Quasilocality and Efficient Simulation of Markovian Quantum Dynamics

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We consider open many-body systems governed by a time-dependent quantum master equation with short-range interactions. With a generalized Lieb-Robinson bound, we show that the evolution in this very generic framework is quasilocal; i.e., the evolution of observables can be approximated by implementing the dynamics only in a vicinity of the observables' support. The precision increases exponentially with the diameter of the considered subsystem. Hence, time evolution can be simulated on classical computers with a cost that is independent of the system size. Providing error bounds for Trotter decompositions, we conclude that the simulation on a quantum computer is additionally efficient in time. For experiments and simulations in the Schrödinger picture, our result can be used to rigorously bound finite-size effects.

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In Lorentz-invariant theories, a maximum speed for the propagation of information is, by construction, the speed of light. In nonrelativistic quantum theory, the existence of a maximum propagation speed results more indirectly and for different reasons. For nonpathological models, this maximum speed is much smaller than the speed of light. The seminal paper by Lieb and Robinson [1] and further contributions like [2–13] cover isolated systems.

Here, we consider the evolution of a more general and, experimentally, extremely relevant class of systems—open quantum many-body systems governed by a quantum master equation [14,15] with short-range Liouvillians that are allowed to be time dependent. Prominent experimental examples are presented in Refs. [16–20], and recent theoretical advances on quantum computation, nonequilibrium steady states, and phase transitions in open systems can, for example, be found in Refs. [21–24]. Going beyond the existence of a finite maximum propagation speed and the existence of a well-defined thermodynamic limit [1,25], we show that the time evolution of such systems is quasilocal. This means that, up to an exponentially small error, the diameter of the support of any evolved local observable grows at most linearly in time, or, put differently, that the evolution of the local observable can be approximated to arbitrary precision by applying the propagator of a spatially truncated version of the Liouvillian, as seen in Fig. 1(b). For the special case of isolated systems, where the evolution is given by a unitary transformation, the corresponding question has been addressed in Ref. [9]. As a tool for the proof of quasilocality, we derive and employ a Lieb-Robinson-type bound very similar to the recent results of Poulin [26] and Nachtergaele *et al.* [25]. All constants in the bounds are given explicitly in terms of the system parameters.

The quasilocality of Markovian quantum dynamics has several crucial consequences. It implies that the evolution of observables with a finite spatial support can be simulated efficiently on classical computers, in the sense that the computation cost is independent of the system size, irrespective of the desired accuracy. This can, for example, be exploited in an exact diagonalization approach for a sufficiently large vicinity of the support of the considered observable, as illustrated in Fig. 1(b). For more sophisticated simulation techniques, we provide, in extension of Ref. [27], error bounds for Trotter decompositions [28] of the subsystem propagator into a circuit of local channels, as shown in Fig. 1(c). The Trotter error is polynomial in the time, at most linear in the size of the time step, and can hence be made arbitrarily small. Importantly, the subsystem Trotter decompositions allow for the efficient simulation of the time evolution on a quantum computer as envisaged by Feynman. For any required accuracy, the simulation can be implemented with a cost that is independent of the system size and polynomial in the time.

Experimental and numerical physicists who study nonequilibrium systems in the Schrödinger picture can use our result on quasilocality to rigorously bound finite-size effects. This is, for example, relevant for experiments with ultracold atoms in optical lattices [29] and numerical investigations employing time-dependent density-matrix renormalization group methods [30–33].

Setting.—Let us consider lattice systems, where each site $z \in \Lambda$ is associated with a local Hilbert space $\mathcal{H}_z$. Subsystem Hilbert spaces are denoted by $\mathcal{H}_V := \bigotimes_{z\in V}\mathcal{H}_z \,\forall_{V\subset\Lambda}$ and $\mathcal{H} := \mathcal{H}_\Lambda$. Let $\rho(t)$ denote the system state at time t. Markovian dynamics of an open quantum system, i.e., the evolution under a linear differential equation that generates a completely positive and trace-preserving map for ρ, can always be written in the form of a Lindblad equation [34–36]:

$$\partial_t\rho = -i[H,\rho] + \sum_\nu\Big(L_\nu\rho L_\nu^\dagger - \frac{1}{2}(L_\nu^\dagger L_\nu\rho + \rho L_\nu^\dagger L_\nu)\Big),$$

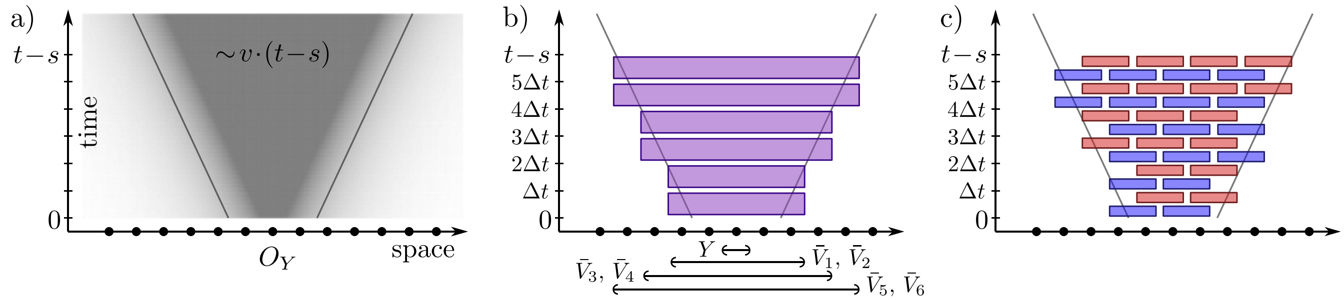

FIG. 1 (color online). (a) An evolved local operator $\tau(s,t)O_Y$ behaves almost like the identity outside its associated space-time cone. (b) Approximating $\tau(s,t)O_Y$ by application of subsystem propagators to O_Y. The errors decrease exponentially with the subsystem sizes. (c) For one-dimensional systems, approximating $\tau(s,t)O_Y$ by a Trotter decomposition yields an error scaling as $(t-s)^2\Delta t$. Note that the Trotter circuit can be trimmed off at the boundary of the Lieb-Robinson space-time cone.

where the arbitrary Lindblad operators L_ν and the Hermitian Hamiltonian H may depend on time. This equation captures, for example, in the framework of the Born-Markov approximation, the evolution of a system that interacts with an environment [14,15] and isolated systems as a special case. Let us switch from the Schrödinger picture, where expectation values are evaluated according to $\langle O\rangle_{s\to t} = \mathrm{Tr}[\rho(t)O]$ with $\rho(s)=\rho$ to the Heisenberg picture, where $\langle O\rangle_{s\to t} = \mathrm{Tr}[\rho O(s)]$ with $O(t)=O$. The corresponding time-dependence of an observable $O(s)\in\mathcal{B}(\mathcal{H})$ is then given by the quantum master equation $\partial_s O(s) = -\mathcal{L}(s)O(s)$, where $\mathcal{L}(t)\in\mathcal{B}(\mathcal{B}(\mathcal{H}))$ is a superoperator, the so-called Liouvillian, with the Lindblad representation

$$\mathcal{L}\, O = i[H,O] + \sum_\nu \left(L_\nu^\dagger O L_\nu - \frac{1}{2}(L_\nu^\dagger L_\nu O + O L_\nu^\dagger L_\nu)\right).$$

The set of Liouvillians with spatial support $V\subset\Lambda$ will be denoted by $\mathbb{L}_V \subset \mathcal{B}(\mathcal{B}(\mathcal{H}_V))$.

In order to be able to use Lieb-Robinson bound techniques, we need to restrict ourselves to Liouvillians with norm-bounded short-range interaction terms. Let us hence assume that $\mathcal{L}$ is a sum of local Liouville terms ℓ_Z with norm bound $|\ell|$, maximum range a, and a maximum number $\mathcal{Z}$ of nearest neighbors [37]. Specifically,

$$\mathcal{L}(t) = \sum_{Z\subset\Lambda} \ell_Z(t), \qquad \ell_Z(t)\in\mathbb{L}_Z, \tag{1}$$

$$|\ell| := \sup_{t,Z\subset\Lambda} \|\ell_Z(t)\|, \tag{2}$$

$$a := \sup_{Z:\ell_Z\neq 0} \mathrm{diam}(Z), \tag{3}$$

$$\mathcal{Z} := \max_{Z:\ell_Z\neq 0} |\{Z'\subset\Lambda | \ell_{Z'}\neq 0, Z'\cap Z\neq\varnothing\}|, \tag{4}$$

where $\mathrm{diam}(Z) := \max_{x,y\in Z} d(x,y)$ is the diameter of Z and d is a metric on the lattice Λ. In Eq. (2), we have used the superoperator norm [38,39] defined by $\|T\| := \sup_{O\in\mathcal{B}(\mathcal{H})} \|TO\|/\|O\|$. In the Heisenberg picture, this is the physically relevant norm as induced by the operator norm $\|O\|$. For notational convenience, we define for every subsystem $V\subset\Lambda$ the corresponding extension $\bar{V}$, volume $\mathrm{Vol}(V)$, and truncated Liouvillian $\mathcal{L}_V$,

$$\bar{V} := \bigcup_{\substack{Z:\ell_Z\neq 0\\ Z\cap V\neq\varnothing}} Z, \tag{5}$$

$$\mathrm{Vol}(V) := |\{Z\subset V | \ell_Z\neq 0\}|, \tag{6}$$

$$\mathcal{L}_V(t) := \sum_{Z\subset V} \ell_Z(t). \tag{7}$$

Propagators $\tau_V(s,t)$ are superoperators that map observables to time-evolved observables. They are defined as the unique solutions of

$$\partial_s \tau_V(s,t) = -\mathcal{L}_V(s)\tau_V(s,t), \quad \tau_V(t,t) = \mathrm{id} \quad \forall_{s\le t}. \tag{8}$$

With $\tau(s,t) := \tau_\Lambda(s,t)$, one has indeed $O(s) = \tau(s,t)O(t)$. Propagators obey the composition rule $\tau(r,s)\tau(s,t) = \tau(r,t)\ \forall_{r\le s\le t}$. Furthermore [38], the derivative with respect to the second time argument is given by

$$\partial_t \tau_V(s,t) = \tau_V(s,t)\mathcal{L}_V(t), \tag{9}$$

and the propagators are norm-decreasing,

$$\|\tau(s,t)O\| \le \|O\| \quad \forall\ \mathcal{L}\in\mathbb{L}_\Lambda, s\le t, O\in\mathcal{B}(\mathcal{H}). \tag{10}$$

Quasilocality of the evolution.—Given an operator $O_Y\in\mathcal{B}(\mathcal{H}_Y)$ with support $Y\subset\Lambda$, we would like to show that the exactly time-evolved operator $\tau(r,t)O_Y$ with $r\le t$ can be approximated by the evolution with respect to a spatially truncated Liouvillian, i.e., by $\tau_{\bar{V}}(r,t)O_Y$ with $Y\subset V\subset\Lambda$. Indeed, our main result, Theorem 2, states that the approximation error is exponentially small, in the distance of $\Lambda\setminus V$ to the time-r slice of a space-time cone originating from the operator's support Y at time t, as depicted in Fig. 1(b). More precisely, the error decays exponentially in $d(Y,\Lambda\setminus V)/a - v(t-r)$, where $d(X,Y) := \inf_{x\in X, y\in Y} d(x,y)$ is the distance of two subsystems $X, Y\subset\Lambda$, and $v = e\mathcal{Z}|\ell|$ is the so-called Lieb-Robinson velocity.

To prove this, we can write the difference of the evolved operators in the form

$$\begin{aligned}
&\tau(r,t)O_Y - \tau_{\bar{V}}(r,t)O_Y \\
&\quad = -\int_r^t ds\partial s[\tau_{\bar{V}}(r,s)\tau(s,t)]O_Y \\
&\quad = \int_r^t ds\tau_{\bar{V}}(r,s)\underbrace{[\mathcal{L}(s) - \mathcal{L}_{\bar{V}}(s)]}_{=\mathcal{L}_{\Lambda\setminus V}(s)}\tau(s,t)O_Y
\end{aligned}$$

due to the fundamental theorem of calculus and Eqs. (8) and (9). Using the triangle inequality and the fact that the propagators are norm-decreasing, it follows that

$$\|\tau(r,t)O_Y - \tau_{\bar{V}}(r,t)O_Y\| \le \sum_{X\subset\Lambda\setminus V}\int_r^t ds\|\ell_X(s)\tau(s,t)O_Y\|. \tag{11}$$

In the case of unitary dynamics ($\ell_X(s)O = i[h_X, O]$), the integrand would be of the form $\|[h_X, \tau(s,t)O_Y]\|$, and the standard Lieb-Robinson bound [1–5] would be applicable. To proceed in our more general case, however, we use a Lieb-Robinson bound for Markovian quantum dynamics, similar to recent results in Refs. [25,26].

Theorem 1 (Lieb-Robinson bound for Markovian quantum dynamics).—Let the Liouvillian $\mathcal{L}(t) = \sum_{Z\subset\Lambda}\ell_Z(t)$ for the lattice Λ be of finite range a, with a finite maximum number $\mathcal{Z}$ of nearest neighbors, and $|\ell|$ as defined in Eqs. (1)–(4). Also, let $\mathcal{K}_X \in \mathbb{L}_X$, $O_Y \in \mathcal{B}(\mathcal{H}_Y)$, and $r \le t \in \mathbb{R}$. Then

$$\|\mathcal{K}_X\tau(r,t)O_Y\| \le \mathcal{V}_{X,Y}\|\mathcal{K}_X\|\|O_Y\|e^{v(t-r)-d(X,Y)/a}, \tag{12}$$

where $v := \exp(1)\mathcal{Z}|\ell|$ and $\mathcal{V}_{X,Y} := \min\{\frac{Vol(\bar{X})}{\mathcal{Z}}, \frac{Vol(\bar{Y})}{\mathcal{Z}}\}$.

The proof is given in the Supplemental Material [38]. With the Lindblad representation $\mathcal{K}_X O = i[k,O] + \sum_\nu[K_\nu^\dagger O K_\nu - \frac{1}{2}(K_\nu^\dagger K_\nu O + O K_\nu^\dagger K_\nu)]$ of the Liouvillian $\mathcal{K}_X$, one has in Eq. (12) that $\|\mathcal{K}_X\|/2 \le \|k\| + \sum_\nu\|K_\nu\|^2$. The theorem tells us that an evolved observable $\tau(r,t)O_Y$ remains basically unchanged when we evolve it with respect to a Liouvillian that is supported at a distance $R \gg v(t-r)$ away from Y, i.e., that $\tau(r,t)O_Y$ behaves like the identity outside the corresponding space-time cone. In the special case $\mathcal{K}_X O = i[O_X, O]$, Eq. (12) yields a Lieb-Robinson bound for $\|[O_X, \tau(r,t)O_Y]\|$ as in Ref. [26].

This theorem can now be employed to proceed from Eq. (11) in our proof of quasilocality. Let us restrict ourselves to the typical case of Liouvillians $\mathcal{L}(t)$ for which the number of terms $\ell_X(t)$ with distance $d(y,X)/a \in [n, n+1)$ from any site $y \in \Lambda$ is bounded by a power law,

$$\begin{aligned}
&|R_{n,y}| \le Mn^\kappa \quad \forall_{y\in\Lambda, n\in\mathbb{N}_+}, \\
&R_{n,y} := \left\{X\subset\Lambda | \ell_X \ne 0, \frac{d(y,X)}{a} \in [n, n+1)\right\},
\end{aligned} \tag{13}$$

for some constants $M, \kappa > 0$. Now, choose a point $y_0 \in Y$ that is closest to $\Lambda\setminus V$, i.e., $d(y_0, \Lambda\setminus V) = d(Y, \Lambda\setminus V)$. With $D := \lceil d(Y, \Lambda\setminus V)/a\rceil$, we can exploit that the support of every term in $\mathcal{L}_{\Lambda\setminus V}$ is an element of exactly one of the sets R_{n,y_0} with $n \ge D$ to obtain

$$\begin{aligned}
&\|\tau(r,t)O_Y - \tau_{\bar{V}}(r,t)O_Y\| \\
&\quad \le \sum_{n=D}^\infty \sum_{X\in R_{n,y_0}} \int_r^t ds\|\ell_X(s)\tau(s,t)O_Y\| \\
&\quad \le \sum_{n=D}^\infty Mn^\kappa|\ell|\|O_Y\| \int_r^t ds e^{v(t-r)-n} \\
&\quad \le M|\ell|\|O_Y\|\frac{e^{v(t-r)}}{v}\sum_{n=D}^\infty n^\kappa e^{-n}.
\end{aligned}$$

In the second step, Theorem 1 and $\mathcal{V}_{XY} \le \mathrm{Vol}(\bar{X})/\mathcal{Z} \le 1$ have been used. With the bound $\sum_{n=D}^\infty n^\kappa e^{-n} \le 2eD^\kappa e^{-D}\ \forall_{D>2\kappa+1}$, we arrive at the central result of this work.

Theorem 2 (Quasilocality of Markovian quantum dynamics).—Let the Liouvillian $\mathcal{L}(t) = \sum_{Z\subset\Lambda}\ell_Z(t)$ for the lattice Λ be of finite range a, with a finite maximum number $\mathcal{Z}$ of nearest neighbors, and $|\ell|$ as defined in Eqs. (1)–(4). Further, let constraint Eq. (13) be fulfilled for some constants $M, \kappa > 0$. Also, let $Y \subset V \subset \Lambda$, $O_Y \in \mathcal{B}(\mathcal{H}_Y)$, and $r \le t \in \mathbb{R}$. Then one has with $D := \lceil d(Y, \Lambda\setminus V)/a\rceil$

$$\begin{aligned}
&\|\tau(r,t)O_Y - \tau_{\bar{V}}(r,t)O_Y\| \\
&\quad \le \frac{2M}{\mathcal{Z}}\|O_Y\|D^\kappa e^{v\cdot(t-r)-D} \quad \forall_{D>2\kappa+1},
\end{aligned} \tag{14}$$

where v is the Lieb-Robinson speed from Eq. (12).

The full dynamics can be approximated with exponential accuracy by subsystem dynamics. In a sense, the constraint Eq. (13) requires the lattice to have a finite spatial dimension. A $\mathcal{D}$-dimensional hypercubic lattice with finite-range interactions fulfills Eq. (13) with $\kappa = \mathcal{D} - 1$. An interesting observation is that short-range models on a Bethe lattice [40] have a finite Lieb-Robinson speed according to Theorem 1 but do not fulfill Eq. (13) and are thus not covered by Theorem 2. Hence, for such systems, it is conceivable that a quench of the Liouvillian starting at time $t = 0$ with a distance of at least aD from some point y causes a perceptible effect at y for a time $t^* \ll D/v$.

Trotter decomposition of the evolution.—The quasilocality of the dynamics, Theorem 2, implies that the evolution of observables with a finite spatial support can be simulated efficiently on classical computers, in the sense that the computation cost is independent of the system size, irrespective of the desired accuracy. However, exploiting this, in an exact diagonalization approach that stores the approximated time-evolved observable $\tau_{\bar{V}}(r,t)O_Y$ in a full basis of $\mathcal{H}_{\bar{V}}$ exactly, requires resources that are exponential in the size $|\bar{V}|$ of the considered subsystem. There are more sophisticated numerical techniques; e.g., one can use matrix-product operators [41–43] for the representation of (an approximation to) $\tau_{\bar{V}}(r, t)O_Y$ or sampling algorithms. In such schemes, it is typically not possible to address the differential equation for $\tau_{\bar{V}}(r, t)O_Y$ directly, but one can use Trotter decompositions [28] instead, where propagators $\tau_{\bar{V}}(r, t)$ are decomposed into a circuit of local (diameter-a) channels.

Using the quasilocality, Theorem 2, and techniques as in Ref. [27], we can derive a Trotter decomposition with an error that is polynomial in time, at most linear in the time step, and, in extension of Ref. [27], system-size independent. Furthermore, implementing such a Trotter circuit on a quantum computer [27] yields a simulation that, additionally to being independent of the system size, is efficient in time. In this case, the physically relevant norm for superoperators T is the subsystem-seminorm

$$\|T\|_Y := \sup_{O_Y \in \mathcal{B}(\mathcal{H}_Y)} \|T O_Y\| / \|O_Y\|. \tag{15}$$

Theorem 3 (Efficient Trotter decomposition of time-evolved observables).—With the preconditions of Theorem 2, a sequence of times $t_0 \leq t_1 \leq \ldots \leq t_N$ and a sequence of subsystems $Y \subset V_1 \subset V_2 \subset \ldots \subset V_N \subset \Lambda$ such that $D_n := \lceil d(Y, \Lambda \setminus V_n)/a \rceil > 2\kappa + 1 \; \forall_n$, the Trotter decomposition

$$\tilde{\tau} := \prod_{n=1}^{N} \prod_{Z \subset \bar{V}_n : \ell_Z \neq 0} \tau_Z(t_{n-1}, t_n) \tag{16}$$

into propagators τ_Z for local Liouville terms ℓ_Z approximates the full system propagator $\tau(t_0, t_N)$ up to an error

$$\|\tau(t_0, t_N) - \tilde{\tau}\|_Y \leq \sum_{n=1}^{N} \left(\frac{2M}{Z} D_n^{\kappa} e^{v(t_n - t_0) - D_n} + \varepsilon_n \right),$$

$$\varepsilon_n := (t_n - t_{n-1})^2 Z \, \mathrm{Vol}(\bar{V}_n) |\ell|^2 e^{(t_n - t_{n-1})|\ell|} \tag{17}$$

with the Lieb-Robinson speed v from Eq. (12).

In the Trotter decomposition $\tilde{\tau}$, we used the convention $\prod_{n=1}^{N} T_n = T_1 T_2 \ldots T_N$, and the ordering of the channels τ_Z in the second product of Eq. (16) can be chosen arbitrarily. As in Ref. [27], one can use averaged Liouvillians, i.e., $\tau_Z(r, t) \mapsto e^{\int_r^t ds \ell_Z(s)}$, without changing the scaling of the error bound. Choosing a constant time step, $t_n = n\Delta t$, and subsystems V_n such that $D_n = D_0 + vn\Delta t$, for sufficiently large D_0, the bound (17) is dominated by the Trotter errors ε_n. The subsystems can be chosen such that $\mathrm{diam} V_n \leq \mathrm{diam}(Y) + aD_n$, as shown in Fig. 1(c). For this case, the total error is in $\mathcal{O}(\Delta t (\mathrm{diam}(Y)/a + D_0 + vt)^{\kappa+2})$. Higher-order Trotter-Suzuki decompositions [44] can be used to further improve the scaling in Δt.

To prove Theorem 3, one can first apply Theorem 2, the inequality $\|T_1 T_2 - \tilde{T}_1 \tilde{T}_2\| \leq \|T_1\| \|T_2 - \tilde{T}_2\| + \|T_1 - \tilde{T}_1\| \|\tilde{T}_2\|$, and Eq. (10) iteratively N times, to obtain

$$\|\tau(t_0, t_N) - \tau^V\|_Y \leq \frac{2M}{Z} \sum_{n=1}^{N} D_n^{\kappa} e^{v(t_n - t_0) - D_n} \tag{18}$$

with $\tau^V := \prod_{n=1}^{N} \tau_{\bar{V}_n}(t_{n-1}, t_n)$. For every time-step propagator $\tau_{\bar{V}_n}(t_{n-1}, t_n)$, we can then employ a Trotter decomposition similar to Ref. [27], yielding

$$\|\tau_{\bar{V}}(r, t) - \prod_{Z \subset \bar{V}, \ell_Z \neq 0} \tau_Z(r, t)\|_Y \leq (t - r)^2 Z \, \mathrm{Vol}(\bar{V}) |\ell|^2 e^{(t-r)|\ell|}. \tag{19}$$

See the Supplemental Material [38] for details. Combining Eqs. (18) and (19) with the triangle inequality proves Theorem 3.

Conclusion.—We have shown that the evolution of an observable with support Y under a quantum master equation with a short-range Liouvillian can be approximated by the evolution with respect to the truncation of the Liouvillian to a subsystem $V \supset Y$. The error decreases exponentially in the distance of Y from the complement of V. With this tool, we derived an error bound for Trotter decompositions of the propagator. Those results correspond to efficient simulation techniques for open-system dynamics on classical and quantum computers and provide rigorous bounds to finite-size effects.

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[38] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.108.230504 for a brief discussion of the employed superoperator norms and properties of the propagators, a proof of the dissipative Lieb-Robinson bound (Theorem 1), the employed bounds on some elementary series, and the Trotter decomposition for a single time step.
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