Quantum Algorithm for Linear Systems of Equations

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***Index Terms*—component, formatting, style, styling, insert**

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- Use a zero before decimal points: "0.25", not ".25". Use "cm^3", not "cc".)

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Number equations consecutively. To make your equations more compact, you may use the solidus (/), the exp function, or appropriate exponents. Italicize Roman symbols for quantities and variables, but not Greek symbols. Use a long dash rather than a hyphen for a minus sign. Punctuate equations with commas or periods when they are part of a sentence, as in:

$$a + b = \gamma \tag{1}$$

Be sure that the symbols in your equation have been defined before or immediately following

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IV. Overview of the algorihtm

The following section will describe how the algorithm works in general. Firstly, it will specify the problem statement. After that, it will describe a short mathematical explanation. Then, it will sketch out the steps of the algorithm.

A. Problem statement

Given an NxN hamiltonian matrix A and $\vec{a}$ vector $\vec{b}$, we want to solve for the vector $\vec{x}$ such that,

$$A\vec{x} = \vec{b} \tag{2}$$

To solve for x the equation can be rewritten as

$$\vec{x} = A^{-1}\vec{b} \tag{3}$$

Note that to encode $\vec{b}$ we need $\mathcal{O}(log_2 N)$ qubits.

As described earlier the hermitian matrix A^{-1} can be split into its spectral decomposition. A can be represented in terms of its eigenvalues $U_1 ... U_n$ and eigenvectors $\lambda_1 ... \lambda_n$.

$$A = UDU^\dagger = \begin{pmatrix} U_1 & ... & U_n \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \dots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix} \begin{pmatrix} U_1^\dagger \\ ... \\ U_n^\dagger \end{pmatrix} \tag{4}$$

This means, if we can find the eigenvalues and eigenvectors of A we can then solve the linear equation quite easily. Classical solutions involving spectral decomposition are not faster than other standard algorithms such as Gaussian Elimination. Though, estimating eigenvalues and eigenwerte can be performed quite efficiently by quantum methods. Via amplitude amplification, QPE can be accelerated to generate the eigenvalues and eigenvectors in $\mathcal{O}(log_2 N)$ steps.

In the quantum version the linear equation looks like this

$$|x\rangle = A^{-1} |b\rangle \tag{5}$$

where $|b\rangle$ and $|x\rangle$ are the quantum state of the $\vec{b}$ and $\vec{x}$ vectors respectively. Note that $|x\rangle$ is just a quantum state. We can not read every element to achieve the vector $\vec{x}$. So far we were able to perform everything in $\mathcal{O}(log_2 N)$. Reading out every entry of $\vec{x}$ would take $\mathcal{O}(N)$ steps which would destroy our speed up. But, as we are only interested in an approximation, we can compute an expectation value $\langle x| M |x\rangle$, where M is some linear operator. With this method we can extract many statistical features like normalization, distribution of weights, moments, etc.

B. Mathematical Overview

We will now look at a mathematical overview of what is happening in the quantum circuit. We will also assume that the matrix A is hermitian. If A is not hermitian, we can write A as a hermitian like this

$$A^\dagger = \begin{pmatrix} 0 & A \\ A^T & 0 \end{pmatrix} \tag{6}$$

As already mentioned the matrix can now be described as a linear combination of its outer products of its eigenvectors and its eigenvalues. In the quantum version the formula looks like this

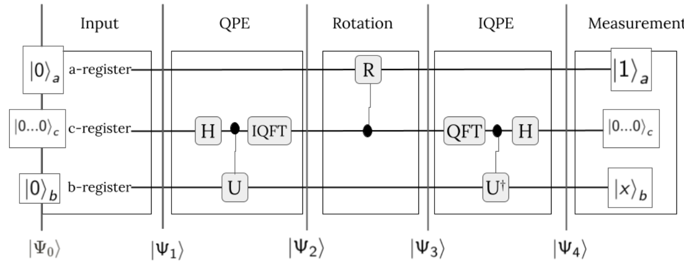

Fig. 1. Example Circuit

$$A = \sum_{i=0}^{N-1} \lambda_i |u_i\rangle \langle u_i| \tag{7}$$

where $|u\rangle_i \langle u|_i$ are the outer products of A and λ_i are the eigenvalues of A. N is the size of the matrix A. We can rewrite the formula for the inverse A^{-1} as such

$$A^{-1} = \sum_{i=0}^{N-1} \lambda_i^{-1} |u_i\rangle \langle u_i| \tag{8}$$

Similary $|b\rangle$ can be expressed in the eigenbasis of A like this

$$|b\rangle = \sum_{j=0}^{N-1} b_j |u_j\rangle \tag{9}$$

We now have all the tools to solve the equation by inserting the definition of A^{-1} and $|b\rangle$ into our original equation,

$$\begin{aligned} |x\rangle &= A^{-1} |b\rangle \\ &= \left(\sum_{i=0}^{N-1} \lambda_i^{-1} |u_i\rangle \langle u_i|\right) \left(\sum_{j=0}^{N-1} b_j |u_j\rangle\right) \\ &= \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \lambda_i^{N-1} |u_i\rangle \langle u_i| b_j |u_j\rangle \\ &= \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \lambda_i^{-1} b_j |u_i\rangle \langle u_i|u_j\rangle \\ &= \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \lambda_i^{-1} b_j |u_i\rangle \delta_{ij} \\ &= \sum_{i=0}^{N-1} \lambda_i^{-1} b_j |u_j\rangle \end{aligned}$$

As we can see we can encode the solution $|x\rangle$ of our linear system into our quantum system quite nicely. That means, $|x\rangle$ can be calculated, only by determinining the eigenvectors and eigenvalues of A. Using Quantum Phase Estimation, calculating the eigenvalues and eigenvectors for a unitary U can be very efficient.

C. Quantum Circuit

We will now look at how the algorithm is implemented in the quantum circuit. We will firstly look at the sets of qubits need for the algorithm. Then, we will describe the phases of the procedure.

1) Registers: Fig. 1 shows the scheme of a simple quantum circuit for the HHL algorithm. We have three registers which describe three different sets of qubits in the quantum circuit.

The a-register contains the ancilla qubit. It is used for the inversion of the eigenvalues and will be explained in detail later on.

The c-register, oftentimes refered to as the clock-register, is used for the quantum phase estimation part. It is related to the time (clock) of the controlled rotation of the qubits and will store the eigenvalues after performing QPE.

The b-register contains the $\vec{b}$ vector which is encoded into a quantum state $|b\rangle$. After the whole HHL procedure is done the b-register will contain the solution state $|x\rangle$.

2) Phases: The procedure of the quantum circuit can be split into 5 phases:

- State preparation
- Quantum phase estimation (QPE)
- Inversion of eigenvalues
- Inverse quantum phase estimation (IQPE)
- Measurement of $|x\rangle$

In the state preparation phase, the vector $\vec{b}$ will be encoded into a quantum state $|b\rangle$ and the A matrix will be encoded as a hamiltonian, which is a unitary operator $U = e^{iAt}$ into the QPE and IQPE operations.

The Quantum Phase Estimation will then calculate the eigenvalues and eigenvectors of the A matrix.

Then, we perform the rotation and invert the eigenvalues through rotary operations. Unfortunately, these operations have a probability to fail, as they are not unitary operators. The ancilla will detect wether the rotation was successfull or not. It will either collapse to $|0\rangle$ or $|1\rangle$ for failure and success respectively. If the rotation is not successfull, the procedure has to be repeated from the beginning. If the rotation was successfull we can continue the procedure. The problem is, that the qubits in the b-register and c-register are entangled. This means that we cannot factorize the result into a tensor product of the c-register and b-register. As a result, we cannot convert the b-register into the $|0\rangle$ / $|1\rangle$ measurement basis with the desired amplitudes. We will need to uncompute the state so that it gives the right results in the $|0\rangle$ / $|1\rangle$ measurement during which the b-register and c-register will be unentangled. That means we have undo all operations until now to unentangle the states, keeping the inverted eigenvalues though.

This is achieved by the Inverse Quantum Phase Estimation which undos all steps we performed in the QPE phase, leaving us with the a $|0...0\rangle$ state in the c-register and the $|x\rangle$ state in the b-register.

Lastly, the $|x\rangle$ state is to be measured. As mentioned earlier, we can only read out an approximation of an expectation value $\langle x| M |x\rangle$.

V. The HHL Algorithm

The next section will give a more detailed walkthrough of the HHL algorithm. Thereby, it will go through all the 5 phases namely, state preperaration, QPE, inversion of eigenvalues, IQPE and lastly the measurement.

A. State Preparation

In total we have $n_b + n + 1$ qubits. In the beginning they are all initialized in their zero state as

$$\begin{aligned} |\Psi_0\rangle &= |0\ldots0\rangle_b \ |0\ldots0\rangle_c \ |0\rangle_a \\ &= |0\rangle_b^{\otimes n_b} \ |0\rangle_c^{\otimes b} \ |0\rangle_a \end{aligned} \tag{10}$$

We now have to load the vector $\vec{b}$ into the b-register. This is achieved by amplitude encoding.

Todo

insert formula here

The state $|b\rangle$ is then loaded into the b-register. Therefore

$$|\Psi_1\rangle = |b\rangle_b \ |0\ldots0\rangle_c \ |0\rangle_a \tag{11}$$

We have successfully encoded the $\vec{b}$ into our b-register. We now continue with the QPE.

B. Quantum Phase Estimation

We will only briefly go through the specifics of the QPE and will not discuss each step in detail, as this is not the main topic of this paper. For further explanations refer to this paper. As already mentioned, the QPE is a procedure to evalute an estimate of eigenvalues. It consists of three phases, namely the superpositions of the clock-bits via Hadamard gate, controlloed rotation via unitary U and the IQFT. After QPE we will have an estimate of the eigenvalues of the unitary U. As we have encode A as as a Hamiltonian $U = e^{iAt}$, the phase of the eigenvalue of U is proportional to the eigenvalue of A. We have to define a scaled version of our eigenvalues λ_j.

$$\widetilde{\lambda_j} = \frac{N\lambda_j t}{2\pi} \tag{12}$$

where t can be choosen freely so that the scaled eigenvalues $\widetilde{\lambda_j}$ are integers.

Thus, the eigenvalues of A will be stored in the c-register after QPE as

$$\begin{aligned} |\Psi_2\rangle &= |b\rangle_b \, |\widetilde{\lambda}\rangle_c \, |0\rangle_a \\ &= \sum_{j=0}^{N-1} b_j \, |u_j\rangle_b \, |\widetilde{\lambda_j}\rangle_c \, |0\rangle_a \end{aligned} \tag{13}$$

Notice, that the b-register is now a representation of the $|b\rangle$ state in the eigenbasis $|u_j\rangle$ of A.

C. Inversion of the eigenvalues

In the next step we want to invert the eigenvalues in our state. This is achieved by the rotation of the ancilla qubit in the a-register by the eigenvalues in the c-register. The state of the registers after the rotation looks like this

$$|\Psi_3\rangle = \sum_{j=0}^{N-1} b_j |u_j\rangle_b |\widetilde{\lambda_j}\rangle_c \left(\sqrt{1 - \frac{C^2}{\widetilde{\lambda}_j^2}} |0\rangle_a + \frac{C}{\widetilde{\lambda_j}} |1\rangle_a \right) \tag{14}$$

where C is a constant that should be chosen to be as large as possible to increase the success probability. Currently, the state of the a-register can either collapse into $|1\rangle$ or $|0\rangle$. The probability of the state collapsing to $|1\rangle$ is $\left|\frac{C}{\widetilde{\lambda_j}}\right|^2$. If the ancilla bit collapses to $|0\rangle$, the whole procedure has to be repeated from the beginning. As mentioned earlier this has to be done, because the rotation process is not unitary and has a probability to fail.

We assume that our rotation process was successfull and the ancilla bit collapses to $|1\rangle$. The registers will look as such

$$|\Psi_4\rangle = \frac{1}{\sqrt{\sum_{j=0}^{N-1} \left|\frac{b_j C}{\widetilde{\lambda_j}}\right|^2}} \sum_{j=0}^{N-1} b_j |u_j\rangle_b |\widetilde{\lambda_j}\rangle_c \frac{C}{\widetilde{\lambda_j}} |1\rangle_a \tag{15}$$

Note that term in front of the sum is just a factor to normalize the state. Lets call this normalization factor D. We see that we now have a term $\frac{C}{\widetilde{\lambda_j}}$ that represents the inverted eigenvalues. This term can be moved around freely as it is just a scalar and can be moved, such that it is applied to the b-register

$$|\Psi_4\rangle = D \sum_{j=0}^{N-1} \frac{C}{\widetilde{\lambda_j}} b_j |u_j\rangle_b |\widetilde{\lambda_j}\rangle_c |1\rangle_a \tag{16}$$

If we go back to our idea from the mathematical overview section, our b-register is in the same form as our solution state

$$|x\rangle = \sum_{i=0}^{N-1} \lambda_i^{-1} b_j |u_j\rangle \tag{17}$$

That means our solution is already encoded in our registers. The problem here is, that we cannot read the solution out yet. This has to with the states in the b-register and c-register being entangled with each other. That means we cannot convert the b-register into a $|0\rangle / |1\rangle$ measurement. In the following we have to undo all operations to unentangle the state in the b-register and c-register, to achieve the correct result.

D. Inverse Quantum Phase estimation.

The unentangling of the registers is achieved throught the IQPE which just backtracks all calculations of the QPE. We are left with the following state

$$\begin{aligned} |\Psi_5\rangle &= \frac{1}{\sqrt{\sum_{j=0}^{N-1} \left|\frac{b_j C}{\lambda_j}\right|^2}} \sum_{j=0}^{N-1} \frac{C}{\lambda_j} b_j |u_j\rangle_b |0\rangle_c^{\otimes n} |1\rangle_a \\ &= \frac{C}{\sqrt{\sum_{j=0}^{2^{n_b}-1} \left|\frac{b_j C}{\lambda_j}\right|^2}} |x\rangle_b |0\rangle_c^{\otimes n} |1\rangle_a \end{aligned} \tag{18}$$

The a-register is untouched and still hold the $|1\rangle$ state as before. The c-register however is reset to the zero state $|0\rangle_c^{\otimes n}$ as in the beginning of the process. It is now unentangled from the b-register. The b-register now contains the solution $|x\rangle$ after the uncomputation and can be measuremed correctly.

We can furthermore simplify the term as we assume that C is real and that the eigenvectors $|u_i\rangle$, and the $|b\rangle$ state are normalized. Then we can simplify to

$$\begin{aligned} |\Psi_5\rangle &= \frac{1}{\sqrt{\sum_{j=0}^{N-1} \left|\frac{b_j}{\lambda_j}\right|^2}} |x\rangle_b |0\rangle_c^{\otimes n} |1\rangle_a \\ &= |x\rangle_b |0\rangle_c^{\otimes n} |1\rangle_a \end{aligned} \tag{19}$$

We can now read out the result $|x\rangle$ in the b-register.

E. Measurement

As mentioned earlier, we cannot obtain the whole solution for the $\vec{x}$ as reading out all the entries would cost us $\mathcal{O}(N)$ steps. This would ommit our speedup of $\mathcal{O}(logN)$. That means that by measuring, we will only obtain an estimate of specific features of $|x\rangle$. Using a linear operator M we can perform various measurements on $|x\rangle$ by calculating the inner product as such

$$\langle x| M |x\rangle \tag{20}$$

With this we can extract various statistical features of $|x\rangle$ like the norm of the vector, the average of the weight of the components, moments, probability distributions, localization and concentration in specific regions, etc.