Fourier-based quantum signal processing

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Implementing general functions of operators is a powerful tool in quantum computation. It can be used as the basis for a variety of quantum algorithms including matrix inversion, real and imaginary-time evolution, and matrix powers. Quantum signal processing is the state of the art for this aim, assuming that the operator to be transformed is given as a block of a unitary matrix acting on an enlarged Hilbert space. Here we present an algorithm for Hermitian-operator function design from an oracle given by the unitary evolution with respect to that operator at a fixed time. Our algorithm implements a Fourier approximation of the target function based on the iteration of a basic sequence of single-qubit gates, for which we prove the expressibility. In addition, we present an efficient classical algorithm for calculating its parameters from the Fourier series coefficients. Our algorithm uses only one qubit ancilla regardless the degree of the approximating series. This contrasts with previous proposals, which required an ancillary register of size growing with the expansion degree. Our methods are compatible with Trotterised Hamiltonian simulations schemes and hybrid digital-analog approaches.

I. INTRODUCTION

Quantum signal processing (QSP) was originally developed as a technique to design real-variable functions from single-qubit rotations [1]. It has attracted a lot of attention in the last few years after the discovery that it can be extended to realize also functions of operators, initially only for Hermitian operators [2, 3] and culminating in the general formalism of quantum singular value transformations (QSVT) [4, 5]. Using single-qubit rotations and having controlled black-box access to the operator to be transformed, QSVT provides a circuit structure and error control that reduces the problem of operator-function synthesis to that of real-variable function approximation, regardless the dimension of the underlying Hilbert space, the input operator, and the state on which the operator function is to be applied.

Basically, the \( N \)-qubits operator \( H \) is embedded in a unitary operator – the oracle – acting on an enlarged Hilbert space. A powerful model of oracle is the so called block-encoding oracle, which has the (necessarily normalized) non-unitary operator \( H \) as a block [3, 4]. The QSVT circuit applying an approximation to a target operator function \( f[H] \) is obtained by interspersing the action of the oracle with qubit rotations on an ancilla control. The particular sequence of qubit gates in each call to the oracle allows for certain achievable functions, and the specific rotation angles determine the final function implemented. In the case of block-encoding oracles, Chebyshev series approximations of the target function have been extensively studied. The (usually non-unitary) operator function is then obtained after post-selection on the control ancilla.

Several algorithms have been proposed using QSVT with block-encoding oracles for many different tasks such as Hamiltonian simulation [2], imaginary time evolution [6], matrix inversion [7], to give few examples [4]. Although very versatile and, in principle, possible to implement for any normalized operator (not necessarily a Hermitian or even square matrix), this kind of oracle requires a large number of ancillas, besides requiring for QSVT a further transformation called qubitization, which uses an extra ancilla and \( O(N) \) extra gates in each oracle call [3].

Here, we assume \( H \) to be Hermitian and explore an alternative type of oracle, namely the unitary evolution oracle, in which we have black-box access to the unitary \( e^{-iHt} \) with adjustable time \( t \). We apply the QSP ideas to implement operator functions via their truncated Fourier expansion. Previous algorithms were already proposed that use the time evolution given by a Hermitian operator to implement functions of that operator. Remarkable examples are the HHL algorithm for matrix inversion [8] (and subsequent improvements of it [9, 10]), and imaginary-time evolution for preparing thermal Gibbs states [11]. Other algorithms were also put forward for more general smooth functions of Hermitian operators [12, 13]. In common all these algorithms have the fact that they rely on the implementation of the unitary evolution operator for several values of time and use the technique of linear combination of unitaries [14, 15] to obtain a Fourier-like sum from it. It requires a number of ancillas that is logarithmic with the degree of the Fourier expansion. Our algorithm is a novel QSP variant that demands Hamiltonian simulation with a fixed time. It is superior to previous
Fourier-based approaches in that, remarkably, it makes use of only one ancillary qubit, which is the minimum number of qubits necessary to state-independently implement non-unitary operators. Moreover, this method does not require qubitization [3], which is a significant experimental simplification in view of intermediate scale implementations. The method formalizes and expands on a technique that we introduced in a summarized fashion in Ref. [6]. There, we applied it to the specific case of an exponential function.

Realizing the unitary $e^{-iH}$ – a problem known as Hamiltonian simulation – can be a hard task in itself. In fact, it is a BQP-complete problem [16]. Nevertheless, one may for instance apply product formulae [17–19] to implement the oracle with gate complexities that, for intermediate-scale systems, can be considerably smaller than for block-encoding oracles [6]. Furthermore, the real-time evolution oracle naturally arises in hybrid analogue-digital platforms [20–22], for which QSP schemes have already been studied [23].

The basic sequence of single-qubit gates we use to assemble the Fourier series has been proposed in a previous work [24] in the context of single-qubit variational circuits for approximating real-variable functions. Here, we formally prove that this sequence is able to implement any normalized Fourier series of a real variable. Part of the proof is a generalization of the results in Ref. [25], removing the restriction over the series parity. Moreover, we provide an efficient classical algorithm to analytically calculate the rotation angles from the target series. This removes the need for optimizing a large number of parameters present in Ref. [24], a task that becomes impractical as the number of rotation angles grows with the order of the series. This single-qubit construction is the basis of our operator-valued function algorithm. The complexity of the algorithm is dominated by the truncation order of the Fourier series and by the probability of success – the correct operator-function is obtained after post-selecting the state of the ancilla register. On one hand, standard Fourier series present convergence issues for approximating non-periodic functions – the so-called Gibbs phenomenon. On the other hand, methods used to improve the convergence rate might incur in a reduction of the success probability. Here, we compare two techniques for obtaining Fourier series of non-periodic functions. The first was introduced in Ref. [12], which obtains the Fourier series from a power series of the target function. The second is an analytical extension of the target function [26]. While the former provides an analytical bound for the error of the approximation, the latter has the advantage of avoiding a decrease of the success probability.

The paper is organized as follows: in Sec. II we give some preliminary definitions and formally establish the problem we will tackle. In Sec. III we present our results, starting with the construction for real-variable function approximation using qubit rotations in Sec. III A, which is extended to operator function design in Sec. III B. In Secs. III C and III D we discuss two alternatives for obtaining Fourier approximations of non-periodic functions and compare them for the case of imaginary-time evolution. The proofs of the theorems and lemmas are left to Sec. IV. Finally, we discuss our results in Sec. V.

II. PRELIMINARIES

From calls to a block-encoding oracle for a multi-qubit Hermitian operator $H$, QSP yields an operator which has the same eigenvectors as $H$, but eigenvalues transformed by a polynomial function. This requires the use of qubit ancilllas on which a sequence of rotations is applied. The basic QSP circuit has the oracle as an input and the function being realized solely depends on the values of the parameters for the ancilla rotations. The achievable functions can be determined by analysing an $SU(2)$ operator as a function of a single real variable. By using the ancillary system to control the action of the operator oracle, it is possible to promote a real-variable function $f$ to an operator function $f[H]$ by applying $f$ to each eigenvalue of $H$. QSVT generalizes this procedure to include non-Hermitian operators $H$. In this case, eigenvalues and eigenvectors should be substituted by singular values and singular vectors.

We consider an $N$-qubit system $S$, with Hilbert space $\mathbb{H}_S$. A Hamiltonian operator $H$ on $\mathbb{H}_S$ with eigenvalues $\lambda \in [\lambda_{\min}, \lambda_{\max}]$ is given by a unitary oracle $O$. For simplicity, we assume $\lambda_{\min} \geq -1$ and $\lambda_{\max} \leq 1$, such that $\|H\| \leq 1$. Contrary to other oracle types, for which the normalization is mandatory [3], here it is merely a convenience. Our goal is to approximately implement an operator function $f[H] = \sum_{\lambda} f(\lambda) |\lambda\rangle\langle \lambda|$ on $\mathbb{H}_S$ from calls to $O$, where $f : \mathbb{R} \to \mathbb{C}$ and $|\lambda\rangle$ is the eigenvector of $H$ corresponding to eigenvalue $\lambda$. In general, $f[H]$ is not unitary and its implementation via a unitary circuit is achieved by enlarging the Hilbert space to include an ancillary register $\mathcal{A}$, whose Hilbert space we denote by $\mathbb{H}_\mathcal{A}$. We denote by $\mathbb{H}_{S,\mathcal{A}} := \mathbb{H}_S \otimes \mathbb{H}_\mathcal{A}$ the joint Hilbert space of $S$ and $\mathcal{A}$, and by $\|\mathcal{A}\|$ the spectral norm of an operator $\mathcal{A}$. The oracle model that we consider is formally defined below. It encodes $H$ through the real-time unitary evolution it generates for a
fixed but tunable time value.

**Definition 1.** (Real-time evolution Hamiltonian oracle). We refer as a real-time evolution oracle for a Hamiltonian $H$ on $\mathbb{H}_S$ at a time $t \in \mathbb{R}$ to a controlled-$e^{-itH}$ gate $O = 1 \otimes |0\rangle \langle 0| + e^{-itH} \otimes |1\rangle \langle 1|$ on $\mathbb{H}_{SA}$.

The target operator function is obtained via post-selection on the ancilla state after applying a unitary operator $U_{f[H]}$ on $\mathbb{H}_{SA}$ that encodes $f[H]$ in one of its matrix blocks [3, 4, 13]. $U_{f[H]}$ is called a block-encoding of $f[H]$, as defined below for a general operator $A$ on $\mathbb{H}_S$ [6]:

**Definition 2.** (Block encodings). For sub-normalization $0 \leq \alpha \leq 1$ and tolerated error $\varepsilon > 0$, a unitary operator $U_A$ on $\mathbb{H}_{SA}$ is an $(\varepsilon, \alpha)$-block-encoding of a linear operator $A$ on $\mathbb{H}_S$ if $\|\alpha A - |0\rangle \langle 0| A |0\rangle \langle 0|\| \leq \varepsilon$, for some $0 \in \mathbb{H}_A$. For $\varepsilon = 0$ and $(\varepsilon, \alpha) = (0, 1)$ we use the short-hand terms perfect $\alpha$-block-encoding and perfect block-encoding, respectively.

The need for a subnormalization comes from the unitarity of $U_A$, whose blocks must therefore necessarily have spectral norm below unit. If the system and the ancilla are prepared in the joint state $|\Psi\rangle |0\rangle$, then the target operator $A$ on $\mathbb{H}_S$ is obtained after measuring the ancilla whenever its state is projected onto $|0\rangle$ successfully. This happens with a success probability given by $P_0(\alpha A) = \|\alpha A |\Psi\rangle\|^2$. Therefore, the larger the subnormalization, the best for the algorithm, since it will have a higher probability of getting a successful run.

In the usual QSP method, the target function $f(\lambda)$ is approximated by a finite-order power series $f(\lambda)$ such that $|f(\lambda) - f(\lambda)| \leq \varepsilon$ for all $\lambda \in \lambda_{\min}, \lambda_{\max}$. This ensures that the operator-function spectral-norm error is bounded by the same $\varepsilon$. Similarly, here we use a truncated Fourier series to approximate the target function. The standard measure of complexity used in oracle based algorithms is the number of calls to the oracle needed to implement an approximation of $f[H]$ up to spectral error $\varepsilon$, which we denote by $g_f(\varepsilon)$. As we show later, $q_f(\varepsilon)$ equals double the truncation order of the approximating series. In the next section, we show how it is possible to generate an arbitrary Fourier series from single-qubit rotations. The exact same construction can be used to implement functions at the level of the eigenvalues of an operator encoded in the oracle of Def. 1. This is due to the fact that each eigenvalue $\lambda$ of $H$ is naturally attributed a two-dimensional subspace spanned by $\{|\lambda\rangle |0\rangle, |\lambda\rangle |1\rangle\}$.

### III. RESULTS

#### A. Single-qubit rotation synthesis of Fourier series

Consider a Fourier series $\tilde{g}_q(x) = \sum_{m=-q/2}^{q/2} c_m e^{imx}$ such that $|g(x) - \tilde{g}_q(x)| \leq \varepsilon_0$ for all $x \in [-\pi, \pi]$, where $g : \mathbb{R} \to \mathbb{C}$ is such that $|g(x)| \leq 1$ on the interval $[-\pi, \pi]$. The function $g$ will serve to approximate the target $f$ in a reduced interval as to avoid the so called Gibbs phenomenon, as we explain later. For now, the important thing is that we would like to build a unitary single-qubit operator

$$U_{\tilde{g}_q h_q}(x) = \begin{pmatrix} \tilde{g}_q(x) & h_q(x) \\ -h_q^*(x) & \tilde{g}_q^*(x) \end{pmatrix}$$

having $\tilde{g}_q(x)$ as one of its entries with an arbitrary Fourier series $h_q(x)$ of order $q/2$ as the complementary entry. The operator should be obtained by repeatedly applying a basic gate $R(x, \xi)$ with the variable $x$ as input, such that, for a convenient choice of parameters $\xi_k$, $U_{\tilde{g}_q h_q}(x) = \prod_{k=0}^{q/2} R(x, \xi_k)$ for any $x \in [-\pi, \pi]$ given as input.

Inspired by a construction in Ref. [24], here we consider the basic single-qubit gate $R(x, \omega, \xi) = e^{i\xi Z} e^{-i\omega Y} e^{\frac{i}{2q} \sum_{k=0}^{q-1} \omega k \xi}$, which has five adjustable parameters $\{\omega, \xi\} \in \mathbb{R}^5$, where $\xi := \{\zeta, \eta, \zeta, \kappa\}$. $X$, $Y$ and $Z$ are the Pauli operators. The input variable $x \in \mathbb{R}$ is the signal to be processed and $e^{i\omega x Z}$ is called iterate. In Ref. [24], it was observed that the gate sequence $R(x, \omega, \Phi) := \prod_{k=0}^{q/2} R(x, \omega_k, \xi_k)$, with $\omega := \{\omega_0, \cdots, \omega_q\} \in \mathbb{R}^{q+1}$ and $\Phi := \{\xi_0, \cdots, \xi_q\} \in \mathbb{R}^{4(q+1)}$, can encode certain finite Fourier series into its matrix components. There, the authors numerically find the sequence of pulses for some examples of real functions. However, they do not prove the existence of a complementary Fourier series $h_q(x)$, nor provide an analytical mean of calculating the pulses, relying on numerical optimizations of the rotation parameters and thus limiting the order of the actual implementable series. Here, not only do we formally prove that $U_{\tilde{g}_q h_q}(x) = R(x, \omega, \Phi)$ can encode any target series but also we provide an explicit, efficient recipe for finding the adequate choice of pulses $\Phi$. This is the content of the following theorem, whose proof can be found in Sec. IV A. A circuit representation of $R(x, \omega, \Phi)$ can be found in Fig. 1.a.

**Theorem 1.** [Single-qubit Fourier series synthesis] Given $\tilde{g}_q(x) = \sum_{m=-q/2}^{q/2} c_m e^{imx}$, with $q \in \mathbb{N}$ even, there exist $\omega$ and $\Phi$ such that $\langle 0 | R(x, \omega, \Phi) | 0 \rangle = \tilde{g}_q(x)$ for all $|x| \leq \pi$
iff \( |\hat{g}_q(x)| \leq 1 \) for all \( |x| \leq \pi \). Moreover, \( \omega \) can be taken such that \( \omega_\ell = 0 \) and \( \omega_k = (-1)^k/2 \), for all \( 1 \leq k \leq q \), and \( \Phi \) can be calculated classically from \( \{c_m\}_m \) in time \( O(poly(q)) \).

The power of Theo. 1 relies on that it allows for the implementation of any complex Fourier series, assuming only that it is properly normalized. Moreover, as is usual in QSP, the number of pulses is determined solely by the order of the implemented series. Now, as a Fourier series can be used to approximate any complex function \( g(x) \) on a finite interval, we have a way to approximately obtain any complex function from qubit rotations. Moreover, the error of the approximat is exactly the error made in the series approximation, that is \( \epsilon = \max_{x \in [-\pi, \pi]} |g(x) - \hat{g}_q(x)| \). Notice that if it is guaranteed that \( |g(x)| \leq 1 \), then at most \( \hat{g}_q(x)/(1 + \epsilon) \) satisfies Theo. 1 with error of at most \( 2\epsilon \).

The proof presented in Sec. IV A follows a similar strategy to that of Refs. [25, 27]. The first step is to prove the existence of \( \hat{h}_q(x) \), which leads to a method to obtain it from the coefficients of \( \hat{g}_q(x) \). It is easy to see that a unitary operator can always be built from \( \hat{g}_q(x) \) by taking \( \hat{h}_q(x) = \sqrt{1 - |\hat{g}_q(x)|^2} \). However, this choice is not unique and it is not obvious that \( \hat{h}_q(x) \) could also be chosen as a Fourier series with the same order as \( \hat{g}_q(x) \), neither it is obvious how to obtain this complement. The next step is to show that indeed the sequence of pulses produce all the frequencies of the Fourier series. Finally, this two elements are combined in a constructive method to show that \( U \) in Eq. (1) can be obtained as the sequence of gates \( R(x, \omega, \Phi) \). It directly furnishes a way to calculate \( \Phi \) from \( \hat{g}_q(x) \).

### B. Operator function design

Here, we elaborate on the technique introduced in Sec. V-C of Ref. [6]. We synthesize an \((\varepsilon, \alpha)\)-block-encoding of \( f[H] \) from an oracle for \( H \) as in Def. 1. We build a circuit \( C \) generating a perfect block-encoding \( V_\Phi \) of a target Fourier expansion \( \hat{g}_t[Ht] := \sum_{m=-q/2}^{q/2} c_m e^{imHt} \) that \( \varepsilon \)-approximates \( \alpha f[H] \), for some \( 0 < \varepsilon < 1, \alpha \leq 1, \) and a suitable \( t > 0 \). This is done by adjusting \( \Phi \) according to Theorem 1. Similarly, an algorithm for Fourier synthesis could be devised from the basic single-qubit gate \( R(x, \phi) = e^{i\phi x} e^{i\phi Z} \), the usual pulse sequence used in QSP [1]. However, it would require one extra qubit ancilla and decrease the subnormalization by half (meaning a decrement of the success probability by 1/4), as we show in App. A.

The function \( \hat{g}_q \) is taken as a Fourier approximation of an intermediary function \( g \) such that \( |g(x) - \hat{g}_q(x)| \leq \varepsilon_0 \) \( \forall x \in [-\pi, \pi], \) and \( |g(x) - \alpha f(\lambda)| \leq \varepsilon_1 \) for all \( x \lambda := \lambda t \in [-x_0, x_0], \) with \( x_0 \leq \pi \) and \( \varepsilon_0 + \varepsilon_1 \leq \varepsilon. \) Since we are interested in approximating \( f(\lambda) \) for all \( \lambda \in [-1, 1], \) we can take \( t = x_0 \) so that \( x_\lambda = \lambda t \) is in \([ -x_0, x_0] \) for all the eigenvalues of \( H \). The function \( g \) is, up to \( \varepsilon_1 \)-approximation, a periodic extension of \( f \). The reason for this intermediary step here is to circumvent the well-known Gibbs phenomenon, by virtue of which convergence of a Fourier expansion cannot in general be guaranteed at the boundaries. In turn, the sub-normalization factor \( \alpha \) might take a value strictly smaller than \( 1 \) even if \( |f(\lambda)| \leq 1 \) in \([-1, 1], \) because our \( \hat{g}_q \) converges to \( \alpha f \) only for \( |x_\lambda| \leq x_0, \) whereas Theorem 1 requires that \( |\hat{g}_q(x_\lambda)| \leq 1 \) for all \( |x_\lambda| \leq \pi. \) This forces one to sub-normalize the expansion so as to guarantee normalization over the entire domain. (The inoffensive sub-normalization factor \((1 + \varepsilon)^{-1} \) is neglected.)

Next, we explicitly show how to generate \( V_\Phi \). We define \( V_\Phi := \left(V_{\xi_1} V_{\xi_2} \ldots V_{\xi_4} W_{in}\right) \), where the basic QSP blocks are given as

\[
V_{\xi_k} := \left[\mathbb{1} \otimes \left(e^{i\zeta_k + \eta_k Z} e^{-i\varphi_k Y} e^{i\phi_z - \eta_k Z}\right)\right] O \left[\mathbb{1} \otimes e^{-i\xi_k Y}\right]
\]

(2a)

and

\[
V_{\xi_k} := \left[\mathbb{1} \otimes \left(e^{i\zeta_k + \eta_k Z} e^{-i\varphi_k Y} e^{i\phi_z - \eta_k Z}\right)\right] O^\dagger \left[\mathbb{1} \otimes e^{-i\xi_k Y}\right],
\]

(2b)

with \( \xi_k := \{\zeta_k, \eta_k, \varphi_k, \phi_k\} \). \( V_{\xi_k} \) and \( V_{\xi_k} \) play a similar role to \( R(x, \omega, \xi_k) \) in Sec. III A. The iterate is taken as the oracle: \( O = \mathbb{1} \otimes |0\rangle \langle 0| + e^{-iHt} \otimes |1\rangle \langle 1| \) (with \( x_\lambda \) inside \( O \) playing the role of \( x \) in Sec. III A for each \( \lambda \)). Notice that \( O \) readily acts as an \( SU(2) \) rotation on each 2-dimensional subspace \( \{\langle \lambda|0\rangle, \langle \lambda|1\rangle\} \). Here, qubitization [3] is not required. We take

\[
W_{in} = \mathbb{1} \otimes \left[e^{i\phi_z + \alpha Z} e^{-i\phi Y} e^{i\phi_z - \alpha Z} e^{-i\phi Y}\right].
\]

(3)

The following pseudocode summarizes the entire procedure to implement \( V_\Phi \).
Figure 1. Circuit for generic operator-function design.
(a) Single-qubit circuit implementing the unitary transformation $\mathcal{R}(x)$ which contains $\tilde{g}_q(x)$ as a block. Here we use the short-hand notation $R_k(x) := R(x, \omega_k, \xi_k)$. b) The circuit $C$ from Alg. 1 uses the register $A$ as an ancilla. If the ancilla is initialised and post-selected in $|0\rangle$, the circuit prepares the system state $|\Psi\rangle$. The detailed components of $C$ are shown in part c). $W_m$ is the basic blocks $V_{\xi_k}$ in panel b) represent the gates $V_{\xi_k}$ in c). Each $V_{\xi_k}$ involves one query to the oracle $O$. $V_k$ is defined as $V_k$ but with $O^+$ substituting $O$. Hence, the query complexity of $C$ is $q$. The approximating function $\tilde{g}_q$ is determined by the rotation angles $\Phi = \{\xi_0, \cdots, \xi_q\}$. $R_m(\phi)$ with $\alpha = x, y, z$ denotes a rotation in the $\alpha$ direction and $R_m(\xi_k) := R_x(\xi_k + \eta_k) R_y(2\varphi_k) R_z(\zeta_k + \eta_k)$, with $\xi_k = \{\zeta_k, \eta_k, \varphi_k, \xi_k\}$. These angles are chosen such that $\tilde{g}_q$ is a high-precision Fourier approximation of $f$ in the interval $[-1, 1]$.

Algorithm 1: Operator-valued Fourier series from real-time evolution Hamiltonian oracles

**input:** Fourier coefficients $c := \{c_m\}_{|m| \leq q/2}$, oracle $O$ for $H$ at a time $t = x_0$, and its inverse $O^+$.

**output:** unitary quantum circuit $C$.

1. calculate the rotation angles $\Phi$ (Sec. IV A);
2. begin construction of $C$;
3. \hspace{1em} apply $W_m$ from Eq. (3) on $A$;
4. \hspace{1em} for $k = 1$ to $k = q$ do
5. \hspace{2em} if $k$ is odd then apply $V_{\xi_k}$ from Eq. (2a);
6. \hspace{2em} else apply $V_{\xi_k}$ from Eq. (2b);
7. end
8. end

For each eigenvalue $\lambda$ of $H$, the operator $V_\Phi$ realizes the rotation operator $\mathcal{R}(x, \lambda, \omega, \Phi)$ on the ancillary register $A$, as in Theorem 1. Therefore, the choice of $\Phi$ allows us to block-encode any normalized Fourier series of $H$. This is the content of the next theorem. The circuit realizing $V_\Phi$ is depicted in Figs. 1.b) and 1.c).

**Theorem 2.** (Operator-valued Fourier series from real-time evolution oracles) Let $\tilde{g}_q : [-\pi, \pi] \rightarrow \mathbb{C}$, with $\tilde{g}_q(x) = \sum_{m=-q/2}^{q/2} c_m e^{i m x}$, be such that $|\tilde{g}_q(x)| \leq 1$ for all $x \in [-\pi, \pi]$. Then there is a pulse sequence $\Phi = \{\xi_0, \cdots, \xi_q\} \in \mathbb{R}^{4q+1}$, with $\xi_k = \{\zeta_k, \eta_k, \varphi_k, \xi_k\}$, such that the operator $V_\Phi$ on $\mathbb{H}_{SA}$ implemented by Alg. 1 is a perfect block-encoding of $\tilde{g}_q[H\lambda]$, i.e.

$$\langle 0|V_\Phi|0 \rangle = \sum_{\lambda} \tilde{g}_q(x, \lambda) \langle \lambda | \lambda \rangle,$$  \hspace{1em} (4)

with $x = \lambda t$. Moreover, the pulse sequence can be obtained classically in time $O(poly(q))$.

Let us further discuss the convergence of $\tilde{g}_q$. When $g$ is a periodic function with period $2\pi$, with a finite number of jump discontinuities, the standard partial Fourier series $\tilde{g}_q(x) = \sum_{m=-q/2}^{q/2} c_m e^{i m x}$ with $c_m = 1/\pi \int_{-\pi}^{\pi} g(x) e^{-i m x} dx$ converges to $g(x)$ when $g$ goes to infinity for all $x$ except for the discontinuities, where the series converges to the average value of the function at both sides of the discontinuity. Besides, the convergence close to the discontinuities is slow due to the so-called Gibbs phenomenon. If $g$ is obtained by the simple periodic repetition of the values taken by $f$ – usually a non-periodic continuous function – inside the interval $[-\pi, \pi]$, then the borders of that interval present jump discontinuities. In that case, $\tilde{g}_q(x)$ is a good approximation for $g(x)$ only in the sense that, given $\varepsilon > 0$ and $\delta \in (0, \pi)$, there is a large enough truncation order $q/2$ such that $|g(x) - \tilde{g}_q(x)| \leq \varepsilon$ for all $x \in [-\pi + \delta, \pi - \delta]$. Moreover, this approach does not have a closed expression relating the error to $\delta$ and to the truncation order $q/2$, and a case-by-case analysis is required. This discussion justifies taking $g$ as equal to $\alpha f$ in a limited interval, as $f$ in general is not periodic. Outside $[-x_0, x_0]$, $g$ can take any values, provided it remains normalized and continuous. For instance, one could define $g$ as the periodic repetition of the continuous function $h : \mathbb{R} \rightarrow \mathbb{C}$ defined as

$$h(x) = \begin{cases} h_1(x) & x \in [-\pi, -x_0] \\ \alpha f(x/t) & x \in [-x_0, 0] \\ h_2(x) & x \in [0, \pi] \\ \end{cases}$$  \hspace{1em} (5)
with $h_1$ and $h_2$ any continuous functions satisfying $h_2(\pi) = h_1(-\pi)$, $h_1(-x_0) = \alpha f(-x_0/t)$, and $h_2(x_0) = \alpha f(-x_0/t)$, such that $g$ itself is continuous. Nevertheless, in this case, possibly the first derivative of $g(x)$ in $x = -x_0$ and $x = x_0$ would present jump discontinuities, compromising the convergence of $\tilde{g}_q$.

In what follows, we present two ways of obtaining a Fourier series that approximates the target function. The first one does not use the standard Fourier integral to obtain the series coefficients, while the second method uses a filter to produce an analytical function $g$. While the first method has the advantage of providing analytical bounds for the complexity $q$ as a function of the error $\varepsilon$, the second one is classically much less expensive.

### C. Bounded-error Fourier series

Consider that a power series $\hat{f}_L(\lambda) = \sum_{l=0}^{L} a_l \lambda^l$ is given such that $|f(\lambda) - \hat{f}_L(\lambda)| \leq \varepsilon/(4\alpha)$ for all $\lambda \in [-1, 1]$. For the method presented in this section we do not need to specify $g$ outside the interval $[-x_0, x_0]$ and we take $\varepsilon_1 = 0$, such that

$$g(x) - \alpha \sum_{l=0}^{L} a_l \lambda^l \lambda^l \leq \varepsilon/4,$$

for all $x \in [-x_0, x_0]$ with $t = x_0$. We employ a construction from Ref. [12] that, given $0 < \delta < \pi/2$, $\alpha \hat{f}_L(\lambda)$, and

$$q \geq \frac{2\pi}{\delta} \ln \left( \frac{4}{\varepsilon} \right)$$

yields $c = \{c_m\}_{|m| \leq q/2}$ such that $g \varepsilon$-approximates $g$ for all $x \in [-x_0, x_0]$ with $x_0 = \pi/2 - \delta$. The important features of this construction are given in a slightly modified version of Lemma 37 of Ref. [12]:

**Lemma 3.** (Lemma 37 of Ref. [12]) Let $\delta \in (0, \pi/2)$, $\varepsilon \in (0, 1)$, and $g : \mathbb{R} \to \mathbb{C}$ be such that

$$|g(x) - \sum_{l=0}^{L} q_l \left( \frac{\pi}{2} x \right)^l | \leq \varepsilon/4 \text{ for all } x \in \left[ -\frac{\pi}{2} + \delta, \frac{\pi}{2} - \delta \right].$$

Then $\exists c \in \mathbb{C}^{q+1}$ such that

$$|g(x) - \tilde{g}_q(x)| \leq \varepsilon$$

for all $x \in \left[ -\frac{\pi}{2} + \delta, \frac{\pi}{2} - \delta \right]$, where $\tilde{g}_q(x) = \sum_{m=-q/2}^{q/2} c_m e^{imx}$, $q = \max \left[ \frac{2\pi}{\delta} \ln \left( \frac{4||d||_1}{\varepsilon} \right) \right]$, 0, and $||c||_1 \leq ||d||_1$. Moreover, $c$ can be efficiently calculated on a classical computer in time $\text{poly}(L, q, \log(1/\varepsilon))$.

For $f$ analytical, one can obtain the power series of $g$ from a truncated Taylor series of $f$ using that $g(x) = \alpha f(\lambda)$. The truncation order $L$ can be obtained from the remainder:

$$\frac{\varepsilon}{4} \leq \max_{\lambda \in [-1, 1]} |\alpha f(\lambda)|.$$  \hspace{1cm} (9)

In addition, we may bound the sub-normalization constant $\alpha$ in terms of the Taylor coefficients $a := \{a_l\}_{0 \leq l \leq L}$ of $f$ as follows. Lemma 3 can be applied to build a Fourier series for $g(\lambda)$, identifying $d_l = \alpha a_l/(2t/\pi)^l = \alpha a_l/(1 - \frac{2\delta}{\pi})^l$ since $t = x_0 = \pi/2 - \delta$. The expansion $\tilde{g}_q(x)$ converging to the target function only in $[-\pi/2 + \delta, \pi/2 - \delta]$, although the period of $\tilde{g}_q$ is still $2\pi$. To implement $\tilde{g}_q$ using Theorem 2, we need to chose $\alpha$ as to guarantee the normalization $|\tilde{g}_q(x)| \leq 1$ in the whole interval $[-\pi, \pi]$. For that, notice that $|\tilde{g}_q(x)| = \left| \sum_{m=-q/2}^{q/2} c_m e^{imx} \right| \leq \sum_{m=-q/2}^{q/2} |c_m| = ||c||_1$ for all $x \in [-\pi, \pi]$. On the other hand, according to Lemma 3, the vector of coefficients satisfies $||c||_1 \leq ||d||_1$, ensuring that $|\tilde{g}_q(x)| \leq 1$ is attained in the whole interval $[-\pi, \pi]$ if $||d||_1 = \sum_{l=0}^{L} |d_l| = \alpha \sum_{l=0}^{L} |a_l/(1 - \frac{2\delta}{\pi})^l| \leq 1$. Therefore, it suffices to take $\alpha$ such that

$$\sum_{l=0}^{L} |a_l/(1 - 2\delta/\pi)|^l \leq \alpha^{-1}.$$  \hspace{1cm} (10)

Note that $L$ and $\alpha$ are inter-dependent. One way to determine them is to increase $L$ and iteratively adapt $\alpha$ until Eqs. (9) and (10) are both satisfied. Alternatively, if the expansion converges sufficiently fast (e.g., if $\lim_{L \to \infty} |a_{L+1}| < 1 - \frac{2\delta}{\pi}$), one can simply substitute $L$ in Eq. (10) by $\infty$, simplifying the analysis. Finally, the obtained $c$ can be input to Alg. 1 in order to produce the desired operator function.

We experimented applying Lemma 3 in the context of imaginary-time evolution [6]. The desired function to be implemented there is $f(\lambda) = e^{-\beta(\lambda+1)}$, where $\beta$ is the inverse temperature. While Lemma 3 does indeed provide a theoretically efficient recipe to obtain a Fourier-series approximation, and it also guarantees a controlled approximation error, it proved prohibitively time consuming to evaluate said coefficients numerically. This happens due to the $1/\delta$ dependence in the expansion order of the desired series - actually, the number of operations to obtain the coefficients from Lemma 3 scales as $O(1/\delta^3)$. In essence, we want $\delta$ to be small so that the parameter $\alpha^{-1}$ in Eq. (10) is also small, which will have implication in the success probability of the block-encoding implementation. For imaginary-time evolu-
tion, we [6] obtain $\delta = O(1/\beta)$ for large $\beta$, as the $\delta$ that optimizes the overall number of calls to the oracle, so that the truncation order will increase linearly with $\beta$ and the computational complexity as $O(\beta^3)$. Since one is usually interested in the low temperature regime, the construction turned out to be too expensive for large $\beta$. An alternative to this construction is provided below.

D. Analytic-extension Fourier series

It is known [28] that the Fourier series of an analytical, periodic function converges exponentially fast, i.e., the error $\varepsilon$ made in the approximation goes asymptotically as $\varepsilon = \varepsilon \text{[1]}$, $c = 0$, where $q$ is the truncation order. Our goal is to obtain a periodic extension of $f$ which is analytic in the whole interval $[-\pi, \pi]$. The advantage of this method is that there will be no unnecessary sub-normalization. This would correspond to $\delta = 0$ in Lemma 3, which is only possible there if we consider the exact, infinite series. For simplicity, we consider $t = 1$ such that $x_\lambda = \lambda t = \lambda$ and, in a slight abuse of notation, we use the variable $\lambda$ everywhere, even outside the interval $[-1, 1]$ of eigenvalues of $H$. Suppose $f(\lambda)$ is analytic for $\lambda \in [-\pi, \pi]$ and $|f(\lambda)| \leq 1$ for $\lambda \in [-1, 1]$, then the function $g(\lambda) := \tilde{g}(\lambda, L, \chi) = f(\lambda)b(\lambda, L, \chi)$, with

$$b(\lambda, L, \chi) = \frac{erf[L(\lambda + \chi)] - erf[L(\lambda - \chi)]}{2},$$

where $erf$ is the error function, $1 < \chi < \pi$, is an approximate, analytic [26] extension of $f$ in the interval $\lambda \in [-\pi, \pi]$. Before we make this statement more precise, note that in the limit of $L \to \infty$, $b(x, L, \chi)$ is a perfect step function which equals 1 in the interval $[-\chi, \chi]$ and zero otherwise. For a finite $L$, $b(\lambda, L, \chi)$ will then be a smooth step function and therefore, $g(\lambda)$ will only approximate $f(\lambda)$ over $[-\chi, \chi]$. By bounding Eq. (11) one can see that

$$|f(\lambda) - g(\lambda)| < \frac{1}{2}erf[L(\lambda + \chi)] - 1$$

$$< \frac{1}{2}erfc[L(\lambda - 1)]$$

$$< \frac{1}{2}e^{-L^{2}(\chi-1)^{2}},$$

for all $\lambda \in [-1, 1]$, where $erfc$ is the complementary error function. Thus, if we take

$$L_\epsilon \geq \frac{1}{\chi-1}\sqrt{\ln \left(\frac{3}{2\varepsilon}\right)},$$

it is guaranteed that

$$|f(\lambda) - g(\lambda)| < \varepsilon \frac{3}{3}.$$  

Moreover, because $g(\lambda) \to 0$ for $\lambda \to \pm \pi$, the periodic extension of $g$ with period $2\pi$ has no jump discontinuities.

From Eq. (13), we see that for $\chi \to 1$, one would need

![Figure 2. Comparison among different Fourier approximations for the real exponential function.](image)
\( L \to \infty \) to satisfy the error bound in Eq. (14) – in fact, in that case, with \( \varepsilon = 0 \). This happens because, although in the open interval \((-1,1)\) error \( \varepsilon = 0 \) can be obtained, at the boundaries we have \( b(\pm \chi, L, \chi) \approx 1/2 \). To fix this, we consider \( \chi \) such that \([-1,1] \in (-\chi, \chi)\). Also, because \( g \) must be bounded by one – up to given error – in the closed interval \([-1,1]\), we fix \( \chi = \chi_\varepsilon \) through the equation

\[
\max_{\lambda \in [-\chi, \chi]} |f(\lambda)| = 1 + \varepsilon/3. \tag{15}
\]

Here we are assuming that the filter \( b(\lambda, L, \chi) \) decays faster than \( f \) for \( |\lambda| > \chi \). One can see, with an analysis similar to (12), that this would hold as long as \( f \) does not grow faster than \( L(|\lambda| - \chi)e^{L^2(|\lambda| - \chi)^2} \) for \( |\lambda| > \chi \). In the end, we implement the truncated standard Fourier expansion of the function \( g(\lambda) = \tilde{g}(\lambda, L, \chi) \) with the guarantee of exponential convergence. Say that \( \tilde{g}_q \) is such an expansion with error \( \varepsilon_0 = \varepsilon/3 \), i.e., \( |\tilde{g}_q(\lambda) - g(\lambda)| \leq \varepsilon/3 \) for \( \lambda \in [-1,1] \). If we take \( L_\varepsilon \) as in Eq. (13) and \( x \) as in Eq. (15), we have

\[
|\tilde{g}_q(\lambda) - f(\lambda)| < \varepsilon, \tag{16}
\]

and just an insignificant sub-normalization factor over the whole interval, i.e., \( |\tilde{g}_q(\lambda)| \leq 1 + \varepsilon, \forall \lambda \in [-\pi, \pi] \).

The downside of this method is that we do not provide an algorithm to compute the coefficients of the series \( \tilde{g}_q(\lambda) \), nor do we provide an analytical way to obtain the truncation order \( q \) as a function of the desired error \( \varepsilon \). At first sight this might seem to invalidate the whole construction. However, as was already mentioned, this method came about precisely because Lemma 3 becomes infeasible for small \( \delta \). Even having to evaluate the Fourier coefficients explicitly from its integral definition, and having to brute-force search the truncation order \( q \), this construction turned out to outperform the previous one in terms of classical computation time for the particular studied case of the exponential function. Since one of the most important metrics of oracle-based methods is the number of queries to the oracle, which here is the truncation order of the series used to approximate the desired function, a natural comparison to make between this method and the one presented in Lemma 3 is the truncation order necessary to achieve the same error guarantee. In Fig. 2 we can see how the methods compare to each other in this aspect. Note that for Lemma 3 we can only use the upper-bound since the construction of the series for large \( \beta \) was too expensive to be carried out, let alone construct many of them in order to binary search [29] the minimum truncation order that would guarantee the desired error. In Fig. 2 one can also see the comparison with a non-analytic extension as well.

IV. PROOFS OF THEOREMS

A. Real-variable function design: Proof of Theorem 1 and classical algorithm for pulse angles

Before proceeding with the proof of Theo. 1, we state and prove a lemma that provides an algorithm to find a unitary operator that has the target Fourier series \( \tilde{g}_q(x) \) as one of its entry. This also generalizes the results in Ref. [25] in the sense of removing the parity constraint required there.

**Lemma 4.** [Complementary Fourier series] Given \( \tilde{g}_q(x) = \sum_{m=-q/2}^{q/2} c_m e^{im\pi x}, q \in \mathbb{N} \) even, satisfying \(|\tilde{g}_q(x)| \leq 1\) for all \(|x| \leq \pi\), there is a Fourier series \( \tilde{h}_q(x) = \sum_{m=-q/2}^{q/2} b_m e^{im\pi x} \) (with the same order \( q/2 \)), such that

\[
U_{\tilde{g}_q \tilde{h}_q}(x) = \begin{pmatrix} \tilde{g}_q(x) & \tilde{h}_q(x) \\ -\tilde{h}_q^*(x) & \tilde{g}_q^*(x) \end{pmatrix} \tag{17}
\]

is an SU(2) operator. Moreover, the coefficients \( \{b_m\}_m \) can be calculated classically in time \( \mathcal{O}(\text{poly}(q)) \).

**Proof.** In order to \( U_{\tilde{g}_q \tilde{h}_q}(x) \) be unitary, its entries must satisfy

\[
|\tilde{g}_q(x)|^2 + |\tilde{h}_q(x)|^2 = 1 \quad \forall x \in \mathbb{R}. \tag{18}
\]

Let us define the Laurent polynomial \( G(z) = \sum_{k=-q}^{q} a_k z^k \) such that for \( z \in U(1) \) we have \( G(z) = e^{i\pi x} = 1 - |\tilde{g}_q(x)|^2 \). The coefficients of \( G(z) \) can be obtained as

\[
a_k = \begin{cases} 
-\sum_{l=-q/2}^{q/2} e^{i|l|^2}, & k > 0 \\
1 - \sum_{l=-q/2}^{q/2} |c_l|^2, & k = 0 \\
-\sum_{l=-q/2}^{q/2} e^{i|l|^2}, & k < 0
\end{cases} \tag{19}
\]

\( G(z) \) is such that, if the aimed \( \tilde{h}_q(x) \) does exist, then for \( z \in U(1) \) we have \( G(z) = e^{i\pi x} = |\tilde{h}_q(x)|^2 \). Therefore, the goal is to identify \( G(z) \) with the product of a function with its complex conjugate in the unit circle.

Finally, take \( p(z) \) as the degree-2q polynomial such that \( G(z) = z^{-q} p(z) \). If \( \mathcal{L} = \{r_k\}_{k \in [2q]} \) is the list of all roots of \( p(z) \) with their multiplicities ordered by increasing modulus,
then we can express
\[ G(z) = a_q z^{-q} \prod_{k=1}^{2q} (z - r_k) \]

\[ = \left[ a_q \prod_{k=1}^{q} r_k \right] \left[ \prod_{k=1}^{q} \left( \frac{1}{z} - \frac{1}{r_k} \right) \right] \left[ \prod_{k=q+1}^{2q} (z - r_k) \right]. \tag{20} \]

Now, notice that \( G(z) \) is a real polynomial and it is zero or positive for \( z \) in the unit circle. In particular, the former property, when applied to the unity circle (\( z^* = 1/z, z \in U(1) \)) gives that

\[ G^*(z) = \left[ a_q \prod_{k=1}^{q} r_k \right] \left[ \prod_{k=1}^{q} \left( z - \frac{1}{r_k} \right) \right] \left[ \prod_{k=q+1}^{2q} \left( \frac{1}{z} - \frac{1}{r_k} \right) \right] \tag{21} \]

must be equal to Eq. (20). Comparing the two equations leads to the conclusion that for each root \( r_k \in \mathcal{L} \), \( 1/r_k^* \) is also in \( \mathcal{L} \). This also automatically ensures that the constant \( [a_q \prod_{k=1}^{q} r_k] \) is a real number by noticing that \( a_q \prod_{k=1}^{q} r_k / r_k^* \) is the constant term in \( p(z) \) since the product contains all its roots. Whereas the constant term is \( a_{-q} = c_{-q}/2e^{\pi i/2} q \).

At last, we can use the positiveness of \( G(z) \) in the unit circle:

\[ G(z) = \left[ a_q \prod_{k=1}^{q} r_k \right] \left[ \prod_{k=1}^{q} \left( z - \frac{1}{r_k} \right) \left( z - \frac{1}{r_k^*} \right) \right] \geq 0, \tag{22} \]

for \( z \in U(1) \), to conclude that \( [a_q \prod_{k=1}^{q} r_k] \geq 0 \). Here we used that \( z^* = 1/z \) and assumed that the second half of \( \mathcal{L} \) is composed by \( 1/r_k^* \) for each \( r_k \) in the first half.

Finally, still for \( z \in U(1) \) we can write

\[ G(z) = \left[ a_q \prod_{k=1}^{q} r_k \right] \left[ z^{-q/2} \prod_{k=1}^{q} \left( z - \frac{1}{r_k^*} \right) \right] \]

\[ \quad + \left[ a_q \prod_{k=1}^{q} r_k \right] \left[ z^{q/2} \prod_{k=1}^{q} \left( z^* - \frac{1}{r_k} \right) \right], \tag{23} \]

and identify \( \hat{h}_q(x) \) as the polynomial in the first line for \( z = e^{ix} \), such that \( G(z = e^{ix}) = \hat{h}_q(x) \bar{h}_q^*(x) \). The complexity of calculating the coefficients of \( \hat{h}_q(x) \) is basically given by the complexity of finding the roots of the polynomial \( G(z) \) and thus is \( O(\text{poly}(q)) \).

Now that the operator \( U_{\hat{g}_q}(x) \) has been built, we can prove Theorem 1. The main idea is to show that \( U_{\hat{g}_q}(x) \) can be expressed as a product of the basic qubit gates \( R(x, \omega, \xi) \).

**Proof of Theo. 1.** First of all, we prove that the matrix elements of \( R(x, \omega, \Phi) \) are indeed Fourier series in \( x \) with the correct frequency values. The basic QSP gate \( R(x, \omega, \xi) = e^{i\xi Z} e^{-i\omega Y} e^{i\xi Z} e^{i\omega x Z} e^{-i\omega Y} \) with \( \xi = \{\xi, \eta, \varphi, \kappa\} \) can be conveniently represented as [24]

\[ R(x, \omega, \xi) = \left( a_+ e^{i\omega x} + a_- e^{-i\omega x} b_+ e^{i\omega x} + b_- e^{-i\omega x} \right) \]

\[ a_- = -\sin \varphi \sin \kappa e^{i\eta} \]

\[ b_- = -\cos \varphi \sin \kappa e^{i\eta} \tag{25} \]

We first use mathematical induction to prove that, for any even \( q \), \( R(x, \omega, \Phi) \) is a Fourier series with frequencies \( \{-(q-1)/2, -(q-3)/2, \ldots, 0, \ldots, (q-1)/2\} \). Let us define \( R^{(m)}(x, \omega, \Phi) \) as the partial product up to the \( m \)-th term of \( R(x, \omega, \Phi) \). We are taking \( \omega_0 = 0, \omega_k = (-1)^{-m/2} \) for all \( k \neq 0 \) even. Therefore, the entries of \( R^{(0)}(x, \omega, \Phi) \) are 0-order Fourier series is obtained, i.e complex constants. Moreover, if none of the QSP parameters in Eq. (25) is order-1 with the frequencies \( \{-1, 0, 1\} \). In particular, \( \langle 0 | R^{(2)}(x, \omega, \Phi) | 0 \rangle \) is an order-1 Fourier series. Proceeding with the induction, we now assume that, for \( m \geq 4 \) even, the components of \( R^{(m-2)}(x, \omega, \Phi) \) are order-\((m-2)/2\) Fourier series with all terms with frequencies \( \{-(m-1)/2, \ldots, 0, \ldots, (m-1)/2\} \). Multiplying the next two iterators \( R(x, \omega_{m-1}, \xi_{m-1}) \) and \( R(x, \omega_m, \xi_m) \) will add or subtract 1 to the frequencies, or keep the same frequency of the terms in \( R^{(m-2)}(x, \omega, \Phi) \). This implies that \( R^{(m)}(x, \omega, \Phi) \) is a also a Fourier series with the due frequencies. Therefore, we conclude that this is true for \( R(x, \omega, \Phi) \) with any \( q \) even.

We still need to prove that, we can always find QSP pulses \( \Phi \) such that the upper left-hand matrix entry of \( R(x, \omega, \Phi) \) gives the desired Fourier series \( \hat{g}_q(x) \). From Lem. 4 we know how to obtain the complementary Fourier series \( \hat{h}_q \). The right-hand side of Eq. (18) is constant, implying that all the coefficients of oscillating terms in the left-hand side must vanish. In particular, the highest-frequency term gives
\[ c_q/2C_q^{\ast}/2 + d_q/2d_q^{\ast}/2 = 0. \] Our strategy is to successively multiply \( U_{\xi_q} \) by the inverse of the QSP fundamental gates, finding the pulse \( \xi_q \) that reduces the frequency of its components in each turn, until we obtain the identity operator. This will at the same time show that \( U_{\xi_q} = R(x, \omega, \Phi) \) and find the desired \( \Phi \). We start by multiplying Eq. (17) from the left by \( R^{-1}(x, \omega_q, \xi_q) \), obtaining

\[
U_{\tilde{\xi}_q} : = R^{-1}(x, \omega_q, \xi_q)U_{\tilde{\xi}_q} = \left( \begin{array}{c}
\tilde{g}_{q-1}(x) \\
\tilde{h}_{q-1}(x)
\end{array} \right),
\]

where

\[
\tilde{g}_{q-1}(x) = \sum_{m=-q/2}^{q/2} \left( \begin{array}{c}
a_q^{\ast}e^{-i\tilde{x}/2} + a_qe^{i\tilde{x}/2} \\
b_qe^{i\tilde{x}/2} + b_q^{\ast}e^{-i\tilde{x}/2}
\end{array} \right) cm e^{imx}
\]

and

\[
\tilde{h}_{q-1}(x) = \sum_{m=-q/2}^{q/2} \left( \begin{array}{c}
a_q^{\ast}e^{-i\tilde{x}/2} + a_qe^{i\tilde{x}/2} \\
b_qe^{i\tilde{x}/2} + b_q^{\ast}e^{-i\tilde{x}/2}
\end{array} \right) dm e^{-imx}.
\]

The terms oscillating with frequencies \((q+1)/2\) and \((-q+1)/2\) must vanish, since they increase the frequencies present in \( U_{\tilde{\xi}_q} \). This leads to the two linear systems

\[
\begin{align*}
a_q^{\ast}c_q/2 + b_q + d_q^{\ast}/2 &= 0 \\
a_q^{\ast} - d_q/2 - b_q + c_q^{\ast}/2 &= 0
\end{align*}
\]

and

\[
\begin{align*}
a_q^{\ast}c_q/2 + b_q^{\ast} - d_q^{\ast}/2 &= 0 \\
a_q^{\ast} - d_q^{\ast}/2 - b_q + c_q/2 &= 0
\end{align*}
\]

that must be solved for the variables \( \{a_q, a_q^{\ast}, b_q, b_q^{\ast}\} \). This leads to the QSP angles of the \( q \)-th pulse via Eq. (25). The unitarity condition in Eq. (18) implies that \( c_q/2c_q^{\ast}/2 + d_q/2d_q^{\ast}/2 = 0 \). This guarantees that both linear systems (29) and (30) admit non-trivial solutions. Using Eq. (25), it can be directly verified that both (29) and (30) lead to \( \tan \varphi_q = -e^{i(\xi_q + \eta_q)}d_q^{\ast}/c_q/2 \) and \( \zeta_q + \eta_q = -\text{Arg} \left( \frac{d_q^{\ast}/c_q/2}{e^{i(\xi_q + \eta_q)}} \right) \). Equations (29) and (30) impose no restriction over \( \kappa_q \), which we fix as \( \pi/4 \). Also, one rotation can be eliminated by choosing \( \eta_q = \zeta_q \).

The \((q-1)\)-th pulses are obtained in the exact same way from the highest-order coefficients of \( \tilde{g}_{q-1}(x) \) and \( \tilde{h}_{q-1}(x) \). Because the frequency of the \((q-1)\)-th iterate is \( \omega_{q-1} = -1/2 \), the solution found for the angles is slightly different: \( \tan \varphi_{q-1} = e^{i(\xi_{q-1} + \eta_{q-1})}d_{q-1}/c_{q-1}/2 \) and \( \zeta_{q-1} + \eta_{q-1} = \text{Arg} \left( \frac{c_{q-1}}{d_{q-1}/2} \right) \), where \( c_{q-1}/2 \) is the coefficient of \( e^{-i(\pi/2)x} \) in \( \tilde{f}_{q-1}(x) \) and \( \tilde{d}_{q-1}/2 \) accompanies \( e^{-i(\pi/2)x} \) in \( \tilde{g}_{q-1}(x) \). After the \((q-1)\)-th inverse gate, we are left with an order-\( (q-2) \) Fourier series. We can repeat this process until we get an order-0 Fourier series, which determines the parameters of the last gate with frequency \( \omega_0 = 0 \) to be \( \kappa_0 = 0, \xi_0 = \text{Arg}(\tilde{g}_0), \eta_0 = \text{Arg}(\tilde{h}_0), \) and \( \tan \varphi_0 = -e^{i(\xi_0 - \eta_0)}/\tilde{h}_0 \). To obtain the pulses, \( \mathcal{O}(q^2) \) arithmetic operations are used. \( \square \)

B. Operator function design: proof of Theorem 2

**Proof of Theorem 2.** The proof consists of showing that the operator \( V_\Phi = \left( \tilde{V}_\xi \tilde{V}_\xi^{\ast} \cdots \tilde{V}_\xi^{\ast} \tilde{V}_\xi \right) \) is the single-qubit operator \( R(x, \omega, \Phi) \) satisfies Theorem 1. Therefore, given a Fourier series \( \tilde{g}_q(x) \), with \(|\tilde{g}_q(x)| \leq 1 \) for all \( x \in [-\pi, \pi] \), it is possible to efficiently find \( \Phi \) from \( c = \{c_m\}_m \) such that

\[
\langle 0 | V_\Phi | 0 \rangle = \sum_\lambda |\lambda\rangle \langle \lambda | \otimes R(x, \omega, \Phi) | 0 \rangle
\]

reduces to Eq. (4) with \(|\langle 0 | \mathcal{R}(x, \omega, \Phi) | 0 \rangle \rangle = \tilde{g}_q(x) \).

First of all, notice that Eq. (3) can be written, using the definition of \( R(x, \omega, \xi) \), as

\[
W_\mathcal{R} = \sum_\lambda |\lambda\rangle \langle \lambda | \otimes R(x, \omega, 0, \xi_0).
\]

Using the spectral decomposition of the Hamiltonian \( H \), the oracle \( O \) can be written as

\[
O = \sum_\lambda |\lambda\rangle \langle \lambda | \langle 0 \rangle \langle 0 | + e^{-ix\lambda} |1\rangle \langle 1 |,
\]
or, alternatively, \( O = \sum \lambda e^{-i \frac{x}{2} \lambda} |\lambda\rangle \otimes e^{i \frac{x}{2} \lambda} Z \), which directly implies that Eq. (2a) can be expressed as

\[
V_{\xi_k} = \sum_{\lambda} |\lambda\rangle \langle \lambda| \otimes R(x_{\lambda}, \omega = 1/2, \xi_k).
\]  

(35)

Analogously, from Eq. (2b) it holds

\[
\tilde{V}_{\xi_k} = \sum_{\lambda} |\lambda\rangle \langle \lambda| \otimes R(x_{\lambda}, \omega = -1/2, \xi_k).
\]  

(36)

Because of the orthogonality between distinct eigenvectors of \( H \), Eq. (31) follows straightforwardly from the product of Eq. (33) and the alternated iteration of the operators in Eqs. (35) and (36), as desired.

Finally, let us make a last comment about the mapping of Hamiltonian eigenvalues to the convergence interval of the target Fourier series. Notice that taking \( t = x_0 \) maps any \( \lambda \in [-1, 1] \) to the convergence interval \([-x_0, x_0]\) of the Fourier series. However, we can map any interval of eigenvalues \([\lambda_+, \lambda_-]\) to \([-x_0, x_0]\). This is done by replacing the oracle \( O \) with the iterate \( V_0 = I \otimes |0\rangle\langle 0| + e^{-i \Delta} e^{-i H t} \otimes |1\rangle\langle 1| \), which can be obtained from \( O \) using one query. We can write \( V_0 = \sum_{\lambda} e^{-i \frac{x}{2} \lambda} |\lambda\rangle \langle \lambda| \otimes e^{i \frac{x}{2} \lambda} Z \), now with \( x_{\lambda} = \lambda t + \Lambda \), and again a function \( \alpha f(\lambda) = g(x_{\lambda}) \) can be \( \varepsilon \)-block-encoded into \( V_0 \). The eigenvalues interval \([\lambda_+, \lambda_-]\) is then mapped into the convergence interval if we take \( t = x_0 / \Delta \lambda \) and \( \Lambda = -x_0 \frac{\lambda_+}{\Delta \lambda} \), with \( \Delta \lambda = (\lambda_+ - \lambda_-) / 2 \) and \( \lambda = (\lambda_+ + \lambda_-) / 2 \).

V. DISCUSSION

We presented a novel quantum signal processing variant able to produce any Fourier series of a Hermitian operator \( H \). The algorithm assumes access to a Hamiltonian oracle given by a single-qubit controlled version of the unitary operator \( e^{-i H t} \). Remarkably, this is the only ancilla required throughout the algorithm. The evolution time \( t \) in the oracle is fixed at a tunable value. By interspersing oracle calls with parameterized single-qubit rotations on the ancilla, the target operator function is encoded into a block of the resulting joint-system unitary transformation. The operator function is then physically realized on the system by a measurement postselection on the ancilla.

More technically, the problem of synthesizing a Fourier series of an operator is reduced to applying a single-qubit pulse sequence that realizes the corresponding real-variable series as a matrix element of an \( SU(2) \) operator. We provided an explicit efficient classical algorithm for determining the parameters in such sequence from the target Fourier-series coefficients, and rigorously proved that any (normalized) finite Fourier series can be implemented. Hence, our method is able to implement arbitrarily good approximations to any Hamiltonian function with a finite number of jump discontinuities. The tunable evolution time in the oracle gives us freedom to map the range of eigenvalues of \( H \) to an effective interval of interest shorter than the period of the approximation series, which allows us to control the convergence in a practical way and avoid the Gibbs phenomenon at the boundaries.

Another important task we considered is how to find the best Fourier approximation to be used, given a fixed target function. We presented two such classical sub-routines for such approximations. The first one is based on Lemma 37 of Ref. [12] and comes guaranteed error bounds. The second one is obtained from an analytic periodic extension of the target function to Fourier-approximate that has guaranteed asymptotic convergence but no closed-form expression for the approximation error. However, while the former is so computationally intensive that it becomes in practice prohibitive already for moderate applications, the former is consistently observed to be numerically very efficient. Moreover, the second method circumvents the sub-normalization required by the first method, thus leading also to significantly higher post-selection probabilities.

Our findings provide a versatile tool-box for generic operator-function synthesis, relevant to a plethora of modern quantum algorithms, with the advantages of reduced number of ancillary qubits, compatibility with Trotterised Hamiltonian simulations schemes, and relevance both for digital as well as hybrid digital-analog quantum platforms.

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upper-half and again, repeats the process. Convergence happens after at most $\lceil \log_2(n) \rceil$ steps, where $n$ is the size of the array. Note that the naive one-by-one comparison used in the linear search requires $n$ steps in the worst-case scenario.

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Appendix A: Another algorithm for operator function design using Fourier series

In this appendix we show that it is possible to implement Fourier series of Hermitian operators using the standard QSP pulses. Nevertheless, this approach has achievability guaranteed only for real Fourier series. Moreover, it requires one extra qubit ancilla and extra subnormalization of $1/2$.

1. Real-function design with single-qubit rotations

We start by reviewing the design of functions of one real variable with single-qubit pulses presented in Ref. [1].

The basic single qubit rotation in this method is given by $R(x, \phi) = e^{ixX}e^{i\phi Z}$, where $X$ and $Z$ are the first and third Pauli matrices, respectively, and $\phi \in [0, 2\pi]$. The angle $x \in [-\pi, \pi]$ is the signal to be processed and the rotation $e^{ixX}$ is now the iterate. For a given even number $q$, the sequence of rotations $\mathcal{R}(x, \phi) = e^{i\phi_{q+1}Z} \prod_{k=2}^{q/2} R(-x, \phi_{2k}) R(x, \phi_{2k-1})$ results in an operator with matrix representation [1]

$$\mathcal{R}(x, \phi) = \begin{pmatrix} B(\cos x) & i \sin x D(\cos x) \\ i \sin x D^*(\cos x) & B^*(\cos x) \end{pmatrix},$$

(A1)

whose entries contain polynomials $B$ and $D$ in $\cos x$ with complex coefficients determined by the sequence of rotation angles $\phi = (\phi_1, \cdots, \phi_{q+1}) \in \mathbb{R}^{q+1}$.

Given target real functions $\mathcal{B}(x)$ and $\mathcal{D}(x)$ satisfying

$$\mathcal{B}^2(x) + \sin^2 x \mathcal{D}^2(x) \leq 1$$

(A2)

for all $x$ and having the form

$$\mathcal{B}(x) = \sum_{k=0}^{q/2} b_k \cos(2kx)$$

(A3)

$$\sin x \mathcal{D}(x) = \sum_{k=1}^{q/2} d_k \sin (2kx),$$

with $b_k$ and $d_k$ arbitrary real coefficients, then there is a pulse sequence $\phi$ that generates $B(\cos x)$ and $D(\cos x)$ with $\mathcal{B}(x)$ and $\mathcal{D}(x)$ as either their real or imaginary parts, respectively.

Given that the desired polynomials are achievable by QSP, the rotation angles $\phi$ can be computed classically in time $O(poly(q))$ [1, 25, 27, 30].

2. Multiqubit operator-function design

We again assume that the Hermitian operator $H$ is encoded in the real-time evolution oracle of Def. 1 and show how to apply the QSP pulses of Sec. A 1 in order to implement an operator Fourier series. As the pulses already produce sine and cosine series, we use an extra ancilla denoted by $A_P$ to combine the two opposite parity series into an arbitrary real Fourier series. Denoting by $A_O$ the oracle ancilla, the total Hilbert space for the ancillas is now $H_A = H_{A_O} \otimes H_{A_P}$.

Defining $O' = (1 \otimes O)(1 \otimes M)$, the basic QSP blocks $V_{\phi^{(j)}} = O'(1 \otimes e^{i\phi^{(j)} Z})$ and $\bar{V}_{\phi^{(j)}} = O'(1 \otimes e^{i\bar{\phi}^{(j)} Z})$ can be obtained from one call to the oracle $O$ or its inverse. Here the qubit rotations are applied on the oracle ancilla. Depending on the preparation and post-selection of this ancilla, Eq. (A3) allows for a sine or a cosine series on the input $x$. The addition of the second qubit ancilla makes possible to implement a series with undefined parity. With $V_{\phi} = W_{out} V_{\phi_0} V_{\phi_1} \cdots V_{\phi_2} V_{\phi_1} W_{in}$, for this algorithm we take input and output ancillary unitaries as

$$W_{in} = 1 \otimes M \otimes M,$$

(A4)

where $M$ is a qubit Hadamard gate, and

$$W_{out} = W_{in} \left[ 1 \otimes \left( e^{i\phi^{(1)} Z} \otimes |0\rangle \langle 0| + (Ze^{i\bar{\phi}^{(1)} Z} \otimes |1\rangle \langle 1|) \right) \right],$$

(A5)

and the basic QSP blocks are defined as

$$V_{\phi} = V_{\phi^{(1)}} \otimes |0\rangle \langle 0| + V_{\phi^{(1)}} \otimes |1\rangle \langle 1|,$$

(A6)

$$\bar{V}_{\phi} = \bar{V}_{\phi^{(1)}} \otimes |0\rangle \langle 0| + \bar{V}_{\phi^{(1)}} \otimes |1\rangle \langle 1|,$$

(A7)

with $\phi = (\phi^{(1)}, \bar{\phi}^{(1)})$. The following lemma summarizes the method:
Lemma 5. (Fourier series from real-time evolution oracles - second approach) Let \( \bar{g}_q : [-\pi, \pi] \rightarrow \mathbb{R} \) be the Fourier series \( \bar{g}_q(x) = b_0 + \sum_{k=1}^{q/2} (b_k \cos kx + d_k \sin kx) \), with \(|\bar{g}_q(x)| \leq 1 \) for all \( x \in [-\pi, \pi] \). Then there is a pulse sequence \( \Phi = (\phi_1, \ldots, \phi_{q+1}) \in \mathbb{R}^{2q+2} \), with \( \phi_k = (\phi_k^{(c)}, \phi_k^{(s)}) \), such that the operator \( V_\Phi \) on \( \mathbb{H}_{S,A} \) with \( W_{in}^* \) and \( W_{out} \) and \( V_{\phi_k} \) and \( V_{\phi_k} \) given by Eqs. (A4), (A5), (A6), and (A7), respectively, is a perfect block-encoding of \( \bar{g}_q \) for all \( x \in [-\pi, \pi] \). Moreover, the pulse sequence can be obtained classically in time \( O(\text{poly}(q)) \).

Proof. Consider the operator \( V_{\phi^{(j)}} \) on \( \mathbb{H}_{S,A_0} \), where \( \phi^{(j)} \in \mathbb{R}^{q+1} \) is the set of angles \( \{\phi_{q+1}^{(j)}, \ldots, \phi_1^{(j)}\} \), with \( j = c \) or \( j = s \). Using Eq. (34), it is straightforward to see that

\[
V_{\phi^{(j)}} = \sum_\lambda |\lambda\rangle \langle \lambda| \otimes \mathcal{R} \left( \frac{x}{2}, \phi^{(j)} \right),
\]

with the concatenated qubit-rotations operator \( \mathcal{R} \left( \frac{x}{2}, \phi \right) \) given by Eq. (A1). Considering \( A_0 \) to be initialized and afterwards projected on state \( |+\rangle \), the resulting operator on \( \mathbb{H}_S \) is obtained as

\[
|+\rangle V_{\phi^{(j)}} |+\rangle = \sum_\lambda \left( \mathcal{R}(x) + i \mathcal{R}(x) \right) |\lambda\rangle \langle \lambda|.
\]

By setting \( \mathcal{R}(x) = \text{Re}[B(x)] \) and \( \mathcal{R}(x) = \text{Re}[\sin x D(x)] \), A real sine series can also be implemented through

\[
\langle + | (1 \otimes Z) V_{\phi^{(j)}} |+\rangle = \sum_\lambda \left( iB(x) + D(x) \right) |\lambda\rangle \langle \lambda|.
\]

by setting \( B(x) = 0 \). Here we defined \( \mathcal{B}(x) = \text{Im}[B(x)] \) and \( \mathcal{D}(x) = -\text{Im}[\sin x D(x)] \). Moreover, adding an extra control qubit \( A_P \) allows to perform a combination of them by applying \( V_{\phi^{(j)}} = V_{\phi^{(c)}} \otimes |0\rangle \langle 0|_{A_P} + (1 \otimes Z) \mathcal{V}_{\phi^{(s)}} \otimes |1\rangle \langle 1|_{A_P} \), since

\[
A_P \left( |+\rangle V_{\phi^{(j)}} |+\rangle \right) A_P = \frac{1}{2} (V_{\phi^{(c)}} + (1 \otimes Z) V_{\phi^{(s)}}).
\]

In order to meet the achievability conditions, both cosine and sine series must be normalized according to Eq. (A2). Since \(|\bar{g}_q(x)| \leq 1 \) and all \( x \in [-\pi, \pi] \) then and

\[
\left| \sum_{k=0}^{q/2} b_k \cos x \right| \leq \left| \frac{\bar{g}_q(x) + \bar{g}_q(-x)}{2} \right| \leq 1
\]

\[
\left| \sum_{k=1}^{q/2} d_k \sin x \right| \leq \left| \frac{\bar{g}_q(x) - \bar{g}_q(-x)}{2} \right| \leq 1
\]

such that the achievability conditions of QSP are satisfied by the cosine and sine series individually. Therefore, there are two sets of angles \( \phi^{(c)} \) and \( \phi^{(s)} \) that realize the sine and the cosine series through the QSP operators (A10) and (A11), respectively. Notice that setting \( \mathcal{R}(\theta) = 0 \) and \( \mathcal{R}(\theta) = 0 \) does not compromise the achievability conditions to be fulfilled. The final result in Eq. (A8) comes from the observation that \( V_{\phi^{(j)}} = W_{in}^* V_{\phi} W_{in} \). The ancillas unitary \( W_{in} \) serves only to change the ancillas projection to the computational basis.