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Quantum Circuit Design for Solving Linear Systems of Equations

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Recently, it has been demonstrated that quantum computers can be used for solving linear systems of algebraic equations with exponential speedup compared with classical computers. Here, we present a generic quantum circuit design for implementing the algorithm for solving linear systems. In particular, we show the detailed construction of a quantum circuit which solves a 4×4 linear system with 7 qubits. It consists of only the basic quantum gates that can be realized with present physical devices, implying great possibility for experimental implementation. Furthermore, the performance of the circuit is numerically simulated and its ability to solve the intended linear system is verified.

Quantum computers are devices that take direct advantage of quantum mechanical phenomena such as superposition and entanglement to perform computations [1]. Because they compute in ways that classical computers cannot, for certain problems quantum algorithms provide exponential speedups over their classical counterparts. For example, in solving problems related to factoring large numbers [2] and simulation of quantum systems [3–15], quantum algorithms are able to find the answer exponentially faster than classical algorithms. Recently, A. W. Harrow, A. Hassidim and S. Lloyd [16] proposed a quantum algorithm for solving linear systems of equations with exponential speedup over the best known classical algorithms.

With the theoretical potential of the algorithm, an equally important issue is to render the algorithm viable for experimental implementation. Therefore, in this Letter we present a generic quantum circuit design based on the theoretical framework outlined by the algorithm. In particular, we choose a specific linear system (described by a matrix A of dimension 4×4) as the numerical example for of the algorithm. Since our circuit involves only 7 qubits and is composed of only basic quantum gates, our work bridges the theoretical development of the algorithm with the possibility of physical implementation by experimentalists.

The algorithm[16] solves the problem $A\vec{x} = \vec{b}$ where A , a Hermitian s -sparse $N \times N$ matrix and \vec{b} , a unit vector are given. The major steps of the algorithm can be summarized as the following: (1) Represent the vector \vec{b} as a quantum state $|b\rangle = \sum_{i=1}^N b_i |i\rangle$, stored in a quantum register (termed b). In a separate quantum register (termed C) of t qubits, initialize the qubits by transforming the register to state $\sum_{\tau} |\tau\rangle$ from $|0\rangle$; (2) Apply the conditional Hamiltonian evolution $\sum_{\tau=0}^{T-1} |\tau\rangle\langle\tau|^C \otimes e^{iA\tau t_0/T}$; (3) Apply the quantum inverse Fourier transform to the register C . Denote the basis states after quantum Fourier transform as $|k\rangle$. At this stage, the amplitudes of the basis states are concentrated on k values that satisfy $\lambda_k \approx \frac{2\pi k}{t_0}$, where λ_k is the k -th eigenvalue of the matrix A ; (4) Add an ancilla qubit and apply conditional rotation on it, controlled by the register C with $|k\rangle \approx |\lambda_k\rangle$. The rotation transforms the qubit to $\sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle$. This is a key step of the algorithm and it involves finding the reciprocal of the eigenvalue λ_j quantum mechanically, which is not a trivial task on its own; (5) Uncompute the registers b and C , and (6) Measure the ancilla bit. If it returns 1, the register b of the system is in the state $\sum_{j=1}^n \beta_j \lambda_j^{-1} |u_j\rangle$ up to a normalization factor, which is equal to the solution $|x\rangle$ of the linear system $A\vec{x} = \vec{b}$. Here $|u_j\rangle$ represents the j -th eigenvector of the matrix A

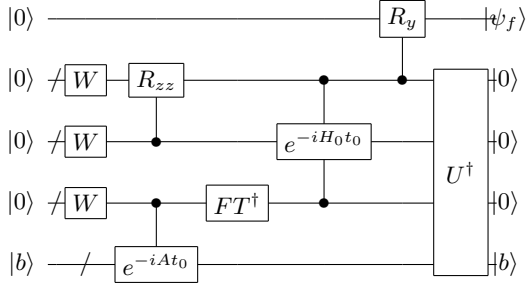


FIG. 1: Generic quantum circuit for implementing the algorithm for solving linear systems of equations. The registers from bottom up are respectively register b , C , m , l and ancilla bit. $|\psi_f\rangle = \sqrt{1 - \frac{C^2}{\lambda_j^2}}|0\rangle + \frac{C}{\lambda_j}|1\rangle$. U^\dagger represents uncomputation.

and let $|b\rangle = \sum_{j=1}^n \beta_j |u_j\rangle$.

Based on the theoretical framework of the algorithm outlined above, here we present a generic quantum circuit design that implements the algorithm to find the solution $|x\rangle$ to the linear equation $A|x\rangle = |b\rangle$. The circuit contains registers b , C , m , l and an ancilla bit (Figure 1). Register b is used to store the value of $|b\rangle$. Register C , m and l contain t , m and l qubits respectively. the Walsh-Hadamard transform on Register C , the controlled Hamiltonian simulation and the inverse Fourier transform ideally gives a state $\sum_j \beta_j |u_j\rangle |\lambda_j\rangle$ [16] in Register b and C . After the inverse Fourier transform is executed on register C , we use its $|\lambda_j\rangle$ states as a control for a Hamiltonian simulation $\exp(iH_0 t_0)$ that is applied on register m . Here H_0 is defined as $\text{diag}(1, 2, \dots, M)$ where $M = 2^m$. Due to the unitary nature of $\exp(iH_0 t_0)$, the operation $\exp(iH_0 t_0)$ can be readily decomposed into a quantum circuit [17, 18] that consists of only basic quantum gates.

We establish the control relationship between Register l and the $\exp(iH_0 t_0)$ by using the k_l -th qubit of the register l to control a $\exp[-ip(\frac{\lambda_j}{2^m} \frac{1}{2^{l-k_l}} t_0)]$ gate that acts on register m . The values of binary number stored in register l are then able to determine the time pa-

rameter t in the overall Hamiltonian simulation $\exp(-iH_0 t)$. Following such construction, after the Hamiltonian simulation $\exp(-iH_0 t_0)$ the state of the system is $\sum_{j=1}^n \sum_{p=0}^{2^m-1} \sum_{s=0}^{2^l-1} \beta_j |u_j\rangle |\lambda_j\rangle \exp[i\frac{p}{2^{m+l}} t_0 (2^l - \lambda_j s)] |p\rangle |s\rangle \otimes |0\rangle$. Ideally, only $s = \frac{2^l}{\lambda_j}$ survive in the above expression.

Denote such $|s\rangle$ states as $|\frac{2^l}{\lambda_j}\rangle$. Rotate the ancilla bit with the angle shift controlled by the $|\frac{2^l}{\lambda_j}\rangle$ states stored in register l : $R_y(\frac{2^l}{\lambda_j})|0\rangle \approx \sqrt{1 - \frac{C^2}{\lambda_j^2}}|0\rangle + \frac{C}{\lambda_j}|1\rangle$ with C being a constant. Uncomputing the three registers (Figure 1), we are left with a state in register b with the ancilla qubit proportional to $\sum_{j=1}^n \beta_j |u_j\rangle \left[\sqrt{1 - C^2/\lambda_j^2} |0\rangle + C/\lambda_j |1\rangle \right]$

Measuring the ancilla qubit and if we obtain $|1\rangle$, the state of the system will collapse to $\sum_{j=1}^n \beta_j \lambda_j^{-1} |u_j\rangle \otimes |1000\rangle$, where $|u_j\rangle$, where the first register represents the solution. If the ancilla bit measures $|0\rangle$, the system is back to its original state $|b0000\rangle$. If the ancilla bit measures $|1\rangle$, the state stored in the register b is proportional to the solution of the linear system of equations $A|x\rangle = |b\rangle$ and the register b is no longer entangled with any other registers in the system. Therefore we have obtained the solution of the linear system of equations in form of a quantum superposition state stored in the register b .

With the generic circuit model outlined above, now we present a 7-qubit circuit for solving a system with A of dimension 4×4 as a numerical example. For the numerical example we specifically choose the form of matrix A such that it allows for a very simple *ad hoc* design of the circuit for finding the binary reciprocal. For this example we choose

$$A = \frac{1}{4} \begin{pmatrix} 15 & 9 & 5 & -3 \\ 9 & 15 & 3 & -5 \\ 5 & 3 & 15 & -9 \\ -3 & -5 & -9 & 15 \end{pmatrix} \quad (1)$$

Hence A is a Hermitian matrix with the eigenvalues $\lambda_i = 2^{i-1}$ and corresponding eigenvectors

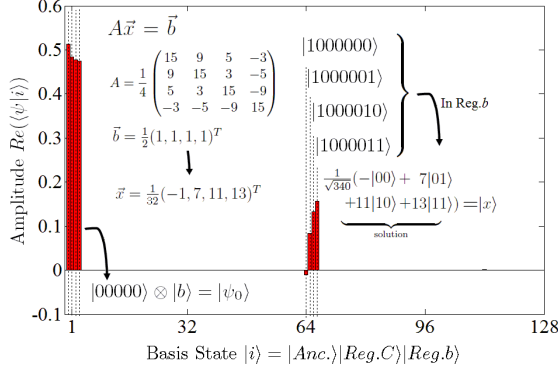


FIG. 2: The final state of the algorithm for solving the 4×4 system. The horizontal axis represents the decimal value that corresponds to a basis state of the seven-qubit system. The vertical axis represents the real parts of the probability of amplitudes that corresponds to a certain basis.

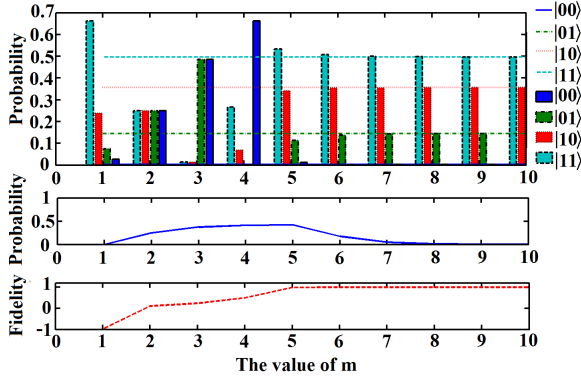


FIG. 3: Simulation results on the dependence of final state on the value of the parameter m .

The first barplot shows the probability distributions over the four basis states of Register b with different values of m in the controlled rotation gates acted upon the ancilla bit. The horizontal dashed lines show the analytical values of the probabilities. The two plots following show the probability of getting the solution as well as the fidelity $\langle x'|x \rangle$ as functions of m .

tor $|u_i\rangle = \frac{1}{2} \sum_{j=1}^4 (-1)^{\delta_{ij}} |j\rangle^C$, where $|j\rangle^C$ represents the state of register C which encode the number j in binary form, δ_{ij} is the Kronecker delta, and the index i runs from 1 to 4. Furthermore, we let $\vec{b} = \frac{1}{2}(1, 1, 1, 1)^T$. Therefore, $|b\rangle = \sum_{j=1}^4 \beta_j |u_j\rangle$ and each $\beta_j = \frac{1}{2}$. To compute the reciprocals of the eigenvalues, a quantum *swap* gates is used (Figure 4) to exchange the values of the first and third qubit. Therefore there is no need for specific auxiliary registers m and l (Figure 1) in this example. The eigenvalues are inverted to their reciprocals with the *swap* gate in the following fashion. For example, the eigenvalue $\lambda_4 = 8$ is encoded as $|1000\rangle$ in register C , after applying the *swap* gates it is transformed to $|0010\rangle$, which is equal to $\frac{1}{8} \times 2^4 = 2$.

Figure 4 shows the circuit. We use Group Leader Optimization Algorithm [17, 18] to find the circuit decomposition of the Hamiltonian simulation operator $e^{iA \frac{2\pi}{16}}$, where $t_0 = 2\pi$. The resulting quantum circuit for $e^{iA \frac{2\pi}{16}}$ is shown in Figure 4. With the decomposition of $e^{iA \frac{2\pi}{16}}$ readily available, the operators $e^{iA \frac{2\pi}{8}}$, $e^{iA \frac{2\pi}{4}}$ and $e^{iA \frac{2\pi}{2}}$ can be obtained with minimum modification [17].

The final state of system, conditioned on obtaining $|1\rangle$ in the ancilla bit, is $\frac{1}{\sqrt{85}}(8|u_1\rangle + 4|u_2\rangle + 2|u_3\rangle + |u_4\rangle) \otimes |0000\rangle \otimes |1\rangle$. Written in the standard bases, it becomes $\frac{1}{\sqrt{340}}(-|00\rangle + 7|01\rangle + 11|10\rangle + 13|11\rangle)$, which is proportional to the exact solution of the system $\vec{x} = \frac{1}{32}(-1, 7, 11, 13)^T$ (Figure 2). The quantum circuits (Figure 4) outlined above is then simulated and the statistics of final states that are computed from the simulations (Figure 3). The results show that the circuit is able to solve the 4-dimensional linear equation to satisfactory accuracy when the value of m is properly determined. Therefore this letter may motivate experimentalists with the capability of addressing 7 qubits and execute basic quantum gates on their setups to implement the algorithm and verify its results. Future work regarding the improvement upon the algorithm needs to be focused on topics such as extending the algorithm

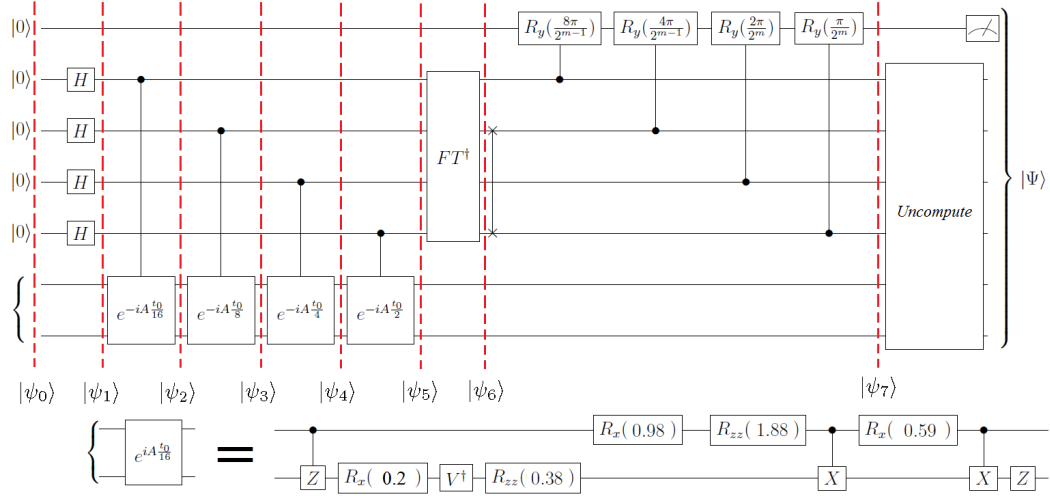


FIG. 4: Quantum Circuit for solving $A\vec{x} = \vec{b}$ with $A_{4 \times 4}$ being the matrix shown in equation (1). The first qubit at the top of the figure is the ancilla bit. The four qubits in the middle stand for the register C . The two qubits at the bottom is the register that stores the vector \vec{b} .

to cases where the matrix A has a low condition number [19].

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BIBLIOGRAPHY

- * Corresponding author:kais@purdue.edu
- [1] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, United Kingdom, 2000).
 - [2] P.W.Shor, in *Proc. 35th Annu. Symp. Found. Comp. Sci.*, edited by S.Goldwasser (IEEE Computer Society Press, New York, 1994) pp. 124–134.
 - [3] S. Lloyd, *Science* **273**, 1073 (1996).
 - [4] D. S. Abrams and S. Lloyd, *Phys. Rev. Lett.* **83**, 5162 (1999).
 - [5] D. S. Abrams and S. Lloyd, *Phys. Rev. Lett.* **79**, 2586 (1997).
 - [6] A. Papageorgiou, I. Petras, J. F. Traub, and C. Zhang, (arXiv:1008.4294v2).
 - [7] A. Papageorgiou and C. Zhang, (arXiv:1005.1318v3).
 - [8] H. Wang, S. Kais, A. Aspuru-Guzik, and M. R. Hoffmann, *Phys. Chem. Chem. Phys.* **10**, 5388 (2008).
 - [9] A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, and M. Head-Gordon, *Science* **309**, 1704 (2005).
 - [10] D. Lidar and H. Wang, *Phys. Rev. E* **59**, 2429 (1999).
 - [11] H. Wang, S. Ashhab, and F. Nori, *Phys. Rev. E*, arXiv:1108.5902.
 - [12] J. You and F. Nori, *Nature* **474**, 589 (2011).
 - [13] J. You and F. Nori, *Phys. Today* **58**, 42 (2005).
 - [14] I. Buluta and F. Nori, *Science* **326** (2009).
 - [15] J. Dowling, *Nature* **439**, 919 (2006).
 - [16] A. W. Harrow, A. Hassidim, and S. Lloyd, *Phys. Rev. Lett.* **15**, 150502 (2009).
 - [17] A. Daskin and S. Kais, *J. Chem. Phys.* **134** (2011).
 - [18] A. Daskin and S. Kais, *Mol. Phys.* **109**, 761 (2011).
 - [19] A. M. Childs, *Nature Phys.* **5**, 861 (2009).