All You Need is Trotter

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arXiv:2311.01533v6 [quant-ph] 31 Oct 2026

The work here enables a cost scaling of $\tilde{O}\left(\frac{T^{1+o(1)}\log^2(1/\epsilon)}{\varepsilon}\right)$ and maximum depth $\tilde{O}\left(\frac{T^{1+o(1)}\log(1/\epsilon)}{\varepsilon}\right)$ for estimating observables after some Hamiltonian evolution e^{iHT} using no extra block-encoding qubits, where ϵ is the algorithmic error of the target Hamiltonian evolution and ε is the statistical error from the observable estimation. Throughout, $\tilde{O}$ suppresses factors that are doubly logarithmic in $1/\epsilon$ (i.e. polyloglog$(1/\epsilon)$), which are subdominant to the displayed polylog$(1/\epsilon)$ factors. This is achieved through product formulas, stable interpolation (Chebyshev), and to calculate the needed fractional queries, cardinal sine interpolation is used. This is an improvement over similar work using interpolation methods which have a superlinear scaling of the form $5^p T^{1+1/p}$, where p is the order of the product formula used and an improvement on required qubits over Quantum Signal Processing methods while maintaining scaling with polylog$1/\epsilon$. This is accomplished through an optimized and variable (with T) order p. The slightly better $\log^2(1/\epsilon)$ compared to $\log^3(1/\epsilon)$ comes from the use of cardinal sine interpolation compared to other methods using Chebyshev interpolation and product formulas. The work presented here also provides an alternative to Quantum Signal Processing techniques to calculate observables or amplitudes after a fractional query evolution with a cost $O(T\log 1/\epsilon)$ through this cardinal sine interpolation.

1 Introduction

A central task in quantum simulation is the estimation of observables following Hamiltonian evolution: given a Hamiltonian H, an evolution time T, and an observable or amplitude of interest, one wishes to estimate a quantity such as $\langle\psi_1|e^{iHT}|\psi_2\rangle$ to a target accuracy. Product formulas (Trotterization) are the most hardware-frugal route to this task, using no block-encoding ancillas, but they suffer from a poor dependence on the algorithmic error ϵ: the Trotter step size must shrink polynomially in $1/\epsilon$. Post-Trotter methods such as Quantum Signal Processing achieve the desirable polylog$(1/\epsilon)$

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dependence, but at the cost of additional ancilla qubits and circuit-depth overhead from block-encoding. The question we address is whether one can retain the low qubit footprint of product formulas while attaining polylog$(1/\epsilon)$ accuracy and a near-linear dependence on T.

This work answers the question in the affirmative. We give an algorithm for estimating observables after Hamiltonian evolution with a cost scaling of $\tilde{O}\Big(T^{1+o(1)}\ \log^2(1/\epsilon)/\varepsilon\Big)$ and maximum depth $\tilde{O}\Big(T^{1+o(1)}\ \log(1/\epsilon)/\varepsilon\Big)$, using no extra block-encoding qubits, where ϵ is the algorithmic error and ε is the statistical error of the observable estimation; here and throughout, $\tilde{O}$ hides factors doubly logarithmic in $1/\epsilon$, which are subdominant to the displayed polylogarithmic ones. Informally, the algorithm proceeds in three steps. (i) The Trotterized evolution is run at several step sizes chosen at stable (Chebyshev) interpolation nodes, and the corresponding amplitudes are estimated. (ii) Because these nodes require non-integer powers of the product formula, the needed fractional queries are reconstructed *classically*, as a post-processing step, from the amplitudes of nearby integer-power product formulas via cardinal sine interpolation. (iii) The amplitudes are extrapolated in the Trotter step size to the zero-step-size limit, recovering the un-Trotterized result. The two design choices that yield the stated scaling are the use of cardinal sine interpolation for the fractional queries (which gives a $\log^2(1/\epsilon)$ dependence, an improvement over the $\log^3(1/\epsilon)$ of product-formula-plus-Chebyshev-interpolation methods) and an order p that is optimized and allowed to vary with T, which produces the quasi-linear $T^{1+o(1)}$ dependence. As a byproduct, step (ii) is itself a self-contained method for evaluating amplitudes after a fractional-query evolution, at a cost $O(T \log 1/\epsilon)$ and without any signal processing on the quantum computer.

The remainder of this introduction places these ideas in the context of prior work on fractional queries and Trotter-error mitigation.

Fractional queries on a quantum computer are of great importance for quantum algorithms like Grover search and its variations. And they were difficult to come by up to 2006 according to Scott Aaronson's "The ten most annoying questions in quantum computing"[1]. They were later proven to be implementable by Sheridan et al. in [2]. Later, an exponential improvement was achieved in the query model in the work of [3]. These techniques combined with linear combination of unitaries and amplitude amplification authors of [4] achieve an exponential improvement on Hamiltonian simulation.

After this, there was a flurry of works using Quantum Signal Processing [5, 6] which achieved exponential precision improvements on several operations like inversion of a matrix, Hamiltonian simulation, and also fractional queries [7]. There has been a recent paradigm shift in regards to what has to be done in a quantum computer and what can be relegated to classical post-processing [8] using the power of stable interpolation. Here, it is shown how to implement fractional queries by using cardinal sine interpolation which is closely related to the sampling theorem [9, 10, 11, 12], while preserving optimal error scaling and requiring no signal processing on the quantum computer.

Moreover, fractional queries have emerged as a necessity when using well-conditioned interpolation methods for interpolating to zero Trotter-step size[8] of the Hamiltonian evolution operator as feasible alternative to block-encoding. These methods are competitive in the sense that they accomplish polylog$(1/\epsilon)$ scaling, where ϵ is the algorithmic error. The scaling achieved for the evolution operator with respect to the time evolution t was $O(t^2)$, and thus here an attempt to improve this is made.

It is useful to situate the present work among existing approaches to Hamiltonian simulation and observable estimation. Product formulas[13] are simple and use no ancilla qubits, but a p-order formula incurs an algorithmic error scaling as $T(T/r)^p$, so reaching error ϵ requires a step count growing polynomially in $1/\epsilon$. Post-Trotter methods — linear combination of unitaries[4], quantum signal processing and qubitization[5, 6, 14], and the quantum singular value transformation[7] — achieve the exponentially better polylog$(1/\epsilon)$ dependence and (for QSP/qubitization) optimal joint scaling in T and ϵ, but they require block-encoding the Hamiltonian, which introduces ancilla qubits and additional circuit depth. When the goal is the estimation of time-evolved observables rather than the evolution operator itself, a complementary line of work mitigates the Trotter error in classical post-processing: Richardson extrapolation and polynomial (Chebyshev) interpolation of observables computed at several Trotter step sizes[8, 15, 16], and multi-product formulas[17, 18]. These retain the low qubit footprint of product formulas while recovering a polylog$(1/\epsilon)$ accuracy dependence; the underlying amplitudes are read out by amplitude estimation[19, 20]. The algorithm presented here belongs to this last family. Relative to the Chebyshev-interpolation methods[8, 15] on which it builds, it improves the accuracy dependence from $\log^3(1/\epsilon)$ to $\log^2(1/\epsilon)$ through cardinal sine interpolation of the fractional queries, and improves the dependence on T to quasi-linear $T^{1+o(1)}$ through an order p that varies with T; relative to the multi-product approach of [17], discussed next, it forms the required combination classically rather than coherently, avoiding the associated qubit overhead.

We note that the well-conditioned multi-product formulas of [17] also confront the non-integer powers that arise from interpolation nodes, and do so by rounding them to integers while preserving a well-conditioned linear combination. The key distinction of the present work is where and how this combination is formed. In [17] the linear combination of (integer-power) product formulas is realized *coherently and in situ* on the quantum device, through a linear combination of unitaries together with oblivious amplitude amplification; the rounding to integer powers is precisely what keeps this on-device combination well-conditioned. By contrast, the fractional queries here are never formed coherently: they are reconstructed *classically, as a post-processing step*, from the amplitudes of integer-power product formulas via cardinal sine interpolation. Consequently, the Trotterization bias is corrected without the ancilla register and amplitude-amplification overhead required by an in-situ combination, that is, with no extra block-encoding qubits beyond those used for amplitude estimation.

In the next section (see section 2), we illustrate how the necessity of fractional queries emerge in the approach of interpolating away Trotter error in a stable manner. In the section after (section 3), we show how to obtain fractional queries through

a classical addition of amplitudes of integer queries as a post-processing step using cardinal sine interpolation. Next (section 4), bounds are obtained on the convergence rate of Chebyshev interpolation of the Trotterized evolution operator assuming access to efficient fractional queries. Finally (section 5), the results are combined to obtain an algorithm that achieves quasi-linear cost-scaling with t while keeping polylog$(1/\epsilon)$.

The stability analysis for the cardinal sine interpolation is left to Section A and the reader is pointed to [8] for an analysis on the stability of Chebyshev interpolation.

2 Setup of the problem

Suppose one wants to estimate:

$$\langle\psi_1|\prod_j^M V_j e^{iT_j H_j}|\psi_2\rangle, \tag{1}$$

where V_i are unitary matrices. Suppose each Hamiltonian H_j on a collection of n qubits can be decomposed into a sum of m_j terms.

$$H_j = \sum_{\gamma=1}^{m_j} H_{j,\gamma}. \tag{2}$$

Notice that both the Hamiltonian and decomposition are specified, as the decomposition is not unique. Throughout this work, $\sum_\gamma^{m_j} \|H_{j,\gamma}\| \leq 1$ is assumed.

In order to implement the unitary evolution operators

$$e^{iT_j H_j} \tag{3}$$

we wish to approximate them first through p-order product formulas. Standard examples of product formulas include the Trotter first-order formula

$$S_{1,j}(t) := \prod_{\gamma=1}^{m_j} e^{iH_{j,\gamma}t}, \tag{4}$$

the second-order symmetric formula

$$S_{2,j}(t) := e^{iH_{j,1}t/2}\ldots e^{iH_{j,m_j}t/2}e^{iH_{j,m-j}t/2}\ldots e^{iH_{j,1}t/2}, \tag{5}$$

and more generally, the order $2k$ symmetric Suzuki-Trotter formula, defined recursively as

$$S_{2k,j}(t) := [S_{2k-2,j}(u_k t)]^2 S_{2k-2,j}\left((1-4u_k)t\right)[S_{2k-2,j}(u_k t)]^2 \tag{6}$$

for every $k \in \mathbb{Z}_+ \setminus \{1\}$, where $u_k := (4 - 4^{1/(2k-1)})^{-1}$ [13].

Thus, one calculates

$$\langle\psi_1|\prod_j^M V_j S_{p,j}^{g/s}(st_j)|\psi_2\rangle = \langle\psi_1|\prod_j^M V_j \left(e^{i(st_j)\tilde{H}_{p,j}(st_j)}\right)^{(g/s)}|\psi_2\rangle, \tag{7}$$

where $g = T_j/t_j$, for certain values of s and then interpolates to $s \to 0$ to recover the desired result. Here,

$$\tilde{H}_{p,j}(st_j) = \frac{\log\left(S_{p,j}(st_j)\right)}{ist_j}, \tag{8}$$

where $\tilde{H}_{p,j}(st_j)$ will be a single-valued analytic function of s provided that

$$t_j \leq \pi. \tag{9}$$

The values of s chosen are those at optimal collocation of nodes, s_k, and set of interpolating polynomials such that the error does not blow up (see [8, 21, 22, 17]). This, however, introduces the necessity of using fractional queries since g/s_k will not be in general an integer. This was an obstacle which authors in [15] ran into. Typically, fractional queries are assumed to be calculated through Quantum Signal Processing techniques ([7, 5, 14]) because this is the most efficient approach in terms of error. However, fractional queries using this technique require extra ancillary qubits and additional circuit depth overhead. For that reason, we propose to use close-to-optimal interpolation techniques by estimating nearby integer powers

$$\langle\psi_1|\prod_j^M V_j S_{p,j}^{m+n}(s_k t_j)|\psi_2\rangle, \tag{10}$$

where $m = \lfloor g/s_k \rfloor$ for $n \in \{-q, -q+1, \ldots, q\}$.

In the next section, we will detail how to obtain the fractional queries through cardinal sine interpolation and estimate upper-bounds on the resource requirements. Following that, we will estimate the uncertainty propagation to the interpolant due to cardinal sine interpolation. Finally, we explain the Trotter interpolation to the limit $s \to 0$.

3 Fractional Queries using Cardinal Sine Interpolation

In this section, we will explain how one can use cardinal sine interpolation to obtain the fractional queries required by Trotter step interpolation. Here is the main theorem regarding fractional queries interpolation:

Theorem 1. *In order to give an estimate of* $\langle\psi_1|\prod_j^M V_j S_{p,j}^{g/s_k}(s_k t_j)|\psi_2\rangle$ *within an error* $\tilde{\varepsilon}_{\text{interp}}$ *using*

$$\frac{\sum_{n=-q}^{q} \operatorname{sinc}(r-n)\, w(n) \langle\psi_1|\prod_j^M V_j S_{p,j}^{n+m}(s_k t_j)|\psi_2\rangle}{w(r)},$$

where $w(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\sigma^2}\right)$, $m = \lfloor g/s_k \rfloor$, *and* $r = g/s_k - \lfloor g/s_k \rfloor$, *one needs to choose any*

$$q \geq \frac{6}{\pi}\left(\log \frac{4\sqrt{2\pi}+8}{\pi e^{1/3+\pi/12}\tilde{\varepsilon}_{\text{interp}}}\right)$$

and enforce $\sum_{j=1}^{M} |t_j| \leq \pi$.

The proof occupies the remainder of this section and proceeds in three stages. We first cast the integer-power amplitudes as samples of a windowed signal $x(t)$ (Equation (11)), so that recovering the fractional query becomes a band-limited interpolation problem. The interpolation error then splits, by the triangle inequality, into a *spectral* part (from windowing a signal that is not exactly band-limited) and a *truncation* part (from using finitely many samples). We bound these two contributions separately in Theorem 2 and Theorem 4, and finally combine them to solve for the number of samples q stated above.

To prove this theorem, we first make the following definition for the signal:

$$\tilde{x}(t) = \langle\psi_1| \prod_j^M V_j S_{p,j}^{t+m}(s_k t_j) |\psi_2\rangle = \langle\psi_1| \prod_j^M V_j \left(e^{i(s_k t_j)\tilde{H}_{p,j}(s_k t_j)}\right)^{t+m} |\psi_2\rangle. \tag{11}$$

Now, one defines the following windowed function:

$$x(t) = w(t)\tilde{x}(t), \tag{12}$$

where

$$w(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\sigma^2}\right). \tag{13}$$

By triangle inequality, one can estimate the total error by looking at both the truncation error and the spectral error separately

$$\begin{aligned}\varepsilon_{\text{interp}} = \max_t |x(t) - x_{\text{interp},2q+1}(t)| \leq \overbrace{\max_t |x(t) - x_{\text{interp},\infty}(t)|}^{\varepsilon_{\text{spectral}}} \\ + \underbrace{\max_t |x_{\text{interp},\infty}(t) - x_{\text{interp},2q+1}(t)|}_{\varepsilon_{\text{trunc}}}.\end{aligned} \tag{14}$$

Here,

$$x_{\text{interp},\infty}(t) = \sum_{n=-\infty}^{\infty} x(n)\,\text{sinc}\,(t-n)\,, \tag{15}$$

and

$$x_{\text{interp},2q+1}(t) = \sum_{n=-q}^{q} x(n)\,\text{sinc}\,(t-n)\,. \tag{16}$$

Let us first bound the spectral error, $\varepsilon_{\text{spectral}}$. Our result is expressed in the following lemma:

Lemma 2. *Let Δ_{pad} denote the guard band between the maximum normalized frequency of the signal, $\max_{\vec{l}}|\mu_{\vec{l}}|$, and the Nyquist edge $1/2$, that is, $\Delta_{\text{pad}} = 1/2 - \max_{\vec{l}}|\mu_{\vec{l}}|$. Provided that $\Delta_{\text{pad}} = 1/4$ and $\sigma \geq 1/(4\pi)$, then*

$$\varepsilon_{\text{spectral}} \leq \left(\frac{8}{\sqrt{2\pi}} + 2\right) \exp\left(-\frac{\pi^2\sigma^2}{2}\right).$$

To prove this, we start by re-expressing the operators in Equation (11) terms of the eigen-states $|j,l\rangle$, defined through $\tilde{H}_{p,j}(s_k t_j)|j,l\rangle = E_l^{(j)}|j,l\rangle$, thus

$$e^{i(s_k t_j)\tilde{H}_{p,j}(s_k t_j)} = \sum_l |j,l\rangle\langle j,l| \exp\left(i(s_k t_j)E_l^{(j)}\right), \tag{17}$$

$$V_j = \sum_{l',l''} |j,l'\rangle\langle j,l'|V_j|j,l''\rangle\langle j,l''|. \tag{18}$$

We insert these expressions into Equation (11) to obtain

$$\begin{aligned}
\tilde{x}(t) &= \langle\psi_1| \prod_j^M V_j \left(e^{i(s_k t_j)\tilde{H}_{p,j}(s_k t_j)}\right)^{t+m} |\psi_2\rangle \\
&= \langle\psi_1| \left(\prod_j \sum_{l',l''} |j,l'\rangle\langle j,l'|V_j|j,l''\rangle\langle j,l''| \sum_l |j,l\rangle\langle j,l| \exp\left(i(t+m)(s_k t_j)E_l^{(j)}\right)\right) |\psi_2\rangle \\
&= \langle\psi_1| \left(\prod_j \sum_{l,l'} |j,l'\rangle\langle j,l'|V_j|j,l\rangle\langle j,l| \exp\left(i(t+m)(s_k t_j)E_l^{(j)}\right)\right) |\psi_2\rangle.
\end{aligned} \tag{19}$$

Here, it will be more convenient to define separate indices l' and l for each j, that is, l'_j and l_j. This way, we can write the previous expression the following way:

$$\tilde{x}(t) = \sum_{l'_1,l'_2,\ldots,l'_M}^{2^n-1} \sum_{l_1,l_2,\ldots,l_M}^{2^n-1} \langle\psi_1| \left(\prod_j |j,l'_j\rangle\langle j,l'_j|V_j|j,l_j\rangle\langle j,l_j| \exp\left(i(t+m)(s_k t_j)E_{l_j}^{(j)}\right)\right) |\psi_2\rangle. \tag{20}$$

With this labeling we can now factorize the phase factor:

$$\tilde{x}(t) = \sum_{l'_1,l'_2,\ldots,l'_M}^{2^n-1} \sum_{l_1,l_2,\ldots,l_M}^{2^n-1} \exp\left(\sum_{j'} i(t+m)(s_k t_{j'})E_{l_{j'}}^{(j')}\right) \langle\psi_1| \left(\prod_j |j,l'_j\rangle\langle j,l'_j|V_j|j,l_j\rangle\langle j,l_j|\right) |\psi_2\rangle, \tag{21}$$

as long as we introduce the new dummy index j'. We can now regroup it

$$\tilde{x}(t) = \sum_{l_1,l_2,\ldots,l_M}^{2^n-1} \exp\left(\sum_{j'} i(t+m)(s_k t_{j'})E_{l_{j'}}^{(j')}\right) \sum_{l'_1,l'_2,\ldots,l'_M}^{2^n-1} \langle\psi_1| \left(\prod_j |j,l'_j\rangle\langle j,l'_j|V_j|j,l_j\rangle\langle j,l_j|\right) |\psi_2\rangle. \tag{22}$$

We now define

$$o_{\vec{l}} = \sum_{l'_1, l'_2, \ldots, l'_M}^{2^n - 1} \langle \psi_1 | \left(\prod_j |j, l'_j\rangle\langle j, l'_j | V_j | j, l_j\rangle\langle j, l_j | \right) |\psi_2\rangle, \tag{23}$$

and

$$\mu_{\vec{l}} = \frac{1}{2\pi} \sum_{j=1}^{M} (s_k t_j) E_{l_j}^{(j)}, \tag{24}$$

such that

$$\tilde{x}(t) = \sum_{\vec{l}} o_{\vec{l}}\, \tilde{x}^{(\mu_{\vec{l}})}(t), \tag{25}$$

where $\tilde{x}^{(\mu_{\vec{l}})}(t) = e^{i2\pi(t+m)\mu_{\vec{l}}}$. A similar decomposition for the windowed function will also be useful:

$$x(t) = \sum_{\vec{l}} o_{\vec{l}}\, x^{(\mu_{\vec{l}})}(t), \tag{26}$$

where $x^{(\mu_{\vec{l}})}(t) = w(t)\tilde{x}^{(\mu_{\vec{l}})}(t)$, more explicitly, for any μ, each individual windowed signal looks like:

$$x^{(\mu)}(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\sigma^2}\right) \exp\left(i2\pi t\mu\right) \exp\left(i2\pi m\mu\right). \tag{27}$$

We also have that

$$\sum_{\vec{l}} \left| o_{\vec{l}} \right| \leq 1, \tag{28}$$

thus, bounding the interpolation error for the worst-case $x^{(\mu)}(t)$ should also be an upper bound for the interpolation error for $x(n)$. Simply put,

$$\varepsilon_{\text{spectral}} = \max_t \left| x(t) - x_{\text{interp},\infty}(t) \right| \leq \max_{\mu,t} \left| x^{(\mu)}(t) - x^{(\mu)}_{\text{interp},\infty}(t) \right|, \tag{29}$$

where

$$x^{(\mu)}_{\text{interp},\infty}(t) = \sum_{n=-\infty}^{\infty} x^{(\mu)}(n) \operatorname{sinc}\left(t - n\right). \tag{30}$$

Moreover,

$$\begin{aligned} x^{(\mu)}_{\text{interp},\infty}(t) &= \mathcal{F}_f^{-1}\left\{ \mathcal{F}_{t'}\left\{ \sum_{n=-\infty}^{\infty} x^{(\mu)}(n) \operatorname{sinc}\left(t' - n\right) \right\}(f) \right\}(t) \\ &= \mathcal{F}_f^{-1}\left\{ \sum_{n=-\infty}^{\infty} x^{(\mu)}(n) \mathcal{F}_{t'}\left\{ \operatorname{sinc}\left(t' - n\right) \right\}(f) \right\}(t) \\ &= \mathcal{F}_f^{-1}\left\{ \sum_{n=-\infty}^{\infty} x^{(\mu)}(n) \operatorname{rect}\left(f\right) \exp\left(2\pi i f n\right) \right\}(t) \\ &= \mathcal{F}_f^{-1}\left\{ \operatorname{rect}\left(f\right) X_1^{(\mu)}(f) \right\}(t). \end{aligned} \tag{31}$$

The discrete-time Fourier transform $X_1^{(\mu)}(f)$ can be written in terms of the Fourier transform

$$\begin{aligned} X^{(\mu)}(f) &= \mathcal{F}_t\left\{x^{(\mu)}(t)\right\}(f) \\ &= \frac{1}{\sigma_f\sqrt{2\pi}}\exp\left(-\frac{1}{2}(f-\mu)^2/\sigma_f^2\right), \end{aligned} \tag{32}$$

where $\sigma_f = \frac{1}{4\pi\sigma}$, in the following way:

$$\begin{aligned} X_1^{(\mu)}(f) &= \sum_{n=-\infty}^{\infty} x^{(\mu)}(n)\exp\left(2\pi i f n\right) \\ &= \int \text{Ш}\left(t\right) x^{(\mu)}(t)\exp\left(2\pi i f t\right)\mathrm{d}t \\ &= \mathcal{F}\left\{\text{Ш}\left(t\right)\right\} \star \mathcal{F}\left\{x^{(\mu)}(t)\right\} \\ &= \text{Ш}\left(f\right) \star X^{(\mu)}(f) \\ &= \sum_k X^{(\mu)}(f-k). \end{aligned} \tag{33}$$

Here, Ш is the Dirac comb function

$$\text{Ш}(t) = \sum_{k=-\infty}^{\infty}\delta(t-k).$$

Now, the error between $x_{\text{interp},\infty}(t)$ and $x(t)$ is

$$\begin{aligned} \varepsilon_{\text{spectral}} &\leq \max_\mu \left|\mathcal{F}^{-1}\left\{X^{(\mu)}(f)\right\} - \mathcal{F}^{-1}\left\{\text{rect}\left(\frac{f}{f_s}\right)X_s^{(\mu)}(f)\right\}\right| \\ &\leq \max_\mu\left(\int\sum_{k\neq 1}|X^{(\mu)}(f-kf_s)|\,\text{rect}(f/f_s)\mathrm{d}f\right) \\ &+ \max_\mu\left(\int|X^{(\mu)}(f)|(1-\text{rect}(f/f_s))\mathrm{d}f\right). \end{aligned} \tag{34}$$

If one assumes

$$\frac{1}{2\pi}\sum_{j=1}^{M} t_j \leq 1/4, \tag{35}$$

we then know that $|\mu_{\vec{l}}| \leq 1/4$. Thus, one can bound the error by letting μ be in the worst case scenarios defined by

$$|\mu| = 1/4. \tag{36}$$

This means that the term in the last line of Equation (34) is bounded as

$$\begin{aligned}
&\int |X^{(1/4)}(f)|(1-\mathrm{rect}(f/f_s))\mathrm{d}f \\
&\leq 2\int_{f=1/2}^{\infty} \frac{1}{\sigma_f\sqrt{2\pi}} \exp\left(-\frac{1}{2}(f-1/4)^2/\sigma_f^2\right)\mathrm{d}f \\
&= 2\,\mathrm{erfc}\left(\frac{1}{\sqrt{32}\sigma_f}\right) \\
&\leq 2\exp\left(-\frac{1}{32\sigma_f^2}\right). \qquad (37)
\end{aligned}$$

For the term in the second-to-last line of Equation (34), the μ that maximizes it is $\mu = -1/4$, giving us:

$$\begin{aligned}
&\int \sum_{k\neq 1} |X^{(-1/4)}(f-kf_s)|\,\mathrm{rect}(f/f_s)\mathrm{d}f \\
&\leq \max_f \left(\sum_{k\neq 1} |X^{(-1/4)}(f-kf_s)|\right) \overbrace{\int \mathrm{rect}(f/f_s)\mathrm{d}f}^{1} \\
&= 2\sum_{k=1}^{\infty} \frac{1}{\sigma_f\sqrt{2\pi}} \exp\left(-\frac{1}{2}(1/2+1/4-k)^2/\sigma_f^2\right) \\
&= 2\sum_{k=0}^{\infty} \frac{1}{\sigma_f\sqrt{2\pi}} \exp\left(-\frac{1}{2}(k+1/4)^2/\sigma_f^2\right) \\
&= 2\sum_{k=0}^{\infty} \frac{1}{\sigma_f\sqrt{2\pi}} \exp\left(-\frac{1}{2}(k^2+\frac{1}{2}k+1/2)/\sigma_f^2\right) \\
&= \frac{2\exp\left(-\frac{1}{2}(1/2)/\sigma_f^2\right)}{\sigma_f\sqrt{2\pi}} \sum_{k=0}^{\infty} \left(\exp\left(-\frac{1}{4}1/\sigma_f^2\right)\right)^{(2k^2+k)}. \qquad (38)
\end{aligned}$$

Now, if we assume $\exp\left(-\frac{3}{4\sigma_f^2}\right) \leq 1$ we can state the following

$$\begin{aligned}
&\int \sum_{k\neq 1} |X^{(-1/4)}(f-kf_s)|\,\mathrm{rect}(f/f_s)\mathrm{d}f \\
&\leq \frac{2\exp\left(-\frac{1}{2}(1/2)/\sigma_f^2\right)}{\sigma_f\sqrt{2\pi}} \sum_{k=0}^{\infty} \left(\exp\left(-\frac{1}{4}1/\sigma_f^2\right)\right)^{(2k^2+k)} \\
&\leq \frac{2\exp\left(-\frac{1}{4\sigma_f^2}\right)}{\sigma_f\sqrt{2\pi}} \sum_{k=0}^{\infty} \left(\exp\left(-\frac{3}{4\sigma_f^2}\right)\right)^{k} \\
&= \frac{2\exp\left(-\frac{1}{4\sigma_f^2}\right)}{\sigma_f\sqrt{2\pi}} \frac{1}{1-\exp\left(-\frac{3}{4\sigma_f^2}\right)}. \qquad (39)
\end{aligned}$$

If one further assumes

$$\exp\left(-\frac{3}{4\sigma_f^2}\right) \leq 1/2, \tag{40}$$

then

$$\begin{aligned}&\int \sum_{k\neq 1} |X^{(-1/4)}(f - kf_s)| \operatorname{rect}(f/f_s)\mathrm{d}f \\ &\leq \frac{4\exp\left(-\frac{1}{4\sigma_f^2}\right)}{\sigma_f\sqrt{2\pi}}.\end{aligned} \tag{41}$$

We note that

$$\frac{\exp\left(-\frac{1}{4\sigma_f^2}\right)}{\sigma_f} = 2\sigma_f^2 \frac{\partial \exp\left(-\frac{1}{4\sigma_f^2}\right)}{\partial \sigma_f}, \tag{42}$$

which leads us to introduce the following necessary lemma:

Lemma 3 (Derivative bound)**.** *If the function $f(z)$ is analytic on the complex disc of radius r centered at z_0, then*

$$|f^{(n)}(z - z_0)| \leq \frac{Mn!2^n}{r^n}, \tag{43}$$

for $|z - z_0| \leq \frac{r}{2}$, where $M = \max_{|z'-z_0|\leq r} |f(z' - z_0)|$.

Now, using this last lemma for $z - z_0 = \sigma_f$, $z_0 = 2\sigma_f > 0$ and $r = 2\sigma_f$ one obtains

$$M = \max_{|z'-z_0|\leq 2\sigma_f} \exp\left(-\frac{1}{4(z' - 2\sigma_f)^2}\right) = \exp\left(-\frac{1}{4(4\sigma_f - 2\sigma_f)^2}\right) = \exp\left(-\frac{1}{16\sigma_f^2}\right). \tag{44}$$

With this, we obtain the following bound:

$$2\sigma_f^2 \frac{\partial \exp\left(-\frac{1}{4\sigma_f^2}\right)}{\partial \sigma_f} \leq 2\sigma_f^2 \frac{2}{2\sigma_f} \exp\left(-\frac{1}{16\sigma_f^2}\right) = 2\sigma_f \exp\left(-\frac{1}{16\sigma_f^2}\right). \tag{45}$$

Finally, if we restrict ourselves to considering $\sigma_f \leq 1$,

$$\frac{\exp\left(-\frac{1}{4\sigma_f^2}\right)}{\sigma_f} \leq 2\exp\left(-\frac{1}{16\sigma_f^2}\right). \tag{46}$$

Thus,

$$\int \sum_{k\neq 1} |X^{(-1/4)}(f - kf_s)| \operatorname{rect}(f/f_s) \mathrm{d}f$$
$$\leq \frac{8}{\sqrt{2\pi}} \exp\left(-\frac{1}{16\sigma_f^2}\right) \leq \frac{8}{\sqrt{2\pi}} \exp\left(-\frac{1}{32\sigma_f^2}\right). \tag{47}$$

Putting together the bounds on the last two terms in Equation (34), one gets

$$\varepsilon_{\text{spectral}} \leq \left(\frac{8}{\sqrt{2\pi}} + 2\right) \exp\left(-\frac{1}{32\sigma_f^2}\right). \tag{48}$$

Thus, we have proven Theorem 2.

Now, we wish to obtain a bound on the truncation error, $\varepsilon_{\text{trunc}}$. This is summarized in the following lemma:

Lemma 4.

$$\varepsilon_{\text{trunc}} = \max_t |x_{\text{interp},\infty}(t) - x_{\text{interp},2q+1}(t)| \leq 2 \exp\left(-\frac{(q+2)^2}{2\sigma^2}\right).$$

Proof.

$$\begin{aligned}
\varepsilon_{\text{trunc}} &= \max_t |x_{\text{interp},\infty}(t) - x_{\text{interp},2q+1}(t)| \\
&\leq \max_{t,\mu} \left|x^{(\mu)}_{\text{interp},\infty}(t) - x^{(\mu)}_{\text{interp},2q+1}(t)\right| \\
&\leq \sum_{n\notin\{k|-q\leq k\leq q\}} \left|x^{(\mu)}(t) \operatorname{sinc}(t-n)\right| \\
&\leq \sum_{n\notin\{k|-q\leq k\leq q\}} \left|x^{(\mu)}(t)\right| \\
&\leq \sum_{n\notin\{k|-q\leq k\leq q\}} |w(t)| \\
&\leq \sum_{n\notin\{k|-q\leq k\leq q\}} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{n^2}{2\sigma^2}\right) \\
&= 2\sum_{n=q+1}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{n^2}{2\sigma^2}\right) \\
&\leq 2\int_{n=q+2}^{\infty} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{n^2}{2\sigma^2}\right) \\
&= 2\operatorname{erfc}\left(\frac{(q+2)}{\sqrt{2}\sigma}\right) \leq 2\exp\left(-\frac{(q+2)^2}{2\sigma^2}\right).
\end{aligned} \tag{49}$$

□

Now, we set equal the exponentials on the bounds for $\varepsilon_{\text{spectral}}$ and $\varepsilon_{\text{trunc}}$ from Theorem 2 Theorem 4 respectively:

$$\exp\left(-\frac{(q+2)^2}{2\sigma^2}\right) = \exp\left(-\frac{\pi^2\sigma^2}{2}\right), \tag{50}$$

which gives

$$\sigma_f = \frac{1}{4\sqrt{\pi}}\frac{1}{\sqrt{q+2}}. \tag{51}$$

With this, $\varepsilon_{\text{interp}}$ can be bounded through

$$\varepsilon_{\text{interp}} \leq \left(4 + \frac{8}{\sqrt{2\pi}}\right)\exp\left(-\frac{\pi(q+2)}{2}\right). \tag{52}$$

Thus, solving for q, we obtain an upper bound for it:

$$q \leq \frac{2}{\pi}\log\frac{\left(4+\frac{8}{\sqrt{2\pi}}\right)}{\varepsilon_{\text{interp}}} - 2. \tag{53}$$

The interpretation of this bound is the following: "If we have an error $\varepsilon_{\text{interp}}$, the value of q must be at most $\frac{2}{\pi}\log\frac{\left(4+\frac{8}{\sqrt{2\pi}}\right)}{\varepsilon_{\text{interp}}} - 2$".

At this point, the error $\varepsilon_{\text{interp}}$ is with respect to the windowed function

$$\tilde{w}(t) := w(t)\langle\psi_1|\prod_j^M V_j S_{p,j}^{t+m}(s_k t_j)|\psi_2\rangle. \tag{54}$$

Now, the bounds on q with respect to the error

$$\tilde{\varepsilon}_{\text{interp}} = |\tilde{w}(r) - x_{\text{interp},2q+1}(r)| = \varepsilon_{\text{interp}}/w(r). \tag{55}$$

After making the substitution the upper bound for q becomes:

$$\begin{aligned}
q &\leq \frac{2}{\pi}\log\frac{\left(4+\frac{8}{\sqrt{2\pi}}\right)}{w(r)\tilde{\varepsilon}_{\text{interp}}} - 2 \\
&\leq \frac{2}{\pi}\log\frac{\sigma\left(4\sqrt{2\pi}+8\right)}{\exp\left(-\frac{r^2}{2\sigma^2}\right)\tilde{\varepsilon}_{\text{interp}}} - 2 \\
&\leq \frac{2}{\pi}\log\frac{\sigma\left(4\sqrt{2\pi}+8\right)}{\tilde{\varepsilon}_{\text{interp}}} + \frac{2}{\pi}\frac{1}{2\sigma^2} - 2 \\
&\leq \frac{2}{\pi}\log\frac{\left(4\sqrt{2\pi}+8\right)}{\pi\sigma_f\tilde{\varepsilon}_{\text{interp}}} + \frac{2}{\pi}\frac{16\pi^2\sigma_f^2}{2} - 2 \\
&\leq \frac{2}{\pi}\log\frac{\sqrt{q+2}\left(4\sqrt{2\pi}+8\right)}{\sqrt{\pi}\tilde{\varepsilon}_{\text{interp}}} + \frac{2}{\pi}\frac{\pi}{2(q+2)} - 2 \\
&\leq \frac{1}{\pi}\log\frac{(q+2)\left(4\sqrt{2\pi}+8\right)^2}{\pi\tilde{\varepsilon}_{\text{interp}}^2} + \frac{1}{\pi}\frac{\pi}{(q+2)} - 2
\end{aligned} \tag{56}$$

If we assume that $q \geq 0$, we can loosen the bound to

$$(q+2) \leq \frac{1}{\pi} \log \frac{(q+2)\exp(\pi/2)\left(4\sqrt{2\pi}+8\right)^2}{\pi\tilde{\varepsilon}_{\text{interp}}^2} \tag{57}$$

Solving for q one obtains

$$(q+2) \leq -\frac{1}{\pi} W_{-1}\left(-\frac{\pi^2\tilde{\varepsilon}_{\text{interp}}^2}{\exp(\pi/2)\left(4\sqrt{2\pi}+8\right)^2}\right), \tag{58}$$

provided $0 \leq \frac{\pi^2\tilde{\varepsilon}_{\text{interp}}^2}{\exp(\pi/2)\left(4\sqrt{2\pi}+8\right)^2} \leq 1/e$. Now, we use $-W_{-1}(-e^{-u-1}) \leq 1+\sqrt{2u}+u \leq 1+3u$ for $u > 0$ We are now able to identify

$$u = \log \frac{\exp(\pi/2)\left(4\sqrt{2\pi}+8\right)^2}{e\pi^2\tilde{\varepsilon}_{\text{interp}}^2}, \tag{59}$$

which means $\frac{\pi^2\tilde{\varepsilon}_{\text{interp}}^2}{\exp(\pi/2)\left(4\sqrt{2\pi}+8\right)^2} < 1/e$. Using the aforementioned bound, one obtains

$$q \leq \frac{6}{\pi}\left(\log \frac{4\sqrt{2\pi}+8}{\pi e^{1/3+\pi/12}\tilde{\varepsilon}_{\text{interp}}}\right). \tag{60}$$

This means that, for a given target error $\tilde{\varepsilon}_{\text{interp}}$ we need only choose any:

$$q \geq \frac{6}{\pi}\left(\log \frac{4\sqrt{2\pi}+8}{\pi e^{1/3+\pi/12}\tilde{\varepsilon}_{\text{interp}}}\right). \tag{61}$$

Thus, we have proven Theorem 1.

4 Optimally-conditioned Trotter Interpolation

After having solved the issue interpolating to fractional queries with powers g/s_k we will now discuss the interpolation of the amplitudes

$$f(s) = \langle\psi_1|\prod_j^M V_j S_{p,j}^{g/s}(st_j)|\psi_2\rangle = \langle\psi_1|\prod_j^M V_j \left(e^{i(st_j)\tilde{H}_{p,j}(st_j)}\right)^{(g/s)}|\psi_2\rangle \tag{62}$$

to $s \to 0$. These results will be summarized at the end of the section in Theorem 7.

The interpolant we use is the following linear combination of orthogonal polynomials

$$P_{n-1}f(s) = \sum_{j=0}^{n-1} c_j p_j(s). \tag{63}$$

One samples f at certain values s_k and solves the following system of linear equations

$$y = \mathbf{V}c \tag{64}$$

where $y = (f(s_1), f(s_2), \ldots, f(s_n))$, and

$$\mathbf{V} := \begin{pmatrix} p_0(s_1) & p_1(s_1) & \ldots & p_{n-1}(s_1) \\ p_0(s_2) & p_1(s_2) & \ldots & p_{n-1}(s_2) \\ \vdots & \vdots & \ddots & \vdots \\ p_0(s_n) & p_1(s_n) & \ldots & p_{n-1}(s_n) \end{pmatrix}. \tag{65}$$

Thus, one can obtain the coefficients, c_j, with $c = \mathbf{V}^{-1}y$. Like in [8], the choice of interpolating nodes s_k and the interpolating set of polynomials are the Chebyshev nodes and polynomials. In that case, p_j is defined by

$$p_j(s) := \begin{cases} \sqrt{\frac{1}{n}} T_0(s), & j = 0 \\ \sqrt{\frac{2}{n}} T_j(s), & j = 1, 2, \ldots \end{cases} \tag{66}$$

where T_j is the standard jth Chebyshev polynomial.

$$T_j(x) := \cos\Big(n \cos^{-1} x\Big). \tag{67}$$

The node collocation is described by

$$s_i = \cos\left(\frac{2i-1}{2n}\pi\right). \tag{68}$$

These polynomials fulfill the discrete orthonormality condition [23] with respect to the collocation nodes, that is,

$$\sum_{k=1}^{n} p_i(s_k) p_j(s_k) = \delta_{ij} \tag{69}$$

for all $0 \leq i, j < n$. Instead of estimating the coefficients c_i intermediately to estimate $f(0)$, one knows from [8], that

$$P_{n-1}f(0) = \sum_{k=1}^{n} d_k f(s_k), \tag{70}$$

where

$$d_k(0) = \frac{1}{n}(-1)^{k+n/2} \tan\left(\frac{2k-1}{2n}\pi\right). \tag{71}$$

We define

$$\epsilon_{\text{cheb}} = |f(0) - P_{n-1}f(0)|. \tag{72}$$

Now, to get estimates on the Trotter interpolation error bounds, we need to introduce some methods of complex analysis. For each $\rho > 1$, let $B_\rho \subset \mathbb{C}$ be the Bernstein ellipse, which is an ellipse with foci at ± 1 and the semimajor axis is $(\rho + \rho^{-1})/2$. The following lemma bounds the Chebyshev interpolation error for analytic functions on B_ρ.

Lemma 5. *Let $f(z) \in \mathbb{C}$ be an analytic function on B_ρ, and suppose $C \in \mathbb{R}_+$ is an upper bound such that $|f(z)| \leq C$, for all $z \in B_\rho$. Then the Chebyshev interpolation error on $[-1,1]$ satisfies*

$$\|f - P_n f\|_\infty \leq \frac{4C\rho^{-n}}{\rho - 1}$$

for each degree $n > 0$ of the interpolant through the $n+1$ Chebyshev nodes.

Proof. Theorem 8.2 of Ref. [24]. □

With this lemma in place, we now wish to upper bound the corresponding norm of the amplitude $f(z)$ on the Bernstein ellipse by promoting the real variable s to $z \in B_\rho$.

First, like in Section 2, we assume a sufficiently small $|\tau_i|$, where $\tau_i = zt_j$, such that

$$\tilde{H}_j(\tau_j) = \frac{\log\left(S_{p,j}(\tau_j)\right)}{i\tau_j} \tag{73}$$

is single valued. Now, recalling, with slight modifications, Lemma 14 from [8]:

Lemma 6. *Let $\tilde{H}_j(\tau_j)$ be the effective Hamiltonian associated with a complex-time pth order product formula $S_{p,j}(\tau_j)$, where $\tau_j = zt_j$ with $z \in \mathbb{C}$ and $t_j \in \mathbb{R}_+$, which is analytically continued to an open neighborhood containing $z \in [-1,1]$. The norm of operator error can upper bounded as*

$$\left\|H_j - \tilde{H}_j\right\| \leq \frac{5}{2} \sum_{(\upsilon,m)} \alpha_{\text{comm}}\Big(H_{j,\pi_\Upsilon(\Gamma)}, \ldots, H_{j,\pi_\upsilon(m+1)}, H_{j,\pi_\upsilon(m)}\Big) \cdot \frac{|\tau|^p}{(p+1)!} e^{2|\tau_j| \sum_j^m \|H_j\|}$$

provided that $\left\|H - \tilde{H}_j\right\| \leq 15$, $|\tau| \leq 1/8$, and

$$\sum_{(\upsilon,m)} \alpha_{\text{comm}}\Big(H_{j,\pi_\Upsilon(\Gamma)}, \ldots, H_{j,\pi_\upsilon(m+1)}, H_{j,\pi_\upsilon(m)}\Big) \frac{|\tau|^p}{(p+1)!} e^{2|\tau_j| \sum_{m_j} \left\|H_{j,m_j}\right\|} \leq 1.$$

Here, $\alpha_{\text{comm}}\Big(A_s, \ldots, A_1, B\Big) := \sum_{q_1+\cdots+q_s=p} \binom{p}{q_1 \cdots q_s} \Big\|\text{ad}_{A_s}^{q_s} \cdots \text{ad}_{A_1}^{q_1}(B)\Big\|$. This means that, for a pth-order product formula one has that for $L_j(\tau_j) = \tilde{H}_j(\tau_j) - H_j$

$$\|L_j(\tau_j)\| = O\left(\frac{|\tau_j|^p \alpha_j}{(p+1)!}\right), \tag{74}$$

provided the constraints of Lemma 14 of [8] are fulfilled. Here,

$$\alpha_j = \sum_{(\upsilon,m)} \alpha_{\text{comm}}\Big(H_{j,\pi_\Upsilon(\Gamma)}, \ldots, H_{j,\pi_\upsilon(m+1)}, H_{j,\pi_\upsilon(m)}\Big). \tag{75}$$

We specifically look at each evolution operator that one obtains from Trotterization with a step τ_j is

$$e^{iT_j(H_j+L_j(\tau_j))}. \tag{76}$$

We split this operator (or equivalently raise to a real fractional power Δ/T_j) into sufficiently small steps of length Δ, such that one can use the Zassenhauss formula. That is, we first look at the following expression and use the Zassenhauss formula:

$$e^{-i\Delta H_j}e^{i\Delta(H_j+L_j(\tau_j))} = e^{i\Delta L_j(\tau_j)}e^{\Delta^2[H_j,L_j(\tau_j)]}\dots \tag{77}$$

Thus, applying $e^{i\Delta H_j}$ on the left, we finally obtain:

$$e^{i\Delta(H_j+L_j(\tau_j))} = e^{i\Delta H_j}e^{i\Delta L_j(\tau_j)}e^{\Delta^2[H_j,L_j(\tau_j)]}\dots. \tag{78}$$

With this, one has that

$$\|e^{i\Delta(H_j+L_j(\tau_j))}\| \leq \left\|e^{i\Delta H_j}\right\| O\left(e^{\Delta|\tau_j|^p\alpha_j/(p+1)!}\right) = O\left(e^{\Delta|\tau_j|^p\alpha_j/(p+1)!}\right), \tag{79}$$

which finally gives us, for the full evolution length T_j, after exponentiating $e^{i\Delta(H_j+L_j(\tau_j))}$ by T_j/Δ, a real number, we can bound the following norm through:

$$\left\|e^{iT_j(H_j+L_j(\tau_j))}\right\| = O\left(e^{T_j|\tau_j|^p\alpha_j/(p+1)!}\right). \tag{80}$$

This means that,

$$\max_{z\in B_\rho}\left|\langle\psi_1|\prod_i^M V_i S_p^{g/z}(zt_i)|\psi_2\rangle\right| = O\left(e^{\frac{g}{(p+1)!}\sum_j t_j\alpha_j(rt_j)^p}\right) \tag{81}$$

with $g = T_j/t_j$. Here, $r = O(1)$ is the radius of the smallest disc containing B_ρ. The relationship between ρ and r is

$$\rho = r + \sqrt{r^2-1}. \tag{82}$$

Now, using Theorem 5, one knows the interpolation error is

$$\begin{aligned}\epsilon_{\text{cheb}} &= O\left(\frac{e^{\frac{g}{(p+1)!}\sum_j \alpha_j t_j(rt_j)^p}}{r^n}\right)\\ &= O\left(\frac{e^{\frac{g}{(p+1)!}\sum_j \alpha_j t_j(rt_j)^p}}{e^{n\log r}}\right).\end{aligned} \tag{83}$$

Solving for n one gets

$$n = \frac{1}{\log r}O\left(\log 1/\epsilon_{\text{cheb}} + \frac{g}{(p+1)!}\sum_j \alpha_j t_j(rt_j)^p\right). \tag{84}$$

This is summarized in the following theorem:

Theorem 7. *In order to get a error*

$$\epsilon_{\text{cheb}} = \left| \langle \psi_1 | \prod_j^M V_j e^{iT_j H_j} | \psi_2 \rangle - P_{n-1} f(0) \right|, \tag{85}$$

where $f(s) = \langle \psi_1 | \prod_j^M V_j S_{p,j}^{g/s}(st_j) | \psi_2 \rangle$, $g = T_j/t_j$, *and*

$$P_{n-1} f(0) = \sum_{k=1}^{n} d_k f(s_k), \tag{86}$$

where $d_k(0) = \frac{1}{n}(-1)^{k+n/2} \tan\left(\frac{2k-1}{2n}\pi\right)$, *and* $s_i = \cos\left(\frac{2i-1}{2n}\pi\right)$, *one needs*

$$n = \frac{1}{\log r} O\left(\log 1/\epsilon_{\text{cheb}} + \frac{g}{(p+1)!} \sum_j \alpha_j t_j (r t_j)^p \right),$$

where

$$\alpha_j = \sum_{(\upsilon,m)} \alpha_{\text{comm}}\Big(H_{j,\pi_\Upsilon(\Gamma)}, \ldots, H_{j,\pi_\upsilon(m+1)}, H_{j,\pi_\upsilon(m)} \Big),$$

and m_j *runs over all the non-commuting terms of the product-formula decomposition for* H_j, *and provided that*

$$t_j \leq \pi. \tag{87}$$

5 Combined Results

In this work, a distinction between algorithmic and statistical error is made. We call statistical error, ε, the error that comes from estimating amplitudes on the quantum computer. We call algorithmic error, ϵ, the error stemming from the use of finite interpolations, assuming that the underlying amplitudes are estimated exactly. In turn, from triangle inequality, we know that the algorithmic error is

$$\epsilon \leq \epsilon_{\text{cheb}} + \epsilon_{\text{sinc}}. \tag{88}$$

For convenience, we set $\epsilon_{\text{cheb}} = \epsilon_{\text{sinc}} = \epsilon/2$. Now, we bring to your attention that the number of queries required for Trotter interpolation is proportional to

$$\text{total cost} = O\left(\frac{\log q \log n}{\varepsilon} 5^p M \sum_i^n q \frac{g}{|s_i|} \right), \tag{89}$$

and a maximum circuit depth that goes like:

$$\text{max depth} = O\left(\frac{\log q \log n}{\varepsilon} 5^p M \frac{g}{\min_i |s_i|} \right), \tag{90}$$

where s_i is defined in eq. (68), and the factor 5^p is coming from the number of stages in the Suzuki product formulas. The $1/\varepsilon$ factor is on account of the amplitude estimation algorithm needed to extract the underlying amplitudes [19, 20]. One need only estimate the underlying amplitudes with statistical error $O\left(\frac{\varepsilon}{\log q \log n}\right)$ to get a statistical error ε on the final interpolant. This is due to the stability of the cardinal sine interpolation (see Section A) and the stability of Chebyshev interpolation (see lemmas 4 and 5 of [15]). The factor $g/|s_i|$ is the number of queries needed to achieve an evolution time $O\left(T_j\right)$ for each Chebyshev sample point s_i, and q are the number of integer queries around $\lceil g/|s_i| \rceil$ needed to interpolate to an evolution time T_i. From [8], one knows that $\sum_i 1/|s_i| = O(n \log n)$, and $1/\min_i |s_i| = O(n)$, thus, finally, the number of queries is proportional to

$$\text{total cost} = O\left(5^p M g n \frac{q \log q \log^2 n}{\varepsilon}\right), \tag{91}$$

and the maximum circuit depth is

$$\text{max depth} = O\left(5^p M g n \frac{\log q \log n}{\varepsilon}\right). \tag{92}$$

From these we take the factor $5^p M g n$ and define the following cost function:

$$L = 5^p M g n. \tag{93}$$

Replacing n from Theorem 7 we get

$$L = O\left(5^p M g \frac{1}{\log r}\left(\log 1/\epsilon_{\text{cheb}} + \frac{g}{(p+1)!}\sum_j \alpha_j t_j (r t_j)^p\right)\right). \tag{94}$$

We can simplify this using:

$$t_j = T_j/g \leq \frac{\max_j T_j}{g}, \tag{95}$$

we define $T_{\max} = \max_j T_j$ and $\alpha_{\max} = \max_j \alpha_j$, and thus write the cost function as:

$$L = O\left(5^p M g \frac{1}{\log r}\left(\log 1/\epsilon_{\text{cheb}} + \frac{M \alpha_{\max} T_{\max} (r T_{\max}/g)^p}{(p+1)!}\right)\right). \tag{96}$$

For a moment, we treat p as a continuous variable and optimize this bound with respect to g to obtain:

$$g_{\text{opt}} = r\left(\frac{(p-1) M \alpha_{\max} T_{\max}^{p+1}}{(p+1)!\,\log(1/\epsilon_{\text{cheb}})}\right)^{\frac{1}{p}}. \tag{97}$$

However, for simplicity, we choose a close optimum

$$\tilde{g}_{\text{opt}} \sim r \left(\frac{M \alpha_{\max} T_{\max}^{p+1}}{(p+1)!} \right)^{\frac{1}{p}} \tag{98}$$

If we replace this back into the cost function, we get:

$$L = O\left(\frac{5^p (M T_{\max})^{1+1/p} r}{\log r} \left(\log \frac{1}{\epsilon_{\text{cheb}}} \right) (\alpha_{\max})^{\frac{1}{p}} \right). \tag{99}$$

Here, we now assume we use any $r > 1$ for which $r/\log r = O(1)$. Here, we will now optimize the cost with respect to the order, p. If we optimize this expression with respect to p, we obtain:

$$p_{\text{opt}} = \sqrt{\frac{\log M T_{\max} \alpha_{\max}}{\log 5}}. \tag{100}$$

However, to avoid any problems for when $\alpha_{\max} \ll 1$, we simply choose a near optimal scaling for p that scales only with $M T_{\max}$ (or optimize again, but without the factor $\alpha_{\max}^{1/p}$):

$$\tilde{p}_{\text{opt}} = \sqrt{\frac{\log M T_{\max}}{\log 5}}. \tag{101}$$

Replacing this choice for p in the bound for the cost function L, we obtain:

$$L = O\left((M T_{\max})^{1+o(1)} \alpha_{\max}^{\Theta\left(\sqrt{\frac{1}{\log(M T_{\max})}}\right)} e^{\Theta\left(\sqrt{\log(M T_{\max})}\right)} \log \frac{1}{\epsilon_{\text{cheb}}} \right). \tag{102}$$

We replace this cost function bound in the previous total gate cost bounds and maximum circuit depth:

$$\begin{aligned} \text{total cost} &= O\left((M T_{\max})^{1+o(1)} \alpha_{\max}^{\Theta\left(\sqrt{\frac{1}{\log(M T_{\max})}}\right)} e^{\Theta\left(\sqrt{\log(M T_{\max})}\right)} \log \frac{1}{\epsilon_{\text{cheb}}} \frac{q \log q \log^2 n}{\varepsilon} \right), \\ \text{max depth} &= O\left((M T_{\max})^{1+o(1)} \alpha_{\max}^{\Theta\left(\sqrt{\frac{1}{\log(M T_{\max})}}\right)} e^{\Theta\left(\sqrt{\log(M T_{\max})}\right)} \log \frac{1}{\epsilon_{\text{cheb}}} \frac{\log q \log n}{\varepsilon} \right). \end{aligned} \tag{103}$$

We recall that $q = O(\log(1/\epsilon_{\text{sinc}}))$ from theorem 1 and note that $n = O(\log(1/\epsilon_{\text{cheb}}))$ after our choice of g and p. If we set both target error tolerances equal: $\epsilon_{\text{sinc}} = \epsilon_{\text{cheb}} =$

$\epsilon/2$, we have:

$$\text{total cost} = \tilde{O}\left(\frac{(MT_{\max})^{1+o(1)}\alpha_{\max}^{\Theta\left(\sqrt{\frac{1}{\log(MT_{\max})}}\right)}}{\varepsilon}\log^2\left(\frac{1}{\epsilon}\right)\right)$$
$$\text{max depth} = \tilde{O}\left(\frac{(MT_{\max})^{1+o(1)}\alpha_{\max}^{\Theta\left(\sqrt{\frac{1}{\log(MT_{\max})}}\right)}}{\varepsilon}\log\left(\frac{1}{\epsilon}\right)\right), \tag{104}$$

where, by triangle inequality, the algorithmic error is going to be less than the tolerance ϵ. We have also grouped the term $e^{\Theta\left(\sqrt{\log(MT_{\max})}\right)}$ into $(MT_{\max})^{1+o(1)}$ since the exponent $o(1)$ already encompasses all sub-polynomial growth terms. We do something similar to the bound on the exponent of $\alpha_{\max}$ and replace it with $o(1)$:

$$\text{total cost} = \tilde{O}\left(\frac{(MT_{\max})^{1+o(1)}\alpha_{\max}^{o(1)}}{\varepsilon}\log^2\left(\frac{1}{\epsilon}\right)\right),$$
$$\text{max depth} = \tilde{O}\left(\frac{(MT_{\max})^{1+o(1)}\alpha_{\max}^{o(1)}}{\varepsilon}\log\left(\frac{1}{\epsilon}\right)\right). \tag{105}$$

We also note that with our choices for g and p, the number of Chebyshev nodes for interpolation are:

$$n = O\left(\log 1/\epsilon\right). \tag{106}$$

We can summarize these results in the following theorem:

Theorem 8. *We can estimate*

$$\langle\psi_1|\prod_j^M V_j e^{iT_j H_j}|\psi_2\rangle,$$

with an algorithmic error of at most ϵ and a statistical error of at most ε, with a query cost of

$$\tilde{O}\left(\frac{(MT_{\max})^{1+o(1)}\alpha_{\max}^{o(1)}}{\varepsilon}\log^2\frac{1}{\epsilon}\right),$$

and maximum circuit depth going like:

$$\tilde{O}\left(\frac{(MT_{\max})^{1+o(1)}\alpha_{\max}^{o(1)}}{\varepsilon}\log\frac{1}{\epsilon}\right),$$

using the following interpolation:

$$\sum_{k=1}^{n} d_k \frac{\sum_{o=-q}^{q}\operatorname{sinc}\left(r-o\right)w(o)\langle\psi_1|\prod_j^M V_j S_{p,j}^{o+m_k}(s_k t_j)|\psi_2\rangle}{w(r_k)},$$

where $w(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2}{2\sigma^2}\right)$, $\sigma = \sqrt{\frac{q+2}{\pi}}$, $m_k = \lfloor g/s_k \rfloor$, $r_k = g/s_k - \lfloor g/s_k \rfloor$, $g = T_j/t_j$, $s_i = \cos\left(\frac{2i-1}{2n}\pi\right)$, *and* $d_k = \frac{1}{n}(-1)^{k+n/2} \tan\left(\frac{2k-1}{2n}\pi\right)$. *Here,*

$$\alpha_j = \sum_{(\upsilon,m)} \alpha_{\text{comm}}\Big(H_{j,\pi_\Upsilon(\Gamma)}, \ldots, H_{j,\pi_\upsilon(m+1)}, H_{j,\pi_\upsilon(m)}\Big),$$

$T_{\max} = \max_j T_j$ *and* $\alpha_{\max} = \max_j \alpha_j$. *This is, while choosing* $n = \tilde{O}\left(\log \frac{1}{\epsilon}\right)$, $q = O\left(\log \frac{1}{\epsilon}\right)$,

$$g = \Theta\left(\left(\frac{M\alpha_{max}T_{max}^{p+1}}{p!}\right)^{\frac{1}{p}}\right),$$

and

$$p = \Theta\left(\sqrt{\frac{\log MT_{\max}}{\log 5}}\right),$$

and $\sum_j t_j \leq \pi/2$. *Also, this is provided that* $|\prod_j^M V_j S_{p,j}^{o+m_k}(s_k t_j)|\psi_2\rangle$ *are estimated with* $O\left(\varepsilon/\log^2(1/\epsilon)\right)$ *precision through amplitude estimation.*

Now, we look at the case $M = 1$:

Corollary 9. *There exists a quantum algorithm for Hamiltonian evolution whose query cost scales like* $\tilde{O}\left(\min\left(T^{1+o(1)}\alpha^{o(1)}\log^2(1/\epsilon)/\varepsilon, 1\right)\right)$ *and a maximum query depth that scales like* $\tilde{O}\left(\max\left(T^{1+o(1)}\alpha^{o(1)}\log(1/\epsilon)/\varepsilon, 1\right)\right)$, *while only using two extra ancilla qubits.*

One extra qubit requirement is coming from the Hadamard test to block-encode both the real and imaginary parts of the complex amplitudes, and the other extra qubit is for the amplitude estimation algorithm.

6 Discussion and outlook

We have provided an alternative method for the calculation of fractional queries by using a cardinal sine interpolation in conjunction with amplitudes of integer power queries. The algorithmic error from the query interpolation alone converges exponentially with the number of amplitudes used. Cardinal sine interpolation also proves to be very stable and does not propagate uncertainty significantly when using confidence intervals or normally-distributed random variables. Provided also here is a method to interpolate Trotterized evolution to zero Trotter-step-size.

The scaling with all relevant parameters is almost optimal for static Hamiltonian evolution. The expected quadratic scaling $\log^2(1/\epsilon)$ of the method presented here is still asymptotically worse than the state-of-the-art $\log(1/\epsilon)$. Extending these kind of methods for time-dependent simulation is also of great importance, however, no attempts at

this were made in this work. Quantum signal processing methods are not good at this either, however there are some new methods available using virtual clock registers and multi-product formulas [18] which achieve polylog$(1/\epsilon)$. More importantly, the algorithm obtained here has, for the first time, an exponentially small algorithmic error in terms of computational resources while having a quasi-linear cost-scaling with respect to the evolution time compared to similar methods using product formulas plus stable interpolation (see for example [16]). This was allowed by the variable order in p we proposed. This could be quite possibly extended to other works using stable interpolation with product formulas.

The results here, combined with low-weight Fourier expansion, Lemma 37, from [25] or Fourier series accelerators/mollifiers ([26]) open up the possibility for efficient offloading of a great extent of quantum signal processing into a classical post-processing (for the $M = O(1)$ case) for Hermitian operators. Such examples include Gibbs sampling ($f(H) = \exp(-\beta H)$), and matrix inversion $f(H) = H^{-1}$. This, while keeping competent cost scaling with respect to state-of-the-art methods. All that is left for the quantum computer is to estimate the matrix element amplitudes for unitary operators. If the amplitude of these operators with respect to two quantum states is expected to be small, one is better off estimating these coherently as there is a quadratic advantage lost if one estimates the amplitudes of unitaries incoherently and then added up. In this regard, quantum signal processing remains better as well.

7 Acknowledgements

The author would like to acknowledge the useful comments by Rutuja Kshirsagar, Bibhas Adhikari, and Taozhi Guo for their useful comments on the earlier versions. GR would also like to thank James Watson and Jacob Watkins for pointing out an important error introduced in the second version of the manuscript. In particular GR would like to thank Jacob Watkins for his generous input on the write-up of the overall manuscript. GR thanks the 2025 QIP reviewers for useful feedback as well as the useful feedback from Quantum Journal reviewers. The author used large language models to assist with language editing, formatting, and bibliography preparation; all scientific content, derivations, and results are the author's own, and the author takes full responsibility for the final manuscript.

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A Uncertainty propagation

In this section, we provide bounds on the uncertainty propagation to the cardinal sine interpolant coming from errors on integer queries estimates. First, we estimate how the uncertainty propagates when the estimates come in the form of confidence intervals. This is summarized in the following lemma:

Lemma 10. *Given an error vector $\epsilon \in \mathbb{C}^{2q+1}$, where $\|\epsilon\|_\infty \leq \varepsilon_{\text{estimate}}$. The error tolerance on the interpolated quantity is*

$$\max_t \|\epsilon s(t)\|_1 \leq \varepsilon_{\text{estimate}} \left(3 + \frac{2}{\pi} \log(2q)\right). \tag{107}$$

Here,

$$\|s(t)\|_1 = \sum_{n=-q}^{q} |\text{sinc}(t-n)| \tag{108}$$

Proof. Using Hölder's inequality, one obtains that the error tolerance on the interpolated quantity is

$$\max_t \|\epsilon s(t)\|_1 \leq \|\epsilon\|_\infty \max_t \|s(t)\|_1. \tag{109}$$

Now, we would like to upper-bound $\max_t \|s(t)\|_1$. First note

$$\max_t \|s(t)\|_1 = \sum_{n=-q}^{q} |\mathrm{sinc}\,(\tau - n)|\,. \tag{110}$$

With this, we note that one can split the sum into two parts

$$\max_\tau \|s(\tau)\|_1 \leq \sum_{n=\lfloor\tau\rfloor+1}^{q} |\mathrm{sinc}\,(n-\tau)| + \sum_{n=-q}^{\lfloor\tau\rfloor} |\mathrm{sinc}\,(n-\tau)| \tag{111}$$

We now upper-bound the terms $|\,\mathrm{sinc}(\lfloor\tau\rfloor+1-\tau)|$, $|\,\mathrm{sinc}(\lfloor\tau\rfloor-\tau)|$, and $|\,\mathrm{sinc}(\lfloor\tau\rfloor-1-\tau)|$ with 1, obtaining

$$\max_\tau \|s(\tau)\|_1 \leq 3 + \sum_{n=\lfloor\tau\rfloor+2}^{q} |\mathrm{sinc}\,(n-\tau)| + \sum_{n=-q}^{\lfloor\tau\rfloor-2} |\mathrm{sinc}\,(n-\tau)| \tag{112}$$

We can now upper bound the summands with

$$\begin{aligned}
\max_\tau \|s(\tau)\|_1 &\leq 3 + \frac{1}{\pi}\sum_{n=\lfloor\tau\rfloor+2}^{q} \left|\frac{1}{n-\tau}\right| + \frac{1}{\pi}\sum_{n=-q}^{\lfloor\tau\rfloor-2} \left|\frac{1}{n-\tau}\right| \\
&\leq 3 + \frac{1}{\pi}\sum_{n=-q+2}^{q} \left|\frac{1}{n+q}\right| + \frac{1}{\pi}\sum_{n=-q}^{q-2} \left|\frac{1}{n-q}\right| \\
&= 3 + \frac{2}{\pi}\sum_{n=2}^{2q} \frac{1}{n}.
\end{aligned} \tag{113}$$

Following that, we use right-Riemann sum approximation of an integral to upper bound the last term, finally getting

$$\begin{aligned}
\max_\tau \|s(\tau)\|_1 &\leq 3 + \frac{2}{\pi}\int_1^{2q} \frac{1}{x}\mathrm{d}x \\
&\leq 3 + \frac{2}{\pi}\log(2q)\,.
\end{aligned} \tag{114}$$

□

Now, if we were to estimate the amplitudes for integer queries sampling a Gaussian distribution, the variance on the interpolated quantity would be

Lemma 11. *Suppose one has $2q+1$ independent random variables $X_n \sim \mathcal{N}(\mu_n, \sigma_n^2)$, where $n \in \{-q, -q+1, \ldots, q\}$. One has that the interpolating quantity is the random variable*

$$X_{\text{interp}}(t) = \sum_{n=-q}^{q} \text{sinc}\,(t-n)\, X_n.$$

For such, the variance $\sigma^2(t)$ is calculated through

$$\sigma(t)^2 = s^T(t) C s(t)$$

where $C = \text{diag}(\sigma_{-q}^2, \sigma_{-q+1}^2, \ldots, \sigma_q^2)$ and $(s(t))_n = \text{sinc}\,(t-n)$ and it can be bounded through

$$\sigma(t)^2 \leq \left(3 + \frac{4}{\pi^2}\right) \max_n(\sigma_n^2).$$

Proof.

$$\begin{aligned} \sigma(t)^2 &= s^T(t) C_x s(t) \\ &= \|\sigma^2 s^2\|_1 \leq \|\sigma^2\|_\infty \|s^2\|_1 = \|\sigma^2\|_\infty \|s\|^2 \end{aligned} \tag{115}$$

$$\begin{aligned} \|s\|^2 &= \sum_{n=-q}^{q} |\text{sinc}\,(t-n)|^2 \\ &\leq \sum_{n=-\infty}^{\infty} |\text{sinc}\,(t-n)|^2 \\ &\leq \max_{\tau\in[-1,1]} \sum_{n=-\infty}^{\infty} |\text{sinc}\,(\tau-n)|^2 \\ &\leq \max_{\tau\in[-1,1]} \left(\text{sinc}^2(\tau) + 2\sum_{n=1}^{\infty} |\text{sinc}\,(n-\tau)|^2\right) \\ &\leq \max_{\tau\in[-1,1]} \left(\left(\text{sinc}^2(\tau) + 2\,\text{sinc}^2(\tau-1)\right) + \frac{2}{\pi^2}\sum_{n=2}^{\infty} \frac{1}{(n-\tau)^2}\right) \\ &\leq 3 + \frac{4}{\pi^2} \end{aligned} \tag{116}$$

□