EVALUATION OF EXPONENTIAL SUMS AND Riemann Zeta Function on Quantum Computer

SANDEEP TYAGI

Abstract. We show that exponential sums (ES) of the form

\[ S(f, N) = \sum_{k=0}^{N-1} \sqrt{w_k} e^{2\pi i f(k)}, \]

can be efficiently carried out with a quantum computer (QC). Here \( N \) can be exponentially large, \( w_k \) are real numbers such that \( \sum_{k=0}^{N-1} w_k = 1 \) and \( f(x) \) is a real function, that is assumed to be easily implementable on a QC. As an application of the technique, we show that Riemann zeta (RZ) function, \( \zeta(\sigma + it) \) in the critical strip, \( \{0 \leq \sigma < 1, t \in \mathbb{R}\} \), can be obtained in \( \text{polyLog}(t) \) time. In another setting, we show that RZ function can be obtained with a scaling \( t^{1/D} \), where \( D \geq 2 \) is any integer. These methods provide a vast improvement over the best known classical algorithms; best of which is known to scale as \( t^{4/13} \). We present an alternative method to find \( |S(f, N)| \) on a QC directly. This method relies on finding the magnitude \( A = |\sum_{k=0}^{N-1} a_k| \) of a \( n \)-qubit quantum state \( |\psi_n\rangle = \sum_{k=0}^{N-1} a_k |k\rangle \). We present two different ways to do obtain \( A \). Finally, a brief discussion of phase/amplitude estimation methods is presented.

1. Introduction

An exponential sum (ES) is defined as

\[ S(f, N) = \sum_{k=0}^{N-1} \sqrt{w_k} e^{2\pi i f(k)}, \]

where \( f(x) \) is a real function, and real weights \( w_i \) are such that \( \sum_{i=0}^{N-1} w_i = 1 \). A particular case of the ES is when \( f(x) \) is a polynomial function \( p_d(x) \) of order \( d \) with real coefficients. We call such an ES, ES of polynomial order. ES have been used, mostly with \( w_i = 1/\sqrt{N} \) and \( f(x) = p_d(x) \) in solving a number of problems in number theory. They have found applications in congruence, theory of Diophantine equations and in particular establishing the upper limit of the magnitude of the RZ function, \( \zeta(s) \), with complex argument \( s \). Recently they have been used in devising efficient ways to calculate \( \zeta(s) \) on the critical line \( s = 1/2 + it \). They have also been used in number factorization where the factorization of a large number with two prime factors is cast into a problem that requires the evaluation of ES with quadratic polynomial as argument. Peaks of these sums at certain argument values indicate the possible factors of the number being factorized \[ \text{WMS}^{+11}, \text{MWS}^{+11}. \]

Date: February 26, 2020.

2010 Mathematics Subject Classification. Primary 11M06, 11Y16; Secondary 68Q25.

Key words and phrases. Exponential sums, Gauss sums, Riemann zeta function, Quantum Computer, Dirichlet L-functions, algorithms.
In general an ES with \( N \) terms requires an explicit addition of the terms and thus scales as \( N \). However for some special cases such as when \( p_d(x) \) is a quadratic polynomial and \( w_i = 1/\sqrt{N} \), they can be calculated in polyLog\((N)\) time classically \[\text{Hia11b}\]. In general, evaluation of ES for cubic and higher polynomials is a very difficult problem, especially when \( N \) is exponentially large \[\text{Hia11a}\]. We show in this paper that ES can be evaluated on a QC assuming that a unitary operator for function \( f(.) \) can be efficiently implemented. In particular, ES of polynomial order \( d \), \( f(x) = p_d(x) \), can be obtained.

The implementation of ES on a QC leads to efficient numerical evaluation of the RZ function, \( \zeta(s) \), in the critical region. Here \( s = \sigma + it \) where \( \sigma \) and \( t \) are real numbers and critical region is defined as \( 0 \leq \sigma < 1 \). The \( \zeta(s) \) function is defined in the whole complex plane \[\text{Edw74, TTHB}^+86\] by an analytical continuation of the following convergent sum which is valid for \( s > 1 \):

\[
\zeta(s) = \sum_{k=1}^{\infty} k^{-s}. \tag{2}
\]

The \( \zeta(s) \) function is intimately connected to the distribution of the prime numbers. The number of primes smaller than a given integer \( n \) can be accurately determined in terms of zeros of the function \( \zeta(s) \) in the critical region \[\text{Edw74, TTHB}^+86\]. It is conjectured that all non-trivial zeros of RZ fall on the critical line. This conjecture which is known as Riemann hypothesis has not yet been proved despite numerous efforts over the last 150 years. There are hundreds of theorems whose validity depend on the assumption that the Riemann hypothesis is true \[\text{MNR17}\].

Among many different approaches that have been proposed to prove the hypothesis, the most direct method depends on explicit numerical evaluation of the function for different values of \( \sigma \) and \( t \). A single instance of non-trivial zero of \( \zeta(s) \) at \( \sigma \) different from \( 1/2 \) will lead to the disproof of the hypothesis. The first such attempt was made by Riemann himself who manually calculated a few non-trivial zeros of the function and found they all fall on the real line \( \sigma = 1/2 \) \[\text{Edw74}\].

For the calculation of \( \zeta(s) \) in the critical region, the main difficulty encountered is that there is no fast way to numerically evaluate the function for large \( t > 10^{30} \). All known methods to evaluate RZ for large \( t \) are based on Riemann-Siegel (RS) formula \[\text{Edw74, TTHB}^+86\]. The RS formula allows one to calculate \( \zeta(s) \) with a complexity proportional to \( t^{1/2} \). Based on this method, it is known that there is no non-trivial zero off the critical line up to \( t = 10^{24} \) \[\text{CD04}\]. The RS formula consists of two parts, a series sum and an integral. While the integral can be estimated using a Saddle point approach, the series sum poses significant problem. This is because the total number of terms in the series scale as \( t^{1/2} \) and thus an explicit evaluation of the series scales as \( t^{1/2} \). In general there are no closed form or polyLog complexity methods known to evaluate this series.

Recently, progress has been made in this direction by Hiary \[\text{Hia11a}\] who has shown that if we break the series sum in blocks of size \( t^{\beta} \) with a total of \( t^{1/2-\beta} \) blocks and if each of the blocks can be calculated efficiently in polyLog time or better than one can achieve an overall scaling of \( t^{1/2-\beta} \) for the series sum. In particular, he has shown that the series can be divided in \( t^{1/3} \) blocks each of size \( t^{1/6} \) and the sum of terms in each such block can be computed efficiently by approximating these sums with ES with quadratic polynomial as exponent. ES of \( N \) terms with quadratic polynomial as exponent can be calculated in polyLog\((N)\) time classically,
thus leading to an overall $t^{1/3}$ scaling \cite{HiaI11a}. Further, He develops a method to obtain a scaling of $t^{4/13}$ for the series sum. This $t^{4/13}$ scaling assumes that one can approximate each block with ES sums of cubic order. The main difficulty encountered in applying this approach for even larger $\beta$, thus leading to even better $t^{1/2-\beta}$ scaling is that the numerical calculation of ES of cubic order is very difficult and of even higher orders is almost impossible. Even for cubic ES, one needs to take recourse to a number of approximations and this puts significant requirements on the pre-computations and temporary storage of the results. With these methods, it is possible to explore RZ function near $t = 10^{36}$ \cite{BH18}.

ES allow us to compute $\zeta(s)$ in polyLog($t$) time assuming that the logarithm function can be implemented on a QC \cite{WWl+20}. Working with a different method that involves ES of polynomial order $D$ and following Hiary \cite{HiaI11a} one can obtain $\zeta(s)$ with a scaling $t^{1/D}$ where $D$ can be any reasonable integer $D \geq 2$.

Rest of the paper is organized as follows. First in section 2, we consider the problem of evaluating general ES on a QC. In section 3, we discuss how we can apply one qubit rotations based on a general function and in particular based on polynomial functions. We then apply the idea of section 2 and section 3 in section 4 to show that RZ function be evaluated efficiently on a QC. In section 6, we present a method to find the magnitude of the ES directly. We discuss phase estimation methods in section 7. Finally, conclusions are provided in section 8.

2. General Exponential Sums

In the context of ES, very few quantum algorithms are known. An efficient algorithm to evaluate Gauss sums over a finite field was given by van Dam and Seroussi \cite{VDS02}. We present a method to obtain real and imaginary parts of ES in Equation 1 on a QC. We first show this for the real part:

$$\Re[S(f, N)] = \sum_{k=0}^{N-1} \sqrt{w_k} \cos(2\pi f(k)).$$

The imaginary part of the sum can be obtained by applying a constant offset of $1/4$ to function $f$:

$$\Im[S(f, N)] = \Re[S(f - 1/4, N)].$$

We start with a state

$$|\psi\rangle_n = \sum_{k=0}^{N-1} \sqrt{w_k} |k\rangle_n,$$

where $|k\rangle_n$ is a $n$ qubit state, $N = 2^n$ and $w_i$ are real weights as described following Equation 1. Such a state can be prepared on a QC if we can implement a unitary operator that corresponds to rotating a single qubit with the rotation angle being a function of $S_w(K) = \sum_{i=0}^{K-1} w_i$ for various levels $K = 2^0, 2^1, \ldots, 2^n$ that the algorithm needs \cite{GR02}. Note the power of this method lies in creating superposition of states $|k\rangle_n$ with weights $w_i$ in polyLog($N$). This is not possible for any arbitrary $w_k$. The requirement is that one should be able to implement $S_w(K)$ efficiently in classical and quantum settings.

The state $|\psi\rangle_n |0\rangle$ where $|0\rangle$ is an ancillary qubit, is then transformed to a suitable state with the help quantum unitary operators so that the resultant state contains the desired ES, Equation 3 as the amplitude of finding the ancillary qubit in state
For this purpose, let us assume that there is a controlled-$k$ unitary operator $U_f$ that acts as
\begin{equation}
U_f |k\rangle_n |0\rangle = |k\rangle_n (\cos(\pi f(k)) |0\rangle + \sin(\pi f(k)) |1\rangle).
\end{equation}
We will discuss in section 3 how such a function $f$ dependent rotation can be performed on an ancillary qubit. An application of the $U_f$ to state $|\psi\rangle_n |0\rangle$ gives
\begin{equation}
|\xi\rangle_{n+1} = U_f |\psi\rangle_n |0\rangle = \sum_{k=0}^{N-1} \sqrt{w_k} |k\rangle (\cos(\pi f(k)) |0\rangle + \sin(\pi f(k)) |1\rangle).
\end{equation}
The state $|\xi\rangle_{n+1}$ can be written as
\begin{equation}
|\xi\rangle_{n+1} = a |\phi_1\rangle_n |0\rangle + \sqrt{1-a^2} |\phi_2\rangle_n |1\rangle,
\end{equation}
where $|\phi_1\rangle_n$ and $|\phi_2\rangle_n$ are some properly normalized state vectors and
\begin{equation}
a^2 = \sum_{k=0}^{N-1} w_k \cos^2 (\pi f(k)).
\end{equation}
There are a number of methods that have been proposed to estimate the amplitude $a$. For example, one can use phase estimation method due to Kitaev \cite{Kitaev95} that can estimate $a$ to an exponential accuracy but this requires operators like $U_f$ to be applied an exponentially large number of times. To overcome this difficulty, faster methods based on classical post processing, rather than QFT, have been proposed [AR20, SUR+20, SHF13]. These methods allow a significant reduction in the number of times $U_f$ need to be applied. We discuss these methods in subsection 7.2. Following the estimation of $a$, the real part of the ES, Equation 3 is simply given by $(2a^2 - 1)$.

3. Applying rotations based on a function

For our algorithm to work, we should be able to apply rotations based on a given function $f$ as argument [Equation 6]. This is easy to achieve if
\begin{equation}
f(k) = \sum_{i=-m_2}^{m_1} q_{k,i} 2^i
\end{equation}
for different $k$ are implemented in a helper quantum state as
\begin{equation}
|f(k)\rangle = |q_{k,m_2}, q_{k,m_2-1}, \ldots, q_{k,1}, q_{k,0}, q_{k,-1}, q_{k,-2}, \ldots, q_{k,-m_2+1}, q_{k,-m_2}\rangle,
\end{equation}
where $q_{k,i} \in \{0,1\}$ for $i \in \{-m_1, -m_1+1, \ldots, -1, 0, 1, \ldots, m_2-1, m_2\}$. The form [Equation 10] suggests that a rotation by $f(k)$ can be written in terms of $q_{k,i}$-conditional rotations by angles $2^i$. In particular, it is easy to apply a controlled-$k$ rotation with angle $f(k) \cdot t$, where $t$ can be any real number. An example of this rotation for 2-qubit state $(m_1 = 2, m_2 = 2)$ is shown in Figure 1. When $f(x)$ is a polynomial function $p_d(x)$ with real coefficients, there is an alternative way to apply rotation of $p_d(x) \cdot t$ directly by using multi-qubit controlled rotations [WE19]. For example assuming that $f(x)$ is a polynomial of degree 2:
\begin{equation}
p_d(x) = ax^2 + bx + c,
\end{equation}
Figure 1. Circuit to perform the rotation given by \( f \times t \), where \( f \) is stored in a qubit state as \(|q_2, q_1, q_0, q_{-1}, q_{-2}\rangle\) and \( t \) is a real constant.

Figure 2. Circuit to perform the rotation given by \((ax^2 + bx + c) \cdot t\), where \( x \) is stored in a qubit state as \(|q_2, q_1, q_0, q_{-1}, q_{-2}\rangle\) and \( t \) is a real constant. We have shown only 1 out of total 5 one qubit controlled operations and similarly just 3 out of total of 20 two qubit controlled rotations. In addition the constant rotation by \( c \cdot t \) is shown.

and \(|x\rangle = |q_2, q_1, q_0, q_{-1}, q_{-2}\rangle\) represents the value \( x = 2^2q_2 + 2q_1 + 2^0q_0 + 2^{-1}q_{-1} + 2^{-2}q_{-2}\), we have

\[
p_d(x) = \sum_{k=-2}^{2} q_k(2^{2k}a + b) + \sum_{k,j=-2,k>j}^{2} q_j q_k(2^{j+k}a) + c,
\]

where we have used \( q_k^2 = q_k \). An implementation of this quantum circuit is shown in Figure 2. We note that in general a polynomial of degree \( d \) will lead to a total of about \( n^d \) controlled rotations and thus this method scales badly compared to first method that is based on calculating and storing the result of \( p_d(x) \) in a helper state and then rotating the ancillary qubit based on this helper state as shown in Figure 1 for the special case with \( m_1 = 2, m_2 = 2 \).

4. Riemann Zeta Function

Here we briefly describe two methods to evaluate the RZ function. Both methods have limitations for the evaluation of RZ with large \( t \). The first method is based on Euler-Maclaurin summation [Edw74, Rub05]

\[
\sum_{n=a}^{b} g(n) = \int_{a}^{b} g(t)dt + \sum_{k=1}^{K} \frac{(-1)^k B_k}{k!} + \frac{(-1)^{K+1}}{K!} \int_{a}^{b} B_K(\{t\})g^{(K)}(t)dt,
\]

(14)
where $B_k(t)$ are Bernoulli numbers defined by
\[ \frac{ze^{zt}}{e^z - 1} = \sum_{k=0}^{\infty} B_k(t) \frac{z^k}{k!}, \]

$B_k = B_k(0)$ and $\{t\}$ represents the fractional part of $t$. $B_K(\{t\})$ have the property
\[ |B_K(\{t\})| \leq \frac{K!}{(2\pi)^K} 2\zeta(K). \]

RZ function for $\Re(s) > 1$ can be obtained from the convergent series
\[ \zeta(s) = \sum_{n=1}^{\infty} n^{-s} = \sum_{n=1}^{N} n^{-s} + \sum_{n=N+1}^{\infty} n^{-s}, \]

where $N$ is a free integer. The first part on the rhs of Equation 16 is to be evaluated explicitly and the second part is to be determined by Euler-Maclaurin summation
\[ \sum_{n=1}^{\infty} n^{-s} = \frac{N^{1-s}}{s-1} + \sum_{k=1}^{K} \left( \frac{s+k-2}{k-1} \right) B_k k \frac{N^{-s-k+1}}{K} \left( \frac{s+K-1}{K} \right) \int_{N}^{\infty} B_K(\{t\}) t^{-s-K} dt. \]

By analytic continuation, the sum Equation 17 remains valid for all $s \neq 1$ and thus Equation 16 and Equation 17 define the $\zeta(s)$ on the whole complex plane except $s = 1$ which has a pole of order one. Choosing $K$ as an even integer it can be shown [Rub05] that the value of the integral is less than
\[ \frac{\zeta(K) s + K - 1}{\pi N^s} \frac{s+1}{\sigma + K - 1} \prod_{j=0}^{K-2} \frac{|s+j|}{2\pi N}, \]

If we choose $N$ such that $|(s+j)/(2\pi N)| < 1/10$ for all $j$ from 0 to $K - 2$, and assume that $\sigma \geq 1/2$, then it is easy to see that we can achieve a $D$ digit accuracy if
\[ K - 1 > D + \frac{1}{2} \log_{10}(|s + K - 1|). \]

For a general $s$ with large $t$, the limiting factor is that the number of terms $N$ become as large as $|s|$. This limits the use of the method to those cases where $s$ is close to the real line. For such cases, the formula in Equation 17 converges very fast. In particular for $s$ real and $\Re(s) < 1$, we roughly need to set $K = D + 1$ and $N \approx 2K$ for $D$ digits accuracy.

We now consider another well known formula for evaluating the RZ function, that we discussed in section 1. This is known as Riemann-Siegel (RS) formula and it has been widely used to verify RH for large $t$ values [Edw74]. The RS formula is given by :
\[ \zeta(s) = I_0(s) + \chi(s) \overline{I_0(1 - \overline{s})}, \]

where the bar denotes the complex conjugation, $\chi(s)$ is given by
\[ \chi(s) = \pi^{s-\frac{1}{2}} \frac{\Gamma\left(\frac{1-s}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}. \]
Here \( \Gamma \) denotes the Gamma function and \( I_0 \) is defined as a special case of more general \( I_N \):

\[
I_N (s) = \int_{N/\sqrt{N+1}} \int_{N/\sqrt{N+1}} g(z) \, dz
= \int_{N/\sqrt{N+1}} \int_{N/\sqrt{N+1}} e^{i\pi z^2} e^{i\pi z} - e^{-i\pi z} \, dz,
\]

with integration performed in the complex plane along a straight line going from the third quarter to the first quarter and intersecting the x-axis anywhere between \( N \) and \((N + 1)\). It follows from the Residue theorem that

\[
I_N (s) = I_{N-1} (s) - N^{-s}
\]

and this leads to

\[
I_0 (s) = \sum_{k=1}^{N} k^{-s} + I_N (s).
\]

The reason to express \( I_0 (s) \) in terms of \( I_N (s) \) is that for a particular value of \( N = \lfloor \sqrt{t/(2\pi)} \rfloor \) the \( I_N (s) \) develops a saddle point along the integration path making the integral amenable to numerical evaluation.

It is the explicit sums like \( \sum_{k=1}^{N} k^{-s} \) that a QC can compute in polyLog\( (t) \) time and this allows both Euler-Maclaurin and RS methods to achieve polyLog\( (t) \) complexity as we explain in section 5.

5. Riemann zeta on a quantum computer

The main difficulty in applying the Euler-Maclaurin or the RS formula is in calculating the partial series sum like \( \sum_{k=1}^{N} k^{-s} \) which can be written as

\[
S = \sum_{k=1}^{N} k^{-\sigma} \exp(-it \ln k).
\]

However a QC can carry our sums like \( S \) very efficiently as we now explain. We start with preparing the initial state

\[
|\psi\rangle_n = \sum_{k=1}^{N} k^{-\frac{\sigma}{2}} \frac{1}{\sqrt{H_N}} |k\rangle_n,
\]

following Grover’s algorithm for creating superposition [GR02]. Here \( H_k \) denotes the sum:

\[
H_k = \frac{1}{1^\sigma} + \frac{1}{2^\sigma} + \cdots + \frac{1}{k^\sigma}.
\]

To prepare such an initial state, we need a unitary operator that rotates a single qubit by angle \((H_{k_1} - H_{k_2})\) for some integers \( k_1, k_2 \in \{0, N\} \). \( H_k \) can be calculated classically, almost in a closed form, using Euler-Maclaurin summation as shown in section 4 and thus a quantum implementation of \((H_{k_1} - H_{k_2})\) should be achievable. Note that for Grover method to work, \( N \) can be exponentially large and it is this ability to create these superpositions that leads to efficient evaluation of ES on a QC.

Once the initial state has been prepared, we need a unitary operator to apply rotation by \( \theta_k = t/2 \ln(k) \) on an ancillary qubit. Assuming implementation of
such a unitary operator, we prepare a state of \((n + 1)\) qubits \(|\psi\rangle_n|0\rangle\) and apply conditional-\(k\) rotations on the ancillary qubit and this results in an overall state of
\[
|\phi\rangle_{n+1} = \sum_{k=1}^N k^{-\frac{\sigma}{2}} \sqrt{\frac{H_N}{J}} |k\rangle_n (\cos(\theta_k) |0\rangle + \sin(\theta_k) |1\rangle),
\]
Amplitude of \(|0\rangle\) in Equation 35 is given by
\[
S_r = \frac{1}{H_N} \sum_{k=1}^N k^{-\sigma} \cos^2(\theta_k).
\]
Similarly, rotations by angles \((\pi/4 - \theta_k)\) lead to
\[
S_i = \frac{1}{H_N} \sum_{k=1}^N k^{-\sigma} \cos^2(\pi/4 - \theta_k).
\]
Using these sums we can obtain
\[
S = \sum_{k=1}^N k^{-\sigma} \exp(-2i\theta_k)
= H_N ((2S_r - 1) + i(2S_i - 1)).
\]
The \(S_r\) and \(S_i\) can be calculated as discussed in section 2. This method thus allows one to achieve \(\text{polyLog}(t)\) complexity.

We now discuss another implementation of the series sum based on breaking this sum in different blocks and evaluating each block on a QC after approximating it with ES with polynomials exponents. Hiary [Hia11a] has shown that, starting with RS formula, if we break the series sum in blocks of size \(t^{1/2 - \beta}\) with a total of \(t^{1/2 - \beta}\) blocks and if each of the blocks can be calculated efficiently in \(\text{polyLog}(t)\) time or better than one can achieve \(t^{1/2 - \beta}\) scaling. The method relies on approximating each block with a linear combinations of sums
\[
\frac{1}{K^j} \sum_{k=0}^{K-1} k^j \exp(2\pi ip_d(k)), \quad j = 0, 1, \cdots, J,
\]
where polynomial \(p_d(k)\) are of degree \(d = \lfloor 1/(1/2 - \beta) \rfloor - 1\) and the coefficients of \(p_d(k)\) can be easily determined. The \(J\) depends on the accuracy \(\lambda\) sought as \(J = (d + 1)(\lambda + 3) \log(t)\). The error in evaluating each block with the sum of linear combinations Equation 27 is of the order of \(\pm t^{-\lambda}\). The \(K\) is an integer to be chosen such that
\[
Pt^{1/2} < K \leq Pt^{1/2} + 1, \quad P = \lfloor \frac{1}{2} \sqrt{\frac{t}{2\pi}} \rfloor.
\]
To obtain sums Equation 27 we start with preparing the initial state
\[
|\psi\rangle_n = \sum_{k=0}^{K-1} \frac{k^j}{\sqrt{H_{N,j}}} |k\rangle_n,
\]
following Grover’s algorithm for creating superposition [GR02]. Here \(H_{k,j}\) denotes the sum:
\[
H_{k,j} = \sum_{n=1}^k n^j.
\]
$H_{k,j}$ can be calculated classically, in a closed form, using Euler-Maclaurin summation [Edw74]:

$$H_{k,j} = \frac{B_{j+1}(k+1) - B_{j+1}}{j+1},$$  \hspace{1cm} (31)

where

$$B_j(t) = \sum_{m=0}^{j} \left( \begin{array}{c} j \\ m \end{array} \right) B_{j-m}t^m, \quad j \geq 0.$$  \hspace{1cm} (32)

Here $B_j$ denote the Bernoulli numbers. It is clear that $H_{k,j}$ can be calculated in terms of $j$ lower order Bernoulli numbers from $B_0$ to $B_j$. This, a quantum implementation of $(H_{k_1,j} - H_{k_2,j})$ should be achievable.

6. Sum of quantum amplitudes

We now present a method to find the magnitude of the sum of quantum amplitude for a given quantum state. Magnitude of ES will be a special case of this more general method. We would like to estimate the magnitude of the sum of amplitudes, $|\sum_{k=0}^{N-1} a_k|$, in the normalized state $|\psi\rangle_n$:

$$|\psi\rangle_n = \sum_{k=0}^{N-1} a_k |k\rangle_n.$$  \hspace{1cm} (33)

As the state is normalized, we have $\sum_k |a_k|^2 = 1$. The mean of the amplitudes is

$$a = \frac{1}{N} \sum_{k=0}^{N-1} a_k.$$  \hspace{1cm} (34)

We start with the direct product of $|\psi\rangle_n$ with an ancillary qubit in $|1\rangle$:

$$|\phi\rangle_{n+1} = 0 |\psi\rangle_n |0\rangle + |\psi\rangle_n |1\rangle$$

$$= 0 \sum_{k=0}^{N-1} |k\rangle_n |0\rangle + \sum_{k=0}^{N-1} a_k |k\rangle_n |1\rangle.$$  \hspace{1cm} (35)

Now we apply to $|\phi\rangle_{n+1}$ the unitary operator, $U_{\text{Inv}}$, corresponding to an inversion around the mean. This leads to a new state $|\phi'\rangle_{n+1}$

$$|\phi'\rangle_{n+1} = U_{\text{Inv}} |\phi\rangle_{n+1}$$

$$= (2b) \sum_{k=0}^{N-1} |k\rangle_n |0\rangle + \sum_{k=0}^{N-1} (2b - a_k) |k\rangle_n |1\rangle,$$  \hspace{1cm} (36)

where $b$ is the mean of all coefficients in state $|\phi\rangle_{n+1}$:

$$b = \frac{1}{2N} \sum_{k=0}^{N-1} a_k = \frac{a}{2}.$$  

Thus, the new state is

$$|\phi'\rangle_{n+1} = a \sum_{k=0}^{N-1} |k\rangle_n |0\rangle + \sum_{k=0}^{N-1} (a - a_k) |k\rangle_n |1\rangle.$$  \hspace{1cm} (37)
We rewrite Equation 37 in terms of two normalized states, $|\psi_0\rangle_n$ and $|\psi_1\rangle_n$ as

$$|\phi\rangle_{n+1} = \sqrt{N}|a| |\psi_0\rangle_n |0\rangle + \sqrt{1-N|a|^2} |\psi_1\rangle_n |1\rangle .$$

Using Equation 38 we can obtain $|a|$ by the amplitude estimation. In particular, as a special case with $a_k = \sqrt{w_k} \exp(2\pi i f(k))$ and $w_i$ given as in Equation 1, we can obtain the magnitude of the ES. Note that such a state with $a_k = \sqrt{w_k} \exp(2\pi i f(k))$ can be prepared by first using Grover’s method [GR02] to create an initial superposition state with weights $\sqrt{w_i}$, Equation 29 followed by controlled-$k$ unitary operator $U_z$

$$U_z |k\rangle_n \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = |k\rangle_n \frac{1}{\sqrt{2}} (\exp(i\pi f(k)) |0\rangle + |1\rangle).$$

The application of this controlled-$k$ operator $U_z$ to $|\psi\rangle_n 2^{-1/2} (|0\rangle + |1\rangle)$ gives

$$|\xi\rangle_{n+1} = U_z |\psi\rangle_n \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$= \frac{1}{\sqrt{2}} \sum_{k=0}^{N-1} \sqrt{w_k} |k\rangle (\exp(i\pi f(k)) |0\rangle + |1\rangle).$$

State Equation 40 can be written in alternative form as $|\phi\rangle_{n+1}$ in Equation 38. We now present another method arrive at Equation 37. We start with the direct product of $|\psi\rangle_n$ defined in Equation 29 and ancillary qubit $|0\rangle$ as given in Equation 29 and apply Hadamard transform to $|\psi\rangle_n$. This leads to

$$|\phi\rangle_{n+1} = \left( H \sum_{k=0}^{N-1} a_k |k\rangle_n \right) |0\rangle$$

$$= \left( \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} a_k |0\rangle_n + H \sum_{k=0}^{N-1} a_k |k\rangle_n - \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} a_k |0\rangle_n \right) |0\rangle$$

$$= \left( \sqrt{N} a |0\rangle_n + H \sum_{k=0}^{N-1} a_k |k\rangle_n - \sqrt{N} a |0\rangle_n \right) |0\rangle.$$

Note that it is only the first term which contains the state component $|0\rangle_n$. This component cancels out from the last two terms. Applying now a controlled-or gate with control state $|k\rangle_n$ and the target state $|0\rangle$ leads to

$$|\phi\rangle_{n+1} = \sqrt{N} a |0\rangle_n |0\rangle + \left( H \sum_{k=0}^{N-1} a_k |k\rangle_n - \sqrt{N} a |0\rangle_n \right) |1\rangle.$$

We apply the Hadamard gate again on the first $n$ qubits and this leads to

$$|\phi\rangle_{n+1} = \left( \sum_{k=0}^{N-1} a |k\rangle_n |0\rangle + \sum_{k=0}^{N-1} (a_k - a) |k\rangle_n |1\rangle \right),$$

which is the same Equation 37. The rest of the approach is the same as outlined earlier.
7. Phase Estimation

Phase estimation aims to determine the phase $0 \leq \varphi_k < 1$ in the eigenvalue $\lambda_k = \exp(2\pi i \varphi_k)$ of a unitary operator $U$ for a given eigenstate $|\xi_k\rangle$:

$$U |\xi_k\rangle = \lambda_k |\xi_k\rangle.$$  

As shown in [BHMT02], finding $\varphi_k$ is intimately related to finding amplitude $a$ in Equation 38. This is because if we have a unitary operator $A$ acting on $(n+1)$ qubit state as

$$|\phi\rangle_{n+1} = A |\psi\rangle_n |0\rangle$$

(45) $$= \cos(\theta_a) |\psi\rangle_n |0\rangle + \sin(\theta_a) |\psi_1\rangle_n |1\rangle$$

with $\theta_a$ defined as $\cos(\theta_a) = a$, and operators $S_0$ and $S_\chi$ defined as

$$S_0 |\phi\rangle_{n+1} = \cos(\theta_a) |\psi\rangle_n |0\rangle - \sin(\theta_a) |\psi_1\rangle_n |1\rangle$$

$$S_\chi |\phi\rangle_{n+1} = -\cos(\theta_a) |\psi\rangle_n |0\rangle + \sin(\theta_a) |\psi_1\rangle_n |1\rangle,$$

then operator $Q$:

$$Q = -AS_0A^{-1}S_\chi,$$

acts on state $|\phi\rangle_{n+1}$ as

$$Q^m |\phi\rangle_{n+1} = \cos((2m+1)\theta_a) |\psi\rangle_n |0\rangle + \sin((2m+1)\theta_a) |\psi_1\rangle_n |1\rangle.$$  

There are two main methods to find $\varphi_k$ that we discuss in subsection 7.1 and subsection 7.2 below. For further details on phase and amplitude estimation one can refer to [BHMT02, BHMT02, NC02, KSV02, SHF13, Jor08, MOD+19, WG16, SUR+20, AR20].

7.1. QFT based phase estimation: The main idea is to use the Quantum Fourier transform (QFT) to obtain $\varphi_k$. An inverse QFT applied to state to an $n$ qubit state with $N = 2^n$:

$$|\psi(x)\rangle = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} \exp\left(2\pi i \frac{x l}{N}\right) |l\rangle_n,$$

leads to

$$QFT^{-1} |\psi(x)\rangle = |x\rangle.$$  

Now a state like $|\psi(x)\rangle$ with $x = N \varphi_k$ is easy to produce with the help of the original state $|\xi_k\rangle$ and state $|L\rangle$ of $n$ qubits:

$$|L\rangle = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} |l\rangle.$$  

This is because if one starts with the state $|L\rangle |\xi_k\rangle$ and applies $l$-controlled operator $\sum_l |l\rangle \langle l| \otimes U^l$, then the resultant state is

$$|\psi(lN \varphi_k)\rangle |\xi_k\rangle = \frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} \exp(2\pi i \varphi_k l) |l\rangle |\xi_k\rangle.$$  

Now because any $l$ can be written in the bit form as $l = a_{l,n-1}2^{n-1} + a_{l,n-2}2^{n-2} + \cdots + a_{l,0}$ where $a_{l,i} \in 0, 1$, we can write $U^l$ as

$$U^l = a_{l,n-1}U^{2^n-1} + a_{l,n-2}U^{2^n-2} + \cdots + a_{l,0}.$$
Thus the $l$-controlled operator $U^l$ is basically a sum of $a_i$-controlled operators $U^{2^i}$ that are applied to the target state $|ξ_k⟩$ if $i = 1$ and not applied if $i = 0$. The circuit for applying $l$-controlled $U^l$ operator is shown in Figure 3. Now applying inverse $QFT$ to state $|ψ(Nφ_k)⟩$ one gets

$$QFT^{-1} |ψ(Nφ_k)⟩ = |Nφ_k⟩.$$ 

Thus a measurement on the $n$ qubit state will reveal the value of $Nφ_k$ from which the value of $φ_k$ can be obtained. We note that the settings of Figure 3 can be used with Equation 47 with the following substitutions: work with $(n+1)$ qubit state rather than $n$-qubit state, replace input state $|ξ_k⟩$ with $|φ⟩_{n+1}$ and and $U$ with $Q$.

With these substitutions, the output state will correspond to $Nθ_a$.

7.2. Classical post processing based amplitude estimation: There are other alternatives for phase estimation. Rather than working in terms of QFT they depend on classical post processing of a number of measurements carried out using a simpler quantum circuits [SHF13, WG16]. One such circuit is shown in Figure 4.

We have a single control qubit $|0⟩$ and a rotation operator $Z(θ)$:

$$Z(θ) = \begin{bmatrix} 1 & 0 \\ 0 & e^{iθ} \end{bmatrix}.$$ 

Here $U$ acts on $ξ_k$ as in Equation 44. It is easy to see that the quantum circuit transforms the first qubit to

$$|0⟩ \mapsto \left(1 + e^{2πiMφ_k+iθ} \right) |0⟩ + \frac{1 - e^{2πiMφ_k+iθ}}{2} |1⟩.$$ 

Thus, the measurement outcome probabilities for up and down states, conditioned on $ξ_k$, $M$ and $θ$, are given by:

$$P_{M,θ}(0|k) = \left|1 + e^{2πiMφ_k+iθ} \right|^2 = \frac{1 + \cos(2πMφ_k + θ)}{2},$$

Figure 4. Circuit to perform the measurement operator.
and

\begin{equation}
\label{eq:P}
P_{M,\theta}(1|k) = \left|1 - e^{2\pi i M \varphi_k + i \theta}\right|^2 = \frac{1 - \cos(2\pi M \varphi_k + \theta)}{2}.
\end{equation}

If we carry out a large number of experiments for fixed $M = 1$ and $\theta = 0$ then the fractions corresponding to up and down states allow one to estimate $\cos(2\pi \varphi_k)$. However, the estimation of $\varphi_k$ will be ambiguous because if $\varphi_k$ is a solution then so will be $(1 - \varphi_k)$. We thus need to do experiments at an additional value of $\theta$ which is conveniently chosen as $\theta = \pi/2$. This pins down the exact value of $\varphi_k$. It turns out that this algorithm can results in a fixed accuracy that will depend on the number of measurements carried out \cite{SIPT13}. In fact, for a given accuracy $\varepsilon$, it is known \cite{AR20} that one obtain an estimate $\hat{a}$ of $a$ such that

\begin{equation}
\label{eq:accuracy}
a(1 - \varepsilon) < \hat{a} < a(1 + \varepsilon),
\end{equation}

using $O(-\varepsilon^{-1} \log(\delta))$ applications of $U_f$ such that the failure probability of the algorithm will be $\delta$.

If one wants to achieve exponential accuracy under the classical post processing settings, then we can follow Kitaev’s phase estimation algorithm \cite{Kit95}. This algorithm works by estimating $2^{j-1} \varphi_k$ for $j = m, (m-1), (m-2), \cdots, 1$. As one multiplies $\varphi_k$ with bigger and bigger $2^{j-1}$, the information about the integral multiple of $2\pi$ is lost and one recovers the estimation of the $j^{th}$ bit of $\varphi_k$. The algorithm works as before for $M = 1$ and still uses two different angles $\theta \in \{0, \pi/2\}$.

8. Conclusion

We have shown that a QC can efficiently calculate ES for any real function $f$ as exponent that can be implemented on QC. In particular, ES with polynomial functions as exponents can be obtained. ES can also incorporate real weights $w_i$ via Grover’s algorithm for creating superpositions \cite{GR02}. As an application, we have considered the evaluation of RZ function and have shown that our method can evaluate RZ for argument $\sigma + it$ with a scaling of $t^{1/D}$, where $D \geq 2$ is an integer. In addition, we have presented a general algorithm that can calculate RZ in polyLog($t$), assuming that general arithmetic functions and in particular logarithmic function can be efficiently implemented on a QC. We have presented a general method to obtain the magnitude of an ES. All of the methods proposed are based on phase/amplitude estimation and they can evaluate ES to a given preset accuracy. We presented a brief overview of amplitude estimation methods and showed that for a given accuracy $\varepsilon$, amplitude can be estimated with an application of about $1/\varepsilon$ applications of the $Q$ operators \cite{Equation 46}. However, if exponential accuracy is required, then these methods have limitations unless one can figure out an efficient way to implement very high powers of unitary operators. We note that in the context of RZ function, not achieving a very high accuracy is not a limitation for locating non-trivial zeros of RZ. This is because to locate the zeros we just need to calculate $S(t) = \pi^{-1} \arg \zeta(1/2 + it)$, and this does not require the determination of $\zeta(1/2 + it)$ to very high accuracy.

References

\cite{AR20} Scott Aaronson and Patrick Rall. Quantum approximate counting, simplified. In \textit{Symposium on Simplicity in Algorithms}, pages 24–32. SIAM, 2020.
Jonathan W Bober and Ghaith A Hiary. New computations of the riemann zeta function on the critical line. *Experimental Mathematics*, 27(2):125–137, 2018.

Gilles Brassard, Peter Hoyer, Michele Mosca, and Alain Tapp. Quantum amplitude amplification and estimation. *Contemporary Mathematics*, 305:53–74, 2002.

Harold M Edwards. *RiemannÆs zeta function*, volume 58. Academic press, 1974.

Xavier Gourdon and P Demichel. The 1013 first zeros of the riemann zeta function, and zeros computation at very large height. *preprint*, 24, 2004.

Lov Grover and Terry Rudolph. Creating superpositions that correspond to efficiently integrable probability distributions. *arXiv preprint quant-ph/0208112*, 2002.

Ghaith Ayesh Hiary. Fast methods to compute the riemann zeta function. *Annals of mathematics*, 174(2):891–946, 2011.

Ghaith Ayesh Hiary. A nearly-optimal method to compute the truncated theta function, its derivatives, and integrals. *Annals of mathematics*, pages 859–889, 2011.

Stephen P Jordan. Quantum computation beyond the circuit model. *arXiv preprint arXiv:0809.2307*, 2008.

A Yu Kitaev. Quantum measurements and the abelian stabilizer problem. *arXiv preprint quant-ph/9511026*, 1995.

Alexei Yu Kitaev, Alexander Shen, and Mikhail N Vyalyi. *Classical and quantum computation*. Number 47. American Mathematical Soc., 2002.

Hugh Montgomery, Ashkan Nikeghbali, and Michael Th Rassias. *Exploring the Riemann Zeta Function*. Springer, 2017.

Hamed Mohammadbagherpoor, Young-Hyun Oh, Patrick Dreher, Anand Singh, Xianqing Yu, and Andy J Rindos. An improved implementation approach for quantum phase estimation on quantum computers. *arXiv preprint arXiv:1910.11696*, 2019.

Wim Van Dam and Gadiel Seroussi. Efficient quantum algorithms for estimating gauss sums. *arXiv preprint quant-ph/0207131*, 2002.

Stefan Woerner and Daniel J Egger. Quantum risk analysis. *npj Quantum Information*, 5(1):15, 2019.

Nathan Wiebe and Chris Granade. Efficient bayesian phase estimation. *Physical review letters*, 117(1):010503, 2016.

Shengbin Wang, Zhimin Wang, Wendong Li, Lixin Fan, Guolong Cui, Zhiqiang Wei, and Yongjian Gu. Quantum circuits design for evaluating transcendental functions based on a function-value binary expansion method. *arXiv preprint arXiv:2001.00807*, 2020.

E-mail address: tyagi.sandeep@yahoo.com

Bank of America, London, EC1A 1HQ