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 $|i_1 i_2 \cdots i_n\rangle$ with i_j being either 0 or 1, but it is a nontrivial task to construct an *arbitrary* superposed quantum state. 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 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 $|i_1 i_2 \cdots i_n\rangle$ is used and massive parallelism is achieved [1]. For instance, a significant speed up over classical computers, at least theoretically, has been gained in prime factorization [2] and quantum searching [3]. Nevertheless, some simple operations for a classical computer cannot 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 [4] 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 [5]. This universality of quantum computation has been studied by many authors [6–8]. A quantum circuit, which is a network of gate operations for a certain purpose, has been constructed, for example, for basic arithmetic [9] and efficient factorization [10]. 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 Brief Report, we present a general scheme that initializes a quantum register without introducing additional qubits. For some quantum computing tasks, the 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

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

Normalization of this state vector is assumed. The coefficients a_i are in general complex numbers with the requirement $|a_i| \leqslant 1$. Here i is a short notation for a set of indices $\{i_1 i_2 \cdots i_j \cdots i_n\}$, 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 jth qubit. To be concrete, our notation implies

$$i = \begin{cases} 0 \rightarrow \{00 \cdots 00\}, \\ 1 \rightarrow \{00 \cdots 01\}, \\ 2 \rightarrow \{00 \cdots 10\}, \\ \quad \vdots \\ N-1 \rightarrow \{11 \cdots 11\}. \end{cases}$$

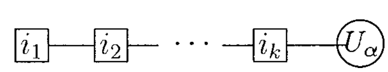
Thus $|\psi\rangle$ in Eq. (1) is a general quantum superposition of N basis states, and each of the basis states is a product state of n qubits.

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_θ:

$$U_\theta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{2}$$

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 $\theta = \pi/4$, U_θ is reduced to the Hadamard-Walsh transformation [12]. Finally, when $\theta = \pi/2$, 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:



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 [7].

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

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

which involves one single-bit rotation α_1 and two controlled^1 operations $U_{\alpha_{2,i}}$ $(i=0,1)$

$$\alpha_1=\arctan\sqrt{\frac{|a_{10}|^2+|a_{11}|^2}{|a_{00}|^2+|a_{01}|^2}},$$

$$U_{\alpha_{2,0}}=\begin{bmatrix}\frac{a_{00}}{\sqrt{|a_{00}|^2+|a_{01}|^2}} & \frac{a_{01}}{\sqrt{|a_{00}|^2+|a_{01}|^2}}\\ \frac{a_{01}^*}{\sqrt{|a_{00}|^2+|a_{01}|^2}} & -\frac{a_{00}^*}{\sqrt{|a_{00}|^2+|a_{01}|^2}}\end{bmatrix},$$

$$U_{\alpha_{2,1}}=\begin{bmatrix}\frac{a_{10}}{\sqrt{|a_{10}|^2+|a_{11}|^2}} & \frac{a_{11}}{\sqrt{|a_{10}|^2+|a_{11}|^2}}\\ \frac{a_{11}^*}{\sqrt{|a_{10}|^2+|a_{11}|^2}} & -\frac{a_{10}^*}{\sqrt{|a_{10}|^2+|a_{11}|^2}}\end{bmatrix}.$$

The quantum circuit of a 3-qubit system transforms the state $|000\rangle$ to an arbitrary superposed state with $N=2^3=8$ basis states. Starting from the $|000\rangle$, a rotation with an angle

$$\arctan[\sqrt{(|a_{100}|^2+|a_{101}|^2+a_{110}|^2+|a_{111}|^2)/(|a_{000}|^2+|a_{001}|^2+|a_{010}|^2+|a_{011}|^2)}]$$

is operated on the first qubit, and this rotation transforms the state to $\sqrt{|a_{000}|^2+|a_{001}|^2+|a_{010}|^2+|a_{011}|^2}|000\rangle + \sqrt{|a_{100}|^2+|a_{101}|^2+|a_{110}|^2+|a_{111}|^2}|100\rangle$. Then two controlled^1 rotations with angles $\arctan\sqrt{(|a_{010}|^2+|a_{011}|^2)/(|a_{000}|^2+|a_{001}|^2)}$ and $\arctan\sqrt{(|a_{110}|^2+|a_{111}|^2)/(|a_{100}|^2+|a_{101}|^2)}$ are applied to the second qubit. The state vector becomes

$$\sqrt{|a_{000}|^2+|a_{001}|^2}|000\rangle+\sqrt{|a_{010}|^2+|a_{011}|^2}|010\rangle + \sqrt{|a_{100}|^2+|a_{101}|^2}|100\rangle+\sqrt{|a_{110}|^2+|a_{111}|^2}|110\rangle.$$

Finally four controlled^2 unitary transformations

$$U_{\alpha_{3,00}}=\begin{bmatrix}\frac{a_{000}}{\sqrt{|a_{000}|^2+|a_{001}|^2}} & \frac{a_{001}}{\sqrt{|a_{000}|^2+|a_{001}|^2}}\\ \frac{a_{001}^*}{\sqrt{|a_{000}|^2+|a_{001}|^2}} & -\frac{a_{000}^*}{\sqrt{|a_{000}|^2+|a_{001}|^2}}\end{bmatrix},$$

$$U_{\alpha_{3,01}}=\begin{bmatrix}\frac{a_{010}}{\sqrt{|a_{010}|^2+|a_{011}|^2}} & \frac{a_{011}}{\sqrt{|a_{010}|^2+|a_{011}|^2}}\\ \frac{a_{011}^*}{\sqrt{|a_{010}|^2+|a_{011}|^2}} & -\frac{a_{010}^*}{\sqrt{|a_{010}|^2+|a_{011}|^2}}\end{bmatrix},$$

$$U_{\alpha_{3,10}}=\begin{bmatrix}\frac{a_{100}}{\sqrt{|a_{100}|^2+|a_{101}|^2}} & \frac{a_{101}}{\sqrt{|a_{100}|^2+|a_{101}|^2}}\\ \frac{a_{101}^*}{\sqrt{|a_{100}|^2+|a_{101}|^2}} & -\frac{a_{100}^*}{\sqrt{|a_{100}|^2+|a_{101}|^2}}\end{bmatrix},$$

$$U_{\alpha_{3,11}}=\begin{bmatrix}\frac{a_{110}}{\sqrt{|a_{110}|^2+|a_{111}|^2}} & \frac{a_{111}}{\sqrt{|a_{110}|^2+|a_{111}|^2}}\\ \frac{a_{111}^*}{\sqrt{|a_{110}|^2+|a_{111}|^2}} & -\frac{a_{110}^*}{\sqrt{|a_{110}|^2+|a_{111}|^2}}\end{bmatrix}$$

are operated on the third qubit to acquire the general superposed state $a_{000}|000\rangle+a_{001}|001\rangle+a_{010}|010\rangle+a_{011}|011\rangle+a_{100}|100\rangle+a_{101}|101\rangle+a_{110}|110\rangle+a_{111}|111\rangle$. This quantum circuit is illustrated in Fig. 1.

For brevity in notation, 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 notation for angles of the controlled^k rotations and in similar notation 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.

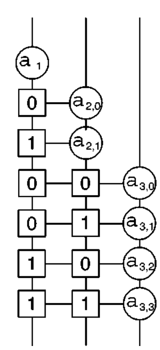


FIG. 1. Quantum circuit for initializing an arbitrary superposed state of Eq. (1) for a 3-qubit register.

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 first qubit, there is a 1-qubit rotation. The rotation angle is

$$\alpha_1 = \arctan\sqrt{\frac{\sum_{i_2 i_3 \cdots i_n}|\alpha_{1 i_2 i_3 \cdots i_n}|^2}{\sum_{i_2 i_3 \cdots i_n}|\alpha_{0 i_2 i_3 \cdots i_n}|^2}}. \tag{3}$$

In the second qubit, there are two controlled[1] rotations

$$\alpha_{2,0} = \arctan\sqrt{\frac{\sum_{i_3 i_4 \cdots i_n}|a_{01 i_3 i_4 \cdots i_n}|^2}{\sum_{i_3 i_4 \cdots i_n}|a_{00 i_3 i_4 \cdots i_n}|^2}}.$$

$$\alpha_{2,1} = \arctan\sqrt{\frac{\sum_{i_3 i_4 \cdots i_n}|\alpha_{11 i_3 i_4 \cdots i_n}|^2}{\sum_{i_3 i_4 \cdots i_n}|a_{10 i_3 i_4 \cdots i_n}|^2}}. \tag{4}$$

In general, in the jth qubit, there are 2^{j-1} controlled^{j-1} 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 jth qubit $(j \neq n)$ is given by

$$\alpha_{j, i_1 i_2 \cdots i_{j-1}} = \arctan\sqrt{\frac{\sum_{i_{j+1} \cdots i_n}|a_{i_1 i_2 \cdots i_{j-1} 1 i_{j+1} \cdots i_n}|^2}{\sum_{i_{j+1} \cdots i_n}|a_{i_1 i_2 \cdots i_{j-1} 0 i_{j+1} \cdots i_n}|^2}}. \tag{5}$$

The fraction in Eq. (5) can be 0/0, 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

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

with

$$A_0 = a_{i_1 i_2 \cdots i_{n-1} 0}, \quad A_1 = a_{i_1 i_2 \cdots i_{n-1} 1}. \tag{7}$$

If the numbers in Eq. (7) are real, the operation is just a usual rotation, and the angle is given by

$$a_{n, i_1 i_2 \cdots i_{n-1}} = \arctan(a_{i_1 i_2 \cdots i_{n-1} 1}/a_{i_1 i_2 \cdots i_{n-1} 0}). \tag{8}$$

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 $O(Nn^2)$, which is still polynomial in N. It is more than the number of steps $[O(Nn)]$ 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 a same task. Barenco *et al.* [7] 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 $O(Nn)$ 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.

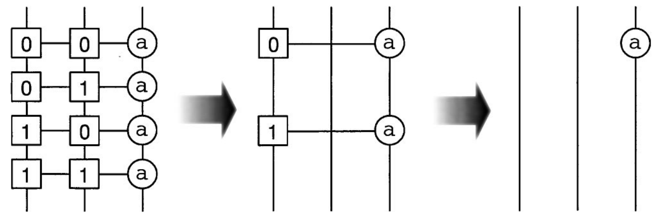


FIG. 2. Example of combining controlled rotations to simplify the circuit.

In many practical cases, the number of controlled gate operations can be reduced and the circuit is accordingly simplified. Figure 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 $|0 \cdots 0\rangle$, 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. (3)–(8) are $\pi/4$, and all gate operations are therefore the Hadamard-Walsh transformation. In each qubit, the controlling qubits exhaust all possible combinations, and hence the 2^{j-1} controlled Hadamard-Walsh gate operations can be reduced to a single Hadamard-Walsh transformation in the jth qubit.

(2) The GHZ state [13] is the maximally entangled state with the form of superposition $(1/\sqrt{2})(|0 \cdots 0\rangle \pm |1 \cdots 1\rangle)$. An example that transforms $|0000\rangle$ to $(1/\sqrt{2})(|0000\rangle + |1111\rangle)$ 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. (3)–(8), the simplification is achieved through the following steps. The rotation in the first qubit is the Hadamard-Walsh transformation. For the two controlled rotations in the

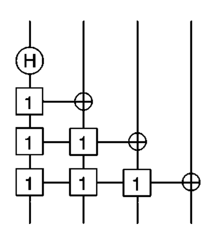


FIG. 3. Quantum circuit for implementing the GHZ state. The circled H represents the Hadamard-Walsh transformation and ⊕ the controlled-NOT gate.

second qubit, $\alpha_{2,0}=0$ means the identity operation which does nothing for the qubit, and $\alpha_{2,1}=\pi/2$ corresponds to the controlled NOT operation. So, effectively, there is only one controlled NOT gate in the second qubit. There are originally four gate operations in the third qubit. $\alpha_{3,11}=\pi/2$ 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 0/0. 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 third qubit: $|11\rangle$-controlled NOT. Similarly, there is only a $|111\rangle$-controlled NOT operation in the fourth qubit. If the circuit consists of more than four qubits, the same analysis applies until the last but 1 qubit. In the last qubit, the rotation is either $\pi/2$ for $(1/\sqrt{2})(|0\cdots0\rangle+|1\cdots1\rangle)$ or $-\pi/2$ for $(1/\sqrt{2})(|0\cdots0\rangle-|1\cdots1\rangle)$.

(3) In Grover's quantum search algorithm [3] 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 $|c\rangle=\Sigma_{i\neq\tau}|i\rangle$. 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 $|\tau\rangle=|i_1 i_2\cdots i_n\rangle$ be the marked state, and we now construct $|\psi\rangle$ from $|0\cdots0\rangle$. The amplitudes of the basis states in Eq. (1) 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 first qubit is

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

with

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

In the kth qubit, the angle for $|i_1 i_2\cdots i_{k-1}\rangle$-controlled rotation is

$$\alpha_{k,i_1 i_2\cdots i_{k-1}}=\begin{cases}\arctan\Omega_k & \text{if}\quad i_k=1,\\ \arctan\dfrac{1}{\Omega_k} & \text{if}\quad i_k=0,\end{cases}$$

with

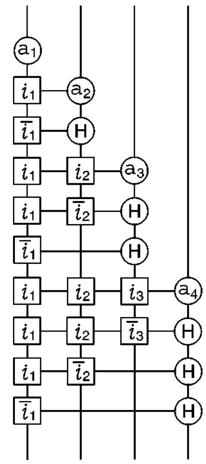


FIG. 4. Quantum circuit for implementing the state vector $|\psi\rangle=\sin\theta|\tau\rangle+\cos\theta|c\rangle$. In the figure, a letter with a bar indicates its NOT value, i.e., $\bar{1}=0$ and $\bar{0}=1$.

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

The other rotation angles in the kth qubit are all equal to $\pi/4$, 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 $|\tau\rangle=|i_1 i_2 i_3 i_4\rangle$ 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 the possibility for simplifying the circuits has been discussed in terms of three well-known superposed states.

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[1] D. Deutsch, Proc. R. Soc. London, Ser. A **400**, 97 (1985).
[2] P. Shor, in *Proceedings of the 35th Annual Symposium on the Foundations of Computer Science*, edited by S. Goldwasser (IEEE Computer Society, Los Alamitos, CA, 1994), p. 124.
[3] L. K. Grover, Phys. Rev. Lett. **79**, 325 (1997).
[4] P. Shor, Phys. Rev. A **52**, R2493 (1995).
[5] D. Deutsch, Proc. R. Soc. London, Ser. A **425**, 73 (1989).
[6] D. P. DiVincenzo, Phys. Rev. A **51**, 1015 (1995).
[7] A. Barenco *et al.*, Phys. Rev. A **52**, 3457 (1995); A. Barenco, Proc. R. Soc. London, Ser. A **449**, 679 (1995).
[8] S. Lloyd, Phys. Rev. Lett. **75**, 346 (1995).
[9] V. Vedral *et al.*, Phys. Rev. A **54**, 147 (1996).
[10] D. Beckman *et al.*, Phys. Rev. A **54**, 1034 (1996).
[11] D. Ventura and T. Martinez, Found. Phys. Lett. **12**, 547 (1999).
[12] D. Deutsch and R. Jozsa, Proc. R. Soc. London, Ser. A **439**, 553 (1992).
[13] D. M. Greenberger *et al.*, in *Bell's Theorem, Quantum Mechanics, and the Conceptions of the Universe*, edited by M. Kafatos (Kluwer, Dordrecht, The Netherlands, 1989), p. 69.
[14] G. L. Long *et al.*, Phys. Lett. A **262**, 27 (1999).