Report:

Hamiltonian Simulation via Quantum Signal Processing

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1 Introduction

Matrix manipulation is a core element of quantum algorithms, specifically matrix functions. Performing various operations efficiently is essential to creating a true quantum advantage in the algorithm space. At the heart of matrix functions and arguably underpinning the idea of quantum computation [Fey82] is the concept of Hamiltonian simulation. Physics 101 teaches the famous Schrödinger equation — the basis for Hamiltonian simulation,

$$H|\psi(t)\rangle = -i\frac{\partial}{\partial t}|\psi(t)\rangle \tag{1}$$

The idea in quantum computation is to simulate the evolution of this system by implementing the matrix exponential,

$$\mathrm{e}^{\mathrm{i}Ht} \tag{2}$$

Such a simple expression is host to a vast array of research and techniques aimed at giving efficient simulation. Lloyd proved that quantum computers can be used to simulate the dynamics of local Hamiltonians [Llo96]. Locality is an innate property of systems in nature [Amb14, CN14] making their study of high interest. The primitive method employed by Lloyd related to the Trotter–Suzuki–Lie method. This decomposes the matrix exponential into smaller steps,

$$\mathrm{e}^{\mathrm{i}Ht} = \left(\mathrm{e}^{\mathrm{i}H_1\frac{t}{n}+\ldots+\mathrm{i}H_m\frac{t}{n}}\right)^n = \left(\mathrm{e}^{\mathrm{i}H_1\frac{t}{n}}\ldots\mathrm{e}^{\mathrm{i}H_m\frac{t}{n}} + \mathcal{E}\right)^n \tag{3}$$

where $\|\mathcal{E}\| = O(m^2t^2/n^2)$. By choosing a sufficient value for n, it can be shown that $U = \left(\mathrm{e}^{\mathrm{i}H_1\frac{t}{n}}\ldots\mathrm{e}^{\mathrm{i}H_m\frac{t}{n}}\right)^n$ approximates eq. (2) within some error ε. The gate complexity scales quadratically with time, while efficient from a theoretical computer science perspective, is not realistically ideal for long time intervals!

The goal of Hamiltonian simulation is to produce a cost efficient simulation of the matrix exponential of some Hamiltonian up to a defined error, specifically, construct some U such that,

$$\left\| U - \mathrm{e}^{\mathrm{i}Ht} \right\| \leq \varepsilon \tag{4}$$

In this essay, we briefly analyse elements of a new approach for Hamiltonian simulation — *quantum signal processing* (QSP) [LC17]; specifically the single ancilla variant. QSP offers an optimal algorithm based on sequential applications of single qubit rotation gates; this systematic method block encodes a desired polynomial function on the eigenvalues.

There are some important prerequisites to this idea. Below, fig. 1, shows a workflow of concepts that lead ultimately to another technique, the quantum singular value transformation [GSLW19]. We do not cover that here; however, we do note that this technique is a further generalisation of QSP (and other ideas). It is a powerful concept that has arguably led to the idea of a 'grand unification' of quantum algorithms [MRTC21].

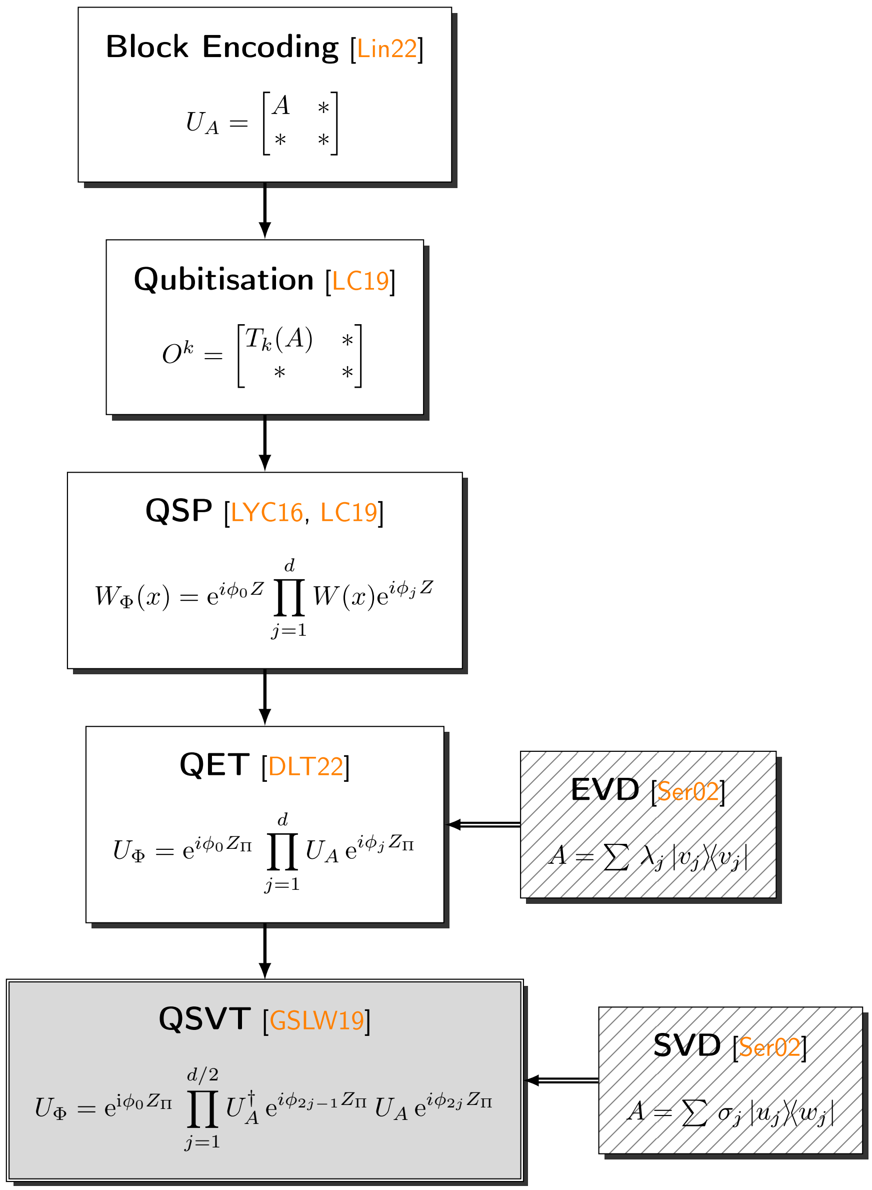

Figure 1: Pipeline of quantum techniques that build from block encoding. Block encoding supports the notion of quantum signal processing, which in turn can be generalised via the quantum eigenvalue transformation. The quantum eigenvalue transformation can be further generalised to the quantum singular value transformation. The final two techniques can be understood as quantum analogous to the robust mathematical concepts of eigenvalue decomposition and singular value decomposition, respectively.

2 Block Encoding

Succinctly described, block encoding is a technique that permits the application of some general matrix $A \in \mathbb{C}^{2^n \times 2^n}$, where A is not necessarily unitary, on a quantum state. Implementation of a gate on quantum hardware requires said gate to be unitary; yet, one may be interested in the dynamics of a state under the influence of a non–unitary matrix. Block encoding, therefore, answers the question: *how could we implement A on a quantum computer*?

At a basic level, this technique embeds A within some larger but unitary matrix, to allow for its implementation on a quantum computer. A trivial example: the CNOT gate, which encodes the action of the Pauli–X gate on some target qubit(s), dictated by the state of the control qubit(s). Block encoding is slightly more general than this but the intuition is analogous, cf. Fig. 2.

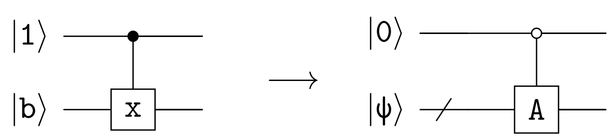

Figure 2: (Right) A trivial example of a block encoded insatnce — the CNOT gate that performs $|b\rangle \mapsto |b \oplus 1\rangle$ upon signal state $|1\rangle$ on the first register. (Left) A generalised block encoding circuit, triggered when the signal state is $|0\rangle$ (eq. (5)).

Assuming this larger unitary $U_A \in \mathbb{C}^{2^\eta \times 2^\eta}$ exists, where $\eta = n + m$ and the state $|0^m, \psi\rangle$ can be efficiently prepared, then,

$$U_A = \begin{bmatrix} A & * \\ * & * \end{bmatrix} \tag{5}$$

block encodes the activity of A onto the state $|\psi\rangle$. The matrix components marked '$*$' are not important for introductory purposes, and so will not be specified but exist in a manner such that U_A is unitary. The action of U_A on $|0^m, \psi\rangle$ can trivially be found as,

$$U_A |0^m, \psi\rangle = |0^m\rangle A |\psi\rangle + |\perp\rangle \tag{6}$$

Additionally, the state $|\perp\rangle$ remains unspecified but is orthogonal with respect to $|0^m\rangle \otimes \mathbb{I}_n$. One subtle condition for the existence of U_A is $\|A\| \leq 1$ [CLBY23]. If, for instance, $\|A\| > 1$, we can just renormalise via a block encoding of A/α, such that $\|A/\alpha\| \leq 1$. Notice that the outcome we desire, i.e. the effect, $A|\psi\rangle$, can be found by a measurement on the first register, see fig. 3. The probability of success is, then,

$$\mathcal{P}(|0^m\rangle) = \frac{\|A|\psi\rangle\|^2}{\alpha^2} \tag{7}$$

With $O\big(1/\sqrt{\mathcal{P}(|0^m\rangle)}\big)$ rounds of amplitude amplification, we can boost the probability of success. Note, the explicit form of a block encoding need not take the exact form shown in eq. (5) and in fact the action of A can be extracted from the encoding U_A via some *signal state* $|G\rangle$. Moreover,

Definition 1 [Lin22, LC19]

Given an n-qubit matrix A, if we can find parameters, $\alpha, \epsilon \in \mathbb{R}^+$ and an $(m+n)$-qubit unitary, U_A, and a signal state $|G\rangle \in \mathbb{C}^{2^m}$, such that,

$$\|A - \alpha\left(\left(\langle G| \otimes \mathbb{I}_n\right) U_A \left(|G\rangle \otimes \mathbb{I}_n\right)\right\| \leq \epsilon \tag{8}$$

Then U_A is the (α, m, ϵ)–BE of A.

Notice that the circuit of fig. 3 can be repeated several times to generate powers of A. This probes the idea of block encoding functions of matrices, i.e. $f(A)$. This is the basis for *qubitisation* [LC19]; qubitisation uses a block encoded iterate in the eigenbasis of a Hamiltonian to craft Chebyshev polynomials on said Hamiltonian. The term qubitisation refers to the 2D space spanned by the states, reminiscent of eq. (6).

It turns out not all possible functions can be constructed exactly; using truncated Taylor expansions, decent approximations can be found. Block encoding strongly overlaps with a technique known as 'linear combination of unitaries' [AMC12]. A simple example of such would be the block encoding of $A + B$ via the LCU method. Figure 4 gives the circuit diagram for this. A quick calculation shows that measuring $|0\rangle$ on the first register produces $(A + B)|\psi\rangle$. Clearly, if $B = A^2$, the function $f(x) = x(1 + x)$ is trivially constructable. By having a longer combination of such unitaries, it is straightforward to see how a truncated series expansion can be implemented.

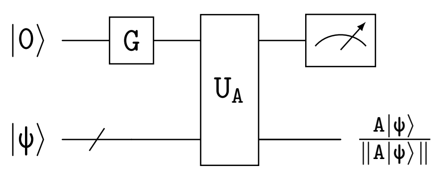

Figure 3: Block encoding of a matrix A with signal state $|G\rangle = G|0\rangle$.

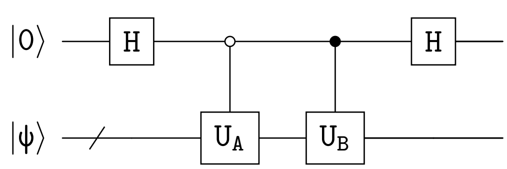

Figure 4: An instance of the linear combination of unitaries technique that encodes the action of $A + B$ on the state $|\psi\rangle$.

There are some apparent bottlenecks to this method. The definition above emphasises the existence of the signal state $|G\rangle$; furthermore, the block encoding of A usually comes in the form of constructing oracles that can efficiently query the elements [BCK15, CKS17]. For specific examples of sparse matrices, such oracles have been explicitly calculated [CLBY23].

3 Single Qubit Rotations

Before an analysis of the quantum signal processing technique, let us briefly discuss the action of a simple single qubit rotation gate — the rotation–X gate,

$$R_{\mathrm{x}}(\theta) = \mathrm{e}^{-\mathrm{i}\theta X} = \cos\frac{\theta}{2}\mathbb{I} - \mathrm{i}\sin\frac{\theta}{2}X \tag{9}$$

Clearly, this just rotates a state around the $|+\rangle\,/\,|-\rangle$ axis of the Bloch sphere. Note that all pure states can be geometrically represented on the boundary of the Bloch sphere, $S^2 = \partial B^3$, via,

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + \mathrm{e}^{\mathrm{i}\phi}\sin\frac{\theta}{2}\,|1\rangle \tag{10}$$

where θ describes a rotation about the $|+\rangle\,/\,|-\rangle$ axis and ϕ a rotation about the $|0\rangle\,/\,|1\rangle$ axis[1]. To a get a more intuitive picture of R_{x}'s effect, imagine rotating the $|0\rangle$ state by some angle θ — it then becomes a superposition of $|0\rangle$ and $|1\rangle$. The addition of the ϕ allows for further rotation along the line of latitude at which the state lies. We would find that all pure states conform to following a circular path under a sequence of R_{x} rotations; fig. 6 shows an example of the effect of sequential R_{x} applications.

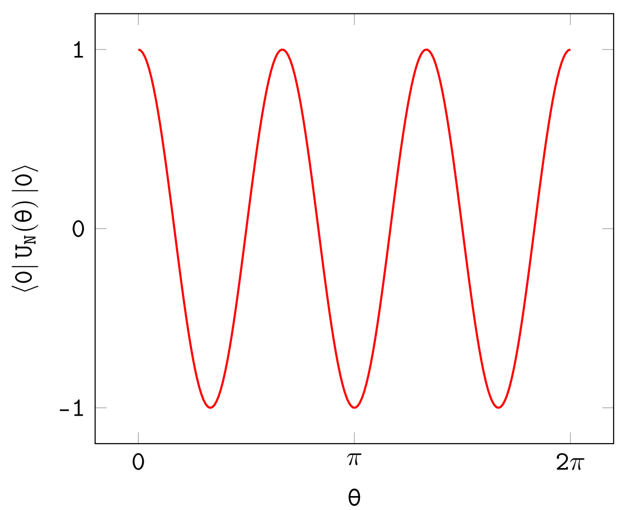

Figure 5: Graphical representation of the function traced by a pure state after a series of $R_{\mathrm{x}}(\theta)$ rotations

More formally, let $U_N(\theta) = R_{\mathrm{x}}(\theta)\ldots R_{\mathrm{x}}(\theta)$ which is generated by N applications of the rotation–X gate. This produces $f(x) = \cos\frac{Nx}{2}$ in the upper right corner of $U_N(\theta)$, namely,

$$\langle 0|\, U_N(\theta)\,|0\rangle = \cos\frac{N\theta}{2} \tag{11}$$

The plots of fig. 6 correlate with the result shown in fig. 5! It is easy to conclude that $U_N(\theta)$ can only give circular

[1] It is common for θ and ϕ to be referred to as the polar and azimuthal angle respectively

paths on ∂B^3. An important question: *how do we impart more control on the system*? This is the basis argument for the QSP technique. By conjugating $R_{\mathrm{x}}(\theta)$ with $R_{\mathrm{z}}(\phi) = \mathrm{e}^{\mathrm{i}\phi Z/2}$ gates we can perform more complex actions!

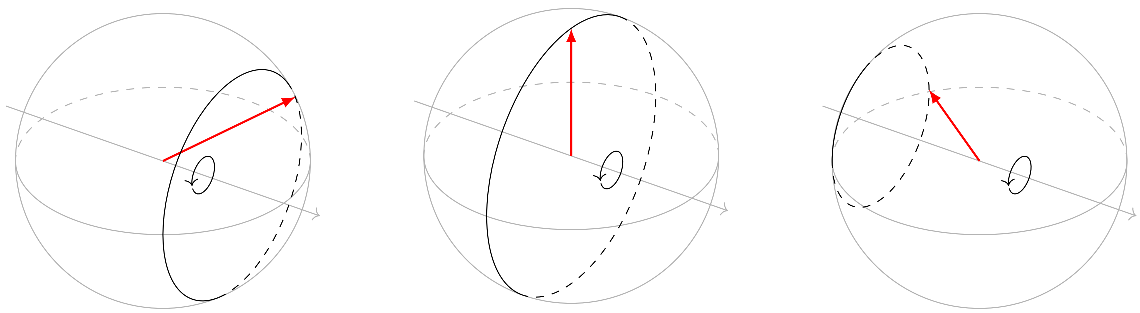

Figure 6: A series of different pure state vectors lying on the surface of the Bloch sphere, ∂B^3, undergoing a sequence of R_{x} rotations. The path ultimately traced out by each is a circular one (given a large enough sequence).

4 Quantum Signal Processing

Consider the following single qubit rotation gate,

$$R_\phi(\theta) = \exp\big(-\mathrm{i}\frac{\theta}{2}(\cos\phi X + \sin\phi Y)\big) \tag{12}$$

Using spectral decomposition, we can express this unitary as,

$$R_\phi(\theta) = \mathrm{e}^{-\mathrm{i}\frac{\theta}{2}} |\eta_+\rangle\langle\eta_+| + \mathrm{e}^{\mathrm{i}\frac{\theta}{2}} |\eta_-\rangle\langle\eta_-| \tag{13}$$

Where $|\eta_\pm\rangle \sim |0\rangle \pm \mathrm{e}^{\mathrm{i}\phi}|1\rangle$. In this manner, we can easily translate the gate into its matrix form as follows,

$$R_\phi(\theta) = \begin{bmatrix} \cos\theta/2 & -\mathrm{i}\mathrm{e}^{-\mathrm{i}\phi}\sin\theta/2 \\ -\mathrm{i}\mathrm{e}^{\mathrm{i}\phi}\sin\theta/2 & \cos\theta/2 \end{bmatrix} \tag{14}$$

When in this form, the identification $R_\phi(\theta) = R_{\mathrm{z}}(-\phi + 2\pi)R_{\mathrm{x}}(\theta)R_{\mathrm{z}}(\phi + 2\pi)$ can be made with a simple calculation and thus the extra control can easily be seen via the presence of ϕ terms! Informally, a sequence of $R_\phi(\theta)$ operations can produce specific polynomials (beyond $\cos x$), figs. 7,8 provide insight into possible functions achievable and ∂B^3 paths.

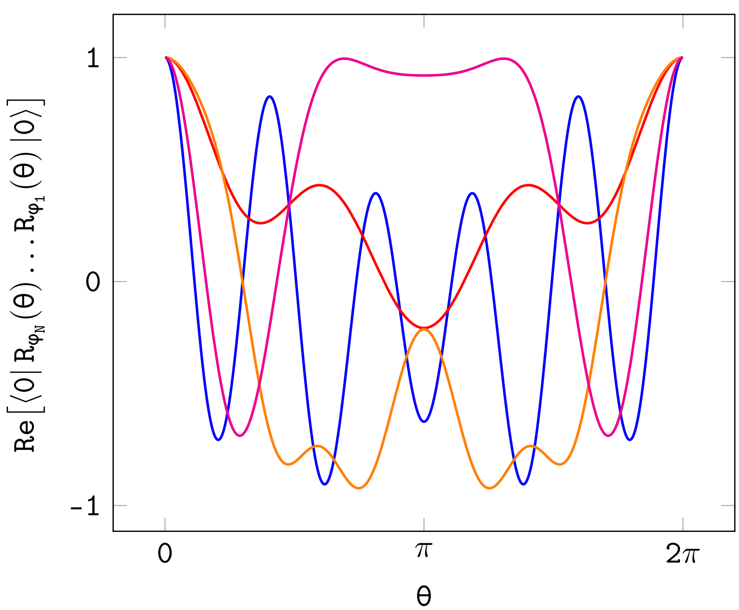

Figure 7: Graphical representation of possible functions constructable via a series of $R_\phi(\theta)$ applications according to different random $\mathbf{\Phi} \in \mathbb{R}^N$

The sequence of $R_\phi(\theta)$'s can be expanded into the Pauli basis such that each Pauli matrix is coupled with some real function. This is the main idea of QSP — to craft approximations to generic functions using simple rotation

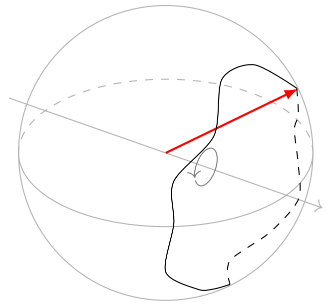

Figure 8: A possible path taken by a vector on ∂B^3 after a sequence of $R_\phi(\theta)$

gates. The decomposition follows [LYC16, LC19],

$$V_{\mathbf{\Phi}}(\theta) = A(\theta)\mathbb{I} + \mathrm{i}B(\theta)Z + \mathrm{i}C(\theta)X + \mathrm{i}D(\theta)Y \tag{15}$$

where $A(\theta), B(\theta), C(\theta), D(\theta)$ are real and $\mathbf{\Phi} \in \mathbb{R}^N$. A neat trick finds that not all functions need to be evaluated, and we can reduce our study to just A, C [LC19]. This gives insight into the particular state we desire for the ancilla. Specifically, $\langle +| V_{\mathbf{\Phi}}(\theta) |+\rangle = A(\theta) + \mathrm{i}C(\theta)$. We now state the theorem underpinning the capabilities of the single ancilla QSP method:

Theorem 1 [LC17, LC19]

For any even $N > 0$ and a choice of real functions, $A(\theta)$, $C(\theta)$, can be implemented by a set of angles, $\mathbf{\Phi} \in \mathbb{R}^N$, if and only if:

(i) $\forall \theta \in \mathbb{R},\ A^2(\theta) + C^2(\theta) \leq 1$

(ii) $A(0) = 1$

(iii) $A(\theta) = \sum_{k=0}^{N/2} a_k \cos(k\theta)$ *gives a real cosine Fourier series of degree at most $N/2$*

(iv) $C(\theta) = \sum_{k=0}^{N/2} c_k \sin(k\theta)$ *gives a real sine Fourier series of degree at most $N/2$*

Given the above theorem and ideas, the QSP technique is aimed at implementing the following transformation,

$$V = \sum_{\lambda} \mathrm{e}^{\mathrm{i}h(\lambda)} |\lambda\rangle\langle\lambda| \tag{16}$$

where $|\lambda\rangle$ are the eigenvectors of some unitary W; moreover,

$$W |\lambda\rangle = \mathrm{e}^{\mathrm{i}\lambda} |\lambda\rangle \tag{17}$$

The circuit for V transforms the eigenphases of $|\lambda\rangle$ according to the real function $h(x)$, created using a sequence of

$R_\phi(\theta)$ gates. Ideally, V uses minimal queries to W. In circuit diagram language, V is a sequence of unitary rotation gates, U_{ϕ_j}, shown in fig. 9.

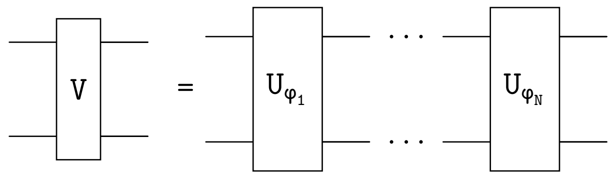

Figure 9: The sequence of U_ϕ gates applied to produce the ideal unitary V which transforms the eigenphases accoring to some real function $h(x)$.

The individual U_ϕ are related to $R_\phi(\theta)$ and a controlled–W gate. The exact form of U_ϕ can be defined as,

$$U_\phi = \sum_\lambda R_\phi(\lambda) \otimes |\lambda\rangle\langle\lambda| \tag{18}$$

With a little bit of work, it can be shown that the circuit diagram of fig. 10 is sufficient for implementing U_ϕ

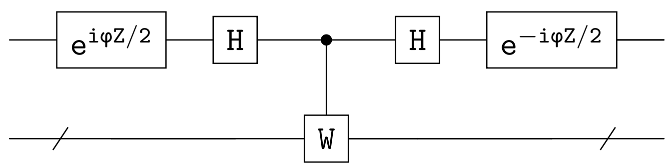

Figure 10: A circuit diagram showing how to construct U_ϕ using a single controlled–W gate and $O(1)$ other single qubit rotation gates.

Notice an eigenstate input renders U_ϕ as $R_\phi(\lambda)$! In this regard, it can be shown,

$$V = \bigoplus_\lambda \left(\mathrm{e}^{\mathrm{i}\varphi_0 Z} \left(\prod_{j=1}^{N} R_{\mathrm{x}}(\lambda) \mathrm{e}^{\mathrm{i}\varphi_j Z} \right) \right) \otimes |\lambda\rangle\langle\lambda| = \begin{bmatrix} f[W] & * \\ * & * \end{bmatrix} \tag{19}$$

By selecting a specific $\mathbf{\Phi}$, an approximation to $\mathrm{e}^{\mathrm{i}h(\lambda)}$ can be implemented according to the rules of Theorem 1. Principally, this is what quantum signal processing does with $O(N)$ queries to W and post–selecting the $|+\rangle$ state on the ancilla qubit. The addition of a single ancilla allows for opposing parity on A and C, whereas the no–ancilla variant [LC19] renders both functions having like parity. In this regard, the single ancilla variant has more freedom.

5 Hamiltonian Simulation Via Quantum Signal Processing

For Hamiltonian simulation it is convenient to decompose the exponential function the following way, to determine a good polynomial approximation,

$$\mathrm{e}^{\mathrm{i}Ht} = \cos Ht + \mathrm{i}\sin Ht \tag{20}$$

By using the Jacobi–Anger expansion [LC17, CMN+18], it can be stated that,

$$\mathrm{e}^{\mathrm{i}Ht} = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t)T_{2k}(H) + 2\mathrm{i}\sum_{k=0}^{\infty}(-1)^k J_{2k+1}(t)T_{2k+1}(H) \tag{21}$$

To approximate the exponential function, via truncation, within some error margin ε for a d–sparse Hamiltonian, it is sufficient to choose,

$$\tilde{A}(H) = \frac{1}{\alpha}\left(J_0(t) + 2\sum_{k=1}^{r}(-1)^k J_{2k}(t)T_{2k}(H)\right) \tag{22}$$

$$\tilde{C}(H) = \frac{1}{\alpha}\left(2\sum_{k=1}^{r}(-1)^k J_{2k+1}(t)T_{2k+1}(H)\right) \tag{23}$$

where α is such that $|A(H)|, |C(H)| \leq 1$ on the interval $[-1, 1]$. This bounds the query complexity as [LC17],

$$r = \Theta\left(dt\|H\|_{\max} + \frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right) \tag{24}$$

showing that $\tilde{A}(H) + \mathrm{i}\tilde{C}(H)$ satisfies,

$$\max_{x\in[-1,1]}\left|\tilde{A}(x) + \mathrm{i}\tilde{C}(x) - \mathrm{e}^{\mathrm{i}xt}\right| \leq \varepsilon \tag{25}$$

By Theorem 1 phase angles, $\mathbf{\Phi}_{\tilde{A}}$ and $\mathbf{\Phi}_{\tilde{C}}$ can be found that produce the functions above! Constructing these functions and using an instance of LCU as shown in fig. 4 will be sufficient to implement the action of $\tilde{A}(H) + \mathrm{i}\tilde{C}(H)$.

6 Scope

The quantum signal processing technique is powerful and likely to be rooted in future quantum algorithms. There is a rich literature surrounding this topic yet, more work must be done to fully appreciate the different contexts where it is useful. The workflow of fig. 1 shows further general ideas, following immediately from QSP. Notably, the quantum singular value transformation [GSLW19] — a very powerful and general technique to encode non–square matrices. Recent work has generalised QSP [MW23], which focuses on using general SU(2) rotations. Furthermore, an example of QSP has been implemented on noisy quantum hardware [KKC+23].

With regards to Hamiltonian simulation, the QSP algorithm provides an optimal query complexity [LC17], beating previous work: [BCK15] based on quantum walks and [BCC+15] using truncated Taylor series. A more robust query complexity was provided in [GSLW19]:

$$\Theta\left(\alpha|t| + \frac{\log(1/\varepsilon)}{\log(\mathrm{e} + \log(1/\varepsilon)/(\alpha|t|))}\right) \tag{26}$$

Aside from hardware and error correction improvements, perhaps hybrid approaches or Hamiltonian structure exploits can achieve sublinear scaling [CHI+20]. However, for a general Hamiltonian, sublinear scaling is impossible [BACS06] implying QSP is likely optimal!

Acknowledgement

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