Modified Grover’s algorithm for an expectation value quantum computer

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The translation of Grover’s search algorithm from its standard version, designed for implementation on a single quantum system amenable to projective measurements, into one suitable for an ensemble of quantum computers, whose outputs are expectation values of observables, is described in detail. A filtering scheme, which effectively determines expectation values on a limited portion of the quantum state, is presented and used to locate a single item for searches involving more than one marked item. A truncated version of Grover’s algorithm, requiring fewer steps than the translated standard version but locating marked items just as successfully, is proposed. For quantum computational devices which only return expectation values, the truncated version is superior to its standard counterpart. This indicates that it is possible to modify quantum algorithms so as to reduce the required temporal resources by using the ensemble’s spatial resources.

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I. INTRODUCTION

The standard formulation of quantum algorithms, such as the Deutsch-Jozsa [1], Shor factorization [2] and Grover search algorithms [3], assumes that the algorithm will eventually be implemented on a single quantum system amenable to projective measurements. Currently, however, the most advanced realizations of quantum algorithms use room temperature solution state NMR, where an entire ensemble of quantum systems must be manipulated and which can only yield expectation values of certain observables [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Consequently various steps of the standard algorithm formulation have to be modified for implementation on such an expectation value quantum computing device. The typical approach has been to translate the operations as literally as possible so that the expectation value quantum computer effectively mimics its single quantum system relative. In this article we consider this process for Grover’s algorithm and report a superior and significantly different version, which effectively uses the ensemble’s spatial resources to reduce the required temporal resources, for implementation on an expectation value quantum computer.

We conclude this introduction with a description of a general scheme for translating the standard version of a quantum algorithm into a form suitable for realization on an expectation value quantum computer. In section II we briefly describe the standard formulation of Grover’s algorithm. The main result of this article is contained in section III which first describes a standard expectation value formulation of Grover’s algorithm for searching a database containing one marked item and then proposes a truncated version requiring fewer steps. Section IV extends these ideas to situations where there is more than one marked item and proposes a scheme of filtered expectation values for extracting the location of a single marked item. Finally in section V we briefly consider initial attempts to apply these techniques to other quantum algorithms.

In the standard formulation of any quantum algorithm the first step is to prepare a single $L$ qubit quantum system in a pure state $|\psi_i\rangle$. This is followed by applying of a sequence of unitary time evolution transformations, $\hat{U}_1, \ldots, \hat{U}_m$, performing $|\psi_i\rangle \rightarrow |\psi_f\rangle := \hat{U}_m \cdots \hat{U}_1 |\psi_i\rangle$. The time evolution transformations collectively form a single algorithm unitary operator, $\hat{U}_{alg} := \hat{U}_m \cdots \hat{U}_1$. Finally a computational basis projective measurement (PM) is performed on an $L'$ qubit subset of the quantum system resulting in $x \in \{0, \ldots, 2^{L'}-1\}$. The corresponding collection of measurement operators are the projectors $\{P_x = |x\rangle \langle x| \mid x = 0, \ldots, 2^{L'}-1\}$ and the output $x$ is produced with probability $\langle \psi_f | P_x | \psi_f \rangle = \langle x | \psi_f \rangle^2$. Typically this is nonzero for more than one value of $x$, some of which may yield incorrect solutions to the problem at hand. However, efficient quantum algorithms have the property that the probabilities of such failures are appropriately small; Shor’s algorithm offers an example [2].

In expectation value quantum computation, such as standard NMR implementations, there are two important differences. First, the single quantum system is replaced by an ensemble and in the case of solution state, room temperature NMR this is in a highly mixed state. However, various pseudo-pure state preparation schemes [4, 18, 19, 20] result in a state that, as far as typical NMR measurements are concerned, resembles a pure state although it may lack the entanglement properties associated with the pure state [21]. Such preparation schemes effectively carry out the same initialization required by the single, pure state quantum system formulation. Second, the most basic outputs which an expectation value quantum computer can provide are expectation values of observables over the entire ensemble; this is the case with NMR quantum computers. This stands in contrast to situations where individual quantum systems are accessible, in which case the basic outputs are the results...
of projective measurements which can then be used to derive expectation values. A translation between the PM and expectation value (EV) protocols is essential for the development of expectation value quantum computation. This is accomplished by considering PMs on an ensemble of identically prepared quantum systems. Firstly a PM can be accomplished in a bitwise fashion via projective measurement in the basis \(|0\rangle, |1\rangle\) for each qubit. The resulting outcomes yield the expectation values of \(\hat{P}_0^{(k)} = |0\rangle \langle 0|\), from which the expectation value of \(\sigma_z^{(k)} = 2\hat{P}_0^{(k)} - \hat{1}^{(k)}\) is easily computed (here \(k\) labels the qubit). The comparative ease with which Pauli operators are manipulated versus computational basis projection operators results in the standard practice of replacing the PM by the EVs of the set of single qubit observables \(\{\sigma_z^{(k)} | k = 1, \ldots, n\}\). Henceforth we assume that it is possible to measure the expectation value of \(\sigma_z^{(k)}\) for an arbitrary qubit. Finally we note that it is generally assumed that the algorithm unitary operator (or at least its constituents) can be translated straightforwardly into a sequence of operations suitable for an expectation value quantum computer. This is certainly the case for standard NMR quantum computers \[14, 15, 19\].

The two protocols are equally powerful for reversible deterministic classical computation, in which case \(|\psi_f\rangle = |s\rangle\) for some \(s = 0, \ldots, 2^n - 1\). The standard EV yields

\[
\langle \sigma_z^{(k)} \rangle \equiv \langle \psi_f \rvert \sigma_z^{(k)} \lvert \psi_f \rangle = (-1)^{s_k}
\]

where \(s = s_n \ldots s_2 s_1\) is the bitwise representation of the algorithm solution. On the other hand, the PM extracts \(s = s_n \ldots s_2 s_1\) directly and the equivalence is clear. The only requirement is the ability to distinguish between \(\langle \sigma_z^{(k)} \rangle = +1\) and \(\langle \sigma_z^{(k)} \rangle = -1\) for each qubit.

In quantum computation \(|\psi_f\rangle\) is often a superposition of computational basis states, each of which contribute to \(|\psi_f\rangle \langle \psi_f | \sigma_z^{(k)} \rangle \rangle\). In some cases, such as those presented in section [15] or ref \[18\], these contributions cancel and inferences such as those offered in Eq. [11] no longer apply. It is not surprising that the single quantum system, pure state versions of algorithms may have to be modified so as to be amenable to implementation via expectation value quantum computers. Indeed, this modification has already been provided for Shor’s algorithm \[18\].

II. GROVER’S SEARCH ALGORITHM

Grover’s quantum algorithm for searching an unstructured database provides a quadratic speedup compared to the classical sequential search \[3, 22\]. The relatively small computational resources required (compared to Shor’s algorithm) has motivated several successful small scale experimental implementations, using NMR quantum computers, for databases which conceal one marked item in one of as many as eight locations \[6, 7, 9, 10, 12, 17\]. The primary focus in these demonstrations appears to have been the successful implementation of the preparation and algorithm unitary operator steps; here the typical measurement operations aimed to verify the accuracy of the aforementioned preceding steps.

As usual the standard version of the algorithm is formulated in terms suitable for single quantum systems amenable to projective measurements. The problem involves a database which conceals \(M\) marked items in \(N\) possible locations, where it is assumed that \(M\) is known (note that there exists a quantum algorithm, which is more efficient than its classical counterparts, for finding \(M\) if it is not known in advance \[23\]). The task is to find the location of any one of the marked items, given an oracle which can answer the question, “Is a marked item located at \(x^*\)” for any possible location denoted \(x\). The database will be represented as \(X = \{0, 1, \ldots, N - 1\}\) and the locations of the marked items form a subset, \(S \subset X\). Querying the oracle is equivalent to evaluating

\[
f(x) := \begin{cases} 0 & \text{if } x \notin S \\text{and } x^* \in S \\text{and } f(x) = 1 \text{ if } x \in S \end{cases}
\]

and it is assumed that this can be done at unit cost for any \(x \in X\). A classical sequential search evaluates \(f(x)\) for a succession of distinct \(x \in X\) until it returns 1. For \(M \ll N\) this requires approximately \(N/(M + 1)\) oracle queries on average to be certain of locating at least one of the marked items.

The standard formulation of Grover’s algorithm \[3, 23\] represents database locations in terms of the computational basis states, \(\{|x\rangle, x = 0, 1, \ldots, 2^L - 1\}\), of an \(L\)

qubit data register, where \(L - 1 \leq \log_2(N) \leq L\). Information about the location of the marked items is supplied via an oracle unitary operation, defined on the computational basis states as

\[
\hat{U}_f |x\rangle := (-1)^{f(x)} |x\rangle
\]

and extended linearly to superpositions of these. The database can be extended to one with \(2^L\) locations by requiring that \(f(x) = 0\) for \(x = N, \ldots, 2^L - 1\;\text{henceforth we assume that } N = 2^L\). The data register is initially prepared in an unbiased superposition of all possible locations, i.e. \(|\psi_i\rangle := 1/\sqrt{2^L} \sum_{x=0}^{2^L-1} |x\rangle\), which is an unentangled state and typically easy to create. Repeated applications of the Grover iterate \(G := \hat{D} \hat{U}_f\) follow the preparation; the crucial oracle unitary operations are interspersed with the unitary “inversion about the average”

\[
\hat{D} \left( \sum_{x=0}^{N-1} c_x |x\rangle \right) := \sum_{x=0}^{N-1} (-c_x + 2 \langle c \rangle) |x\rangle
\]

where \(\langle c \rangle = \sum_{x=0}^{N-1} c_x / N\). Analysis of the algorithm is simplified by noting \[24, 25\] that, after any number of applications of \(G\), the state of the data register has the
form
\[ |\psi\rangle := \frac{\alpha}{\sqrt{M}} \sum_{x \in S} |x\rangle + \frac{\beta}{\sqrt{N-M}} \sum_{x \notin S} |x\rangle \] (5)

where \( \alpha, \beta \in \mathbb{R} \) satisfy \( \alpha^2 + \beta^2 = 1 \). Thus the data register state is conveniently represented by a two dimensional real unit vector \( \mathbf{v} := (\alpha, \beta) \). Accordingly the probability with which a data register PM will locate a marked item is \( \alpha^2 \). After \( m \) applications of \( G \),
\[ \alpha = \sin \left( \frac{(2m+1)\theta}{2} \right) \quad \text{and} \quad \beta = \cos \left( \frac{(2m+1)\theta}{2} \right) \] (6)

where \( \cos \theta = 1 - 2M/N \), and therefore each invocation of the Grover iterate effectively rotates \( \mathbf{v} \) through angle \( \theta \). The algorithm may be regarded as a procedure for rotating the undesirable initial state \( \mathbf{v}_i = (\sqrt{M/N}, \sqrt{1-M/N}) \) as close as possible to the desired final state \( \mathbf{v}_f = (1,0) \). If \( N/M \gg 1 \) then \( \theta \approx 2\sqrt{M/N} \) and thus after \( \sqrt{N/M \pi/4} \) applications of the Grover iterate \( \mathbf{v} \approx (1,0) \), whereupon a PM will yield a marked item with probability close to 1. Rounding errors occur when there is no integer \( m \) such that \( (2m+1)\theta/2 = \pi/2 \) but even in the worst of these cases the probability of success is at least \( 1 - M/N \) [24]. Each application of \( G \) queries the oracle once. Thus Grover’s algorithm provides a quadratic speedup compared to the classical sequential search. We shall refer to this rendition of the algorithm as the standard PM version.

### III. EV VERSIONS OF GROVER’S ALGORITHM: ONE MARKED ITEM

The first attempt to translate Grover’s algorithm to a form suitable for implementation on expectation value quantum computers results in a standard EV version which essentially differs from its standard PM counterpart only in the measurement stage. The translation is considerably simpler whenever there is only one marked item than for the remaining cases (i.e. \( M > 1 \)), and the key ideas behind modifications to the standard EV version are illustrated more clearly in the former. Suppose that there is only one marked item, located at \( s \). In the standard EV version the ensemble is initialized via a preparation scheme which results in a pseudo-pure state corresponding to \( |\psi_s\rangle = 1/\sqrt{2L} \sum_{x=0}^{2L-1} |x\rangle \). The unitary algorithm operator of the standard PM version is retained; only the measurement stage must be altered. In the standard PM version the data register is approximately in the state \( |\psi_f\rangle = |s\rangle \) after \( \lceil \pi/\sqrt{N} \rceil \) applications of \( G \). The algorithm is essentially deterministic and EVs of the single qubit observables, \( \sigma_z^{(k)} \) for \( k = 1, \ldots, L \), yield a bitwise representation of \( s \) as described earlier. Rounding errors result in discrepancies with relative size at most \( 1/N \). Thus if there is only one marked item the translation is accomplished by merely replacing the projective measurements of the standard PM version with expectation values of \( \sigma_z^{(k)} \) and determining the binary representation of the marked item’s location by the sign of \( \langle \sigma_z^{(k)} \rangle \) for each data register qubit. This is the standard EV version of Grover’s algorithm. To date all experimental NMR demonstrations of Grover’s algorithm have taken this approach [1, 7, 11, 12, 17].

The standard EV version of the algorithm does not use the ensemble’s spatial resources (i.e. the replication of the quantum computing device via the ensemble members) in any essential way. However, by considering the effect of terminating the algorithm after significantly fewer than \( \lceil \pi/\sqrt{N} \rceil \) applications of \( G \) since this would leave the data register in a superposition of computational basis states somewhat distant from the ideal, namely \( |\psi_f\rangle = |s\rangle \). At the outset it is unclear whether, for such superpositions, the sign of \( \langle \sigma_z^{(k)} \rangle \) could provide any useful information regarding the location of the marked item. However, as we shall demonstrate below, this is indeed a reasonable strategy. In fact, whenever measurements only yield expectation values the resulting approach will usually be superior to that of the standard EV version.

As with the standard EV version the system must be initialized in the pseudo-pure state corresponding to \( |\psi\rangle = 1/\sqrt{2L} \sum_{x=0}^{2L-1} |x\rangle \). Then suppose that \( G \) is repeatedly applied an arbitrary number of times, resulting in the state of the form given by Eq (3). At this stage data register EVs give (the discussion is presented for an arbitrary number of marked items for later generalization)
\[ \langle \sigma_z^{(k)} \rangle = \frac{\alpha^2}{M} \sum_{x \in S} (-1)^{x_k} + \frac{\beta^2}{N-M} \sum_{x \notin S} (-1)^{x_k}. \] (7)

However,
\[ \sum_{x \in X} (-1)^{x_k} = 0 \Rightarrow \sum_{x \notin S} (-1)^{x_k} = -\sum_{x \in S} (-1)^{x_k} \]
and thus
\[ \langle \sigma_z^{(k)} \rangle = \left( \frac{\alpha^2}{M} - \frac{\beta^2}{N-M} \right) \sum_{x \in S} (-1)^{x_k}. \] (9)

Finally the normalization requirement, \( \alpha^2 + \beta^2 = 1 \), yields
\[ \langle \sigma_z^{(k)} \rangle = \frac{A}{M} \sum_{x \in S} (-1)^{x_k}. \] (10)

where the EV attenuation
\[ A := \frac{\alpha^2 N - M}{N-M} \] (11)
determines the magnitude of the EV. When there is only one marked item and \(G\) has been applied \(m\) times

\[
\langle \sigma_z^{(k)} \rangle = \frac{A_m}{M} (-1)^{s_k}.
\]

(12)

where the EV attenuation is

\[
A_m = \frac{\sin^2 [(2m+1)\theta/2] N - 1}{N - 1}.
\]

(13)

The binary representation of the marked item’s location can still be extracted by the usual process of inspecting the sign of \(\langle \sigma_z^{(k)} \rangle\) for each data register qubit provided that \(A_m\) is sufficiently large. The latter increases monotonically with respect to \(m\) from 0 (for \(m = 0\)) to approximately 1 in the case of the standard EV version (for \(m = [\frac{1}{\sqrt{2}} \sqrt{N}]\)). Thus whenever the basic outputs are EVs it is entirely feasible to modify the algorithm unitary operator so that it uses fewer than \([\frac{1}{\sqrt{2}} \sqrt{N}]\) applications of \(G\) without reducing the probability of successfully locating a marked item. The only effect of this truncation is to reduce the magnitudes of the EVs by a factor of \(A_m\) where \(m\) is the number of applications of \(G\). Therefore we propose a truncated EV version of the algorithm which uses an \(L\) qubit data register initialized in the pseudopure state corresponding to \(|\psi_i\rangle = 1/\sqrt{2^L} \sum_{x=0}^{2^L-1} |x\rangle\) and which terminates after the minimum number of applications of \(G\) such that it is still possible to distinguish reliably between \(\langle \sigma_z^{(k)} \rangle > 0\) and \(\langle \sigma_z^{(k)} \rangle < 0\) for all data register qubits. When there is only one marked item the minimum number of applications of \(G\), \(m\), is based on the ability to distinguish between \(\langle \sigma_z^{(k)} \rangle = +A_m\) and \(\langle \sigma_z^{(k)} \rangle = -A_m\) for all qubits. The resolution in measuring \(\langle \sigma_z^{(k)} \rangle\), and hence the minimum tolerable number of applications of \(G\), usually depends on features of the experimental setup such as the ensemble size and the signal-to-noise ratio of the observed signal. However, in many instances it should be possible to use significantly fewer invocations of the oracle than required by the standard EV version without reducing the probability of locating the marked item. In such cases the truncated EV version is clearly superior to its standard EV predecessor.

Proposals for expectation value quantum computing devices typically assume that each of the required operations will be applied simultaneously to all members of the ensemble; this is true for existing NMR realizations. The truncated EV version of Grover’s algorithm reduces the required number of constituent operations of the unitary algorithm operator, and hence the required temporal resources, by effectively exploiting the ensemble’s spatial resources. In this sense too the truncated EV version represents a greater departure from the standard PM version than the standard EV version does; not only are the measurement stages but also the algorithm unitary operators different.

The truncated EV version may appear to violate the optimality \([24, 25, 26]\) of the standard formulation of Grover’s algorithm. However, it will only work if reliable expectation values can be produced. This requires an ensemble of quantum systems and it can be argued that each oracle invocation, via implementation of \(\hat{G}\), on the ensemble effectively amounts to one oracle query per ensemble member. The truncated EV version of Grover’s algorithm is not intended to substitute the standard PM version. Rather in situations, such as NMR, where the basic measurement quantities are expectation values (in contrast to PMs) it is intended as an improvement on the standard EV version.

IV. EV VERSIONS OF GROVER’S ALGORITHM: MORE THAN ONE MARKED ITEM

Translating the standard PM version of the algorithm to EV versions is significantly more complicated if there is more than one marked item. Here, after \([\sqrt{N/M}\ \pi/4]\) applications of \(\hat{G}\), the data register is approximately in the state \(|\psi_f\rangle = 1/\sqrt{M} \sum_{x \in S} |x\rangle\) (we henceforth ignore the deviation from this approximation, which gives a probability of \(M/N\) of incorrectly locating a marked item, since \(M < N\)). A PM will yield a location of one of the marked items with certainty. However, merely substituting EVs for PMs, as was done for the single marked item case, will sometimes not provide enough useful information. An extreme example is that where there are two marked items, whose locations have binary expansions, \(s = s_L \ldots s_1\) and \(s' = s'_L \ldots s'_1\) where \(s'_k = 1 - s_k\) for all \(k\). In this case \(\langle \sigma_z^{(k)} \rangle = 0\) for all \(k\). If it is known that \(M = 2\) then the only information that this set of EVs provides is that \(s'_k = 1 - s_k\). While it is possible to determine any single bit for some \(s \in S\), it is impossible to infer two or more bits of any \(s \in S\) with certainty. In general the strategy of replacing PMs with EVs only offers the following limited information: if \(\langle \sigma_z^{(k)} \rangle > 0\) then \(s_k = 0\) for some \(s \in S\), while \(\langle \sigma_z^{(k)} \rangle < 0\) implies that \(s_k = 1\) for some \(s \in S\). However, such bitwise EVs ignore crucial inter-qubit correlations, which are effectively exploited in the PM scheme to yield the location of some marked item. The EV outputs for qubits \(j\) and \(k\) only give \(s_j\) and \(s'_k\) for some \(s, s' \in S\). However, as the example above illustrates, there does not necessarily exist any single \(s'' \in S\) whose relevant bits have these values. (i.e. such that \(s'_k = s_j\) and \(s'_k = s'_k\).)

Thus we first develop an EV scheme, which exploits correlations between qubits, to circumvent this obstacle and then use this to provide a truncated EV version for Grover’s algorithm when there is more than one marked item. The key idea, which will eventually allow for a bitwise determination of a marked item’s location using EVs, is a filtered expectation value, i.e. an EV on one
qubit which is conditional on the states of one or more of the remaining qubits. A related technique has been proposed in connection with a logical labeling scheme for pseudo-pure state preparation \[ \text{[...]} \]. However, to the best of our knowledge, application of this to situations such as encountered here has not been described explicitly in the literature and the version offered here is somewhat simpler to that of \[ \text{[...]} \].

To illustrate the filtered EV technique consider an instance where \( \langle \sigma_z^{(1)} \rangle \leq 0 \). Then \( s_1 = 1 \) for some \( s \in S \). The intention is to determine \( s_2 \) for some \( s \in S \) such that \( s_1 = 1 \). The idea now is to repeat the algorithm so that, in the course of measuring \( \langle \sigma_z^{(2)} \rangle \), the final data register state is effectively filtered or restricted to \( |\psi_f\rangle = 1/\sqrt{M} \sum_{x,S,x=1} |x\rangle \). Then the sign of \( \langle \sigma_z^{(2)} \rangle \) gives \( s_2 \), and hence \( s_2 s_1 \) for some \( s \in S \) such that \( s_1 = 1 \). The restriction could be accomplished by redefining the oracle so as to fix \( x_1 = 1 \). However, this can be avoided by comparing the outputs of two runs of the algorithm, the second of which includes an additional unitary operation. First note that after applying \( U_{\text{alg}} \), \( |\psi_f\rangle = 1/\sqrt{M} \sum_{x} |x\rangle \) and

\[
\langle \sigma_z^{(2)} \rangle = \frac{1}{M} \sum_{x,S,x=1} (1-x^2) + \frac{1}{M} \sum_{x,S,x=1} (1-x^2)^2
\]

(14)

Now suppose that \( \hat{U}_{\text{alg}} \) is followed by a correlation operation, defined on computational basis states and extended linearly to superpositions,

\[
\hat{C}_2(s_1 = 1) |x_L...x_1\rangle := \left( \sigma_z^{(2)} \right)^{x_1 \oplus 1} |x_L...x_1\rangle
\]

(15)

where \( x_k \in \{0,1\} \), and addition is modulo 2. The argument of \( \hat{C} \) describes the filtering conditions and the subscript the qubit whose EV will be determined subject to such conditions. Applying this after the unitary algorithm operation gives

\[
|\psi_f\rangle \xrightarrow{\hat{C}_2(s_1 = 1)} 1/\sqrt{M} \sum_{x,S} \left( \sigma_z^{(2)} \right)^{x_1 \oplus 1} |x\rangle
\]

(16)

after which

\[
\langle \sigma_z^{(2)} \rangle = -\frac{1}{M} \sum_{x,S,x=0} (1-x^2) + \frac{1}{M} \sum_{x,S,x=1} (1-x^2)^2
\]

(17)

since \( \sigma_z^{(2)} \sigma_z^{(2)} \sigma_z^{(2)} = -\sigma_z^{(2)} \). Averaging the EVs obtained immediately after applying the algorithm unitary operation, Eq. (14), and immediately after the correlation operation, Eq. (15), gives

\[
\langle \sigma_z^{(2)} \rangle = \frac{1}{M} \sum_{x,S,x=1} (1-x^2)^2
\]

(18)

which is identical to an EV performed on the state \( 1/\sqrt{M} \sum_{x,S,x=1} |x\rangle \). Combining the two runs of the algorithm, one with and the other without the correlation operation applied after the algorithm unitary operation has effectively filtered out the the desired portion of the state.

When \( \langle \sigma_z^{(1)} \rangle \geq 0 \) the filtering is conditional on \( s_1 = 0 \). The only modification to the scheme described above is that the correlation operation is

\[
\hat{C}_2(s_1 = 0) |x_L...x_1\rangle := \left( \sigma_z^{(2)} \right)^{x_1} |x_L...x_1\rangle
\]

(19)

or equivalently \( \hat{C}_2(s_1 = 0) = \sigma_z^{(1)} \hat{C}_2(s_1 = 1) \sigma_z^{(1)} \). The average of the EVs from the two runs will be identical to that performed on \( 1/\sqrt{M} \sum_{x,S,x=1} |x\rangle \).

This first round of filtered EVs will give \( s_2 \) and \( s_1 \) for some \( s \in S \). This procedure can be iterated with appropriate modifications of the correlation operation, eventually yielding the location of a single marked item. The general idea is demonstrated by considering the situation where the filtering is conditional on \( s_k = s_{k-1} = \ldots s_1 = 1 \). The relevant correlation operator is defined via

\[
\hat{C}_{k+1}(s_k = 1, \ldots, s_1 = 1) |x_L...x_1\rangle := \left( \sigma_z^{(k+1)} \right)^{g(x_k...x_1)} |x_L...x_1\rangle
\]

(20)

where

\[
g(x_k...x_1) := x_kx_{k-1}...x_2x_1 \oplus 1.
\]

(21)

Averaging the EVs obtained in the two cases where \( \hat{U}_{\text{alg}} \) and \( \hat{C}_{k+1}(s_k = 1, \ldots, s_1 = 1) \hat{U}_{\text{alg}} \) are applied to \( |\psi_i\rangle \) yields

\[
\langle \sigma_z^{(k+1)} \rangle = \frac{1}{M} \sum_{x,S,x_k=1,\ldots,x_1=1} (1-x)^{k+1}
\]

(22)

and this achieves the desired filtration. Instances where any of the filtering conditions is of the form \( s_j = 0 \) are
accommodated by using
\[C_{k+1}(\ldots, s_j = 0, \ldots) = \sigma_x^{(j)} C_{k+1}(\ldots, s_j = 1, \ldots) \sigma_x^{(j)}.\]
(23)

Note that \(g\) defined in Eq. (24) can be computed with \(k\) multiplications and a single additions, which implies that the filtering procedure requires \(O(\log_2 N)\) additional operations at worst.

This filtered EV technique allows an expectation value quantum computer to use Grover’s algorithm to locate at least one marked item with certainty. The additional cost is that the algorithm must be run repeatedly and the relevant correlation operations must be included. However, the number of runs of the algorithm is not prohibitive since at each level of filtration only one additional run is required (to compare with the results from the previous level). Therefore at most \(\log_2 N\) runs of the algorithm are needed to locate a single marked item with certainty.

This EV version of Grover’s algorithm is also amenable to the treatment which resulted in the truncated EV version of the algorithm with only one marked item. Again suppose that \(U_{\text{alg}}\) is modified so that it terminates after \(m\) applications of \(G\). Applying this to the system in the state \(|\psi_0\rangle = 1/\sqrt{2^L \sum_{x=0}^{2^L-1} |x\rangle\rangle\) and using the filtering procedure to select a subset \(S' \subset S\) is easily shown to result in
\[\langle \sigma_z^{(k)} \rangle = \frac{A_m}{M} \sum_{x \in S'} (-1)^{x_k} \langle \sigma_z^{(k)} \rangle = +A_m/M \text{ and } \langle \sigma_z^{(k)} \rangle = -A_m/M. \text{ If this is true then it will be possible to discern bit values for marked items reliably even when the filtered EV approach leaves more than one marked item. In the standard EV version } A_m \approx 1 \text{ and in order to locate a marked item with certainty the maximum tolerable error is } \epsilon_{\text{stand}} := 1/M. \text{ Now suppose that for a particular realization of the computing device, expectation values are determined to an accuracy of } \epsilon < \epsilon_{\text{stand}}. \text{ Then it will be possible to successfully infer the location of a marked item after } m \text{ applications of } G \text{ provided that } A_m/M > \epsilon. \text{ Equation (25) implies that this is true if } \]
\[m > \frac{1}{\theta} \arcsin \sqrt{\epsilon/\epsilon_{\text{stand}} + (1 - \epsilon/\epsilon_{\text{stand}})M/N} - \frac{1}{2}. \]
(26)

If \(M \ll N\) then \(\theta \approx 2\sqrt{M/N}\) and the minimum number of applications of \(G\) for the truncated EV version is
\[m_{\text{trunc}} \approx \frac{1}{2} \sqrt{\frac{N}{M}} \arcsin \sqrt{\epsilon/\epsilon_{\text{stand}} + (1 - \epsilon/\epsilon_{\text{stand}})M/N}. \]
(27)

The number of applications of \(G\) required for the standard EV version to locate a marked item with certainty is \(m_{\text{stand}} \approx \pi/4\sqrt{N/M}\) and thus
\[m_{\text{trunc}} \approx \frac{2}{\pi} \arcsin \sqrt{\epsilon/\epsilon_{\text{stand}} + (1 - \epsilon/\epsilon_{\text{stand}})M/N}. \]
(28)

One remaining issue is the relationship between the ensemble’s size and it’s ability to estimate expectation values accurately. Determining expectation values requires an ensemble of identically prepared quantum systems, to each member of which the same experiment (i.e. the same sequence of unitary transformations and projective measurements) is applied. In this context, expectation values are identified with sample averages calculated from outcomes of projective measurements, one per member of the ensemble. In particular if the experiment is performed on an ensemble consisting of \(n\) members and the number of times that the PMs on qubit \(k\) return 0 and 1 are \(n_0\) and \(n_1\) respectively then the expectation value \(\langle \sigma_z^{(k)} \rangle\) is equated with the sample average \(\bar{x}_k \approx (n_0 - n_1)/n\). Here the distribution is binomial, in which case Chebyshev’s inequality (23) offers
\[\text{Prob} \left\{ \left| \bar{x}_k - \langle \sigma_z^{(k)} \rangle \right| < \epsilon \right\} > 1 - 1/4nc^2 \]
(30)
where \(c > 0\) bounds the error in the estimate. In realizations such as standard room temperature, solution state NMR, \(n \approx 10^{20}\) and estimates within very small error bounds are easily attained with near certainty. Thus the ensemble size is of little concern for standard NMR approaches although it may become an issue elsewhere.
V. OTHER ALGORITHMS

It remains to ask whether such modifications apply to other quantum algorithms. It is unlikely that the truncation will be applicable elsewhere as it requires an iterated operation, which amongst quantum algorithms is unique to Grover’s algorithm. On the other hand the filtered EV scheme could perhaps be more widely applicable. However, initial attempts to apply it to Shor’s factorization algorithm have been unsuccessful. The quantum part of Shor’s algorithm [4] seeks to find the period, r, of a well defined function of the number to be factorized. For the present discussion the essential details are as follows. After applying the unitary algorithm operator, a computational basis measurement is performed on an L, suitably large, qubit data register. The result of this is, with high probability, an integer $y ≈ 2^L k/r$ for any one of $k = 0, 1, \ldots , r - 1$. All possibilities for $k$ are approximately equally likely (i.e. $≈ 1/r$). An appropriately terminated continued fractions approximation to $y/2^L$ gives $k/r$ and if $k$ and $r$ are relatively prime, which occurs sufficiently often, then the denominator of the continued fractions approximation gives $r$. It is well known that simply substituting EVs for the PMs will not work [8]. One proposed solution is to have the quantum computer perform the continued fractions expansion reversibly and follow this with EVs [15]. Although these additional steps are still computationally efficient, it would be preferable to avoid them. One attempt to do so would be to use filtered EVs to isolate the computational basis states in the region of $y ≈ 2^L k/r$ for some desirable choice of $k$. However, although there is a reasonable hope that, by using a variant of the binary search, this will succeed with an sufficiently small number of additional steps this approach is still futile since the amplitudes of the resulting EVs will scale as $≈ 1/r$ and hence diminish exponentially as the size of $r$ increases. This straightforward approach appears to be doomed and no alternatives are clearly visible.

VI. CONCLUSIONS

In conclusion we have described in detail modifications which translate Grover’s search algorithm from a formulation in terms of single quantum systems amenable to projective measurements into one suitable for ensemble quantum computers where only expectation values are available. This included a thorough exposition of a filtered expectation value technique, which has the potential to be applicable more generally. In the context of Grover’s algorithm, we presented a significantly modified version of the algorithm which, for realizations involving expectation values, is superior to the standard version. The existence of this superior version indicates that it may be worthwhile to investigate similar modifications to other quantum algorithms although our initial attempts to do so have failed.

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[1] R. Cleve, A. Ekert, C. Macchiavello, and M. Mosca, Proc. R. Soc. Lond. A 454, 339 (1998).
[2] P. Shor, SIAM J. Comput. 26, 1484 (1997).
[3] L. K. Grover, Phys. Rev. Lett. 79, 325 (1997).
[4] D. G. Cory, A. F. Fahmy, and T. F. Havel, Proc. Nat. Acad. Sci. 94, 1634 (1997).
[5] I. L. Chuang, N. Gershenfeld, M. G. Kubinec, and D. W. Leung, Proc. R. Soc. Lond. A 454, 447 (1998).
[6] I. L. Chuang, N. Gershenfeld, and M. Kubinec, Phys. Rev. Lett. 80, 3408 (1998).
[7] J. A. Jones, M. Mosca, and R. H. Hansen, Nature 399, 344 (1998).
[8] N. Linden, H. Barjat, and R. Freeman, Chem. Phys. Lett. 296, 61 (1998).
[9] L. M. K. Vandersypen, C. S. Yannoni, M. H. Sherwood, and I. L. Chuang, Phys. Rev. Lett. 83, 3085 (1999).
[10] L. M. K. Vandersypen, M. Steffen, M. H. Sherwood, C. S. Yannoni, G. Breyta, and I. L. Chuang, App. Phys. Lett. 76, 646 (2000).
[11] R. Marx, A. F. Fahmy, J. M. Myers, W. Bermel, and S. J. Glaser, Phys. Rev. A 62, 012310 (2000).
[12] H. K. Cummins and J. A. Jones, New J. Phys. 2, 6 (2000).
[13] D. Collins, K. W. Kim, W. C. Holton, H. Sierzputowska-Grazc, and E. O. Stejskal, Phys. Rev. A 62, 022304 (2000).
[14] J. Kim, J.-S. Lee, and S. Lee, Phys. Rev. A 62, 022312 (2000).
[15] L. M. K. Vandersypen, M. Steffen, G. Breyta, C. S. Yannoni, R. Cleve, and I. L. Chuang, Phys. Rev. Lett. 85, 5452 (2000).
[16] Y. S. Weinstein, M. A. Pravia, E. M. Fortunato, S. Lloyd, and D. G. Cory, Phys. Rev. Lett. 86, 1889 (2001).
[17] G. L. Long, H. Y. Yan, Y. S. Li, C. C. Tu, J. X. Tao, H. M. Chen, M. L. Liu, X. Zhang, J. Luo, L. Xiao, et al., Phys. Lett. A 286, 121 (2001).
[18] N. A. Gershenfeld and I. L. Chuang, Science 275, 350 (1997).
[19] E. Knill, I. Chuang, and R. Laflamme, Phys. Rev. A 57, 3348 (1997).
[20] D. G. Cory, M. D. Price, and T. F. Havel, Physica D 120, 82 (1998).
[21] R. Schack and C. M. Caves, Phys. Rev. A 60, 4354 (1999).
[22] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, 2000).
[23] G. Brassard, P. Høyer, and A. Tapp, Lect. Notes Comp.
[24] M. Boyer, G. Brassard, P. Hoyer, and A. Tapp, Fortschr. Phys. 46, 493 (1998).
[25] C. Zalka, Phys. Rev. A 60, 2746 (1999).
[26] C. H. Bennett, E. Bernstein, G. Brassard, and U. Vazirani, SIAM J. Comput. 26, 1510 (1997).
[27] W. Feller, An Introduction to Probability Theory and Its Applications (Wiley, New York, 1968), 3rd ed.