On the Generalizations of Grover algorithm

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We generalize Grover algorithm with two arbitrary phases in a density matrix set up. We give exact analytic expressions for the success probability after arbitrary number of iteration of the generalized Grover operator as a function of number of iterations, two phase angles \((\alpha, \beta)\) and parameter \(\xi\) introduced in the off diagonal terms of the density matrix in a sense to capture the coherence present in the initial quantum register. We extend Li and Li’s idea and show for the phase matching condition \(\alpha = -\beta = 0.35\pi\) with two iterations and \(\xi = 1\), we can achieve success probability \(\geq 0.8\) only with a knowledge about the lower bound of \(\lambda = 0.166\) where \(\lambda\) is the ratio of marked to total number states in the database. Finally we quantify success probability of the algorithm with decrease in coherence of the initial quantum state against modest noise in this simple model.

I. INTRODUCTION

There has been a constant effort since few decades in order to harness the power of Quantum mechanics in various fields of science and engineering. The subject of Quantum computation is one such example which believe to hold exceptional promises in the sense of solving some of the crucial problems with significantly better computational advantage than its classical counterpart. Quantum algorithms such as Deutsch–Jozsa algorithm [1], Shor’s factorization algorithm [2], Grover’s quantum search algorithm [3, 4] are some of the notable examples in this regard. Grover’s quantum search gives square root speed up over the best available classical algorithm when searching for marked items from an unstructured database.

After this seminal finding, several efforts have been made to extend and improve the quantum search algorithm. Benett et al. [5] proved square root speed up to be computationally optimal [6]. It was shown to be a larger class of quantum amplitude amplification problem by Brassard and Hoyer [7]. Long [8] generalized the algorithm for generic phase angles and gave exact phase expressions for 100% success. Boyer et al. [9] showed how to handle multiple marked states in the database. Biham et al. [10–12] gave success probability for arbitrary iteration with the original phase matching for a general pure and mixed initial state. For some of the further results, see for example [13, 14]. Li and Li [15] reported for \(\lambda \geq 1/3\), where \(\lambda\) is the ratio of the marked to total states in the database, success probability \(P(\lambda) \geq 25/27\) can be achieved with a single iteration. Multi-phase matching condition was proposed and numerical results were given in order to improve the success probability for wide range of \(\lambda\) [16, 17]. Dependence of coherence was studied in [18] using several typical measures of quantum coherence and quantum correlations for pure states using previous results of Biham et al.. Grover iteration can be thought of as a rotation in the two-dimensional hilbert space spanned by marked and unmarked state [19], with each rotation slowly rotates the initial uniform superposition state towards the marked state. Unitarity of the Grover operator implies there will always be so-called ‘overcooking’ of the prepared state if we iterate more than the required number as the eigen values are inherently periodic which often poses difficulty when number of marked items is unknown. To get around this problem, the idea of Fixed point quantum search was proposed by Grover [20] where the success probability always gets an improvement with each iteration as the iteration operator followed a recursion relation implies each iteration is not the identical unitary which would’ve prevented the algorithm to have a fixed point earlier. Fixed point quantum search is useful when \(\lambda\) is unknown at the price of decreased efficiency of the algorithm [21]. Recently Chuang et al all [22] claimed a fixed point search involving a different phase matching condition with optimal number of queries using functions typically used as frequency filters in electronics. Some of the experimental realizations of Grover algorithm are also reported, see for example [21, 23, 24].

In this work, we generalize Grover algorithm in a density matrix set up and find the exact success probabilities for arbitrary iteration as a function of number of iterations, two generic phase angles \((\alpha, \beta)\) and parameter \(\xi\) introduced in the off diagonal terms of the density matrix in order to capture the coherence present in the initial quantum register. We extend the Li and Li’s result [15] and show for the phase matching condition \(\alpha = -\beta = 0.35\pi\) with two iteration, we get success probability \(\geq 0.8\) for \(\lambda \geq 0.166\). This fixes the problem of so-called ‘overcooking’ of state atleast up to the mentioned range as precise knowledge of \(\lambda\) is not required except for a lower bound and also having to do with an user controlled oracle query suggested recently [25]. Finally, We quantify how success probability of the algorithm gets affected with the initial state preparation errors due to modest noise for various phase matching conditions given for different limits of \(\xi\) in this simple model.

The paper is organized as follows. In Section II A, we give a brief overview of the Grover algorithm. Form of the most general operators with two generic phase angles

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originally given by Li and Li [15] is given with their results. In Section II B. In Section III we present our exact analytic results for the success probability for arbitrary number of iteration as a function of the parameters of the algorithm. Section IV contains further results from the success probability expressions particularly extension of the [15] phase matching condition to a lesser lower bound on $\lambda$. We end the paper with a discussion on the result in Section V.

II. PRELIMINARIES

We review Grover algorithm in its original form. We point out the two dimensional subspace spanned by the marked and unmarked state which simplifies the discussion of the algorithm. Proper generalization of the algorithm in terms of two generic phase angles and the result of [15] is discussed after that.

A. Overview of Grover Algorithm

Suppose we have an unstructured database of size $N = 2^n$ and want to search for $M$ marked items from the database. Classically, query complexity of the problem scales as $O(N/2M)$ with the size of the database. Quantumly, as Grover showed in his remarkable paper [3], we can achieve quadratic speed up over the classical case. Grover algorithm consists of initialization of the $n$ qubit $|0\rangle^\otimes n$ to equal superposition state using $n$-qubit Hadamard gate as $|\psi\rangle = H^\otimes n |0\rangle^\otimes n = \frac{1}{\sqrt{N}} \sum_{x=1}^{2^n} |x\rangle$.

Applying the following two operators, 1. Oracle query $O = (1 - 2 \sum_{x=0}^{M-1} |x\rangle \langle x|)$, 2. Diffuser operator $D = (2 |\psi\rangle \langle \psi| - 1)$ iteratively $k_{opt} = (\pi/2\theta - 1/2)$ times with $\theta$ given by the expression $\theta = 2 \arcsin \sqrt{\lambda}$. Defining Grover operator $G$ as $DO$, effect of $G$ on $|\psi\rangle$ is essentially captured by the rotation matrix written in the basis $|R\rangle, |T\rangle$ as,

$$G = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}$$

with the bases $|R\rangle$ and $|T\rangle$ given by,

$$|T\rangle = \frac{1}{\sqrt{M}} \sum_{x=1}^{M} |x\rangle, \quad |R\rangle = \frac{1}{\sqrt{N-M}} \sum_{x=M+1}^{N} |x\rangle$$

respectively the uniform superposition of marked and unmarked states. In terms of these bases, initial state can be written as,

$$|\psi\rangle = \sqrt{1-\lambda} |R\rangle + \sqrt{\lambda} |T\rangle$$

Application of Grover operator has the effect of rotating $|\psi\rangle$ towards $|T\rangle$ through an angle $\theta$ in each iteration taking $k_{opt}$ iteration in total before measurement can be done in the computational basis completing the quantum search process. Exact knowledge of $\lambda$ is required as otherwise we would end up with decreased success probability because of the inherent periodicity of the rotation matrix if iteration is done for more than the optimal number.

B. Generalization of the algorithm with generic phases

The most general operators was given here [15], written in the basis of $|R\rangle, |T\rangle$ as,

$$U(\alpha) = I - (1-e^{i\alpha}) |T\rangle \langle T|$$

$$V(\beta) = I e^{i\beta} + (1 - e^{i\beta}) |\psi\rangle \langle \psi|$$

where $U$ selectively shifts the phases of the marked states by an angle $\alpha$ and $V$ shifts the phase by angle $\beta$ around the fixed state $|\psi\rangle$ each time. This reduces to the original Grover algorithm for the choice $\alpha = \beta = \pi$.

Li and Li gave their new phase matching condition as $\alpha = -\beta = \frac{\pi}{2}$. This gives the result that with single iteration, we get success probability $P(\lambda) \geq \frac{\pi}{4\lambda}$ for $1/3 \leq \lambda \leq 1$. In this paper we show we can handle even smaller values of $\lambda$ than that as well with one more iteration without the exact knowledge of $\lambda$ beforehand except for a lower bound on $\lambda$ which fixes the problem of both ‘overcooking’ of the state and having user controlled oracle recently suggested [25] as shown in the next section.

III. EXACT SUCCESS PROBABILITY WITH GENERALIZED PHASE ANGLES

Matrix representation of the operator $G(\alpha, \beta) = U(\alpha)V(\beta)$ as,

$$
\begin{pmatrix}
(1 - e^{i\beta})(1-\lambda) & e^{i\alpha}(1-e^{i\beta})\sqrt{\lambda(1-\lambda)} \\
(1 - e^{i\beta})\sqrt{\lambda(1-\lambda)} & e^{i\alpha}(1-e^{i\beta})\lambda + e^{i(\alpha+\beta)}
\end{pmatrix}
$$

Let the initial density matrix be given by,

$$\rho_{initial} = (1 - \lambda) |R\rangle \langle R| + \lambda |T\rangle \langle T| + \xi \sqrt{\lambda(1-\lambda)} (|R\rangle \langle T| + |T\rangle \langle R|)$$

where $\xi$ is a generic parameter introduced to quantify the coherence present in the initial density matrix. Density matrix after $m^{th}$ iteration is given by,

$$\rho_m = G^m \rho_{initial} (G^t)^m$$

The success probability can be given as the $\langle T| \rho_m |T\rangle$ matrix element of the final density matrix. We raise the $G(\alpha, \beta)$ to the $m^{th}$ power using the standard method of expanding the matrix in the basis of $I$ and the Pauli matrices [25]. We get the success probability as a function of number iteration $m$, $\xi$ and two generic angles $\alpha$ and $\beta$ as,

$$P(\lambda, \xi, \alpha, \beta) = \lambda + \sin^2(m\phi)[1 - n_3^2 - 2\lambda(1 - n_3^2)]$$

$$- 2\xi \sqrt{\lambda(1-\lambda)} \sin^2(m\phi)[n_1 n_3 + n_2 \cot(m\phi)]$$
with
\[
\cos(\phi) = \cos\left(\frac{\alpha + \beta}{2}\right) + 2\lambda \sin(\beta/2) \sin(\alpha/2) \tag{5}
\]
\[
n_1 = -\frac{\sqrt{\lambda(1-\lambda)}}{\sin(\phi)} 2\cos(\alpha/2)\sin(\beta/2) \tag{6}
\]
\[
n_2 = \frac{\sqrt{\lambda(1-\lambda)}}{\sin(\phi)}(2\sin(\alpha/2)\sin(\beta/2)) \tag{7}
\]
\[
n_3 = \frac{1}{\sin(\phi)}\left[-\sin\left(\frac{\alpha + \beta}{2}\right) + 2\lambda \sin(\beta/2)\cos(\alpha/2)\right] \tag{8}
\]
We find this reduces to the Li and Li’s result in the specific limit of \(\alpha = -\beta = \pi/2\) and \(m = 1\) as,
\[
P(m, \lambda, 1, \pi/2, -\pi/2) = 4\lambda^3 - 8\lambda^2 + 5\lambda
\]
This gives success probability \(\geq 0.8\) consistently for \(\lambda > 0.243\) with single iteration. In the next section, we show we can extend Li and Li’s phase matching to handle \(\lambda\) value to be as low as 0.166 with only two iteration with success probability \(\geq 0.8\).

### IV. RESULTS

From the given expression of \(P(\lambda, \xi, \alpha, \beta)\), we get the success probability for \(\alpha = -\beta\) phase matching condition for arbitrary iteration as,
\[
P(\lambda, m, \xi = 1, \alpha = -\beta) = 
\lambda + \sin^2(m\phi)\left[1 - \lambda^2 \sin^2(\phi)\right](1 - 2\lambda)
+ 2\xi(1-\lambda)\sin^2(m\phi)\sin(\phi)\left[\lambda \sin^2(\phi) + 2\sin^2(\alpha/2)\cot(m\phi)\right]
\]

We find from the above expression, for \(m=2\), we get success probability to be \(\geq 0.8\) in the range \(0.166 \leq \lambda \leq 1\) for the above phase matching condition with \(\alpha = 0.35\lambda\). It also gives exact success for \(\lambda = 0.3498\). We can improve the result by increasing the number of iteration. With three iteration, we get success probability profile which is better in the region where \(\lambda \geq 0.2\) with a different phase angle. Thus only knowledge about the lower bound of \(\lambda\) is required in this protocol.

We also find the performance of the algorithm against modest noise captured by the parameter \(\xi\). With \(\xi=0\), we have \(p_{\text{initial}} = (1-\lambda) |R\rangle \langle R| + \alpha |T\rangle \langle T|\). Success probability of the generalized Grover algorithm in this limit comes out to be
\[
P(\lambda, \xi = 0, \alpha, \beta) = 
\lambda + \sin^2(m\phi)[1 - n_3^2 - 2\lambda(1 - n_3^2)]
\]
with the same \(n_3\) and \(\phi\) as earlier. We find decrease in the success of the algorithm for most values particularly for \(\lambda \leq 0.5\) as is generally expected. For example, with this new phase matching, for the value \(\lambda = 0.2\), success probability becomes almost 60% of its value with \(\xi=1\).

### V. DISCUSSIONS

Grover algorithm gives substantially improved computational advantage over the classical algorithms while searching for marked items in an unstructured database which has been extremely useful for solving some of the major problems, such as quantum collision problem, quick exhaustive search over possible solutions to solve a NP hard problem etc. Essentially this can be used generically for speeding up all sorts of existing searching problems. We address the issue of so called ‘overcooking’ of the state exists in the original algorithm where precise knowledge of the ratio \(\lambda\) is required for the algorithm to succeed. Because of the inherent periodicity of the eigen values of the unitary operators, slight deviation from the optimum iteration can give significant decrease in the success probability implies for unknown number of marked states, the original algorithm will not be useful. To get around this difficulty, Fixed point quantum search was proposed where the iteration was not a fixed unitary, thus accumulation of probability amplitude in the marked states is possible with decrease in efficiency of the algorithm as discussed earlier. Multi-phase matching algorithms have been proposed with user controlled oracle as well for better success rate over wide ranges of \(\lambda\). This suffers from the problem that user might not be able to have access to the oracle in order to change the phase angle according to the iteration as has been recently pointed out. In this paper, we give exact closed form expression for success probability as a function of the various parameters of the algorithm for the general case of arbitrary iteration in a density matrix set up which potentially helps to incorporate several state preparation errors present due to decoherence effects. We look for phase matching conditions which gives better success probability profile over wide ranges of \(\lambda\) with minimum iteration without using user based oracle query. We iterate with the phase matching condition \(\alpha = -\beta = 0.35\lambda\) twice and get a success probability profile with \(P(\lambda)\) consistently over 0.8 for lower-bound \(\lambda \geq 0.166\). For \(\lambda \geq 0.213\), we get \(P(\lambda)\) to be more than 0.9 for most of the relevant values of \(\lambda\). With three iteration, success probability profile is improved for slightly higher values of \(\lambda\). This improves the earlier result where \(P(\lambda) \geq 25/27\) for \(1/3 \leq \lambda \leq 1\) was reported in the sense of handling wider range of the ratio between marked to total number of states in the database. We explore methods to handle even smaller values of \(\lambda\) with successive iteration and proper tuning of the phase angle as well as modified phase matching condition as will be reported later on elsewhere.

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