Corrected quantum walk for optimal Hamiltonian simulation

Dominic W. Berry[1] and Leonardo Novo[1,2,3]

[1]*Department of Physics and Astronomy, Macquarie University, Sydney, NSW 2109, Australia*
[2]*Physics of Information and Quantum Technologies Group,*
Instituto de Telecomunicações, Lisbon, Portugal and
[3]*Instituto Superior Técnico, Universidade de Lisboa, Portugal*

We describe a method to simulate Hamiltonian evolution on a quantum computer by repeatedly using a superposition of steps of a quantum walk, then applying corrections to correct the weightings for the numbers of steps of the quantum walk. This correction enables us to obtain efficiency which is the same as the lower bound up to double-logarithmic factors for all parameter regimes. The scaling of the complexity is $O\left(\tau \frac{\log\log\tau}{\log\log\log\tau} + \log(1/\epsilon)\right)$ where $\tau := t\|H\|_{\max}d$, for ϵ the allowable error, t the time, $\|H\|_{\max}$ the max-norm of the Hamiltonian, and d the sparseness. This technique should also be useful for improving the scaling of the Taylor series approach to simulation, which is relevant to applications such as quantum chemistry.

I. INTRODUCTION

The simulation of physical quantum systems is a natural application where quantum computers can achieve an exponential speedup (in the dimension of the system), and was Feynman's original motivation for proposing quantum computers [1]. An algorithm for the case of a physical system composed of low-dimensional subsystems and a Hamiltonian that is a sum of interaction Hamiltonians was proposed by Lloyd [2]. An alternative scenario is that where the matrix representing the Hamiltonian is sparse, and there is a procedure for calculating the positions and values of non-zero entries, which can be regarded as an oracle [3]. The advantage of this approach is that it can be used to not just simulate Hamiltonians corresponding to physical systems, but to design other algorithms [4–7]. There have been many papers providing improved algorithms for simulating sparse Hamiltonians [8–16].

One particular approach is that of a quantum walk [10, 13], where a step of the quantum walk can be implemented using an oracle for the Hamiltonian, and has eigenvalues related to that of the Hamiltonian. In Refs [10, 13], the technique was to use phase estimation to estimate the eigenvalue of the quantum walk step, and use that to apply the appropriate eigenvalue for Hamiltonian evolution. Another approach that has been used in many works is that based on a Lie-Trotter product. A more recent improvement is to use a control qubit for each step in the product, and compress the control qubits [14]. Surprisingly, this turns out to be equivalent to an approach based on a Taylor expansion of the exponential for the Hamiltonian evolution [15]. These approaches provide a scaling in the allowable error ϵ that is logarithmic, in contrast to previous approaches which were polynomial in ϵ. The Taylor series approach has also been applied to quantum chemistry [17, 18].

These results motivated an improved approach to quantum walks, where a superposition of different numbers of steps of the quantum walk is used [16]. This approach enables simulations with computational complexity quantified in terms of the number of calls to the oracle for elements of the Hamiltonian

$$O\left(\tau \frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right), \tag{1}$$

where $\tau := t\|H\|_{\max}d$. Here ϵ is the allowable error for the simulation, t is the time that the Hamiltonian evolution is to be simulated over, $\|H\|_{\max}$ is the max-norm of the Hamiltonian, and d is the sparseness of the Hamiltonian, which is the maximum number of nonzero elements in any row or column. In contrast, the lower bound to the complexity is [16]

$$\Omega\left(\tau + \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right). \tag{2}$$

Hence, although there is optimal scaling (up to a logarithmic factor) in any of the parameters individually, the complexity of the algorithm has a product, whereas the lower bound has a sum, so there is room to improve the complexity in the parameter regime where τ is close to $\log(1/\epsilon)$. Note that there is also a complexity in terms of the number of additional gates. We do not consider that complexity here.

Very recently an improved algorithm was given with complexity close to the lower bound [19]. Here we show a different approach that also reduces the complexity to close to the lower bound. The idea is to use the superposition

of different numbers of steps of the quantum walk as in [16], but correct the weightings. The scaling for our approach is

$$O\left(\tau \frac{\log\log\tau}{\log\log\log\tau} + \log(1/\epsilon)\right). \tag{3}$$

Our technique is flexible enough that it can be applied to the Taylor series approach to quantum walks as well (though we will not provide the proof here). The Taylor series approach is important because it can be used for situations like quantum chemistry [17, 18], where the Hamiltonian naturally decomposes into a sum of terms, but it is difficult to construct an oracle to give elements of the Hamiltonian. Another advantage of the Taylor series approach is that it gives better scaling for the number of additional gates (the above scalings are for the number of calls to the oracle for the entries of the Hamiltonian).

In the next Section we provide the theoretical background and a summary of how our method works. Then, in Section III we explain how to use our method with a single round of error correction. In Section IV we explain how to iterate our method with a second round of error correction, to improve the scaling in τ. We conclude in Section V.

II.   BACKGROUND AND SUMMARY OF METHOD

Let U denote the step of the quantum walk approach of [10, 13]. We will not go into the details of how that step is performed here. The crucial feature of that step is that, for an eigenvalue λ of the Hamiltonian H, the step U has eigenvalues

$$\mu_\pm = \pm e^{\pm i \arcsin(\lambda/Xd)}, \tag{4}$$

where X is a constant which needs to satisfy $X \geq \|H\|_{\max}$, and we can take it equal to $\|H\|_{\max}$ for this analysis. The reason why there are two eigenvalues for each eigenvalue of H is that the algorithm first maps the state into two copies of the Hilbert space, and the steps of the quantum walk act on these two copies of the Hilbert space. The inital eigenstate of H, $|\lambda\rangle$, is mapped to a superposition of the corresponding eigenstates of U, $|\mu_+\rangle$ and $|\mu_-\rangle$.

Using the generating function for Bessel functions, it can be shown that [16]

$$\sum_{m=-\infty}^{\infty} J_m(-tXd)\mu_\pm^m = e^{-i\lambda t}. \tag{5}$$

Equivalently we can write that the following two operators are equivalent:

$$\sum_{m=-\infty}^{\infty} J_m(-tXd)U^m \equiv e^{-iHt}. \tag{6}$$

Note that the Hamiltonian acts on a different space than U, so one would need to map from the original Hilbert space to the two copies of the space, apply the superposition of powers of U, then map back to the original Hilbert space to obtain e^{-iHt}. The approach used in [16] is to divide the time into individual *segments*, and for each segment apply a superposition of powers of U with a finite range of m. This superposition of powers can be achieved via control registers and oblivious amplitude amplification (OAA).

The two crucial features are that:

1. the number of steps of OAA will increase with the size of the segment, and

2. the sum over powers of U needs to be over a large enough range that the final error is no greater than the allowable error ϵ.

It is found that the number of steps of OAA will be $O(1)$ if the step size is small enough that the argument of the Bessel function is $O(1)$. That means that the OAA essentially provides no additional factor to the complexity, but the number of segments needs to be $O(tXd)$. Taking $X = \|H\|_{\max}$, this is $O(\tau)$. Then, for each segment, the error can be no larger than $O(\epsilon/\tau)$. The values of Bessel functions are bounded as

$$|J_m(z)| \leq \frac{1}{m!}\left|\frac{z}{2}\right|^{|m|}. \tag{7}$$

The error in the truncation will correspond to the absolute values of the Bessel functions which are omitted. If we truncate at $M > 0$, then the truncated terms will be bounded as [16]

$$2 \sum_{m=M+1}^{\infty} |J_m(z)| \le 4 \frac{1}{(M+1)!} \left| \frac{z}{2} \right|^{M+1}. \tag{8}$$

Using this expression, the error for the segment can be limited to $O(\epsilon/\tau)$ if the scaling of the cutoff is

$$M = O\left(\frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)} \right). \tag{9}$$

In Ref. [16] the overall complexity is then this cutoff multiplied by the number of segments, $O(\tau M)$, which gives the complexity scaling in Eq. (1). Alternatively, consider the case that we were to perform the simulation with a single segment. Then the error could be bounded as $O(\epsilon)$ with M chosen scaling as $O(\tau + \log(1/\epsilon))$. If we were to attempt simulation via this single segment, then the probability of success would be small, and we would incur a large overhead for OAA.

Our method is to instead perform a number of shorter segments with a weaker constraint on the error, and then perform a correction at the end after the segments in order to adjust the coefficients of the powers of U to be closer to Bessel functions as in Eq. (5). The cutoff for the individual segments need not be large enough to give a final error $O(\epsilon)$, and it is only the correction at the end that needs to have a large cutoff. This eliminates the multiplying factor depending on ϵ from the complexity, giving the same advantage as using a single segment. Moreover, the OAA can still be performed in a single step for each segment, so there is no significant overhead from OAA as there would be if we were to use a single large segment.

The reason why this approach works is that the OAA gives an effective operation which is [15]:

$$\frac{3}{s} \tilde{V} - \frac{4}{s^3} \tilde{V} \tilde{V}^\dagger \tilde{V}, \tag{10}$$

where $\tilde{V}$ is the sum of powers of U used to approximate the Hamiltonian evolution, and $1/s$ is the amplitude for success. The successful application of this operation is flagged by an ancilla in the zero state. The value of s depends on the size of the segment, and we will choose the size of the segment so that $s = 2$. The important thing to note here is that the modified operation is still a sum of powers of U. What this means is that after performing the OAA we have still performed an operation that is a sum of powers of U. As this is done for each segment, at the end the overall operation is still a sum of powers of U. This sum of powers of U is something that we can easily calculate, and we can compare this to the weightings that we would want in order to accurately simulate the Hamiltonian evolution.

At the end we can apply another operation that is a sum of powers of U to correct the weightings, and reduce the error to order ϵ. If the truncation of this sum of powers is of the same order as the maximum power of U for the operations that have been performed so far, then this correction will only give a constant multiplying factor to the complexity. What is more, this correction will have most of its weight on $m = 0$ (the identity), which means that the probability of success is high. This means that only a modest number of steps of OAA are needed, with only an additional constant factor overhead. A limiting factor is that the cutoff for the segments needs to be chosen such that the final correction has most of its weight on the identity, and a single step of OAA is sufficient. This means that the error in the individual segments needs to be $O(1/\tau)$, so the cutoff is

$$M = O\left(\frac{\log \tau}{\log\log \tau} \right). \tag{11}$$

Multiplying by the number of segments, this gives a factor in the complexity of

$$O\left(\tau \frac{\log \tau}{\log\log \tau} \right). \tag{12}$$

Another limiting factor is that the final error needs to be $O(\epsilon)$. In the case where ϵ is small, it may be necessary to increase the cutoff for the final correction. It is also convenient to increase M, though M does not need to scale with ϵ. It turns out that it is sufficient to choose $M\tau = O(\log(1/\epsilon))$, which gives the $O(\log(1/\epsilon))$ term in the final scaling.

The discussion so far is for a single round of error correction, which is addressed in detail in the next Section. It is also possible to repeatedly perform error correction, then perform a final round of error correction at the end. If we perform error correction after $O(\log \tau)$ segments, then the cutoff for each segment need only be

$$M = O\left(\frac{\log\log \tau}{\log\log\log \tau} \right). \tag{13}$$

That is what gives our double-log factor in the final result. The details of this double round of error correction are given in Section IV.

III.   A SINGLE ROUND OF ERROR CORRECTION

The specific results we derive for a single round of correction are as in the following theorem.

Theorem 1. *A d-sparse Hamiltonian H acting on n qubits can be simulated for time t within error ϵ with*

$$O\left(\tau\frac{\log\tau}{\log\log\tau} + \log(1/\epsilon)\right) \tag{14}$$

queries, where $\tau := t\|H\|_{\max}d$.

To compare this result with the results of [16], the algorithm in that work had complexity

$$O\left(\tau\frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right), \tag{15}$$

and a lower bound on the complexity

$$O\left(\tau + \frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right). \tag{16}$$

These bounds differ most significantly in the regime where τ is comparable to $\log(1/\epsilon)$. In this regime the previous algorithm gives complexity approximately $O(\tau^2 \log \tau)$, whereas the complexity from Theorem 1 scales as $\tau \log \tau$, which is close to a square root improvement.

In order to prove this result, we first prove a number of intermediate lemmas. The first lemma shows that the absolute values of the coefficients for the correction may be bounded. This is needed in order to show that the correction only needs a single step of OAA. In the following lemmas we define z_M for $M \geq 2$ to be the first positive solution of

$$\sum_{m=-M}^{M} |J_m(z_M)| = 2. \tag{17}$$

The first few values are $z_2 = 1.2291$, $z_3 = 1.1205$, $z_4 = 1.1096$, $z_5 = 1.1085$. The following lemmas require that these values of z are used.

Lemma 2. *Consider simulating Hamiltonian evolution using r segments, where each segment uses a cutoff of M on the number of steps of the quantum walk and uses OAA. Then the coefficients a_m required for a correction operator of the form*

$$V_C(U) = \sum_{m=-\infty}^{\infty} a_m U^m \tag{18}$$

to yield the exact evolution satisfy

$$\sum_{m=-\infty}^{\infty} |a_m| \lesssim \left(1 - 2\sum_{|m|>M} |J_m(z_M)|\right)^{-r}, \tag{19}$$

where $\lesssim$ indicates that higher-order terms in $\sum_{|m|>M} |J_m(z_M)|$ have been omitted.

Proof. For each segment we use a value z and a cutoff M, so the operation we attempt to perform is

$$\tilde{V}(U) := \sum_{m=-M}^{M} J_m(z_M)U^m. \tag{20}$$

It is convenient to write this operation as a function of U, because we will require particular features of the function. In particular, for a function of the form $F(x) = \sum_n F_n x^n$, we define the functional s by

$$s(F) := \sum_n |F_n|. \tag{21}$$

The choice of the coefficients of the function $\tilde{V}$ ensures that $s(\tilde{V}) = 2$. Similarly, we will write the operation that provides the exact evolution for that time interval as the function

$$V(U) = \sum_{m=-\infty}^{\infty} J_m(z_M)U^m. \tag{22}$$

Because $s(\tilde{V}) = 2$, using a single step of OAA, the operation is $V_{\text{oaa}}(U)$, with

$$V_{\text{oaa}} := \frac{3}{2}\tilde{V} - \frac{1}{2}\tilde{V}\tilde{V}^\dagger\tilde{V}. \tag{23}$$

It is also convenient to define

$$\Delta := V - \tilde{V}. \tag{24}$$

After performing $V_{\text{oaa}}(U)$ a number of times given by r, the actual operation is $[V_{\text{oaa}}(U)]^r$, but the desired operation is $[V(U)]^r$. A correction that will yield the exact operation is given implicitly by

$$V^r = V_C V_{\text{oaa}}^r. \tag{25}$$

This means that we must have

$$V_C = (V^\dagger V_{\text{oaa}})^{-r}$$
$$= \left(\frac{3}{2}V^\dagger\tilde{V} - \frac{1}{2}V^\dagger\tilde{V}(V^\dagger\tilde{V})^\dagger V^\dagger\tilde{V}\right)^{-r}$$
$$= (\mathbb{1} - W)^{-r}$$
$$= \sum_{k=0}^{\infty} \binom{r+k-1}{r-1} W^k, \tag{26}$$

where

$$W = \frac{1}{2}\left(V^\dagger\Delta - \Delta^\dagger\tilde{V} + V^\dagger\Delta V^\dagger\Delta + V^\dagger\Delta\Delta^\dagger\tilde{V}\right) \tag{27}$$
$$= \frac{1}{2}\left[\tilde{V}^\dagger\Delta - \Delta^\dagger\tilde{V} + \Delta^\dagger\Delta + (\tilde{V}^\dagger)^2\Delta^2 + (\Delta^\dagger)^2\Delta^2 + 2\tilde{V}^\dagger\Delta^\dagger\Delta^2 + \tilde{V}^\dagger\tilde{V}\Delta\Delta^\dagger + \tilde{V}\Delta(\Delta^\dagger)^2\right]. \tag{28}$$

It is straightforward to show that the functional s satisfies the properties, for functions of U denoted F and G and α and β scalars,

$$s(\alpha F + \beta G) \leq |\alpha|s(F) + |\beta|s(G) \tag{29}$$
$$s(FG) \leq s(F)s(G). \tag{30}$$

To show the first result, for

$$F(x) = \sum_n F_n x^n, \qquad G(x) = \sum_n G_n x^n, \tag{31}$$

we have

$$s(\alpha F + \beta G) = \sum_n |\alpha F_n + \beta G_n|$$
$$\leq |\alpha|\sum_n |F_n| + \beta\sum_n |G_n|$$
$$= |\alpha|s(F) + |\beta|s(G). \tag{32}$$

For the product,

$$(FG)(x) = \sum_n \sum_k F_{n-k}G_k x^n, \tag{33}$$

so

$$s(FG) = \sum_n \left| \sum_k F_{n-k} G_k \right|$$

$$\leq \sum_n \sum_k |F_{n-k}| \times |G_k|$$

$$= \sum_n |F_n| \sum_m |G_m|$$

$$= s(F)s(G). \tag{34}$$

In addition, if F and G are sums over disjoint sets of powers of U, then

$$s(\alpha F + \beta G) = |\alpha| s(F) + |\beta| s(G). \tag{35}$$

Therefore, we immediately obtain

$$s(\Delta) = s(V - \tilde{V}) = \sum_{|m|>M} |J_m(z_M)|. \tag{36}$$

In addition we have $s(V) = 2$. Therefore, using the expression (28) for W, and the properties of the functional s,

$$s(W) \leq 2s(\Delta) + 9[s(\Delta)]^2 + 6[s(\Delta)]^3 + [s(\Delta)]^4. \tag{37}$$

Hence we have

$$s(V_C) \leq [1 - 2s(\Delta)]^{-r} + O\left(r\,[s(\Delta)]^2\right). \tag{38}$$

Using Eq. (36) we therefore obtain the result (19) required for the Lemma. $\qquad\square$

In reality we will perform a truncated operator $\tilde{V}_C(U)$ which has the higher powers of U truncated, but from the definition $s(\tilde{V}_C) \leq s(V_C)$. Therefore the result in Lemma 2 means that the value of r such that the sum over $|a_m|$ is approximately bounded by 2 is

$$r \approx \frac{\log 2}{2\sum_{|m|>M} |J_m(z_M)|}. \tag{39}$$

Next we prove a lemma bounding the error due to truncating the superposition for the correction.

Lemma 3. *Consider simulating Hamiltonian evolution using r segments, where each segment uses a cutoff of M on the number of steps of the quantum walk and uses OAA. Provided $M \geq 2$, the coefficients a_m required for a correction operator of the form*

$$V_C(U) = \sum_{m=-\infty}^{\infty} a_m U^m \tag{40}$$

to yield the exact evolution satisfy

$$\sum_{|m|>N} |a_m| \lesssim 2^{r+1} \left(\frac{z_M \zeta}{M}\right)^{N+1}, \tag{41}$$

where $\zeta \approx 1.8$ is the solution of $e^{1+1/2\zeta} = 2\zeta$, and N is a non-negative integer.

Proof. There is an important symmetry of the coefficients that appear in all stages of the algorithm: we have sums over powers of U of the form $\sum_n c_n U^n$ where $c_{-n} = (-1)^n c_n$. This symmetry holds for the initial Bessel function weighting, and it must also be true for any products of sums of this form. This may be shown via

$$\sum_m c_m U^m \sum_k d_k U^k = \sum_n \left(\sum_m c_m d_{n-m}\right) U^n$$

$$= \sum_n \left(\sum_m (-1)^m c_{-m} (-1)^{n-m} d_{-(n-m)} \right) U^n$$

$$= \sum_n (-1)^n \left(\sum_m c_{-m} d_{-(n-m)} \right) U^n$$

$$= \sum_n (-1)^n \left(\sum_m c_m d_{n-m} \right) U^{-n}, \tag{42}$$

where in the last line the substitution $m \mapsto -m$ and $n \mapsto -n$ has been made. Because the amplitude amplified operation $V_{\mathrm{oaa}}(U)$ has a sum of products of the original operation with Bessel function weightings, its coefficients also satisfy this symmetry. In turn the coefficients a_m satisfy this symmetry.

A trick to bound the sum over $|a_m|$ is to define a modified function V_C^+, which is the same as V_C except with the absolute values of the coefficients, and consider $V_C^+(x)$, where x is real and positive. Using $|a_m| = |a_{-m}|$ and assuming that $x \geq 1$, we obtain

$$\sum_{|m|>N} |a_m| = 2 \sum_{m=N+1}^{\infty} |a_m|$$

$$\leq \frac{2}{x^{N+1}} \sum_{m=N+1}^{\infty} |a_m| x^m$$

$$\leq \frac{2}{x^{N+1}} V_C^+(x), \tag{43}$$

where $V_C^+(x) := \sum_{m=-\infty}^{\infty} |a_m| x^m$. Note that in this expression we can take N to be any integer ≥ 0. To upper bound $V_C^+(x)$ we can use the expression (26) together with (27), and take the absolute values of all coefficients in Eq. (27). That is,

$$V_C^+(x) \leq \sum_{k=0}^{\infty} \binom{r+k-1}{r-1} [W_+(x)]^k$$

$$= [1 - W_+(x)]^{-r}, \tag{44}$$

where W_+ is the function W modified to take the absolute values of all coefficients.

Using Eq. (27), we obtain

$$W_+(x) \leq \frac{1}{2} \left[\sum_{q=-\infty}^{\infty} |J_q(z_M)| x^{-q} \sum_{|n|>M} |J_n(z_M)| x^n + \sum_{|n|>M} |J_n(z_M)| x^{-n} \sum_{q=-M}^{M} |J_q(z_M)| x^q \right.$$

$$+ \left(\sum_{q=-\infty}^{\infty} |J_q(z_M)| x^{-q} \sum_{|n|>M} |J_n(z_M)| x^n \right)^2$$

$$\left. + \sum_{q=-\infty}^{\infty} |J_q(z_M)| x^{-q} \sum_{|n|>M} |J_n(z_M)| x^n \sum_{|m|>M} |J_m(z_M)| x^{-m} \sum_{p=-M}^{M} |J_p(z_M)| x^p \right]$$

$$\leq \sum_{q=-\infty}^{\infty} |J_q(z_M)| x^q \sum_{|n|>M} |J_n(z_M)| x^n + \left(\sum_{q=-\infty}^{\infty} |J_q(z_M)| x^q \sum_{|n|>M} |J_n(z_M)| x^n \right)^2. \tag{45}$$

We will take $x = M/(z_M \zeta)$, where $\zeta \approx 1.8$ is the solution of $e^{1+1/2\zeta} = 2\zeta$. This number can be obtained as $1/(2 \operatorname{ProductLog}[1/e])$ in Mathematica. It is then easy to check numerically that the right-hand side (RHS) of (45) is no greater than $1/2$. It is equal to 0.215968 for $M = 2$, 0.0557057 for $M = 3$, and decreases thereafter.

To address this bound analytically, we can use the upper bound

$$|J_m(z)| \leq \frac{1}{|m|!} \left| \frac{z}{2} \right|^{|m|}. \tag{46}$$

Using this upper bound gives

$$\sum_{m=-\infty}^{\infty} |J_m(z_M)|x^m \le e^{xz_M/2} + (e^{z_M/2x} - 1), \tag{47}$$

and

$$\sum_{|m|>M} |J_m(z_M)|x^m \le 2\frac{(xz_M/2)^{M+1}}{(M+1)!} + 2\frac{(z_M/2x)^{M+1}}{(M+1)!}, \tag{48}$$

provided that $xz_M \le M + 2$ and $z_M/x \le M + 2$. We take $x = M/(z_M\zeta)$, in which case the inequalities are satisfied. For $M > 2$ the second terms in Eqs (47) and (48) are much smaller and may be omitted. Keeping the lowest-order term in the expansion of $W_+(x)$, Eqs (43) and (44) give

$$\sum_{|m|>N} |a_m| \lesssim \frac{2}{x^{N+1}} \left\{ 1 - 2\frac{(xz_M/2)^{M+1}}{(M+1)!} e^{xz_M/2} \right\}^{-r}. \tag{49}$$

Using $x = M/(z_M\zeta)$ and Stirling's approximation, it can be shown that the second term in the braces decreases with M, and is less than $1/2$. This part of the derivation is for $M > 2$, and for the case $M = 2$ it is easily checked numerically that the expression is no greater than $1/2$. The choise of ζ is so that the asymptotic expression decreases with M. Hence the expression in braces is $\ge 1/2$, so we get Eq. (41), which was required to be demonstrated. □

If we want the correction to give no more than a factor of 2 to the complexity, we can choose $N = 3rM$, so

$$\sum_{|m|>N} |a_m| \lesssim 2^{r+1} \left(\frac{z_M\zeta}{M} \right)^{3rM+1}. \tag{50}$$

Since this sum of terms gives the order of the error when the correction is used, we have an error from this correction that is exponentially small, as expected. If we require higher accuracy, we could increase N so there are more terms in the correction. However, it is also possible to obtain higher accuracy by increasing M. Since that does not increase the complexity (except for a factor of 2) until $N = 3rM$, it is advantageous to simply take $N = 3rM$.

Next we can prove the overall result for the simulation with the correction.

Proof of Theorem 1. The algorithm proceeds by performing r segments, where each segment uses a superposition of powers of the step of the quantum walk with a cutoff of M together with OAA. Then the correction uses a sum over powers of U truncated at $N = 3rM$, with weightings a_m

$$\tilde{V}_C(U) = \sum_{m=-N}^{N} a_m U^m. \tag{51}$$

Then OAA is used on the entire operation to obtain success probability near 1.

The complexity in this Theorem is obtained from two requirements. First, we require M to be sufficiently large that $s(\tilde{V}_C)$ is not larger than 2, so we can perform OAA with a single step. Second, we require that the error at the end is no greater than ϵ.

For the OAA,

$$s(\tilde{V}_C) = \sum_{m=-N}^{N} |a_m|. \tag{52}$$

This is because the operation performed prior to OAA has a $1/s(\tilde{V}_C)$ factor on the amplitude for success. Note also that the correction operation corrects the amplitude. That is, the OAA for each of the individual segments will give amplitudes not exactly equal to 1, because the operation is not exactly unitary. The failures are flagged by an orthogonal state in the ancilla. In the case of success, the correction operation boosts the amplitude for success to near 1, provided we are performing the reflections on the intermediate ancillas for the segments and the correction. Hence $s(\tilde{V}_C)$ takes account of the cost of boosting the success probability for the segments as well as the correction, and these do not need to be considered separately.

Using the result of Lemma 2, there is the upper bound

$$
s(\tilde{V}_C) \lesssim \left(1 - 2 \sum_{|m|>M} |J_m(z_M)| \right)^{-r}
$$

$$
\approx \exp \left(2r \sum_{|m|>M} |J_m(z_M)| \right). \tag{53}
$$

Therefore we may obtain $s(\tilde{V}_C) \lesssim 2$ for

$$
r \lesssim \frac{\log 2}{2 \sum_{|m|>M} |J_m(z_M)|}. \tag{54}
$$

Using the inequality

$$
\frac{\log 2}{2 \sum_{|m|>M} |J_m(z_M)|} \gtrsim \frac{(M+1)! \log 2}{8|z_M/2|^{M+1}}, \tag{55}
$$

we find that provided

$$
r \lesssim \frac{(M+1)! \log 2}{8|z_M/2|^{M+1}} \tag{56}
$$

is satisfied, we still obtain $s(\tilde{V}_C) \lesssim 2$. This is because Eq. (56) together with Eq. (55) implies Eq. (54). In order to obtain a simulation for overall time t, we require $r = \Theta(tXd)$, where X can be taken equal to $\|H\|_{\max}$, and therefore $r = \Theta(\tau)$. According to Eq. (56), we can obtain $s(\tilde{V}_C) \lesssim 2$ with $M = \Theta(\log \tau / \log \log \tau)$.

Next we consider the criterion that the error be no larger than ϵ, which may possibly require a larger value of M. Using Lemma 3, we have

$$
\sum_{|m|>N} |a_m| \lesssim 2^{r+1} \left(\frac{z_M \zeta}{M} \right)^{3rM+1}. \tag{57}
$$

This expression gives the scaling in the error after the correction. Using Eq. (28), the error after OAA is of the same order.

Now, if the RHS is less than the allowable error ϵ for $M = 2$, then we immediately have the error appropriately bounded with complexity $O(\log \tau / \log \log \tau)$. Otherwise we need to increase M, in which case $M > z_M \zeta$. Since $3rM$ is the same as the complexity up to a multiplicative factor, the complexity required to ensure the error is no larger than ϵ is $O(\log(1/\epsilon))$. Together with taking $M = \Theta(\log \tau / \log \log \tau)$ to ensure that $s(\tilde{V}_C) \lesssim 2$, we obtain a complexity of

$$
O \left(\tau \frac{\log \tau}{\log \log \tau} + \log(1/\epsilon) \right). \tag{58}
$$

$\square$

IV. TWO ROUNDS OF ERROR CORRECTION

Next we consider how to perform a second round of correction. That is, we perform multiple segments followed by a correction as in the previous section, and repeat multiple times, then perform a correction. This technique enables the scaling given in the following Theorem.

Theorem 4. *A d-sparse Hamiltonian H acting on n qubits can be simulated for time t within error ϵ with*

$$
O \left(\tau \frac{\log \log \tau}{\log \log \log \tau} + \log(1/\epsilon) \right) \tag{59}
$$

queries, where $\tau := t\|H\|_{\max} d$.

In order to show this result, we again need to show a number of intermediate results. The first is a bound on the magnitudes of the individual coefficients a_m, rather than the sum.

Lemma 5. *Consider simulating Hamiltonian evolution using r repetitions, where each repetition uses a cutoff of M on the number of steps of the quantum walk and uses OAA. For $M \geq 2$, the coefficients a_m required for a correction operator*

$$V_C(U) = \sum_{m=-\infty}^{\infty} a_m U^m \tag{60}$$

to yield the exact evolution satisfy

$$|a_m| \lesssim 2^r \left(\frac{z_M \zeta}{M}\right)^{|m|}, \tag{61}$$

where $\zeta \approx 1.8$ is the solution of $e^{1+1/2\zeta} = 2\zeta$.

Proof. Similar to Eq. (43), for $x \geq 1$,

$$
\begin{aligned}
|a_m| &\leq \sum_{n=|m|}^{\infty} |a_n| \\
&\leq \frac{1}{x^{|m|}} \sum_{n=|m|}^{\infty} |a_n| x^n \\
&\leq \frac{1}{x^{|m|}} V_C^+(x).
\end{aligned} \tag{62}
$$

In exactly the same way as in the proof of Lemma 3, we can take $x = M/(z_M \zeta)$, and $V_C^+(x) \leq 2^r$. We then obtain Eq. (61) as required. $\qquad\square$

This result shows that the $|a_m|$ exponentially decrease, so we can use this to show that the sum over $|a_m|$ is properly bounded, and we can even bound a sum over $|a_m| x^m$. The key relation we have used is Eq. (48), which bounds the difference of the coefficients of the ideal sequence and the sequence we have just performed. Therefore, if we can bound that for the corrected series, then we can show that the recursion works.

The particular result we find is as in the following Lemma.

Lemma 6. *Consider a compound segment composed of r segments and a correction, where each segment uses a cutoff of $M \geq 2$ on the number of steps of the quantum walk and uses OAA. The correction uses coefficients a_m, which are required for a correction operator of the form*

$$V_C(U) = \sum_{m=-\infty}^{\infty} a_m U^m \tag{63}$$

to yield the exact evolution, but these coefficients are truncated at $N = 3Mr$. After performing r' repetitions of this compound segment, we then perform a correction with coefficients a'_m required for a correction operator of the form

$$V'_C(U) = \sum_{m=-\infty}^{\infty} a'_m U^m \tag{64}$$

to yield the exact evolution. Provided M is chosen such that

$$r \leq \frac{\log 2}{2 \sum_{|m|>M} |J_m(z_M)|}. \tag{65}$$

the coefficients satisfy

$$\sum_{m=-\infty}^{\infty} |a'_m| \lesssim \left\{1 - 2 \sum_{|m|>N} |a_m|\right\}^{-r'}. \tag{66}$$

Proof. First we define operators for what is achieved with r steps and correction for the compound segment, in a similar way as we did for the first round of correction. We use primed variables to indicate the new variable names corresponding to those for the first round of correction. The exact operation, if there were perfect correction on the compound segment, is denoted V', and the actual operation performed is denoted $\tilde{V}'$. The difference is denoted Δ', and $\Delta' = \tilde{V}' - V'$. As before these are all functions of the step operator U. These functions may be written as

$$V' = V_C V_{\text{oaa}}^r$$
$$\tilde{V}' = \tilde{V}_C V_{\text{oaa}}^r$$
$$\Delta' = \left(V_C - \tilde{V}_C\right) V_{\text{oaa}}^r. \tag{67}$$

Following exactly the same derivation for these primed quantities as in the proof of Lemma 2, we have

$$V_C' = \sum_{k=0}^{\infty} \binom{r+k-1}{r-1} W'^k, \tag{68}$$

where

$$W' = \frac{1}{2}\left(V'^\dagger \Delta' - \Delta'^\dagger \tilde{V}' + V'^\dagger \Delta' V'^\dagger \Delta' + V'^\dagger \Delta' \Delta'^\dagger \tilde{V}'\right). \tag{69}$$

We can rewrite W' as

$$W' = \frac{1}{2}(V_{\text{oaa}}^\dagger V_{\text{oaa}})^r \left(V_C^\dagger \Delta_C - \Delta_C^\dagger \tilde{V}_C\right) + \frac{1}{2}(V_{\text{oaa}}^\dagger V_{\text{oaa}})^{2r} \left(V_C^\dagger \Delta_C V_C^\dagger \Delta_C + V_C^\dagger \Delta_C \Delta_C^\dagger \tilde{V}_C\right), \tag{70}$$

where $\Delta_C := V_C - \tilde{V}_C$. Next, $V_{\text{oaa}}^\dagger V_{\text{oaa}}$ can be expanded as

$$\begin{aligned}
V_{\text{oaa}}^\dagger V_{\text{oaa}} &= \left[\frac{3}{2}\tilde{V}^\dagger - \frac{1}{2}\tilde{V}^\dagger \tilde{V} \tilde{V}^\dagger\right]\left[\frac{3}{2}\tilde{V} - \frac{1}{2}\tilde{V}\tilde{V}^\dagger \tilde{V}\right] \\
&= \frac{9}{4}\tilde{V}^\dagger \tilde{V} - \frac{3}{2}(\tilde{V}^\dagger \tilde{V})^2 + \frac{1}{4}(\tilde{V}^\dagger \tilde{V})^3 \\
&= \mathbb{1} - \frac{3}{2}\Delta^\dagger \Delta + \frac{3}{4}(\Delta^\dagger \Delta)^2 - \frac{1}{4}(\Delta^\dagger \Delta)^3 - \frac{3}{4}\left((\tilde{V}^\dagger \Delta)^2 + (\Delta^\dagger \tilde{V})^2\right) \\
&\quad - \frac{1}{4}\left((\tilde{V}^\dagger \Delta)^3 + (\Delta^\dagger \tilde{V})^3\right) - \frac{3}{4}\Delta^\dagger \Delta\left(\Delta^\dagger \tilde{V} + \tilde{V}^\dagger \Delta\right).
\end{aligned} \tag{71}$$

Therefore, using the properties of the functional s and $s(\tilde{V}) = 2$,

$$\begin{aligned}
s(V_{\text{oaa}}^\dagger V_{\text{oaa}}) &\leq 1 + \frac{3}{2}[s(\Delta)]^2 + \frac{3}{4}[s(\Delta)]^4 + \frac{1}{4}[s(\Delta)]^6 + 6[s(\Delta)]^2 + 4[s(\Delta)]^3 + 3[s(\Delta)]^3 \\
&= 1 + \frac{15}{2}[s(\Delta)]^2 + 7[s(\Delta)]^3 + \frac{3}{4}[s(\Delta)]^4 + \frac{1}{4}[s(\Delta)]^6.
\end{aligned} \tag{72}$$

Given that we have chosen M so that Eq. (39) holds, we have

$$\begin{aligned}
s\left((V_{\text{oaa}}^\dagger V_{\text{oaa}})^r\right) &\leq \left(1 + \frac{15}{2}[s(\Delta)]^2 + O\left([s(\Delta)]^3\right)\right)^{\frac{\log 2}{2s(\Delta)}} \\
&= 1 + \frac{15}{4}(\log 2)s(\Delta) + O\left([s(\Delta)]^2\right).
\end{aligned} \tag{73}$$

In addition, the choice of r ensures that $s(V_C) \leq 2$. Hence we have

$$s(W') \leq 2s(\Delta_C) + 4[s(\Delta_C)]^2 + O\left([s(\Delta)]^2 s(\Delta_C)\right). \tag{74}$$

Using Eq. (68) we then have

$$s(V_C') \lesssim [1 - 2s(\Delta_C)]^{-r'}. \tag{75}$$

Recognising that $s(\Delta_C) \leq \sum_{|m|>N} |a_m|$, this gives the result required. $\qquad\square$

Using Lemma 3, and taking $N = 3rM$, we then find that we can take r' satisfying

$$r' \lesssim \frac{\log 2}{2^{r+2}} \left(\frac{M}{z_M \zeta} \right)^{3rM+1}, \tag{76}$$

and obtain $s(V_C') \leq 2$. This expression is the equivalent of Eq. (56). Next we prove a Lemma bounding the size of the error.

Lemma 7. *Consider a compound segment composed of r segments and a correction, where each segment uses a cutoff of $M \geq 2$ on the number of steps of the quantum walk and uses OAA. The correction uses coefficients a_m, which are required for a correction operator*

$$V_C(U) = \sum_{m=-\infty}^{\infty} a_m U^m \tag{77}$$

to yield the exact evolution, but these coefficients are truncated at $N = 3Mr$. After performing r' repetitions of this compound segment, we then perform a correction with coefficients a_m' required for a correction operator of the form

$$V_C'(U) = \sum_{m=-\infty}^{\infty} a_m' U^m \tag{78}$$

to yield the exact evolution. These coefficients satisfy

$$\sum_{|m|>N'} |a_m'| \lesssim 2^{r'} \left(\frac{z_M \zeta \zeta' 2^{1/M}}{M} \right)^{N'+1}, \tag{79}$$

where $\zeta \approx 1.8$ is the solution of $e^{1+1/2\zeta} = 2\zeta$ and $\zeta' \approx 1.5$ is a solution of $\zeta'^5 (\sqrt{2} - 2\zeta')^2 = 16\sqrt{2}$.

Proof. In the same way as for Lemma 3, we have

$$\sum_{|m|>N} |a_m'| \leq \frac{2}{x^{N+1}} V_C^{+'}(x), \tag{80}$$

where $V_C^{+'}(x) := \sum_{m=-\infty}^{\infty} |a_m'| x^m$. This function satisfies

$$V_C^{+'}(x) \leq \left[1 - W_+'(x) \right]^{-r}, \tag{81}$$

where W_+' is the function W' modified to take the absolute values of all coefficients.

To bound $W_+'(x)$, we can use Eq. (70) and Eq. (71). For $V_{\text{oaa}}^\dagger V_{\text{oaa}}$ with the absolute values of all coefficients taken, it will be upper bounded by

$$1 + \frac{3}{2}\delta^2 + \frac{3}{4}\delta^4 + \frac{1}{4}\delta^6 + \frac{3}{2}\nu^2\delta^2 + \frac{1}{2}\nu^3\delta^3 + \frac{3}{2}\nu\delta^3, \tag{82}$$

where

$$\nu := \sum_{q=-M}^{M} |J_q(z_M)| x^q, \tag{83}$$

$$\delta := \sum_{|n|>M} |J_n(z_M)| x^n. \tag{84}$$

These expressions are upper bounded in Eqs (47) and (48). It was found that for $x \leq M/(z_M\zeta)$, $\nu\delta < 1/2$. In addition, for this choice of x, $\nu \gg 1$ and $\delta \ll 1$, so the overall value will be no greater than 2. Then, using (70), we obtain

$$W_+'(x) \leq 2^r \sum_{q=-\infty}^{\infty} |a_q| x^q \sum_{|n|>N} |a_n| x^n + \left(2^r \sum_{q=-\infty}^{\infty} |a_q| x^q \sum_{|n|>N} |a_n| x^n \right)^2. \tag{85}$$

Note that we can use $|a_m| = |a_{-m}|$ due to symmetry. Then, using the bound (61), we get

$$\sum_{|n|>N} |a_n| x^n \leq \frac{2^{r+1}}{1 - z_M \zeta x/M} \left(\frac{z_M \zeta x}{M} \right)^{N+1}. \tag{86}$$

Similarly the sum over all powers can be bounded as

$$\sum_{q=-\infty}^{\infty} |a_q| x^q \leq \frac{2^{r+1}}{1 - z_M \zeta x/M} \left(\frac{z_M \zeta x}{M} \right) + 2^r, \tag{87}$$

or alternatively

$$\sum_{q=-\infty}^{\infty} |a_q| x^q \leq \frac{2^{r+1}}{1 - z_M \zeta x/M}. \tag{88}$$

Therefore we have

$$\sum_{|m|>N'} |a'_m| \lesssim \frac{1}{x^{N'+1}} \left\{ 1 - 4 \frac{2^{3r}}{(1 - z_M \zeta x/M)^2} \left(\frac{z_M \zeta x}{M} \right)^{N+1} \right\}^{-r'}. \tag{89}$$

We now wish to take x to be slightly less than $M/(z_M \zeta 2^{1/M})$, so that the expression in braces is $\geq 1/2$. In particular we take $x = M/(z_M \zeta \zeta' 2^{1/M})$, where $\zeta' \approx 1.52937$ is a solution of $\zeta'^5(\sqrt{2} - 2\zeta')^2 = 16\sqrt{2}$. Then we obtain

$$\sum_{|m|>N'} |a'_m| \lesssim \left(\frac{z_M \zeta \zeta' 2^{1/M}}{M} \right)^{N'+1} 2^{r'}. \tag{90}$$

$\square$

We are now in a position to prove the Theorem for the complexity.

Proof of Theorem 4. As described in the previous two Lemmas, the simulation proceeds by using compound segments, where each segment uses r segments and a correction. We perform r' of these compound segments, followed by an overall correction. Now the overall length of the simulation is rr', so we require $rr' = \tau$.

Now we have three requirements:

1. The corrections for the compound segments satisfy $s(V_C) \leq 2$, so OAA can be performed in one step.

2. The final correction satisfies $s(V'_C) \leq 2$, so the final OAA can be performed in one step.

3. The error as obtained in Lemma 7 is upper bounded by ϵ.

Considering the first requirement, let us take

$$M = \Theta \left(\frac{\log \log \tau}{\log \log \log \tau} \right). \tag{91}$$

Then we have Eq. (39) satisfied for $r = \Theta(\log \tau)$, which implies that $s(V_C) \leq 2$. Second, we find that we have Eq. (76) satisfied with $r' = \tau/r$. Then we obtain $s(V'_C) \leq 2$ for the final OAA, and $rr' = \tau$ as required. Because the complexity is $rr'M$ up to multiplying factors, this gives a contribution of

$$O \left(\tau \frac{\log \log \tau}{\log \log \log \tau} \right) \tag{92}$$

to the complexity.

Finally we consider the third requirement. We can choose $N' = 9rr'M$ without changing the complexity. Now if the expression on the RHS of Eq. (79) in Lemma 7 is less than ϵ, then we have satisfied this requirement. Otherwise we can further increase M in order to obtain error no greater than ϵ. The overall complexity is equal to N' up to multiplying factors. We can obtain the RHS of Eq. (79) less than ϵ by taking $N' = O(\log(1/\epsilon))$. Hence the overall complexity sufficient to satisfy both requirements is as given in Eq. (59). $\square$

V. CONCLUSIONS

We have shown how to perform corrections on the superposition of quantum walk steps approach to Hamiltonian simulation from Ref. [16]. This approach gives a result much closer to the lower bound for complexity than Ref. [16], because it has a sum rather than a product in the scaling of the complexity. Our result is very close to the lower bound for the complexity in Ref. [16], except our result differs by double-logarithmic factors for the scaling in τ and ϵ. Our result is also very close to the complexity of the algorithm very recently obtained in Ref. [19]

Our approach to correcting the quantum walk is sufficiently flexible that it can be used to perform an arbitrary number of rounds of correction. That should provide scaling of the complexity with further iterated logarithms of τ, though not strictly linear scaling in τ. Proving the complexity scaling is quite complicated, so we have limited to analyzing two rounds of correction here. Our approach is also flexible enough that it can be applied to correction of the Taylor series approach to Hamiltonian simulation of Ref. [16]. That is another important case, because it seems more useful for quantum chemistry, and also has better scaling in the number of additional gates.

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