{ with } z = x_1 + ix_2$$

where $\partial_{\bar{z}} = \partial_{x_1} + i\partial_{x_2}$ with $D_{\bar{z}} = -i\partial_{\bar{z}}$ and $\partial_z = \partial_{x_1} - i\partial_{x_2}$ with $D_z = -i\partial_z$ such that

$$\begin{aligned} H_P &= \left(D_{x_1} - \frac{B_0 x_2}{2} \right)^2 + \left(D_{x_2} + \frac{B_0 x_1}{2} \right)^2 - B_0 \\ &= -\Delta + B_0(\bar{z}\partial_{\bar{z}} - z\partial_z) + \frac{B_0^2}{4}|z|^2 - 2B_0. \end{aligned}$$

We therefore consider a Trotter-splitting of the Hamiltonian with

$$K = \begin{pmatrix} 0 & 2D_z \\ 2D_{\bar{z}} & 0 \end{pmatrix} \text{ and } P = \begin{pmatrix} 0 & \frac{iB_0}{2}\bar{z} \\ -\frac{iB_0}{2}z & 0 \end{pmatrix}. \quad (3.46)$$

Theorem 3.17. *For kinetic energy K and magnetic potential P as in (3.46) and $G = (-\Delta + |z|^2 - 2)^2$ as in Eq. (3.44), the Trotter splitting for the magnetic Dirac operator satisfies for $\omega := 2\varepsilon \max\{1, B_0\}$, $E_0 := \frac{4}{\varepsilon\omega}(2 + \frac{1}{\varepsilon^2}) \max\{B_0, 1\}$ with $\varepsilon > 0$ arbitrary*

$$\| (e^{-itK/n} e^{-itP/n})^n - e^{-it(K+P)} \|_E^G \leq \frac{t^2 B_0 (\sqrt{6} + 1)}{2n} \sqrt{e^{2\omega t} (E + E_0) + 2 - E_0}. \quad (3.47)$$

In particular, for $\varepsilon = 1/t$, we obtain a global-in time bound of the form

$$\| (e^{-itK/n} e^{-itP/n})^n - e^{-it(K+P)} \|_E^G = \mathcal{O}_{B_0}(t^2(1+t)(1+\sqrt{E})/n) \quad (3.48)$$

Proof. We apply Eq. (3.31) with $A = K$ and $B = P$. The C^2 condition follows from Lemma 3.16. We write $N = -\Delta + |z|^2$ and $G_0 = N - 2$ such that $G_0^2 = G$.

It then suffices, by Theorem 3.4, to compute and bound the relevant commutators: We compute

$$[K, N] = \begin{pmatrix} 0 & -2i\bar{z} \\ -2iz & 0 \end{pmatrix} \quad \text{and} \quad [P, N] = 2B_0 \begin{pmatrix} 0 & -D_{\bar{z}} \\ D_z & 0 \end{pmatrix},$$

so in particular $\|[K, N]\|^2, B_0^{-2}\|[P, N]\|^2 \leq 4N = 4(G_0 + 2)$. Moreover, we recall the identity

$$[K, G] = [K, N]G_0 + G_0[K, N].$$

By this, the Cauchy-Schwarz inequality, Young's inequality for products¹² and by above operator inequalities for the commutators we have for $\varepsilon > 0$ arbitrary and $\delta = \varepsilon^2/2$ that

$$\begin{aligned}
|\langle \psi, [K, G]\psi \rangle| &\leq 2|\langle G_0\psi, [K, N]\psi \rangle| \\
&\leq \varepsilon \|G_0\psi\|^2 + \frac{1}{\varepsilon} \|[K, N]\psi\|^2 \\
&\leq \varepsilon \|G_0\psi\|^2 + \frac{4}{\varepsilon} \langle (G_0 + 2)\psi, \psi \rangle \\
&= \varepsilon \|G_0\psi\|^2 + \frac{4}{\varepsilon} \langle G_0\psi, \psi \rangle + \frac{8}{\varepsilon} \|\psi\|^2 \\
&\leq \varepsilon \|G_0\psi\|^2 + \frac{2\delta}{\varepsilon} \|G_0\psi\|^2 + \frac{2}{\varepsilon\delta} \|\psi\|^2 + \frac{8}{\varepsilon} \|\psi\|^2 \\
&= 2\varepsilon \|G_0\psi\|^2 + \frac{4}{\varepsilon^3} \|\psi\|^2 + \frac{8}{\varepsilon} \|\psi\|^2 \\
&= 2\varepsilon \|G_0\psi\|^2 + 4 \left(\frac{1}{\varepsilon^3} + \frac{2}{\varepsilon} \right) \|\psi\|^2
\end{aligned}$$

and similarly

$$\begin{aligned}
|\langle \psi, [P, G]\psi \rangle| &\leq \varepsilon B_0 \|G_0\psi\|^2 + \frac{1}{\varepsilon B_0} \|[P, N]\psi\|^2 \\
&\leq \varepsilon B_0 \|G_0\psi\|^2 + \frac{4B_0}{\varepsilon} \langle (G_0 + 2)\psi, \psi \rangle \\
&\leq \varepsilon B_0 \|G_0\psi\|^2 + \frac{2\delta B_0}{\varepsilon} \|G_0\psi\|^2 + \frac{2B_0}{\varepsilon\delta} \|\psi\|^2 + \frac{8B_0}{\varepsilon} \|\psi\|^2 \\
&= 2\varepsilon B_0 \|G_0\psi\|^2 + 4B_0 \left(\frac{1}{\varepsilon^3} + \frac{2}{\varepsilon} \right) \|\psi\|^2.
\end{aligned}$$

Thus, we find that e^{itP} and e^{itK} are energy-limited with stability constants $\omega := 2\varepsilon \max\{1, B_0\}$, $E_0 := \frac{4}{\varepsilon\omega} (2 + \frac{1}{\varepsilon^2}) \max\{B_0, 1\}$ with respect to G . We also compute

$$\begin{aligned}
[K, P] &= iB_0 \text{diag}(-(D_z z + \bar{z}D_{\bar{z}}), D_{\bar{z}}\bar{z} + zD_z) \\
&= B_0 \text{diag}(-1 - (z\partial_z + \bar{z}\partial_{\bar{z}}), 1 + (\bar{z}\partial_{\bar{z}} + z\partial_z)) \\
&= B_0 \text{diag}(-1 - (x_1\partial_{x_1} + x_2\partial_{x_2}), 1 + x_1\partial_{x_1} + x_2\partial_{x_2}).
\end{aligned}$$

From (3.37) we conclude that

$$\begin{aligned}
\|[K, P]\psi\| &\leq B_0 (\|\psi\| + \|x_1\partial_{x_1}\psi\| + \|x_2\partial_{x_2}\psi\|) \\
&\leq B_0 (\|\psi\| + \sqrt{6}\|N\psi\|) \\
&\leq B_0 (\sqrt{6} + 1) \|(G + 2)^{1/2}\psi\|.
\end{aligned} \tag{3.49}$$

¹²It holds for $x, y \in \mathbb{R}$, $\lambda > 0$ and $p, q > 1$ with $1/p + 1/q = 1$ that

$$|xy| \leq \frac{\lambda}{p} |x|^p + \frac{\lambda^{1-q}}{q} |y|^q$$

which we apply here for $p = q = 2$ and once for $\lambda = \varepsilon$, resp. $\lambda = B_0\varepsilon$, and once for $\lambda = \delta$.

This shows that in the notation of (3.29)

$$\|[K, P]\psi\|^2 \leq B_0^2(\sqrt{6} + 1)^2(\|G^{1/2}\psi\|^2 + 2\|\psi\|^2),$$

we have $M = B_0(\sqrt{6} + 1)$ and $E_1 = 2$. Thus, the result follows from (3.30). \square

Remark 3.18. *To close the estimate, it seemed necessary to consider again the harmonic oscillator as a reference Hamiltonian in the previous theorem. We were initially considering the Pauli operator too but were unable to bound $[K, P]$ in (3.49) with respect to this reference operator.*

4. NUMERICAL EXAMPLES

In this section, we compare our convergence rates on suitably chosen vectors to the true convergence rates of the Trotter splitting in large finite-dimensional approximations of the full infinite-dimensional Hilbert space. We verified numerically that the dimension of the approximation is sufficiently large in the sense that the Trotter error remains constant when increasing it further. We interpret this as a heuristic confirmation that our numerics capture the convergence rate of the full infinite-dimensional Trotter splitting. A more comprehensive discussion of this latter point can be found in [B+23b].

4.1. Singular potentials. Here, we numerically evaluate the scaling of the Trotter error for the case $A = i\Delta$ on $X = L^2([0, 1])$ and $L = iV$ for some potential $V(x)$. Our focus lies on bounded but non-smooth potentials in which case we expect a slow decay of the Trotter error from our results Theorem 2.7 and Corollary 2.21 as the condition $VD((-\Delta)) \subseteq D((-\Delta)^\beta)$ can only hold true for small values of β . As shown for the considered examples in Figures 1 and 2, this expectation is met supporting the corresponding assumption in Theorem 2.7 and Corollary 2.21.

In particular, we consider the square wave potential over the interval $V(x) = 2(H(2x) - H(2x - 1)) - 1$ where H is the Heaviside function $H(x) = \mathbb{1}_{[0, \infty)}(x)$. When periodically continued, this function has a Fourier series representation

$$V(x) = \frac{4}{\pi} \sum_{n \in 2\mathbb{N}_0+1} \frac{e^{2\pi inx} - e^{-2\pi inx}}{2in}.$$

This implies that with respect to the Fourier basis V can be written as

$$V = \frac{2}{\pi} \sum_{n \in 2\mathbb{N}_0+1} \frac{J^n - (J^*)^n}{in},$$

where J is the right shift. The Fourier series of the Laplacian with respect to the basis $(e^{2\pi inx})_{n \in \mathbb{Z}}$ is

$$-\Delta = \text{diag}(4\pi^2 n^2)_{n \in \mathbb{Z}}.$$

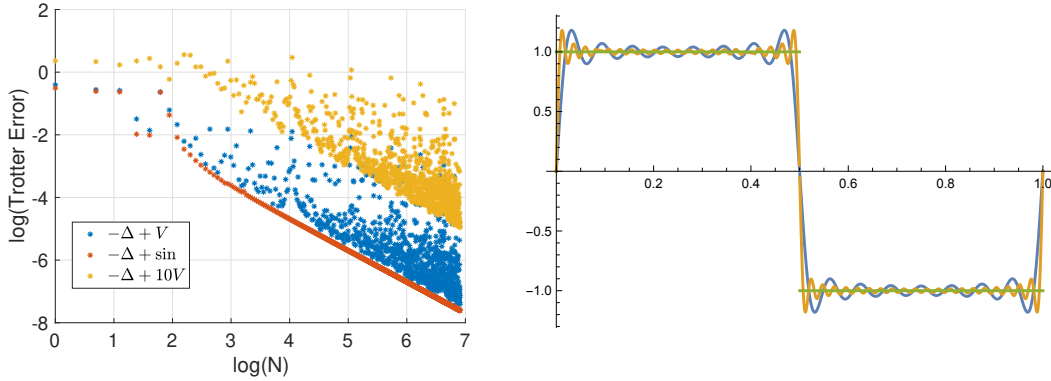


FIGURE 1. Left: Trotter error for the ground state of respective Schrödinger operator (numerically computed with finite matrix truncation in \mathbb{C}^{2M+1} of size $M = 400$) after time $t = 1$. On the right, we see the potential V with its Fourier approximations.

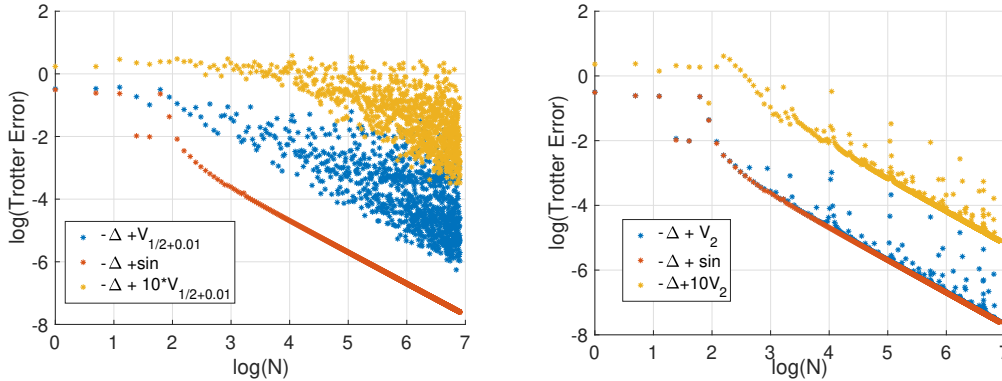


FIGURE 2. Trotter error for ground state of respective Schrödinger operator (numerically computed with finite matrix truncation in \mathbb{C}^{2M+1} of size $M = 400$) after time $t = 1$ (very singular potential on the left, more regular one on the right). N indicates the number of iterations in the Trotter product.

The Trotter error $\|(e^{i\Delta/n}e^{-iV/n})^n\psi - e^{-i(-\Delta+V)}\psi\|$ for V above and $V = \sin(2\pi x)$ on the interval $[0, 1]$ with periodic boundary conditions is shown in Figure 1. Since we use matrix approximations for our numerics, the Trotter error always scales as $\mathcal{O}(n^{-1})$, but the error decays much slower for the singular potential.

We can generalize this by defining the family of potentials

$$V_\alpha(x) = \frac{4}{\pi} \sum_{n \in 2\mathbb{N}_0+1} \frac{e^{2\pi i n x} - e^{-2\pi i n x}}{2i n^\alpha}.$$

This way $V_\alpha \in L^2(\mathbb{R}/\mathbb{Z})$ once $\alpha > 1/2$. Since a slow decay of Fourier coefficients is directly linked to low regularity of V_α , the parameter α directly tunes the regularity. We see in Figure 2 that this directly influences the Trotter error.

4.2. Confining potentials. In Figures 3 and 4, we consider the one-dimensional quantum harmonic oscillator $H = P^2 + Q^2$ with the Trotter splitting into P^2 and Q^2 , which we implement using the usual creation and annihilation operator representation in the Fock basis, where

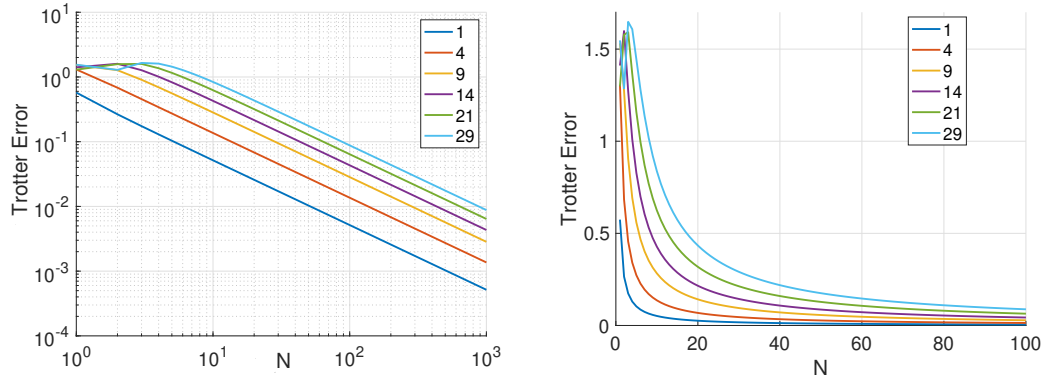


FIGURE 3. Trotter error for eigenstates (Fock states) $\{1, 4, 9, 14, 21, 29\}$ of quantum harmonic oscillator (numerically computed with finite matrix truncation in \mathbb{C}^{400}) after time $t = 1$. (log-log plot (left) and regular plot (right)).

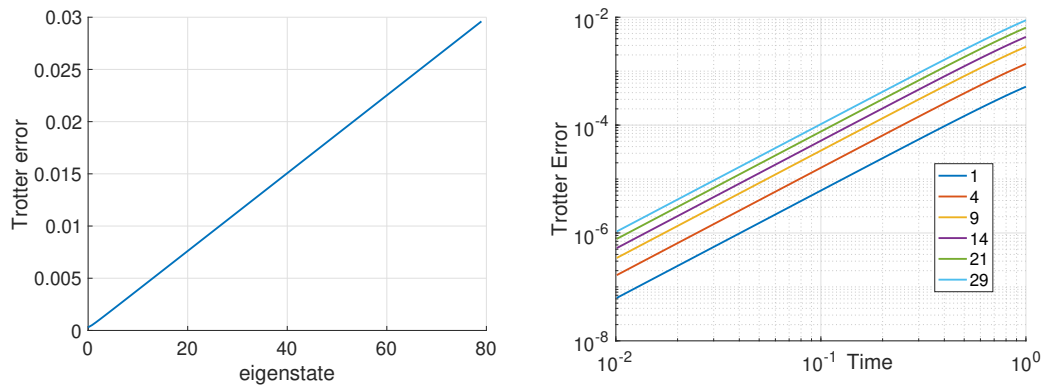


FIGURE 4. On the left, we see the Trotter error at $t = 1$ for all first 81 quantum harmonic oscillator eigenstates (Fock states) after $N = 1000$ Trotter iterations (linear scaling) with matrix truncation in \mathbb{C}^{400} . On the right, we see the time dependence of the Trotter error for eigenstates (Fock states) $\{1, 4, 9, 14, 21, 29\}$.

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots & 0 & \dots \\ 0 & 0 & 0 & 0 & \ddots & \vdots & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \sqrt{n} & \dots \\ 0 & 0 & 0 & 0 & \dots & 0 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

with $Q = \frac{a+a^*}{\sqrt{2}}$ and $P = \frac{a-a^*}{\sqrt{2}i}$. The $\mathcal{O}(n^{-1})$ convergence rate, the linear error in the eigenvalues of the Fock states, and the quadratic time dependence for are correctly predicted by our estimate in Theorem 3.15.

APPENDIX A. PROOFS OF THEOREM 2.2 AND PROPOSITION 2.17

In this section, we prove Theorem 2.2 and Proposition 2.17.

Proof of Theorem 2.2. First of all, note that by (2.8), since the A -bound of L is strictly smaller 1, and $(L, D(L))$ is dissipative [EN00, Proposition II.3.23], we have that $(A + L, D(A))$ generates a strongly continuous contraction semigroup [EN00, Thm. III.2.7]. Hence, we can apply Lemma 2.1 which gives for $x \in D(A^2)$

$$\left\| \left((e^{tL/n} e^{tA/n})^n - e^{t(A+L)} \right) x \right\| \leq t \sup_{s, \tau \in [0, t]} \|[L, e^{sA/n}]x_\tau\|, \quad (\text{A.1})$$

where we denoted $x_\tau = e^{\tau(A+L)}x \in D(A^2)$ and used that since $D(A^2) = D((A + L)^2)$ [P18, Lem. IV.3], the operator $e^{\tau(A+L)}$ leaves $D(A^2)$ invariant. Then, using again that L is relatively A -bounded, we have

$$\begin{aligned} \|[L, e^{sA/n}]x_\tau\| &= \|[L, e^{sA/n} - I]x_\tau\| \\ &\leq \|L(e^{sA/n} - I)x_\tau\| + \|(e^{sA/n} - I)Lx_\tau\| \\ &\leq a \|A(e^{sA/n} - I)x_\tau\| + b \|(e^{sA/n} - I)x_\tau\| + \|(e^{sA/n} - I)Lx_\tau\|. \end{aligned}$$

Furthermore, since for $y \in D(A)$ we have

$$\|(e^{sA/n} - I)y\| = \frac{s}{n} \left\| \int_0^1 e^{rsA/n} Ay \, dr \right\| \leq \frac{s}{n} \|Ay\|,$$

we find, as A and $e^{sA} - I$ commute, that

$$\|[L, e^{sA/n}]x_\tau\| \leq \frac{s}{n} (a \|A^2x_\tau\| + b \|Ax_\tau\| + \|ALx_\tau\|), \quad (\text{A.2})$$

where we have used that by assumption $Ax_\tau, Lx_\tau \in D(A)$. For the term in the middle, we use

$$\begin{aligned} \|Ax_\tau\| &\leq \|(A+L)x_\tau\| + \|Lx_\tau\| \\ &\leq \|(A+L)x\| + \|Lx_\tau\| \\ &\leq \|(A+L)x\| + b\|x\| + a\|Ax_\tau\|. \end{aligned}$$

Using now $a < 1$, we can bring $a\|Ax_\tau\|$ to the other side and get a bound of the form

$$\|Ax_\tau\| \leq \frac{1}{1-a}((1+a)\|Ax\| + 2b\|x\|).$$

By the same argument, we get

$$\|A(A+L)x_\tau\| = \|A[(A+L)x_\tau]\| \tag{A.3}$$

$$\leq \frac{1}{1-a}((1+a)\|A(A+L)x\| + 2b\|x\|). \tag{A.4}$$

Since $A^2 = A(A+L) - AL$ on $D(A^2)$ and by assumption of AL being relatively A^2 -bounded we find

$$\begin{aligned} \|A^2x_\tau\| &\leq \|A(A+L)x_\tau\| + \|ALx_\tau\| \\ &\leq \frac{1}{1-a}((1+a)\|A(A+L)x\| + 2b\|x\|) + \|ALx_\tau\| \\ &\leq \frac{1}{1-a}((1+a+a')\|A^2x\| + (2b+b')\|x\|) + a'\|A^2x_\tau\| + b'\|x\|. \end{aligned} \tag{A.5}$$

Using $a' < 1$ we get

$$\|A^2x_\tau\| \leq \frac{(1+a+a')\|A^2x\| + (2b+(2-a)b')\|x\|}{(1-a)(1-a')}. \tag{A.6}$$

Thus, using relative A^2 -boundedness of AL again in (A.2), we have

$$\begin{aligned} \|[L, e^{sA/n}]x_\tau\| &\leq \frac{s}{n} ((a+a')\|A^2x_\tau\| + b\|Ax_\tau\| + b'\|x\|) \\ &\leq \frac{s}{n} \left((a+a') \frac{(1+a+a')\|A^2x\| + 2b+(2-a)b'}{(1-a)(1-a')} + \frac{b}{1-a}((1+a)\|Ax\| + 2b\|x\|) + b'\|x\| \right) \\ &= \frac{s}{n} (c_2\|A^2x\| + c_1\|Ax\| + c_0\|x\|). \end{aligned}$$

where

$$\begin{aligned} c_0 &= \frac{(a+a')[2b+(2-a)b']}{(1-a)(1-a')} + \frac{2b^2}{1-a} + b', \quad c_1 = \frac{1+a}{1-a}b \\ c_2 &= \frac{(a+a')(1+a+a')}{(1-a)(1-a')}. \end{aligned}$$

Plugging this into (A.1) finishes the proof of (2.10). □

Proof of Prop. 2.17. From the elementary inequality $|z|^\alpha = (|\operatorname{Re}(z)| + |\operatorname{Im}(z)|)^\alpha \leq |\operatorname{Re}(z)|^\alpha + |\operatorname{Im}(z)|^\alpha$, we conclude upon integrating against the spectral measure that by using Lemma 2.15

$$(F_\alpha(\operatorname{Re}(N)) = D(|\operatorname{Re}(N)|^\alpha)) \cap (F_\alpha(\operatorname{Im}(N)) = D(|\operatorname{Im}(N)|^\alpha)) \subset D(|N|^\alpha).$$

Similarly,

$$|\operatorname{Re}(z)|^\alpha \leq |z|^\alpha \text{ and } |\operatorname{Im}(z)|^\alpha \leq |z|^\alpha,$$

implies that $D(|N|^\alpha) \subset D(|\operatorname{Re}(N)|^\alpha)$ and $D(|N|^\alpha) \subset D(|\operatorname{Im}(N)|^\alpha)$ which shows that

$$D(|N|^\alpha) = (F_\alpha(\operatorname{Re}(N)) = D(|\operatorname{Re}(N)|^\alpha)) \cap (F_\alpha(\operatorname{Im}(N)) = D(|\operatorname{Im}(N)|^\alpha)).$$

We conclude that if $x \in D(|N|^\alpha)$, then

$$\begin{aligned} \|(T_t - I)x\| &\leq \|e^{it\operatorname{Im}(N)}(e^{t\operatorname{Re}(N)} - I)x\| + \|(e^{it\operatorname{Im}(N)} - I)x\| \\ &= \|(e^{t\operatorname{Re}(N)} - I)x\| + \|(e^{it\operatorname{Im}(N)} - I)x\| = \mathcal{O}(t^\alpha). \end{aligned}$$

Thus, $x \in F_\alpha(N)$. On the other hand, $F_\alpha(N) = F_\alpha(N^*)$ by normality and $e^{t\operatorname{Re}(N)} = e^{tN/2}e^{tN^*/2}$. Thus, we conclude, since $\|e^{tN/2}\| \leq 1$, that

$$\begin{aligned} \|(e^{t\operatorname{Re}(N)} - I)x\| &\leq \|e^{tN/2}(e^{tN^*/2} - I)x\| + \|(e^{tN/2} - I)x\| \\ &\leq \|(e^{tN^*/2} - I)x\| + \|(e^{tN/2} - I)x\| = \mathcal{O}(t^\alpha), \end{aligned}$$

which shows that $x \in F_\alpha(\operatorname{Re}(N))$. All the previous inclusions follow very directly, yet the inclusion $F_\alpha(N) \subset F_\alpha(\operatorname{Im}(N))$ seems less obvious. Thus, for the final inclusion, we proceed as in Lemma 2.15. Writing $t = t_1 + it_2$ for $t_i \in \mathbb{R}$ we find

$$\|\lambda^r N(\lambda - iN)^{-1}x\|^2 = \lambda^{2r} \int_{\{\operatorname{Re}(t) \leq 0\}} \frac{t_1^2 + t_2^2}{(\lambda - t_1)^2 + t_2^2} d\langle E_N(t)x, x \rangle. \quad (\text{A.7})$$

Optimizing over λ we find

$$\lambda_{\text{opt}} = \frac{t_1(1 - 2r) + \sqrt{t_1^2 + 4t_2^2(1 - r)r}}{2(1 - r)},$$

such that we find the elementary upper bound

$$\lambda_{\text{opt}} \leq \frac{-2rt_1 + 2|t_2|\sqrt{(1 - r)r}}{2(1 - r)} \leq \max\left\{\frac{r}{1 - r}, \sqrt{\frac{r}{1 - r}}\right\}|t|.$$

By establishing a similar lower bound

$$\lambda_{\text{opt}} \geq \sqrt{2}(r - r^2)|t|,$$

we find that $\lambda_{\text{opt}}^{2r}$ in front of the integral in (A.7) behaves like $|t|^{2r}$.

Similar arguments show that the integrand

$$\frac{|t|^2}{(\lambda_{\text{opt}} - t_1)^2 + t_2^2} = \frac{4(1 - r)^2|t|^2}{4(1 - r)^2t_2^2 + (|t_1| + \sqrt{t_1^2 + 4t_2^2(1 - r)r})^2}$$

is uniformly bounded from above and below, i.e., there are $K_r, k_r > 0$ such that for all admissible $t \in (-\infty, 0) \times i\mathbb{R}$

$$k_r \leq \frac{|t|^2}{(\lambda_{\text{opt}} - t_1)^2 + t_2^2} \leq K_r.$$

Thus, arguing as in the proof of the previous Lemma, we conclude that

$$F_\alpha(N) = D(|N|^\alpha).$$

□

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