Grover’s Algorithm with Diffusion and Amplitude Steering

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Abstract

We review the basic theoretical underpinnings of the Grover algorithm, providing a rigorous and well motivated derivation. We then present a generalization of Grover’s algorithm that searches an arbitrary subspace of the multi-dimensional Hilbert space using a diffusion operation and an amplitude amplification procedure that has been biased by unitary steering operators. We also outline a generalized Grover’s algorithm that takes into account higher level correlations that could exist between database elements. In the traditional Grover algorithm, the Hadamard gate selects a uniform sample of computational basis elements when performing the phase selection and diffusion. In contrast, steered operators bias the selection process, thereby providing more flexibility in selecting the target state. Our method is a generalization of the recently proposal pattern matching algorithm of Hiroyuki et al.
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I. INTRODUCTION

Searching an unstructured data base of $N$ elements by classical means takes an average of $N/2$ calls to the database. In contrast, Grover’s algorithm [1] is a quantum search algorithm that requires of order $\sqrt{N}$ calls. While this is only a quadratic improvement, for large values of $N$ this can be a substantial savings. For example, a data base with $N = 10,000$ elements could be searched in just 100 quantum calls, compared to an average of 5,000 classical calls. The essential ingredients of Grover’s algorithm are amplitude selection and the subsequent diffusion of an initial or trial quantum state. Together, these steps constitute a process known as amplitude amplification, first introduced in Refs. [2–4]. In this section, we review the basic theoretical underpinnings of the Grover algorithm and amplitude amplification, providing physically motivated derivations, rather than the traditional proof-theorem construct of computer science and mathematics. We generalize both the method and formalism of the amplitude amplification procedure. We go on to examine a number of variants of the Grover algorithm, and we recast amplitude amplification in such a way as to extract an arbitrary subspace of the $N$-dimensional Hilbert space. We do this by biasing the diffusion operation and phase selection mechanism by unitary steering operators. In the traditional Grover algorithm, the Hadamard gate selects a uniform sample of computational basis elements when performing phase selection and diffusion. In contrast, the steering procedure biases these processes with a well chosen unitary operator, thereby providing more flexibility for the algorithm. We also apply our general formalism to give a concise derivation of the quantum pattern matching algorithm of Hiroyuki et al. [5].

We start our analysis with an overview of Grover’s algorithm, which consists of the following basic operations: (i) a trial wave function is selected and then used as a first guess, (ii) the phase of the wave function in the direction of the target state is inverted, thereby imprinting the target state on the trial wave function, (iii) the resulting state is sent through a diffusion operation to enhance the marked component, and (iv) the process is repeated until the target state is achieved with close to unit probability. In the traditional Grover algorithm, the target state is taken to be one of the computational basis states, and the trial wave function is taken to be the Hadamard state consisting of a uniform superposition of basis elements. While Grover’s algorithm allows one to select a specific quantum state from the multi-qubit Hilbert space, it has proven difficult to translate the algorithm into a realistic search engine. Interestingly, the difficulty of implementing a practical algorithm has led to numerous applications in other fields, such as cryptography and signal processing, but we would like to explore the possibility of using Grover’s algorithm for its original intended purpose of a database search. One of the problems with Grover search involves the difficulty of creating a quantum dictionary that maps the database entries into appropriate quantum states.
states. This is a kind of chicken-and-egg problem: if we knew the basis state corresponding to a specific database entry (and this basis state is precisely the information that Grover’s algorithm returns), then we would in fact already know the database entry, and there would be no need for Grover’s algorithm. We shall call this the dictionary problem. The origin of this problem is that the traditional algorithm has only one preferred state, namely the target state, as the algorithm is initialized with a uniform superposition of basis states, none of which are preferred. If we were to weight these basis states in some preferred direction, then we could avert the dictionary problem. We do this by a mechanism we call steering. Instead of employing a uniform sum over the basis states in selecting the initial guess, we use a non-uniform biased sum determined by a well chosen unitary operator. This biases the state selection, thereby avoiding the chicken-and-egg problem, while simultaneously improving the efficiency of the algorithm.

There are other problems in implementing a practical Grover search. In particular, a database contains an exponential number of gates, and a direct implementation of the database would therefore degrade the quantum advantage of the algorithm. To overcome this exponential gate problem, Ref. [6] introduces a new method called approximate amplitude encoding (AAE). This method approximates the exponentially large database by a constant depth parameterized quantum circuit containing only a polygonal number of gates, and the parameters of the circuit are trained using machine learning. We will discuss this problem throughout this paper, particularly in the last section, where we reproduce the quantum circuit of Hiroyuki et al. from our formalism.

This paper is organized as follows. In Section II A we introduce the general notion of steering operators. In Section II B we derive the traditional Grover’s algorithm, and in Section II C we generalize the algorithm to include what we call steering operators meant to bias the diffusion and amplitude selection processes. Section II D further generalizes Grover’s algorithm to accommodate an arbitrary target set, rather than a target consisting of a single computational basis element. We also generalize the algorithm with a non-separable kernel to account for possible higher order correlations between the search elements, thereby leading to non-planar Grover algorithms with speedups that are potentially better than quadratic. In Section II E we construct several quantum circuits that implement the generalized algorithms, and in Section III we derive the results of the pattern matching algorithm of Hiroyuki et al. from our formalism. Finally, in Section IV we provide some conclusions and closing remarks.
II. STEERED DIFFUSION AND AMPLITUDE AMPLIFICATION

In this section we introduce the notion of steering operators in the context of Grover’s algorithm. These are operators that selectively bias either the diffusion process or the amplitude selection stage of the Grover algorithm, thereby providing for a vast array of amplitude amplification strategies. Choosing the appropriate biasing scheme is of course the critical issue in selecting a steering operator. In a database search, for example, the correct biasing is determined solely by the details of the database itself. In other instances, when something is known a priori about the desired target state, biasing can be used to increase the efficiency of the Grover search.

A. Notation and Context

To establish some context and motivation, let us consider a coherent $n$-qubit system. Recall that the corresponding Hilbert space $\mathcal{H}_n$ has dimension $N = 2^n$, with computational basis states denoted by

$$|x\rangle \equiv |x_{n-1}, \cdots, x_1, x_0\rangle \equiv |x_{n-1}\rangle \otimes \cdots \otimes |x_1\rangle \otimes |x_0\rangle,$$  \hspace{1cm} (2.1)

where $x_\ell \in \{0, 1\}$ are binary observables labeled by the qubit indices $\ell \in \{0, \cdots, n-1\}$. We shall denote the set of computational basis states for an $n$-qubit system by

$$\Omega_n \equiv \left\{ |x\rangle \mid x \in \{0, 1\}^n \right\}.$$  \hspace{1cm} (2.2)

We have ordered the basis states such that the $n$-tuple $x \equiv (x_{n-1}, \cdots, x_1, x_0) \in \{0, 1\}^n$ corresponds to the binary number $x_{n-1} \cdots x_1 x_0$, where $x_0$ is the $2^0$-bit. This is in keeping with OpenQASM syntax [7]. For convenience, we shall use a dual notation in which the binary number $x$ is represented by its corresponding base-10 number between 0 and $N-1$. In other words, we shall index the computational basis state $|x\rangle$ by either a number $x \in \{0, 1, \cdots, N-1\}$, or by the corresponding bit string $x \in \{0, 1\}^n$. Consequently, we can express the set of basis elements in (2.2) by either the index set $\Omega_n = \{0, 1, \cdots, N-1\}$, or by the set of bit string $\Omega_n = \{x \mid x \in \{0, 1\}^n\}$. In this dual notation, we can list the computational basis elements in the order given by their numerical base-10 index,

$$|x_0 = 0\rangle \equiv |0, \cdots, 0, 0\rangle,$$  \hspace{1cm} (2.3)

$$|x_1 = 1\rangle \equiv |0, \cdots, 0, 1\rangle,$$

$$|x_2 = 2\rangle \equiv |0, \cdots, 1, 0\rangle,$$

$$|x_3 = 3\rangle \equiv |0, \cdots, 1, 1\rangle,$$

$$\vdots$$

$$|x_{N-1} = N-1\rangle \equiv |1, \cdots, 1, 1\rangle.$$
Therefore, if we wish to emphasize the order of a basis element, we use the notation $|x_i\rangle$ with the index $i \in \{0, 1, \cdots, N - 1\}$. This new index $i$ should not be confused with the qubit index $\ell \in \{0, 1, \cdots, n - 1\}$ of (2.1), as they are used in different contexts.

The traditional Grover’s algorithm selects a single target state $|\omega\rangle \in \Omega_n$, amplifying this component by the diffusion process. Our goal is to generalize the algorithm to choose an arbitrary subset of basis states $\Omega \subseteq \Omega_n$. We call the subset $\Omega$ the *amplitude steering set*, and the corresponding subspace $\mathbb{H}_\Omega \subseteq \mathbb{H}_n$ will be called the steering subspace. In general, $\mathbb{H}_\Omega$ need not correspond to a multi-qubit system; however, it is of particular interest when it does, and we shall investigate this case in some detail in a future section.

Since the Hadamard vector $|h\rangle$ is so critical to the Grover algorithm, we continue our analysis with a brief review of this state, thereby providing continuity and establishing some notation. The Hadamard state is defined by

$$|h\rangle \equiv H^{\otimes n} |0^n\rangle ,$$

(2.4)

where $H$ is the single-qubit Hadamard gate and $|0\rangle^{\otimes n} \equiv |0^n\rangle \equiv |0, \cdots, 0\rangle$ is the $n$-qubit zero-state. The Hadamard gate acts on the single-qubit computational basis states by

$$H|0\rangle = \frac{1}{\sqrt{2}} \left[ |0\rangle + |1\rangle \right] \equiv |+\rangle$$

(2.5)

$$H|1\rangle = \frac{1}{\sqrt{2}} \left[ |0\rangle - |1\rangle \right] \equiv |-\rangle ,$$

(2.6)

where $|\pm\rangle$ are called the positive and negative Hadamard states, respectively. For an $n$-qubit system we see that $|h\rangle = |+\rangle^{\otimes n}$, and the Hadamard state can therefore be expressed as the uniform sum over all computational basis elements,

$$|h\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle .$$

(2.7)

Our dual qubit ordering convention allows us to change notation to a more convenient form,

$$|h\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle ,$$

(2.8)

and we shall move between the representations (2.7) and (2.8) at will.

The Hadamard state $|h\rangle$ is used in the Grover algorithm in several ways. First, it serves as a trial or initial state upon which the amplitude and diffusion operators act. Then the Hadamard state is passed to the phase oracle, which marks the component of $|h\rangle$ in the direction of the target state $|\omega\rangle$ with a negative phase. The resulting state is finally passed to the diffusion portion of the algorithm, which amplifies the target component of the wave
The idea behind steering is that one can weight certain basis elements that are deemed more relevant, replacing the uniformly weighted Hadamard state \(|h\rangle\) in (2.8) with a biased trial state of the form

\[ |g\rangle = \sum_{x=0}^{N-1} g_x |x\rangle \equiv G|0^n\rangle. \]  

The operator \(G\) is called the diffusion steering operator. The weights \(g_x\) are normalized complex numbers (although they are often taken to be real numbers), so that

\[ \sum_{x=0}^{N-1} g_x g_x^* = 1. \]  

Since \(|g\rangle\) is normalized to unity, the steering operator must be unitary, i.e. \(G^\dagger G = GG^\dagger = 1\). Here, 1 is the \(2^n \times 2^n\) unit matrix for the \(n\)-qubit Hilbert space, although if we wish to emphasize the number of qubits, we shall write the unit operator as \(1_n\). The diffusion operator corresponding to the state \(|g\rangle\) is a simple Householder reflection,

\[ U_g \equiv 2|g\rangle\langle g| - 1 \]
\[ = G \left[ 2|0^n\rangle\langle 0^n| - 1 \right] G^\dagger. \]

When we employ the Hadamard operator \(H^\otimes n\) for the diffusion step, we are using an unbiased linear superposition of computational basis states, whereas the operator \(G\) biases the diffusion in a well chosen manner. This will allow us to steer the diffusion process. We can also bias the amplitude selection in a similar way by expressing the target state as

\[ |\omega\rangle \equiv A_\omega |0^n\rangle, \]

where \(A_\omega\) is a unitary operator called the amplitude steering operator. The phase oracle that marks the state \(|\omega\rangle\) is also a Householder reflection, and takes the form

\[ U_\omega \equiv 1 - 2|\omega\rangle\langle \omega| \]
\[ = A_\omega \left[ 1 - 2|0^n\rangle\langle 0^n| \right] A_\omega^\dagger. \]

Employing well-chosen steering operators \(G\) and \(A_\omega\) can dramatically improve the efficiency and flexibility of the Grover search.

Note that the diffusion and amplitude selection operators (2.12) and (2.15) depend upon the operator \(1 - 2|0^n\rangle\langle 0^n|\), which is a Householder reflection about the zero-state, and it can be implemented in the circuit model by a simple multi-control Z-gate. The steering operators \(G\) and \(A_\omega\), however, require much more care. They are generally (but not always) built...
from an exponential number of gates, thereby potentially degrading the quantum advantage of Grover’s algorithm. As previously noted, this exponential gate problem has plagued the Grover search algorithm since its inception. However, this problem has recently been addressed by Ref. [6], which introduces the notion of approximate amplitude encoding (AAE) in which the steering operators are approximated by a parameterized shallow quantum circuit using only a polynomial number of gates. A machine learning process is then employed, by which the steering operator can be approximated to any desired accuracy. We will return to this point in a later section.

B. Grover’s Algorithm for a Single Basis Element

For continuity and completeness, we now derive the original form of Grover’s algorithm, using well-motivated physical arguments. Our exposition will closely follow the presentation of Ref. [3]. Suppose we wish to find a specific target state $|\omega\rangle$ from among the $N = 2^n$ basis states $|x\rangle$. To proceed, consider the unitary operator $U_\omega$ defined on the basis states by

$$U_\omega |x\rangle \equiv \begin{cases} -|x\rangle & \text{for } x = \omega \\ |x\rangle & \text{for } x \neq \omega \end{cases},$$

(2.16)

as illustrated in the left panel of Fig. 1. Although (2.16) only defines $U_\omega$ on the basis states, since the operator is also linear, its action is in fact defined on any state in the $N$-dimensional quantum Hilbert space $\mathbb{H}_n$,

$$U_\omega |\psi\rangle = U_\omega \left( \sum_{x=0}^{N-1} \psi_x |x\rangle \right) = \sum_{x=0}^{N-1} \psi_x U_\omega |x\rangle.$$

(2.17)

The operator $U_\omega$ is often called an oracle because it can be thought of as black-box that answers the question: “Which state should I chose?” It is called a phase oracle because the answer is encoded by marking the best choice with a negative phase. In other words, the purpose of the phase oracle $U_\omega$ is to insert a negative phase on the target state $|\omega\rangle$, or on the component of the wave function in the target direction. Note that we can express the phase oracle by a simple Householder reflection,

$$U_\omega = 1 - 2|\omega\rangle\langle\omega|,$$

(2.18)

since this satisfies (2.16) on the basis states $|x\rangle$. From (2.18) we see that $U_\omega$ is indeed unitary, $U_\omega^\dagger U_\omega = 1$, and it is therefore a valid gate transformation operator. Furthermore, the operator is self-adjoint or Hermitian, $U_\omega^\dagger = U_\omega$, and so that the unitary condition becomes
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\( U_\omega = 1 - 2 |\omega\rangle \langle \omega | \)
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FIG. 1: Left panel: The phase oracle \( U_\omega \) marks the target state \( |\omega\rangle \) with a negative phase, and therefore the action of the oracle is given by the Householder reflection \( U_\omega = 1 - 2 |\omega\rangle \langle \omega | \). Right panel: The oracle is applied to the Hadamard state \( |h\rangle \). Note that \( U_\omega \) inverts the component of \( |h\rangle \) in the direction of \( |\omega\rangle \), thereby reflecting \( |h\rangle \) across the orthogonal axis \( |h_\perp\rangle \). If the angle between \( |h\rangle \) and \( |h_\perp\rangle \) is defined to be \( \theta \), then the resulting state \( U_\omega |h\rangle \) lies below the orthogonal direction \( |h_\perp\rangle \) by the same angle \( \theta \).

\( U_\omega^2 = 1 \), and we see that \( U_\omega \) is also idempotent. Also note that (2.18) implies that the action of \( U_\omega \) on a general state is given by

\[
U_\omega |\psi\rangle = |\psi\rangle - (2 \langle \omega | \psi \rangle) |\omega\rangle ,
\]

(2.19)
a more concise form than the one given in (2.17). We see explicitly that the component of the wave function in the direction \( |\omega\rangle \) receives a negative phase. Also note that the vector \( U_\omega |\psi\rangle \) always lies in the 2-dimensional subspace spanned by \( |\psi\rangle \) and \( |\omega\rangle \). This fact will allow us to employ a 2-dimensional Euclidean analogy to visualize the algorithm. It is crucial to the Grover algorithm that the action of the oracle in the \( N \)-dimensional quantum Hilbert space reduces to simple reflections in a 2-dimensional subspace of this (potentially quite large) Hilbert space.

The Grover algorithm begins by letting the oracle \( U_\omega \) act on the Hadamard state \( |h\rangle \), thereby forming the marked state \( U_\omega |h\rangle \). Because \( U_\omega \) is a Householder reflection, the vector \( U_\omega |h\rangle \) will lie in the 2-dimensional subspace spanned by \( |\omega\rangle \) and \( |h\rangle \). To visualize this reflection, it is convenient to consider the state \( |h_\perp\rangle \) orthogonal to \( |\omega\rangle \) in this 2-dimensional
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subspace. We can construct $|h_\perp\rangle$ by simply removing $|\omega\rangle$ from $|h\rangle$, and then normalizing the resulting state,

$$|h_\perp\rangle \equiv \frac{1}{\sqrt{N-1}} \sum_{x \neq \omega} |x\rangle .$$  \hfill (2.20)

Note that $\langle h_\perp|h_\perp\rangle = 1$ and $\langle \omega|h_\perp\rangle = 0$, while

$$\langle h|h_\perp\rangle = \sqrt{\frac{N-1}{N}} \hfill (2.21)$$

$$\langle h|\omega\rangle = \frac{1}{\sqrt{N}} . \hfill (2.22)$$

Let $\theta$ be the angle between $|h\rangle$ and $|h_\perp\rangle$ in the 2-dimensional subspace, so that $\cos \theta = \langle h|h_\perp\rangle$ and $\sin \theta = \langle h|\omega\rangle$, and we consequently find

$$\cos \theta = \sqrt{\frac{N-1}{N}} \quad \text{and} \quad \sin \theta = \frac{1}{\sqrt{N}} . \hfill (2.23)$$

Since $U_\omega$ is just a Householder reflection across the $|h_\perp\rangle$ hyperplane, the state $U_\omega|h\rangle$ lies below the axis $|h_\perp\rangle$ at an angle of $\theta$, as illustrated in the right panel of Fig. 1. For $\theta \ll 1$, we have $\theta \approx 1/\sqrt{N}$.

We are now ready for the next step of the algorithm, the so called diffusion operation, which is summarized in Fig. 2. In this step, we start with the state $U_\omega|h\rangle$ in the fourth

![Diagram](image)

FIG. 2: The diffusion portion of the algorithm starts with the state $U_\omega|h\rangle$ in the fourth quadrant, upon which we perform an inversion $-U_\omega|h\rangle$ into the second quadrant. We then perform the Householder reflection $-U_h = 1 - 2|h\rangle\langle h|$ on $-U_\omega|h\rangle$, placing $U_h U_\omega|\omega\rangle$ into the first quadrant. If the angle between $|h\rangle$ and $|h_\perp\rangle$ is $\theta$, then the state $U_h U_\omega|\omega\rangle$ will be inclined at an angle $2\theta$ above the original state $|h\rangle$, and therefore $U_h U_\omega|h\rangle$ lies closer to the target vector $|\omega\rangle$ than does the starting position $|h\rangle$. 

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quadrant of the 2-dimensional subspace spanned by $|\omega\rangle$ and $|h_\perp\rangle$. In other words, we start with $U_\omega|h\rangle$ lying at an angle $\theta$ below the $|h_\perp\rangle$ axis. The inverted state $-U_\omega|h\rangle$ consequently lies in the second quadrant at an angle $\theta$ above the negative $|h_\perp\rangle$ axis. Let us define the diffusion operator

$$U_h \equiv 2|h\rangle\langle h| - 1,$$  \hspace{1cm} (2.24)

and we see that applying $-U_h = 1 - 2|h\rangle\langle h|$ on $-U_\omega|h\rangle$ places $U_h U_\omega|h\rangle$ back into the first quadrant. As the geometry of Fig. 2 reveals, the resulting vector $U_h U_\omega|h\rangle$ is inclined by angle $2\theta$ above the initial choice $|h\rangle$, or an angle $3\theta$ above the horizontal axis $|h_\perp\rangle$. Thus $U_h U_\omega|h\rangle$ is closer to the target state $|\omega\rangle$ than the initial vector $|h\rangle$. Upon repeating these two operations, $U_\omega$ followed by $U_h$, we obtain vectors that lie closer and closer to $|\omega\rangle$. The first such Grover iteration is summarized in Fig. 3.

We must be careful, however, concerning the number of iterations that we employ, as it is possible to overshoot the target vector $|\omega\rangle$. So how many iterations must we perform before we reach the target $|\omega\rangle$? After $r$ iterations, the angle between $|h_\perp\rangle$ and the iterated state $(U_h U_\omega)^r|h\rangle$ is $\theta_r = (2r + 1)\theta$. When $\theta_r = \pi/2$, then we have performed enough iterations to extract the target state $|\omega\rangle$ with unit probability. For $\theta \ll 1$, we must perform $r = r_\ast$ iterations until $2r_\ast \theta \approx \pi/2$, which implies that the number of requisite iterations is

![FIG. 3: The first Grover iteration. We start with the Hadamard state $|h\rangle$ and apply a Householder reflection $U_\omega = 1 - 2|\omega\rangle\langle \omega|$ about the hyperplane orthogonal to $|\omega\rangle$. This inverts the component of $|h\rangle$ that is parallel to $|\omega\rangle$ across the orthogonal direction $|h_\perp\rangle$, as illustrated by the blue dashed arrow. The state $U_\omega|h\rangle$ then undergoes a reflection $U_h = 2|h\rangle\langle h| - 1$, as illustrated by the red dashed line, and this new state $U_h U_\omega|h\rangle$ lies closer to the target state $|\omega\rangle$ than the original vector $|h\rangle$. After $r$ iterations, the state $(U_h U_\omega)^r|h\rangle$ is inclined at an angle $\theta_r = (2r + 1)\theta$ above the horizontal axis $|h_\perp\rangle$, and when $\theta_r = \pi/2$ we obtain the target state $|\omega\rangle$ with unit probability. For $\theta \ll 1$, this corresponds to $r_\ast \approx (\pi/4)\sqrt{N}$ iterations.](image-url)
\[ r_s \approx \pi/4 \theta \approx (\pi/4)\sqrt{N}. \] The fact that the proportionality constant is \( \pi/4 \approx 0.75 < 1 \) is quite fortunate, since a factor like \( 2\pi \approx 6 \) would have required proportionally more iterations.

There is a subtlety that we should mention regarding an overall negative phase factor in Fig. 2. Quantum mechanics cannot distinguish between the action of the two operators 

\[ U_h^{(1)} = 1 - 2|h\rangle\langle h| \quad \text{and} \quad U_h^{(2)} = 2|h\rangle\langle h| - 1 \]

since they differ by a sign (a total phase of \( e^{i\pi} \)). Recall that we first acted on the state \(|h\rangle\) with the operator \( U_\omega \), so that \( U_\omega|h\rangle \) lies in the fourth quadrant. We then inverted the vector to place \(-U_\omega|h\rangle\) into the second quadrant. However, the two states \( U_\omega|h\rangle \) and \(-U_\omega|h\rangle\) are indistinguishable, so we might as well act on \( U_\omega|h\rangle\) with the operator \( U_h^{(1)} = 1 - 2|h\rangle\langle h| \), giving a resultant vector \( U_h^{(1)} U_\omega|h\rangle \) in the third quadrant, as illustrated in Fig. 4. The negative of this vector, \(-U_h^{(1)} U_\omega|h\rangle\), is just the final vector \( U_h^{(2)} U_\omega|h\rangle \) in the first quadrant of Fig. 2. But since quantum mechanics is insensitive to an overall phase, both \( U_h^{(1)} \) and \( U_h^{(2)} \) are represented by the same quantum circuit. We therefore use \( U_h \equiv U_h^{(2)} = 2|h\rangle\langle h| - 1 \) in the text of this manuscript, while we employ \(-U_h = U_h^{(1)} = 1 - 2|h\rangle\langle h| \) in quantum circuits. This is because the quantum circuits for \( U_h^{(1)} \) and \( U_h^{(2)} \) differ by a minus sign, and the circuit implementation of \(-U_h = 1 - 2|\omega\rangle\langle \omega| \) and \( U_\omega = 1 - 2|\omega\rangle\langle \omega| \) will be quite similar.

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\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

\[ U_h^{(1)} U_\omega |h\rangle \]

\[ U_h^{(2)} U_\omega |h\rangle \]

FIG. 4: Since the operators \( U_h^{(1)} = 1 - 2|h\rangle\langle h| \) and \( U_h^{(2)} = 2|h\rangle\langle h| - 1 \) differ by a sign, the states \( U_h^{(1)} U_\Omega|h\rangle \) and \( U_h^{(2)} U_\Omega|h\rangle \) are physically indistinguishable.
C. Grover’s Algorithm with Steering

In the previous section, we can replace the target basis state $|\omega\rangle \in \Omega_n$ by a general target state

$$|\omega\rangle = \sum_{x=0}^{N-1} \omega_x |x\rangle \in \mathcal{H}_n ,$$

(2.25)

and the argument will remain the same. We can write $|\omega\rangle = A_\omega |0^n\rangle$, where $A_\omega$ is the unitary amplitude steering operator, and the oracle takes the form

$$U_\omega = 1 - 2|\omega\rangle\langle\omega|$$

(2.26)

$$= A_\omega \left[ 1 - 2|0^n\rangle\langle0^n| \right] A_\omega^\dagger .$$

(2.27)

The operator $1 - 2|0^n\rangle\langle0^n|$ marks the zero-state, and in the quantum circuit model it can be implemented by a multi-control $Z$-gate. The argument also goes through unscathed if we replace the Hadamard state $|h\rangle$ with the steered state $|g\rangle = G|0^n\rangle$ of (2.9). That is to say, let us start with the trail state $|g\rangle$, apply the oracle $U_\omega$, and then steer the diffusion with the operator

$$U_g = 2|g\rangle\langle g| - 1$$

(2.28)

$$= G \left[ 2|0^n\rangle\langle0^n| - 1 \right] G^\dagger .$$

(2.29)

The form of the steered diffusion operator (2.29) is a special case of Hadamard diffusion,

$$U_h = 2|h\rangle\langle h| - 1 = H^\otimes n \left[ 2|0^n\rangle\langle0^n| - 1 \right] H^\otimes n .$$

(2.30)

Note that the operator $1 - 2|0^n\rangle\langle0^n|$ is an oracle that marks the state $|0^n\rangle$ with a negative phase. The operators $U_\omega$, $U_h$, and $U_g$ can be constructed from a combination of multi-controlled $Z$-gates and single-qubit $X$ and $H$ gates. Let $\theta$ be the angle of inclination of $|g\rangle$, and for $\theta \ll 1$, then the number of Grover iterations required to pull out the target state is

$$r_* \approx \frac{\pi}{4\theta} \approx C\sqrt{N} ,$$

(2.31)

where the prefactor $C$ depends upon the choice of the steering operator $G$. When we take $G = H^\otimes n$, then the prefactor reduces to its previous value $C_h \equiv \pi/4$. For a well-chosen $G$, the prefactor $C$ can be much smaller than $C_h$, and fewer iterations will be required. We therefore arrive at the following algorithm, which is illustrated in Fig. 5.
The Algorithm

1. Initialize the system to the state

\[ |g\rangle = G|0\rangle \otimes_n = \sum_{x=0}^{N-1} g_x |x\rangle , \quad (2.32) \]

and construct the target state

\[ |\omega\rangle = A_\omega|0\rangle \otimes_n = \sum_{x=0}^{N-1} \omega_x |x\rangle . \quad (2.33) \]

2. Perform a Grover iteration on the state vector:
   (a) Apply the phase oracle \( U_\omega = 1 - 2|\omega\rangle \langle \omega | \), where \( |\omega\rangle = A|0\rangle \otimes_n \).
   (b) Apply the diffusion operator \( U_g = 2|g\rangle \langle g | - 1 \), where \( |g\rangle = G|0\rangle \otimes_n \).

3. Repeat this of order \( r_* \approx \pi/4\theta \approx C\sqrt{N} \) times.
4. Measure the resulting state in the computational basis after \( r_* \) iterations. The output will be \( |\omega\rangle \) with probability approaching unity. The numerical value of \( C \) depends upon the steering operator \( G \).

FIG. 5: Steered Grover’s algorithm
D. Grover’s Algorithm for an Arbitrary Target Set

In the last section, we devised a phase oracle $U_\omega$ that marks any given computational basis state $|\omega\rangle$ from among the $N = 2^n$ possible basis states of an $n$-qubit system $\mathcal{H}_n$. That is to say, the phase oracle $U_\omega$ marks a single target vector $\omega \in \Omega_n$, where the set of all computational basis states is represented by $\Omega_n = \{x \mid x \in \{0,1\}^n\}$. In this section we construct a phase oracle $U_\Omega$ that marks an arbitrary subset of target vectors $\Omega \subseteq \Omega_n$. We shall call $\Omega$ the steering set, and assume that it contains $M \leq N$ elements. The Hilbert space associated with $\Omega$ will be denoted $\mathcal{H}_\Omega$, and called the steering subspace, while the orthogonal Hilbert space will be denoted $\mathcal{H}_\perp$. The space $\mathcal{H}_\Omega$ need not be a multi-qubit subspace of $\mathcal{H}_n$, although this is a very interesting case that we will shortly consider.

Recall that we are using a dual notation in which a computational basis vector can be indexed by either a binary number (or bit string) $x \in \{0,1\}^n$, or by the corresponding base-10 number $x \in \{0,1,\ldots,N-1\}$. Thus, if we wish to enumerate the basis elements, we employ the notation $\Omega_n = \{x_0, x_1, \ldots, x_{N-1}\}$ in which $x_i$ is the base-10 representation of the basis element $i \in \{0,1,\ldots,N-1\}$. We can therefore express the set of basis elements by the notation $\Omega_n = \{0,1,\ldots,N-1\}$, or even by the collection of ket vectors $\Omega_n = \{|x_0\rangle, |x_1\rangle, \ldots, |x_{N-1}\rangle\}$, depending upon on the context. We will not necessarily choose the basis elements of $\Omega$ in any specific order, so we express the steering set by $\Omega = \{x_{i_0}, x_{i_1}, \ldots, x_{i_{M-1}}\}$. Adopting the notation $\omega$ to reference a target element, we can also write $\Omega = \{\omega_0, \omega_1, \ldots, \omega_{M-1}\}$, or more precisely, $\Omega = \{|\omega_0\rangle, |\omega_1\rangle, \ldots, |\omega_{M-1}\rangle\}$. Note that there are $2^N = 2^{2^n}$ subsets of $\Omega_n$ (including the empty set), each corresponding to a phase oracle $U_\Omega$.

1. Marking a Subset of the Computational Basis

The phase oracle $U_\Omega$ marks all basis states in the steering set $\Omega \subseteq \Omega_n$ with a negative phase, and its action on a general $x \in \Omega_n$ is therefore given by

$$U_\Omega |x\rangle = \begin{cases} -|x\rangle & \text{for } x \in \Omega \\ |x\rangle & \text{for } x \notin \Omega . \end{cases}$$

Consequently, we can express the oracle by

$$U_\Omega = 1 - 2 \sum_{x \in \Omega} |x\rangle \langle x| ,$$

(2.35)
since (2.35) satisfies (2.34) for every basis element $|x\rangle$. We now decompose the unit operator in terms of basis state projection operators,

$$1 = \sum_{x=0}^{N-1} |x\rangle\langle x| = \sum_{x \in \Omega} |x\rangle\langle x| + \sum_{x \notin \Omega} |x\rangle\langle x| = P_\perp + P_\Omega , \quad (2.36)$$

where the projection operators onto $\mathbb{H}_\Omega$ and the orthogonal subspace $\mathbb{H}_\perp$ are defined by

$$P_\Omega = \sum_{x \in \Omega} |x\rangle\langle x| \quad (2.37)$$

$$P_\perp = \sum_{x \notin \Omega} |x\rangle\langle x| . \quad (2.38)$$

The phase oracle (2.35) now takes a particularly simple form,

$$U_\Omega = \sum_{x \notin \Omega} |x\rangle\langle x| - \sum_{x \in \Omega} |x\rangle\langle x| = P_\perp - P_\Omega . \quad (2.39)$$

The action of the phase oracle on a general state is therefore

$$U_\Omega |\psi\rangle = U_\Omega \left( \sum_{x=0}^{N-1} \psi_x |x\rangle \right) = \sum_{x \notin \Omega} \psi_x |x\rangle - \sum_{x \in \Omega} \psi_x |x\rangle , \quad (2.40)$$

or more specifically, its action on the Hadamard state is

$$U_\Omega |h\rangle = \frac{1}{\sqrt{N}} \sum_{x \notin \Omega} |x\rangle - \frac{1}{\sqrt{N}} \sum_{x \in \Omega} |x\rangle . \quad (2.41)$$

This suggests that we consider the 2-dimensional subspace spanned by the orthonormal states

$$|\Omega\rangle \equiv \frac{1}{\sqrt{M}} \sum_{x \in \Omega} |x\rangle \quad (2.42)$$

$$|h_\perp\rangle \equiv \frac{1}{\sqrt{N-M}} \sum_{x \notin \Omega} |x\rangle . \quad (2.43)$$

One can easily check that the states $|\Omega\rangle$ and $|h_\perp\rangle$ are orthogonal and normalized to unity, i.e. $\langle \Omega | \Omega \rangle = \langle h_\perp | h_\perp \rangle = 1$, and $\langle \Omega | h_\perp \rangle = 0$. Also note that $|\Omega\rangle$ and $|h_\perp\rangle$ have the following overlaps with the Hadamard state $|h\rangle$,

$$\langle \Omega | h \rangle = \sqrt{\frac{M}{N}} \quad \text{and} \quad \langle h_\perp | h \rangle = \sqrt{\frac{N-M}{N}} . \quad (2.44)$$
We shall call the 2-dimensional space spanned by $|\Omega\rangle$ and $|h\rangle$ the $\Omega$-$h$ subspace. The Hadamard state $|h\rangle$ lies within this subspace, and using relations (2.44), it can be decomposed as

$$|h\rangle = \sqrt{\frac{N-M}{N}} |h\rangle + \sqrt{\frac{M}{N}} |\Omega\rangle .$$

(2.45)

Furthermore, the operation of the phase oracle $U_\Omega$ on the Hadamard state remains within this subspace, as applying (2.39) to (2.45) gives

$$U_\Omega |h\rangle = \sqrt{\frac{N-M}{N}} |h\rangle - \sqrt{\frac{M}{N}} |\Omega\rangle .$$

(2.46)

This expression can also be obtained directly from (2.41). Obviously $-U_\Omega |h\rangle$ also lies within the $\Omega$-$h$ subspace, as does the action of the Householder reflection $U_h = 2|h\rangle\langle h| - 1$ on $U_\Omega|h\rangle$,

$$U_h U_\Omega |h\rangle = \left[ 2|h\rangle\langle h| - 1 \right] \left[ \sqrt{\frac{N-M}{N}} |h\rangle - \sqrt{\frac{M}{N}} |\Omega\rangle \right]$$

$$= \sqrt{\frac{N-M}{N}} \left[ 1 - \frac{4M}{N} \right] |h\rangle + \sqrt{\frac{M}{N}} \left[ 3 - \frac{4M}{N} \right] |\Omega\rangle .$$

(2.47)

(2.48)

Further iterations $(\pm U_\Omega U_h)^r |h\rangle$ for $r \geq 1$ also lie within the $\Omega$-$h$ subspace. These results are illustrated in Fig. 6 and provide the basis for a generalized Grover algorithm.

To construct the algorithm, let $\theta$ be the angle between $|h\rangle$ and $|h\rangle$, so that

$$\cos \theta = \langle h\rangle |h\rangle = \sqrt{\frac{N-M}{N}} \quad \text{and} \quad \sin \theta = \langle \Omega \rangle |h\rangle = \sqrt{\frac{M}{N}} ,$$

(2.49)

FIG. 6: The action of $U_\Omega = \mathbb{1} - |h\rangle\langle h| - 1$ remain in the 2-dimensional subspace spanned by $|\Omega\rangle$ and $|h\rangle$. The state $|h\rangle$ lies within this subspace, and is inclined at an angle $\theta$ above $|h\rangle$. The state $U_\Omega|h\rangle$ lies below the $h\rangle$ axis at an angle $\theta$, while the iterated state $U_h U_\Omega|h\rangle$ is inclined at an angle $2\theta$ above $|h\rangle$, or $3\theta$ above $|h\rangle$. 

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and we then expand the Hadamard state as
\[
|h\rangle = \cos \theta |h\rangle + \sin \theta |\Omega\rangle .
\] (2.50)

We see that \(|h\rangle\) lies in the 1-st quadrant of the 2-dimensional \(\Omega-h\) space at an angle \(\theta\) above the \(|h\rangle\) axis, while
\[
U_\Omega |h\rangle = \cos \theta |h\rangle - \sin \theta |\Omega\rangle ,
\]
lies in the 4-th quadrant at an angle \(\theta\) below the \(|h\rangle\) axis. Note, however, that
\[
U_h U_\Omega |h\rangle = \cos \theta \left[ 1 - 4 \sin^2 \theta \right] |h\rangle - \sin \theta \left[ 3 - 4 \sin^2 \theta \right] |\Omega\rangle
\] (2.51)
\[
= \cos 3\theta |h\rangle + \sin 3\theta |\Omega\rangle
\] (2.52)
lies back in the 1-st quadrant only when the coefficients of \(|h\rangle\) and \(|\Omega\rangle\) are both positive, in which case it is inclined by \(2\theta\) above \(|h\rangle\), or \(3\theta\) above the horizontal axis \(|h\rangle\). From (2.48) this corresponds to the region \(0 \leq M/N \leq 1/4\). If the coefficients are both negative, so that \(3/4 \leq M/N \leq 1\), then the Grover iteration places the state \(U_h U_\Omega |h\rangle\) in the 3-rd quadrant, which is equivalent to being in the 1-st quadrant (by a negative inversion). For \(1/4 < M/N < 3/4\) the coefficients have different signs. In fact, the \(|h\rangle\) coefficient is always negative and the \(|\Omega\rangle\) coefficient is positive, placing the state in the 2-nd quadrant. In this case, another Householder reflection of the form
\[
U_\parallel = 2|\Omega\rangle \langle \Omega| - 1
\] (2.53)
is required to bring \(U_\parallel U_h U_\Omega |h\rangle\) back into the first quadrant, inclined at \(2\theta\) above \(|h\rangle\). Figure 7 plots the \(|h\rangle\) and \(|\Omega\rangle\) coefficients of (2.48) as a function of \(M/N\), illustrating that there indeed three regions of interest.

FIG. 7: The coefficients of \(U_h U_\Omega |h\rangle\) from (2.48) as a function of \(M/N\). The blue line is the coefficient of \(|h\rangle\) and the yellow line is the coefficient of \(|\Omega\rangle\). This partitions the ratio \(M/N\) into three regions: (i) \(0 \leq M/N \leq 1/4\), (ii) \(1/4 < M/N < 3/4\), and \(3/4 \leq M/N \leq 1\). Regions (i) and (iii) permit the usual Grover algorithm, while region (ii) requires an extra reflection.
To find the appropriate number of iterations to perform, let us assume \( M/N \ll 1 \). Then from (2.49) we will find the target state \( |\Omega\rangle \) after

\[
r_\ast \approx \frac{\pi}{4\theta} \approx \frac{\pi}{4} \sqrt{\frac{N}{M}}
\]

(2.54) iterations. We see that the factor of \( M \) decreases the number of requisite iterations relative to the factor \( \sqrt{N} \) of the original Grover’s algorithm. This is because the search space becomes smaller as \( M \) increases, and indeed, when \( M = N \) there is in fact no need to perform a search, since all basis vectors lie in \( \Omega_n = \{0, 1, \cdots, N - 1\} \). In fact, the formalism gives \( P_{\Omega_n} = 1 \), \( P_\perp = 0 \), and \( U_{\Omega_n} = -1 \). Since \( U_{\Omega_n} \) introduces a total negative phase, it is equivalent to the unit operator \( 1 \). This formalism is a slight generalization of the amplitude amplification algorithm of Refs. [2] and [3].

2. General Trial State

We can further generalize the initial state of the algorithm from the Hadamard state to an arbitrary normalized vector \( |g\rangle \equiv G|0^n\rangle \), where \( G \) is the corresponding steering operator. Upon decomposing \( |g\rangle \) in terms of the computational basis, we write

\[
|g\rangle = \sum_x g_x |x\rangle = \sum_{x \in \Omega} g_x |x\rangle + \sum_{x \notin \Omega} g_x |x\rangle .
\]

(2.55)

This suggest that we define the (normalized) \( \Omega \)-component and orthogonal-component of \( |g\rangle \) by

\[
|g\rangle_\Omega \equiv N_\Omega^{-1} \sum_{x \in \Omega} g_x |x\rangle \\
|g\rangle_\perp \equiv N_\perp^{-1} \sum_{x \notin \Omega} g_x |x\rangle ,
\]

(2.56, 2.57)

where the normalization factors are

\[
N_\Omega = \left( \sum_{x \in \Omega} g_x^* g_x \right)^{1/2} \equiv \sin \theta
\]

(2.58)

\[
N_\perp = \left( \sum_{x \notin \Omega} g_x^* g_x \right)^{1/2} = \cos \theta .
\]

(2.59)

Furthermore, since \( \langle g_\Omega | g_\perp \rangle = 0 \) and \( \langle g_\perp | g_\perp \rangle = \langle g_\Omega | g_\Omega \rangle = 1 \), we see that \( |g_\Omega\rangle \) and \( |g_\perp\rangle \) form an orthonormal basis for a 2-dimensional subspace, which we shall call the \( \Omega-g \) subspace.
We have expressed the normalization factors \((2.58)\) and \((2.59)\) in terms of an angle \(\theta\), and so the decomposition \((2.55)\) can be expressed as

\[
\langle g \rangle = N_{\perp} \langle g_{\perp} \rangle + N_{\Omega} \langle g_{\Omega} \rangle
\]

\[= \cos \theta \langle g_{\perp} \rangle + \sin \theta \langle g_{\Omega} \rangle.\]  

Thus, \(\theta\) is the angle of inclination of \(\langle g \rangle\) relative to the horizontal axis \(\langle g_{\perp} \rangle\) in the \(\Omega\)-\(g\) subspace. This leads to the following Grover iteration. First, let the phase oracle \(U_{\Omega}\) act upon the trial state \(\langle g \rangle\), giving

\[
U_{\Omega} \langle g \rangle = N_{\perp} \langle g_{\perp} \rangle - N_{\Omega} \langle g_{\Omega} \rangle
\]

\[= \cos \theta \langle g_{\perp} \rangle - \sin \theta \langle g_{\Omega} \rangle;\]  

we then complete the iteration with the diffusion operation, giving

\[
U_{g} U_{\Omega} \langle g \rangle = \left[2 \langle g \rangle \langle g \rangle - \mathbb{1}\right] \left[N_{\perp} \langle g_{\perp} \rangle - N_{\Omega} \langle g_{\Omega} \rangle\right]
\]

\[= N_{\perp} \left[1 - 4 N_{\Omega}^2\right] \langle g_{\perp} \rangle + N_{\Omega} \left[3 - 4 N_{\Omega}^2\right] \langle g_{\Omega} \rangle\]

\[= \cos 3\theta \langle g_{\perp} \rangle + \sin 3\theta \langle g_{\Omega} \rangle.\]  

As before, this vector lies in the 1-st quadrant only when both coefficients of \(\langle g_{\perp} \rangle\) and \(\langle g_{\Omega} \rangle\) are positive (and it lies in the 3-rd quadrant when both are negative), otherwise a further Householder reflection \(U_{\parallel} = 2 \langle g_{\Omega} \rangle \langle g_{\Omega} \rangle - \mathbb{1}\) is required to bring it into the 1-st quadrant. The method reduces to the previous case when the \(g_{x}\) are independent of \(x\), \textit{i.e.} when \(g_{x} = 1/\sqrt{N}\), in which case the target vector becomes \(\langle g_{\Omega} \rangle \equiv |\Omega\rangle\). We now have the following Grover algorithm (we assume for simplicity that both coefficients are positive):

1. Construct the trail state \(\langle g \rangle\) inclined at an angle \(\theta\) above the \(\langle g_{\perp} \rangle\) axis in the \(\Omega\)-\(g\) subspace.
2. Define the diffusion operator \(U_{g} = 2 \langle g \rangle \langle g \rangle - \mathbb{1}\), and the basis selection operator \(U_{\Omega}\).
3. The state \(U_{\Omega} \langle g \rangle\) lies in the 4-th quadrant at an angle \(\theta\) below the \(g_{\perp}\) axis.
4. The state \(U_{g} U_{\Omega} \langle g \rangle\) lies back in the 1-st quadrant, inclined at an angle \(2\theta\) above \(\langle g \rangle\), or a total angle of \(3\theta\) above the \(\langle g_{\perp}\rangle\) axis.
5. After \(r\) iterations, the state \((U_{g} U_{\Omega})^r \langle g \rangle\) is inclined at angle \(\theta_r = (2r + 1)\theta\) above the \(\langle g_{\perp}\rangle\) axis. When \(\theta_r = \pi/2\) we will find the target state \(\langle g_{\Omega} \rangle\) with unit probability. The number of iterations is therefore \(r_* = \pi/4\theta - 1/2\). For \(\theta \ll 1\), then \(r_* \approx C \sqrt{N/M}\).
3. Further Generalization

Let us consider a steering set composed of arbitrary orthonormal basis elements $|y\rangle$, where the relation with the computational basis is given by

$$|y\rangle = \sum_x \Lambda_{yx} |x\rangle .$$  \hspace{1cm} (2.67)

Since both sets of basis elements are orthonormal, the transformation matrix is unitary,

$$\Lambda^\dagger \Lambda = \Lambda \Lambda^\dagger = 1 .$$  \hspace{1cm} (2.68)

Let us now take the steering set to consist of the $M$ elements

$$\Omega = \{|y_0\rangle, |y_1\rangle, \ldots, |y_{M-1}\rangle\} ,$$  \hspace{1cm} (2.69)

and define the phase oracle to be

$$U_\Omega |y\rangle = \begin{cases} -|y\rangle \text{ for } y \in \Omega \\ |y\rangle \text{ for } y \notin \Omega \end{cases} \Rightarrow U_\Omega = 1 - 2 \sum_{y \in \Omega} |y\rangle \langle y| .$$  \hspace{1cm} (2.70)

Upon transforming back to the computational basis, we can write

$$U_\Omega = 1 - 2 \sum_{xx'} \Omega_{xx'} |x\rangle \langle x'| ,$$  \hspace{1cm} (2.71)

where the steering kernel is given by

$$\Omega_{xx'} = \sum_{y \in \Omega} \Lambda_{x'y}^\dagger \Lambda_{yx} .$$  \hspace{1cm} (2.72)

Correlations between the basis elements can be encoded by using a non-separable kernel, which could be used to capture higher order relations between the search elements. Non-separable kernels lead to non-planar Grover algorithms, with the possibility for speed-up beyond quadratic.

E. Circuit Implementation

We now look at the circuit implementations of the Grover algorithms we have discussed, starting with the phase oracle $U_\omega$ that marks an arbitrary basis element $|\omega\rangle$. As we have seen, the phase oracle takes the form of the Householder reflection $U_\omega = 1 - 2|\omega\rangle \langle \omega|$. We have also found it convenient to express the target state $|\omega\rangle$ by the corresponding bit string $\omega$, and we will continue this practice. We shall examine the phase oracles in more detail for
a simple 2-qubit system with computational basis states $\omega = 00, 01, 10, 11$. To pick out the state $\omega = 11$ we can employ the $CZ$ gate, as this marks the target state $|11\rangle$ with a negative phase,

$$U_{11} \equiv \mathbb{1}_2 - |11\rangle\langle 11| = CZ : \begin{cases} 
|00\rangle \rightarrow |00\rangle \\
|01\rangle \rightarrow |01\rangle \\
|10\rangle \rightarrow |10\rangle \\
|11\rangle \rightarrow -|11\rangle .
\end{cases} \quad (2.73)$$

Note that we are using the OpenQASM convention in which the lowest order qubit is the control qubit. In a similar manner, note that $\omega = 00$ is selected by the oracle

$$U_{00} \equiv \mathbb{1}_2 - |00\rangle\langle 00| = (X \otimes X) \cdot CZ \cdot (X \otimes X) : \begin{cases} 
|00\rangle \rightarrow -|00\rangle \\
|01\rangle \rightarrow |01\rangle \\
|10\rangle \rightarrow |10\rangle \\
|11\rangle \rightarrow |11\rangle ,
\end{cases} \quad (2.74)$$

where $X$ is the $2 \times 2$ single-qubit NOT operator. Furthermore, $\omega = 01$ is marked by

$$U_{01} \equiv \mathbb{1}_2 - |01\rangle\langle 01| = (X \otimes I) \cdot CZ \cdot (X \otimes I) : \begin{cases} 
|00\rangle \rightarrow |00\rangle \\
|01\rangle \rightarrow -|01\rangle \\
|10\rangle \rightarrow |10\rangle \\
|11\rangle \rightarrow |11\rangle ,
\end{cases} \quad (2.75)$$

where $I$ is the $2 \times 2$ single-qubit identity operator. In a similar manner, we can mark the state $\omega = 10$ by the oracle

$$U_{10} \equiv \mathbb{1}_2 - |10\rangle\langle 10| = (I \otimes X) \cdot CZ \cdot (I \otimes X) : \begin{cases} 
|00\rangle \rightarrow |00\rangle \\
|01\rangle \rightarrow |01\rangle \\
|10\rangle \rightarrow -|10\rangle \\
|11\rangle \rightarrow |11\rangle ,
\end{cases} \quad (2.76)$$

We can therefore express all four of the 2-qubit phase oracles by

$$U_\omega = A_\omega U_{00} A_\omega , \quad \text{where } \omega \in \{00, 01, 10, 11\} \quad \text{and}$$

$$A_{00} \equiv I \otimes I , \quad A_{01} \equiv I \otimes X , \quad A_{10} \equiv X \otimes I , \quad A_{11} \equiv X \otimes X . \quad (2.78)$$

Note that the steering operator $A_\omega$ is the tensor product of $X$ gates or unit gates $I$, where $X$ corresponds to the 1-bit and $I$ corresponds to the 0-bit of the bit string $\omega \in \{00, 01, 10, 11\}$.  

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This construction generalizes to an arbitrary \( n \)-qubit system. For example, equation (2.74), which marks the zero-state, becomes

\[
U_0^{(n)}(n) \equiv 1_n - 2|0^n\rangle\langle 0^n| = X^{\otimes n} \cdot \underbrace{CC \cdots CZ}_{n-1 \text{ control bits}} \cdot X^{\otimes n}.
\]

Upon expressing the \( n \)-dimensional bit string as \( \omega = \delta_{n-1} \cdots \delta_1 \delta_0 \), where the individual bits are \( \delta_\ell \in \{0,1\} \) for \( \ell \in \{0,1,\cdots,n-1\} \), we define the state selection operators

\[
\Delta_\ell = \begin{cases} 
I & : \delta_\ell = 0 \\
X & : \delta_\ell = 1 
\end{cases}
\]

We then define the steering operator for state \( \omega \) by

\[
A_\omega \equiv \Delta_{n-1} \otimes \cdots \otimes \Delta_1 \otimes \Delta_0 ,
\]

and the \( n \)-qubit phase oracle becomes

\[
U_\omega = A_\omega U_0 A_\omega ,
\]

where we have dropped the superscript from \( U_0^{(n)} \) for ease of notation. In fact, we can generalize the state preparation operator \( A_\omega \) to an arbitrary unitary operator, and define

\[
U_\omega = A_\omega U_0 A_\omega^\dagger ,
\]

where the steering operator \( A_\omega \) depends on \( \omega \) in some functional manner, and the requisite steering set is \( \Omega = \{ A_\omega |0^n\} \). The corresponding quantum circuit is illustrated in Fig. 8.

We now turn to the diffusion portion of the circuit, which performs the Householder reflection \( U_h = 2|h\rangle\langle h| - 1 \). Since \( H^2 = I \) and \( |h\rangle = H^{\otimes n}|0^n\rangle \), the diffusion operator becomes

\[
U_h = -H^{\otimes n}\left[ 1 - 2|0^n\rangle\langle 0^n| \right] H^{\otimes n} .
\]

Note that the diffuser contains the reflection operator \( 1 - 2|0^n\rangle\langle 0^n| \), which marks the \( |0^n\rangle \) state with a negative phase, and we therefore write

\[
U_h = -H^{\otimes n} \cdot X^{\otimes n} \cdot CC \cdots CZ \cdot X^{\otimes n} \cdot H^{\otimes n} .
\]

For steered diffusion, in which \( |g\rangle = G|0^n\rangle \), we find

\[
U_g = -G \cdot X^{\otimes n} \cdot CC \cdots CZ \cdot X^{\otimes n} \cdot G^\dagger .
\]
FIG. 8: Phase oracle $U_\omega = A_\omega \left[ \mathbb{1}_n - 2 |0^n\rangle\langle 0^n| \right] A_\omega^\dagger = A_\omega \cdot X^\otimes n \cdot CC \cdots CZ \cdot X^\otimes n \cdot A_\omega^\dagger$ for target bit string $\omega$ and state selection operator $A_\omega$.

FIG. 9: A diffusion operator $U_g = -G \left[ \mathbb{1}_n - 2 |0^n\rangle\langle 0^n| \right] G^\dagger = -G \cdot X^\otimes n \cdot CC \cdots CZ \cdot X^\otimes n \cdot G^\dagger$. The quantum circuit is insensitive to the overall negative sign.

FIG. 10: A Grover circuit for a phase oracle with steering operator $A_\omega$ and a diffusion oracle with steering operator $G$.
This is just a generalization of the diffusion circuit in Ref. [9], and an example for \(n = 5\) qubits is illustrated in Fig. [9]. Putting all of the pieces together gives the Grover circuit in Fig. [10].

Suppose now that the amplitude steering space \(\mathbb{H}_\Omega\) is an \(m\)-qubit subsystem with \(m < n\), where the \(m\)-qubits are listed first, i.e. we use the OpenQASM convention in which the first \(m\)-qubits start at bit location \(2^0\) and end at bit \(2^{m-1}\). Then the steering space has dimension \(M = 2^m\), and the corresponding Hilbert space will be denoted by \(\mathbb{H}_m \equiv \mathbb{H}_\Omega\). Note that \(\mathbb{H}_m\) is a proper subspace of \(\mathbb{H}_n\), with orthogonal subspace \(\mathbb{H}_{n-m} \equiv \mathbb{H}_\perp\). Letting \(r \equiv n - m > 0\), we see that the orthogonal space has dimension \(R = 2^{n-m} = 2^r\), and from our qubit ordering convention we have \(\mathbb{H}_n = \mathbb{H}_r \otimes \mathbb{H}_m\). Recall that the unit operator has the decomposition \(1_n = 1_r \otimes 1_m\), and that \(\Omega_n, \Omega_r\), and \(\Omega_m\) denote the respective computational basis sets for \(\mathbb{H}_n\), \(\mathbb{H}_r\), and \(\mathbb{H}_m\). Let \(A_{\omega}^m\) be a unitary steering operator on \(\mathbb{H}_m\), i.e. \(A_{\omega}^m A_{\omega}^{m\dagger} = 1_m\). Suppose we wish to mark the state \(A_{\omega}^m |0^m\rangle \in \mathbb{H}_m\) in the \(m\)-qubit system (without regard to the \(r\)-qubit system). The appropriate steering set is therefore

\[
\Omega_{\omega} = \left\{ |y\rangle_n \equiv |x\rangle_r \otimes A_{\omega}^m |0^m\rangle \left| \begin{array}{c} x \in \Omega_r \end{array} \right. \right\}, \tag{2.87}
\]

and the phase oracle can be expressed as (upon replacing \(U_{\Omega_{\omega}}\) by the simpler notation \(U_{\omega}\)):

\[
U_{\omega} \equiv 1_n - 2 \sum_{y \in \Omega_{\omega}} |y\rangle \langle y|_n = 1_r \otimes 1_m - 2 \sum_{x \in \Omega_r} |x\rangle \langle x|_r \otimes A_{\omega}^m |0^m\rangle \langle 0^m| A_{\omega}^{m\dagger} \tag{2.88}
\]

\[
= 1_r \otimes A_{\omega}^m \left[1_m - 2 |0^m\rangle \langle 0^m| \right] A_{\omega}^{m\dagger}. \tag{2.89}
\]

In factoring out the unit matrix \(1_r\) for \(\mathbb{H}_r\), we have used the completeness relation \(\sum_{x \in \Omega_r} |x\rangle \langle x|_r = 1_r\). We consequently find the quantum circuit illustrated in Fig. [11] As we shall see in the next section, this is precisely the circuit developed by Hiroyuki et al.

FIG. 11: Grover circuit in which the amplitude steering operator is composed of an \(m\)-qubit subsystem of the \(n\)-qubit system. We have dropped the index from each of the steering operators for ease of notation, since their dimension is clear from the Figure.
III. QUANTUM PATTERN MATCHING

Hiroyuki et al. [5] have recently provided a working version of Grover’s algorithm that implements an unstructured database search for image pattern matching. Recall that there have been two primary difficulties in creating a practical working Grover search: the dictionary problem and the exponential gate problem. Hiroyuki et al. solve the dictionary problem by mapping the classical database entries into a well chosen quantum multi-qubit system whereby the database entries correspond basic pixel formations. More specifically, they use a 4-pixel binary data structure in which each quadrant can be black or white (on or off), thereby giving $2^4 = 16$ possible pixel choices that form the words of the dictionary. These 16 base structures are then mapped onto the computational bases of 4-qubit subsystems. Even more significantly, they solve the exponential gate problem by employing a new method called \textit{approximate amplitude encoding} (AAE) [6]. This method approximates the exponentially large database by a constant depth \textit{parameterized quantum circuit} containing a polynomial number of gates, and the parameters of the circuit are trained using a machine learning technique. In this section, we derive the quantum circuit used by Hiroyuki et al. as a special case of the steering formalism. Since we use OpenQASM conventions and Hiroyuki et al. employ the standard physics conventions of qubit ordering, one must adjust the quantum circuit for the difference in conventions.

A. Mathematical Statement of the Problem

Before presenting the Grover algorithm, we formulate the search problem in a precise mathematical fashion. Suppose we have a \textit{database} composed of $R$ complex valued data vectors $\mathbf{a}_k$, each of dimension of $M$,

$$
\mathbf{a}_k = (a_{0k}, a_{1k}, \cdots, a_{M-1k})^T \quad \text{with} \quad k \in \{0, 1, \cdots, R-1\},
$$

(3.1)

where the elements $a_{jk}$ are complex numbers that define the entries in the database for $j \in \{0, 1, \cdots, M-1\}$. Let us further suppose that we are given an $M$-dimensional \textit{query vector} of complex numbers

$$
\mathbf{b} = (b_0, b_1, \cdots, b_{M-1})^T.
$$

(3.2)

The query vector represents the target state that we wish to find in the database. Since the vectors $\mathbf{a}_k$ and $\mathbf{b}$ are $M \times 1$ column vectors, we have expressed them by the transpose of $1 \times M$ row vectors (so that the expressions will fit on a single horizontal line of text). Our
goal is to identify the index \( k = k_* \) for which the query vector \( \mathbf{b} \) has the largest overlap with the data vector \( \mathbf{a}_k \),

\[
  k_* = \arg\max_{k} |\mathbf{b}^\dagger \mathbf{a}_k| .
\] (3.3)

Hiroyuki et al. take the database vectors and the query vector to have real entries, but we have generalized them to complex values. The practical reason for restricting \( a_{jk} \) and \( b_j \) to be real is because AAE is only applicable to real-valued circuits. Nonetheless, we feel there is value in generalizing the problem to complex vectors, in which case, AAE must be applied separately to the real and imaginary parts of the steering operator (or a more general approximate amplitude encoding method must be devised).

If we are given a black-box that calculates \( |\mathbf{b}^\dagger \mathbf{a}_k| \), then a classical algorithm would require \( R \) calls to find the maximal index \( k_* \). This is because we would have to compare \( |\mathbf{b}^\dagger \mathbf{a}_k| \) for all \( R \) possible values of \( k \), and then select the index \( k = k_* \) for which \( |\mathbf{b}^\dagger \mathbf{a}_k| \) has the largest value. Note that we have defined the problem in terms of the inner product \( \mathbf{b}^\dagger \mathbf{a}_k \) (rather than using the opposite but equivalent ordering \( \mathbf{a}_k^\dagger \mathbf{b} \)) to remind ourselves that the quantum counterpart of this classical problem involves the transition amplitude \( \mathcal{A} \) from an initial quantum state \( |\mathbf{a}_k\rangle \) determined by the database to a final quantum state \( |\mathbf{b}\rangle \) determined by the query vector, so that \( \mathcal{A} = \langle \mathbf{b}|\mathbf{a}_k\rangle \). Grover’s algorithm maximizes the overlap between the states \( |\mathbf{a}_k\rangle \) and \( |\mathbf{b}\rangle \), finding the correct index \( k_* \) in approximately \( \sqrt{R} \) calls to the database.

**B. Encoding the Database in a Quantum State**

Let us now consider two quantum systems with \( m \) and \( r \) qubits, so that the number of computational basis states in each system is \( M = 2^m \) and \( R = 2^r \). The \( m \)-system is used to store the data entries \( \mathbf{a}_k \), and the \( r \)-system stores the data index \( k \). We order the \( m \)-qubit data system first (the lower order bits), followed by the \( r \)-qubit index system, and we denote the corresponding Hilbert spaces by \( \mathcal{H}_m \) and \( \mathcal{H}_r \). We also denote the respective computational basis states for the data and index spaces by

\[
  |j\rangle_m \quad \text{and} \quad |k\rangle_r ,
\] (3.4)

where the state indices range over

\[
  j \in \Omega_m \equiv \{0, 1, \ldots, M - 1\} \quad \text{and} \quad k \in \Omega_r \equiv \{0, 1, \ldots, R - 1\} .
\] (3.5)

Recall that \( \Omega_m \) and \( \Omega_r \) are the set of all computational basis elements for \( \mathcal{H}_m \) and \( \mathcal{H}_r \), respectively. For clarity we have indicated the qubit space to which the state belongs by an \( m \)- or an \( r \)-subscript, keeping in mind that the index \( j \) is associated with the database entry,
and the index \( k \) corresponds to the database index. Let us now define quantum states in \( \mathcal{H}_m \) that correspond to the \( k \)-th database entry \( a_k \) and to the query vector \( b \) as follows,

\[
|\text{data}(k)\rangle_m \equiv \sum_{j \in \Omega_m} a_{jk} |j\rangle_m \in \mathcal{H}_m \quad \text{for} \quad k \in \Omega_r \tag{3.6}
\]

\[
|\text{query}\rangle_m \equiv \sum_{j \in \Omega_m} b_j |j\rangle_m \in \mathcal{H}_m . \tag{3.7}
\]

Since we have encoded the database and query vectors into quantum states, we assume that

\[
\sum_{j \in \Omega_m} |a_{jk}|^2 = 1 \quad \forall k \in \Omega_r \quad \text{and} \quad \sum_{j \in \Omega_m} |b_j|^2 = 1 . \tag{3.8}
\]

To finish the quantum database construction, we form a composite qubit system from the \( m \)-qubit data space and the \( r \)-qubit index space. Taking \( n = r + m \), we denote this \( n \)-qubit database system by \( \mathcal{H}_n = \mathcal{H}_r \otimes \mathcal{H}_m \), and note that the computational basis elements are given by

\[
|x\rangle_n \equiv |k\rangle_r \otimes |j\rangle_m \in \mathcal{H}_n . \tag{3.9}
\]

To form a database entry in \( \mathcal{H}_n \), we concatenate the state \( |\text{data}(k)\rangle_m \in \mathcal{H}_m \) with the index state \( |k\rangle_r \in \mathcal{H}_r \) to form \( |k\rangle_r \otimes |\text{data}(k)\rangle_m \in \mathcal{H}_n \). Upon taking a uniform sum over \( k \), we arrive at the final form of the quantum database,

\[
|\text{database}\rangle_n \equiv A_n |0\rangle^\otimes n \tag{3.10}
\]

\[
\equiv \frac{1}{\sqrt{R}} \sum_{k \in \Omega_r} |k\rangle_r \otimes |\text{data}(k)\rangle_m \tag{3.11}
\]

\[
= \frac{1}{\sqrt{R}} \sum_{j \in \Omega_m} \sum_{k \in \Omega_r} a_{jk} |k\rangle_r \otimes |j\rangle_m , \tag{3.12}
\]

where we have introduced the unitary steering operator \( A_n \) that generate the database state from the corresponding zero-state. We also introduce a steering operator \( B_m \) for the query state, reexpressing (3.7) as

\[
|\text{query}\rangle_m \equiv B_m |0\rangle^\otimes m \tag{3.13}
\]

\[
\equiv \sum_{j \in \Omega_m} b_j |j\rangle_m . \tag{3.14}
\]

We have used \( n \)- and \( r \)-subscripts on the steering operators to emphasize the Hilbert spaces on which these operators act,

\[
A_n : \mathcal{H}_n \rightarrow \mathcal{H}_n \tag{3.15}
\]

\[
B_m : \mathcal{H}_m \rightarrow \mathcal{H}_m . \tag{3.16}
\]
Unless we wish to stress the dimension of the qubit system, we shall drop the qubit subscripts from $A_n$ and $B_m$, and simply write $A$ and $B$. The overlap in the $m$-qubit space between the query state and a data entry is

$$A_m(k) \equiv \langle \text{query}|\text{data}(k)\rangle_m = \langle 0^m|B^\dagger|\text{data}(k)\rangle_m . \tag{3.17}$$

This suggests that our amplitude steering set $\Omega$ should be chosen to mark the zero-state $|0^m\rangle \equiv |0\rangle^\otimes m$ of the $m$-system (without regard to the $r$-system). However, the state $|\text{data}(k)\rangle_m$ in not directly accessible to us. Instead, we only know the total database state

$$|\text{database}\rangle_n = A|0^n\rangle \in \mathcal{H}_n . \tag{3.18}$$

We also know the $m$-qubit query state $|\text{query}\rangle_m \in \mathcal{H}_m$. To properly compare these states, we define the enlarged query state

$$|\text{query}\rangle_n \equiv (1_r \otimes B)|0^n\rangle \in \mathcal{H}_n . \tag{3.19}$$

We shall express the unit operators on $\mathcal{H}_n$, $\mathcal{H}_m$ and $\mathcal{H}_r$ by $1_n$, $1_m$ and $1_r$, respectively, and because of our qubit ordering, we have $1_n = 1_r \otimes 1_m$. Upon restoring the qubit indices on the steering operators for clarity, the overlap between the database and the enlarged query state is given by

$$A_n \equiv \langle \text{query}|\text{database}\rangle_n = \langle 0^n| (1_r \otimes B^\dagger) A_n |0^n\rangle . \tag{3.20}$$

This suggests that we select the trial state for the first Grover iteration to be

$$|g\rangle = (1_r \otimes B^\dagger) A_n |0^n\rangle \equiv G_n |0^n\rangle , \tag{3.21}$$

where $G_n$ is the steering operator for the $n$-qubit system. Thus, the diffusion operator takes the form

$$U_g = 2|g\rangle\langle g| - 1_n \tag{3.22}$$

$$= -G \left[ 1_n - 2|0^n\rangle\langle 0^n| \right] G^\dagger . \tag{3.23}$$

As we have noted, the amplitude (3.17) suggests that we mark the $m$-qubit zero state $|0\rangle_m$, and so we define the amplitude steering set to be

$$\Omega = \left\{ |k\rangle_r \otimes |0^m\rangle \mid k \in \Omega_r \right\} . \tag{3.24}$$

This steering set marks the zero-state in the $m$-system, and any index element in the $r$-system. From definition (2.35) we see that the phase oracle takes the form

$$U_\Omega = 1_n - 2 \sum_{x \in \Omega} |x\rangle\langle x|_n = 1_n - 2 \sum_{k \in \Omega_r} |k\rangle\langle k|_r \otimes |0^m\rangle\langle 0^m| \tag{3.25}$$

$$= 1_n - 2 1_r \otimes |0^m\rangle\langle 0^m| , \tag{3.26}$$

29
where we have used the completeness relation \( \sum_{k \in \Omega_r} |k\rangle \langle k|_r = 1_r \). Upon decomposing \( 1_n = 1_r \otimes 1_m \), we therefore find

\[
U_\Omega = 1_r \otimes \left[ 1_m - 2|0^m\rangle \langle 0^m| \right].
\] (3.27)

Figure 12 represent the corresponding quantum circuit, which is the same as the circuit presented in Hiroyuki et al. (adjusted for OpenQASM conventions).

We can recast this circuit in a more intuitive manner. Upon replacing the qubit subscripts on the steering operator for clarity, let us select a steering set that marks the query state \( |\text{query}\rangle_m = B_m |0^m\rangle \in H_m \), namely

\[
\Omega = \left\{ |k\rangle_r \otimes B_m |0^m\rangle \middle| k \in \Omega_r \right\},
\] (3.28)

where \( |k\rangle_r \in \Omega_r \) is any computational basis set of the \( r \)-qubit index system. We also choose the initial state to be steered by the database operator \( A_n \),

\[
|g\rangle = A_n |0^n\rangle \in H_n.
\] (3.29)

The steering set (3.28) now gives the phase oracle

\[
U_\Omega = 1_r \otimes B_m \left[ 1_m - 2|0^m\rangle \langle 0^m| \right] B_m^\dagger,
\] (3.30)

which corresponds to the oracle presented in (2.89). Furthermore, (3.29) implies that the diffusion operator is now given by

\[
U_g = 2|g\rangle \langle g| - 1_n
\]

\[
= -A_n \left[ 1_n - 2|0^n\rangle \langle 0^n| \right] A_n^\dagger.
\] (3.32)
FIG. 13: A reorganized Grover circuit for quantum database search, where the amplitude oracle \( U_\Omega = 1_r \otimes B_m [1_m - 2|0^m\rangle\langle 0^m|] B_m^\dagger \equiv U_B \) is steered by the query operator \( B_m \). The trial state \( |g\rangle = A_n |0^n\rangle \) is steered by the database operator \( A_n \), and the diffusion operator is therefore \( U_g = -A_n [1_n - 2|0^n\rangle\langle 0^n|] A_n^\dagger \equiv U_A \). For ease of notation, we have dropped the qubit indices from the operators in the Figure.

The complete Grover circuit for these choices is illustrated in Fig. 13. Note that this is analogous to the circuit of Fig. 11, and that the database operator \( A_n \) fixes the initial state \( |g\rangle \) (along with the diffusion operator), while the query operator \( B_m \) determines the phase oracle \( U_\Omega \). When applying AAE, however, it is more convenient to associate \( A_n \) and \( B_m \) together into a single operator \( G_n = (1_r \otimes B_m^\dagger) A_n \), as Hiroyuki et al. do. However, the second approach makes the roles of \( A_n \) and \( B_m \) physically clear.
IV. CONCLUSIONS

This paper provides an overview of Grover’s original algorithm using well motivated physical arguments. Grover’s algorithm starts by choosing a trial wave function as a first guess. This state is then acted upon by a phase oracle that marks the wave function in the direction of the target state. The resulting state is then sent through a diffusion operation to enhance the marked component, and the process is repeated until the target state is achieved with unit probability. This paper introduces the notion of steering operators meant to bias the diffusion and amplitude selection processes. We provide a number of generalizations to Grover’s algorithm using the steering operator formalism, recasting amplitude amplification in terms of these operators. In particular, our formalism accommodates an arbitrary target set, rather than a target state consisting of a single computational basis element. We also generalize the amplitude oracle to capture higher order correlations that might exist between the dictionary elements. This is performed by introducing a non-separable kernel into the oracle, which leads to non-planar Grover algorithms with the potential for speed-up beyond quadratic. We construct several quantum circuits that implement these generalized algorithms. Finally, we use the steering formalism to derive the quantum pattern matching circuit of Hiroyuki et al. as a special case.
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