Efficient Scheme for Initializing a Quantum Register with an Arbitrary Superposed State

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Preparation of a quantum register is an important step in quantum computation and quantum information processing. It is straightforward to build a simple quantum state such as \(|i_1i_2\cdots i_n\rangle\) with \(i_j\) being either 0 or 1, but is a non-trivial task to construct an arbitrary superposed quantum state. In this Letter, we present a scheme that can most generally initialize a quantum register with an arbitrary superposition of basis states. Implementation of this scheme requires \(O(Nn^2)\) standard 1- and 2-bit gate operations, without introducing additional quantum bits. Application of the scheme in some special cases is discussed.

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Research on quantum computers and quantum information processing has been a fast developing interdisciplinary field over the past years. As a new branch of science overlapping quantum physics and classical information theory, it resembles in some ways both of the subfields, but differs from each of them in many other respects. In quantum computation and quantum information processing, the concept of quantum superposition of basis states \(|i_1i_2\cdots i_n\rangle\) is used and massive parallelism is achieved \([2]\). For instance, a significant speed-up over classical computers, at least theoretically, has been gained in prime-factorization \([3]\) and quantum searching \([4]\). Nevertheless, some simple operations for a classical computer can not be easily implemented in a quantum computer. A vivid example is the need of introducing the quantum error correction scheme to overcome the decoherence problem in quantum computers. This has been obtained with admirable genius \([5]\) whereas the corresponding classical coding scheme is straightforward.

Quantum computing is realized by quantum gate operations. It has been shown that a finite set of basic gate operations can be used to construct any quantum computation gate operation \([6]\). This universality of quantum computation has been studied by many authors \([7,8]\). A quantum circuit, which is a network of gate operations for certain purpose, has been constructed, for example, for basic arithmetic \([9]\) and efficient factorization \([10]\).

Initializing a quantum register to an arbitrary superposition of basis states is a seemingly simple, yet difficult problem. Addition of two numbers in a classical computer could not be easier, but addition of two quantum states \(a_1|\psi_1\rangle + a_2|\psi_2\rangle\) is not easy at all. However, superposition is the basic ingredient in quantum computing and quantum information processing. An efficient scheme for initializing an arbitrary superposition for a quantum register is very much desired. An efficient scheme for initializing a quantum register for a known function of amplitude distribution was given by Ventura and Martinez (VM) with \(n + 1\) additional quantum bits (qubits) \([11]\).

In this Letter, we present a general scheme that initializes a quantum register without introducing additional qubits. For some quantum computing tasks, introduction of additional qubits is not permitted. Thus our scheme may be appreciated by these circumstances. Furthermore, qubits are a precious resource in practice, and any saving is a great relief for existing technology, especially at the present time when researchers are striving to make more qubits available.

Starting with the state \(|0\cdots 0\rangle\), we want to transform this state to a general superposed state having the form

\[
|\psi\rangle = \sum_{i=0}^{N-1} a_i|i\rangle.
\]

Normalization of this state vector is assumed. The coefficients \(a_i\) are in general complex numbers with the requirement \(|a_i| \leq 1\). Here, \(i\) is a short notation for a set of indices \(\{i_1i_2\cdots i_j\cdots i_n\}\) with \(n = \log_2 N\) being the total number of qubits in the register, and \(i_j\) denotes the two possible states (0 or 1) of the \(j\)th qubit. To be concrete, our notation implies

\[
i = \left\{
\begin{array}{c}
0 \rightarrow \{00\cdots 00\} \\
1 \rightarrow \{00\cdots 01\} \\
2 \rightarrow \{00\cdots 10\} \\
\vdots \\
N-1 \rightarrow \{11\cdots 11\}
\end{array}\right.
\]

Thus, \(|\psi\rangle\) in Eq. (1) is a general quantum superposition of \(N\) basis states, and each of the basis states is a product state of \(n\) qubits.

Our scheme involves only two kinds of elementary unitary transformations, or gate operations. The first kind of gate operation is a single-bit rotation \(U_\theta\).
\[
U_\theta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}.
\]
(2)

It differs slightly from an ordinary rotation because it is an ordinary rotation for the \( |0 \rangle \) part only, but has a minus sign for the \( |1 \rangle \) part. Upon operation, a qubit in the state \( |0 \rangle \) is transformed into a superposition in the two state: \( (\cos \theta, \sin \theta) \). Similarly, a qubit in the state \( |1 \rangle \) is transformed into \( (\sin \theta, -\cos \theta) \). It is useful to identify some special cases in Eq. (2). When \( \theta = 0 \), it does not change \( |0 \rangle \), but converts the sign of the state \( |1 \rangle \). When \( \theta = \frac{\pi}{2} \), \( U_\theta \) is reduced to the Hadamard-Walsh transformation \( \frac{1}{\sqrt{2}} \). Finally, when \( \theta = \frac{\pi}{4} \), it serves as the NOT operation: it changes \( |0 \rangle \) to \( |1 \rangle \), and \( |1 \rangle \) to \( |0 \rangle \).

The second kind of gate operation is the controlled \( k \)-operations. As illustrated below, it is an operation that has a string of \( k \) controlling qubits:

\[
\begin{array}{c}
\bullet \\
\bullet \\
\vdots \\
\bullet \\
U\bullet
\end{array}
\]

The squares represent the controlling qubits, and the circle is a unitary operation on the target qubit. The operation is a conditional one that is activated only when the controlling qubits hold the respective values indicated in the squares. Controlled \( k \)-operations can be constructed by \( O(k^2) \) standard 1- and 2-bit gate operations \( \mathcal{H} \).

With these basic gate operations at our disposal, we now proceed from simple examples to the most general case. For a 2-qubit system, the transformation can be expressed as

\[
\begin{align*}
|00\rangle &\rightarrow \sqrt{|a_{00}|^2 + |a_{01}|^2}|00\rangle + \sqrt{|a_{10}|^2 + |a_{11}|^2}|10\rangle \\
&\rightarrow |0\rangle \left[ a_{00}|0\rangle + a_{01}|1\rangle \right] + |1\rangle \left[ a_{10}|0\rangle + a_{11}|1\rangle \right] \\
&= a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle,
\end{align*}
\]

which involves one single-bit rotation \( \alpha_1 \) and two controlled \( 1 \)-rotations with angles arctan \( \sqrt{|a_{00}|^2 + |a_{11}|^2} \) and arctan \( \sqrt{|a_{10}|^2 + |a_{01}|^2} \) are applied to the 2nd qubit.

The state vector becomes

\[
\begin{align*}
\sqrt{|a_{00}|^2 + |a_{01}|^2}|00\rangle &+ \sqrt{|a_{10}|^2 + |a_{11}|^2}|10\rangle \\
&+ |a_{10}|^2 + |a_{11}|^2|10\rangle &+ \sqrt{|a_{10}|^2 + |a_{11}|^2}|11\rangle.
\end{align*}
\]

Finally 4 controlled \( 2 \) unitary transformations

\[
\begin{align*}
U_{\alpha_{3,00}} &= \begin{bmatrix} a_{00} & 0 \\ 0 & a_{00} \end{bmatrix} \\
U_{\alpha_{3,01}} &= \begin{bmatrix} a_{01} & 0 \\ 0 & a_{01} \end{bmatrix} \\
U_{\alpha_{3,10}} &= \begin{bmatrix} a_{10} & 0 \\ 0 & a_{10} \end{bmatrix} \\
U_{\alpha_{3,11}} &= \begin{bmatrix} a_{11} & 0 \\ 0 & a_{11} \end{bmatrix}
\end{align*}
\]

are operated on the 3rd qubit to acquire the general superposed state \( a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle \). This quantum circuit is illustrated in Fig. 1.

For brevity in notations, we use an “angle” to label a controlled \( k \)-operation. If the involved coefficients are all real, it reduces to an ordinary rotation angle. In the above notations for angles of the controlled \( k \)-rotations, and in similar notations hereafter, the first subscript (for example, 3 in \( \alpha_{3,01} \)) refers to the target qubit order number and the following subscripts (01 in \( \alpha_{3,01} \)) indicate the quantum states of the controlling qubits.

In the initialization, operations for the first \( n-1 \) qubits are controlled rotations where each rotation depends only on a single real parameter. The rotation angles take the following general expressions. In the 1st qubit, there is a 1-qubit rotation. The rotation angle is

\[
\alpha_1 = \arctan \sqrt{|a_{10}|^2 + |a_{11}|^2}.
\]
(3)

In the 2nd qubit, there are two controlled \( 1 \)-rotations

\[
\begin{align*}
\alpha_{2,0} &= \arctan \sqrt{|a_{01}|^2 + |a_{11}|^2} \\
\alpha_{2,1} &= \arctan \sqrt{|a_{10}|^2 + |a_{01}|^2}
\end{align*}
\]
(4)

In general, in the \( j \)th qubit, there are \( 2^{j-1} \) controlled \( j \)-rotations, with each of them having \( j-1 \) controlling qubits labeled as \( i_1 i_2 \cdots i_{j-1} \). The rotation angle in the \( j \)th qubit (\( j \neq n \)) is given by
\[
\alpha_{i_1 i_2 \cdots i_{n-1}} = \arctan \sqrt{\frac{\sum_{j_2=1}^{i_2} \cdots \sum_{j_{n-1}=1}^{i_{n-1}} |a_{i_1 i_2 \cdots i_{n-1} j_2 \cdots j_{n-1}}|^2}{\sum_{j_2=1}^{i_2} \cdots \sum_{j_{n-1}=1}^{i_{n-1}} |a_{i_1 i_2 \cdots i_{n-1} j_2 \cdots j_{n-1}}|^2}}.
\] (5)

The fraction in Eq. (5) can be \(\frac{9}{4}\) and the rotation angle in this case is undetermined. If this should happen, a simple analysis is sufficient for us to determine which gate operation should be adopted. Examples will be given later.

For the last qubit with \(j = n\), we have \(2^{n-1}\) controlled\(^{n-1}\) unitary transformations

\[
U_{\alpha_{i_1 i_2 \cdots i_{n-1}}} = \begin{bmatrix}
\frac{A_0}{\sqrt{|A_0|^2 + |A_1|^2}} & \frac{A_1}{\sqrt{|A_0|^2 + |A_1|^2}} \\
\frac{A_0^*}{\sqrt{|A_0|^2 + |A_1|^2}} & \frac{A_1^*}{\sqrt{|A_0|^2 + |A_1|^2}}
\end{bmatrix},
\] (6)

with

\[
A_0 = a_{i_1 i_2 \cdots i_{n-1} 0}, \\
A_1 = a_{i_1 i_2 \cdots i_{n-1} 1}.
\] (7)

If the numbers in Eq. (6) are real, the operation is just a usual rotation, and the angle is given by

\[
\alpha_{i_1 i_2 \cdots i_{n-1}} = \arctan \frac{a_{i_1 i_2 \cdots i_{n-1} 1}}{a_{i_1 i_2 \cdots i_{n-1} 0}}.
\] (8)

In general, the \(N\) amplitudes \(a_i\) in Eq. (6) are complex, and together with the normalization, the total number of real parameters for description of a superposed state is \(2^N - 1\). In our scheme, operations on the first \(n - 1\) qubits are all ordinary rotations, and they provide \(1 + 2 + 4 + \cdots + 2^{n-2} = N/2 - 1\) real parameters. The \(N/2\) operations on the last qubit are generally unitary transformations, and each of them depends on 3 real parameters. Altogether, the total number of real parameters involved in the initialization is \(2N - 1\). This number can be reduced if the state has special properties. For instance, if all the amplitudes are real, the number is reduced to \(N - 1\).

Our scheme requires only \(N - 1\) gate operations to initialize a quantum register. In terms of the standard 1- and 2-bit gate operations, the total number of operations is \(O(Nn^2)\) and still polynomial in \(N\). It is more than the number of steps \(O(N\ln n)\) in the VM protocol [11]. This is the price to be paid for saving \(n + 1\) qubits in the register. The present scheme uses \(n\) qubits, whereas the VM protocol requires \(2n + 1\) qubits to perform the same task. Barenco et al. [12] pointed out that introduction of one more qubit to workspace will reduce the number of controlled\(^m\)-gate operations from \(O(m^2)\) to \(O(m)\). According to this, the number would increase from \(O(N\ln n)\) to \(O(Nn^{n+2})\) if we want to save \(n + 1\) qubits. It is surprisingly seen that the actual number required in our protocol is much less than the estimation.

In many practical cases, the number of controlled gate operations can be reduced and the circuit is accordingly simplified. Fig. 2 shows an example for part of a circuit where the rotation angles are the same. In this case, one can combine the \(|0\rangle\)-controlled Hadamard-Walsh transformation and the \(|1\rangle\)-controlled Hadamard-Walsh transformation as one operation, which is equivalent to one Hadamard-Walsh transformation on the target qubit. Consequently, the four controlled operations are reduced to a single-qubit rotation.

If desired superposition has a special form, the quantum circuit can likely be further simplified. Next, we discuss three well-known cases. Starting with \(\{0 \cdots 0\}\), we initialize quantum superpositions of 1) the evenly distributed state; 2) the GHZ state; and 3) the state vector \(|\psi\rangle = \sin \theta |\tau\rangle + \cos \theta |c\rangle\) which is used in Grover’s quantum search algorithm.

1) The evenly distributed state \(|\psi\rangle = \sum_i |i\rangle\) is widely used in quantum computation. The Hadamard-Walsh gate operation on each qubit generates this form of superposition from the state \(|0 \cdots 0\rangle\). This is also true for our scheme. In this special case, all rotation angles in Eqs. (8) - (8) are \(\frac{\pi}{4}\), and all gate operations are therefore the Hadamard-Walsh transformation. In each qubit, the controlling qubits exhaust all possible combinations, and hence the \(2^{n-1}\) controlled Hadamard-Walsh gate operations can be reduced to a single Hadamard-Walsh transformation in the \(j\)th qubit.

2) The GHZ state \(|\chi\rangle\) is the maximally entangled state with the form of superposition \(|\chi\rangle = \frac{1}{\sqrt{2}}(|001\rangle + |110\rangle)\). An example that transforms \(|0000\rangle\) to \(|\frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)\) is given in Fig. 3. It can be seen that the circuit is much simplified from the most general one in Fig. 1. According to Eqs. (6) - (8), the simplification is achieved through the following steps. The rotation in the 1st qubit is the Hadamard-Walsh transformation. For the two controlled rotations in the 2nd qubit, \(\alpha_{2,0} = 0\) means the identity operation which does nothing for the qubit, and \(\alpha_{2,1} = \frac{\pi}{2}\) corresponds to the controlled NOT operation. So effectively, there is only one controlled NOT gate in the 2nd qubit. There are originally four gate operations in the 3rd qubit. \(\alpha_{3,11} = \frac{\pi}{2}\) is the \(|11\rangle\)-controlled NOT gate and \(\alpha_{3,00}\) is the identity operation. \(\alpha_{3,01}\) and \(\alpha_{3,10}\) are undetermined angles with \(\frac{\pi}{2}\). By analyzing this problem, it is easy to see that the angles should be 0, which corresponds to the identity operation. Therefore, there is only one gate operation in the 3rd qubit: \(|11\rangle\)-controlled NOT. Similarly, there is only \(|111\rangle\)-controlled NOT operation in the 4th qubit. If the circuit consists of more than four qubits, the same analysis applies till the last but one qubit. In the last qubit, the rotation is either \(\frac{\pi}{2}\) for \(|\frac{1}{\sqrt{2}}(|001\rangle + |111\rangle)\), or \(-\frac{\pi}{2}\) \(|\frac{1}{\sqrt{2}}(|000\rangle - |111\rangle)\).

3) In Grover’s quantum search algorithm [13] and its generalizations [14], the state vector is built in a two-dimensional space spanned by the marked state \(|\tau\rangle\) and the “rest” state \(|c\rangle = \sum_{i \neq \tau} |i\rangle\). At any search step, the state vector has the form \(|\psi\rangle = \sin \theta |\tau\rangle + \cos \theta |c\rangle\).
We now give the quantum circuit for initializing such a superposed state. Let $|\tau\rangle = |i_1i_2\cdots i_n\rangle$ be the marked state, and we now construct $|\psi\rangle$ from $|0\cdots 0\rangle$. The amplitudes of the basis states in Eq. (3) are $a_{\tau} = \sin \theta$ and $a_i = \cos \theta/\sqrt{N-1}$ for $i \neq \tau$. According to Eq. (3), the rotation angle in the 1st qubit is

$$\alpha_1 = \begin{cases} \arctan \Omega_1, & \text{if } i_1 = 1 \\ \arctan \frac{1}{\Omega_1}, & \text{if } i_1 = 0 \end{cases}$$

with

$$\Omega_1 = \sqrt{(N-2)\cos^2 \theta + 2(N-1)\sin^2 \theta} / N \cos^2 \theta.$$

In the $k$-th qubit, the angle for $|i_1i_2\cdots i_{k-1}\rangle$-controlled rotation is

$$\alpha_{k,i_1i_2\cdots i_{k-1}} = \begin{cases} \arctan \Omega_k, & \text{if } i_k = 1 \\ \arctan \frac{1}{\Omega_k}, & \text{if } i_k = 0 \end{cases}$$

with

$$\Omega_k = \sqrt{(N-2^k)\cos^2 \theta + 2^k(N-1)\sin^2 \theta} / N \cos^2 \theta.$$

The other rotation angles in the $k$-th qubit are all equal to $\frac{\pi}{2}$, corresponding to the Hadamard-Walsh transformation. Thus, the $2^{k-1} - 1$ controlled gate operations are reduced to $k-1$ controlled Hadamard-Walsh transformations. In Fig. 4, we show an example with the marked state $|\tau\rangle = |i_1i_2\bar{i}_3\bar{i}_4\rangle$ in a 4-qubit-system. In this example, $\cos \theta$ and $\sin \theta$ are all real and positive.

To summarize, we have presented a general scheme for initializing a quantum register to an arbitrary superposed state. The quantum circuits utilize only single-qubit rotations and controlled qubit rotations. General expressions for rotation angles have been derived explicitly, and possibility for simplifying the circuits has been discussed in terms of three well-known superposed states.

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Long and Sun, Fig. 2
Long and Sun, Fig. 3
Long and Sun, Fig. 4