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Iterative quantum phase estimation on an IBM quantum processor

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Abstract. **An elementary algorithm of quantum phase estimation based on the modified Kitaev algorithm is implemented on two qubits of an IBM quantum processor. This algorithm includes adiabatic preparation of the initial state, controlled phase shift with allowance for the results of previous measurements of qubit states, and single measurement of the qubit quantum state in order to obtain each significant bit of the measured phase. Classical error correction is applied to determine the correct sequence of bits, which makes it possible to eliminate the influence of limited accuracy of two-qubit gates.**

Keywords: *quantum processor, quantum phase estimation, modified Kitaev algorithm, two-qubit gate.*

1. Introduction

Quantum simulation of elementary physical processes is of interest for solving many problems in physics of many-body quantum interactions, whose complexity exponentially increases with an increase in the number of interacting particles [1, 2]. Quantum simulation is carried out using a quantum processor capable of performing the quantum Fourier transform, on which the quantum phase estimation algorithm is based [3]. Quantum phase estimation is an important building block for various quantum algorithms. For example, it is used in Shor's algorithm to expand numbers in simple factors, in quantum chemistry to simulate molecules, and in Grover's algorithm [2]. Nevertheless, the implementation of quantum algorithms on modern quantum processors is limited by the low accuracy of quantum gates. In this context, of great interest is the experimental realisation of the simplest quantum algorithms, which makes it possible to estimate the potential of quantum processors for solving elementary physical problems and the prospects for achieving quantum dominance.

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In recent years, there has been a significant progress in the implementation of quantum calculations based on different physical platforms. Primarily, these are Josephson junctions in superconductors [4 – 6], which were chosen as a basis for quantum processors by the largest IT companies (IBM, Google, Microsoft). At the same time, certain success has been achieved on alternative physical systems: ultracold ions [7, 8], photons [9], and ultracold neutral atoms [10 – 13]. To analyse the prospects of implementing quantum algorithms in these systems, it is of great interest to compare their possibilities (by an example of very simple quantum algorithms) with those for superconducting quantum processors.

Of particular interest are the problems related to simulation of molecules [14], including the problem of determining the structure and properties of individual molecules or molecular aggregates. The latter task can be reduced to determination of the energy of the molecule in different states, which is equivalent to the search for eigenstates and eigenvalues of the unitary operator. The phase of the unitary operator is presented as a bit sequence of arbitrary length.

Generally, quantum phase estimation is implemented using the inverse quantum Fourier transform [3], which allows one to find a desired sequence of bits via a single measurement of the quantum register state. The length of the measured bit sequence, which determines the measurement accuracy, is set by the quantum register length. An alternative is the Kitaev algorithm with a single control qubit [15]. In this case, one can obtain a bit sequence of arbitrary length as a result of successive measurements of qubit states.

The Kitaev algorithm can be implemented using an iterative scheme, which makes it possible to calculate each significant bit after a single measurement of the control qubit state. Then, in the next step of sequence, the measurement is preceded by a qubit phase correction with allowance for the results of previous measurements. This scheme was proposed in [16]. A numerical simulation of iterative quantum phase estimation for an ideal quantum processor and for a system of two interacting neutral atoms (excited for a short time into Rydberg states when implementing two-qubit gates) was performed in [17]. It is shown that the influence of the decoherence (related to the finite lifetime of Rydberg atoms) on the measurement results can be eliminated by multiple measurements of the control qubit states, which can to be considered as the classical error correction.

In this study we implemented an iterative quantum phase estimation on an IBM quantum processor and a quantum phase estimation based on the quantum Fourier transform by an example of determining the energy of the hydrogen molecule ground state.

2. Quantum phase estimation algorithms

The general scheme of quantum phase estimation is shown in Fig. 1. Here, two quantum registers are used: register S (state), in which the wave function of the considered state of the system, $|\psi\rangle$, is recorded, and register R (readout), which is necessary to store intermediate information and obtain the operator phase. All qubits of the register R used for measurements were initially prepared in the $|0\rangle$ state. Application of Hadamard gates H turns the register into a superposition of all possible states, denoted as $|n\rangle$.

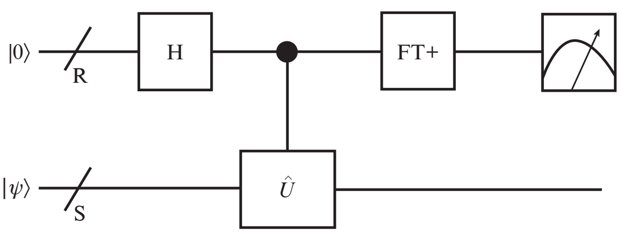

Figure 1. General scheme of quantum phase estimation based on the inverse quantum Fourier transform.

Register S is prepared in the eigenstate of some unitary operator $\hat{U}$, denoted as $|\psi\rangle$. Let φ be the phase of the operator $\hat{U}$, i.e., $\hat{U}|\psi\rangle = \exp(2\pi i\varphi)|\psi\rangle$. Applying successively and controllably operators of the form $\hat{U}_k = \hat{U}^{2^k}$ to register S, we obtain finally the sum of the states of the system:

$$|\mathrm{R}\rangle\otimes|\mathrm{S}\rangle = \sum_n \exp(2\pi i\varphi n)\,|n\rangle\otimes|\psi\rangle. \quad (1)$$

Then we apply an inverse quantum Fourier transform FT+ to the register R and measure its state. This procedure will allow us to estimate the phase with an arbitrary accuracy. Note that the register state is measured once.

Using this method to measure the phase with a high accuracy, one needs a register of sufficiently large length. The Kitaev method [15] makes it possible to solve this problem using only the control qubit. A schematic of this method is shown in Fig. 2. The register consists of one control qubit and a state register, in which the eigenstate $|\psi\rangle$ of the operator $\hat{U}$ is recorded. After carrying out a controlled unitary transformation, the system of two qubits will be in the state

$$\frac{1}{\sqrt{2}}[|0\rangle + \exp(2\pi i\varphi)|1\rangle]\,|\psi\rangle.$$

After the Hadamard gate H the system is in the state

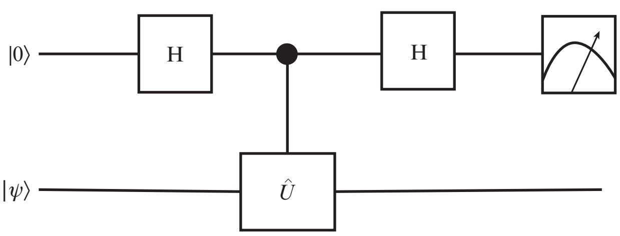

Figure 2. Schematic of the Kitaev algorithm with a single control qubit.

$$\frac{1}{2}[1 + \exp(2\pi i\varphi)]\,|0\rangle\,|\psi\rangle + \frac{1}{2}[1 - \exp(2\pi i\varphi)]\,|0\rangle\,|\psi\rangle. \quad (2)$$

The probability of finding the controlled qubit in the state '0' is $P = \cos^2(\pi\varphi)$. Having measured it, one can determine the phase φ.

Instead of a single measurement of the state of a multiqubit register, multiple measurements of the state of one qubit must be performed to measure the phase with a specified accuracy. Note that multiple measurements are also necessary to measure the probabilities of finding the system in the $|0\rangle$ or $|1\rangle$ state. The modification of this scheme proposed in [16] allows one to determine the kth bit of the phase in one measurement. A schematic of the modified Kitaev algorithm is presented in Fig. 3. In contrast to the methods considered previously, the measurement begins with the low-order bit of the phase. Each iteration includes a single measurement of the control qubit state. Before the measurement, its state is corrected to take into account the results of previous measurements via the phase shift $R_Z(\omega_k)$, i.e., the qubit rotation around the Z axis by an angle ω_k.

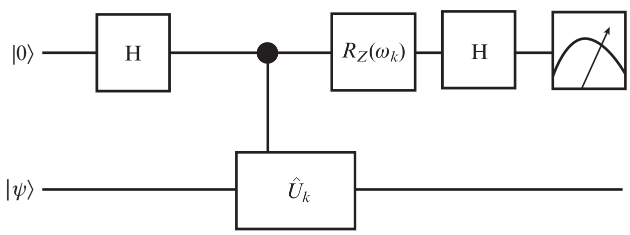

Figure 3. Adaptive phase estimation scheme.

3. Experimental quantum phase estimation using an IBM processor

Similarly to [17], the model problem for quantum phase estimation was chosen to be the determination of the energy of the hydrogen molecule ground state. In accordance with [18], we took the minimum basis set of 1s Slater–Zener orbitals, STO-3G [19]. At a distance of 1.4 au between the nuclei of atoms in the hydrogen molecule, the Hamiltonian matrix has the form (in atomic units) [8]:

$$\hat{H}_{\mathrm{mol}} = \begin{pmatrix} -1.8310 & 0.1813 \\ 0.1813 & -0.2537 \end{pmatrix}. \quad (3)$$

The Hamiltonian eigenstate $|\psi_\lambda\rangle$ corresponds to the eigenvalue λ. The system Hamiltonian $|\hat{H}_{\mathrm{mol}}\rangle$ generates a unitary evolution operator $\hat{U}$ for the time τ:

$$\hat{U}\,|\psi_\lambda\rangle = \exp(-i\hat{H}_{\mathrm{mol}}\tau)\,|\psi_\lambda\rangle = \exp(2\pi i\varphi)\,|\psi_\lambda\rangle = \lambda\,|\psi_\lambda\rangle. \quad (4)$$

Having measured the eigenvalue phase φ, one can find the Hamiltonian eigenvalue (molecule energy) $E_{\mathrm{meas}} = 2\pi\varphi/\tau$.

A program was developed for experimental quantum phase estimation in the IBM Quantum Experience environment, which included adiabatic preparation (similar to that described in [17]) of the initial state $|\psi_\lambda\rangle$, decomposition of the unitary evolution operator in the form of a sequence of single-qubit rotations, measurement of the qubit final state, and correction of the control qubit phase in subsequent measurements. Currently, the IBM company provides access to a quantum simulator and to one 1-qubit, seven 5-qubit, and one 15-qubit quantum processors [4]. A schematic of the 5-qubit quantum processor ibmqx2, which was used in our study, is shown in Fig. 4. The errors in implementing two-qubit gates are about 1.5% [4].

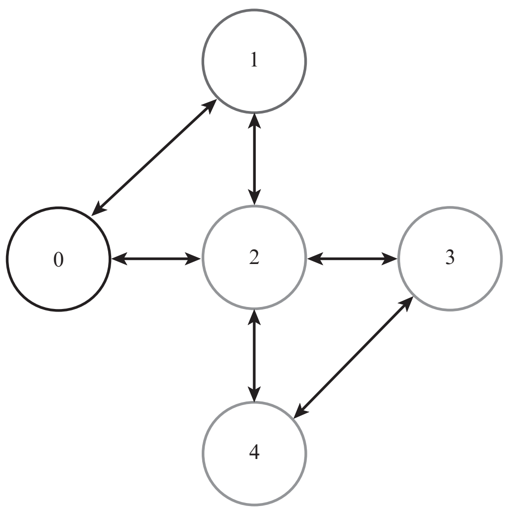

Figure 4. Schematic of a 5-qubit processor ibmqx2. Qubits are shown as circles, and the qubit connections for implementing two-qubit gates are given by arrows.

Figure 5 shows the experimental probabilities of obtaining the correct value of each bit sequence, consisting of 25 significant bits and specifying the phase of unitary evolution operator. For a quantum simulator, the probability of determining the correct value of each low-order bit differs from unity, because the lower order bits of the true phase value (beginning with the 26th bit) cannot be taken into account in the calculations. For the quantum processor ibmqx2, because of the insufficiently high accuracy of two-qubit gates, the average probability of obtaining a correct value for 20 higher order bits of the sequence is $P = 0.91$. Each probability value was found by averaging over 1024 measurements.

This means that a correct sequence of bits cannot be obtained in one measurement at the existing processor accuracy. At the same time, the choice of the most likely value of each bit in repeated measurements makes it possible to find

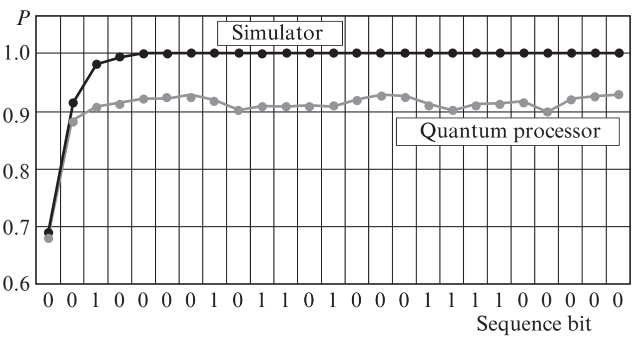

Figure 5. Measured probabilities of obtaining correct values for each bit of the sequence specifying the evolution operator phase (given below). The low-order bits are on the left.

the correct value of the phase-specifying bit sequence presented in Fig. 5.

When carrying out a quantum phase estimation using a quantum inverse Fourier transform, the correct phase value could be obtained only using a quantum simulator. The correct value could not be found using the quantum processor ibmqx2 because of the higher sensitivity of this method to the accuracy of two-qubit gates.

4. Iterative algorithm error

The errors arising when carrying out the iterative Kitaev algorithm were analysed in [16]. In accordance with the notation accepted in the monograph by Nielsen and Chuang [2], we present the phase φ as a sequence of n bits $\varphi_1, \ldots, \varphi_n$ in the form

$$\varphi = 0.\varphi_1\varphi_2\ldots\varphi_n = \frac{\varphi_1}{2} + \frac{\varphi_2}{4} + \ldots + \frac{\varphi_n}{2^n}.$$

It can be seen in Fig. 5 that, even for an ideal quantum processor (quantum simulator), the probability of obtaining the correct value of low-order bits differs from unity. This problem would not arise if the desired phase value had the form $\varphi = 0.\varphi_1\varphi_2 \ldots \varphi_m 0000\ldots$, (the number m of significant bits coincides exactly with the length of measured sequence). In this case, when simulating on a quantum simulator, the probability of determining the correct value is unity for all bits of the sequence, because there is no contribution from the ignored low-order bits.

In fact, the measured sequence of bits $\tilde{\varphi} = 0.\varphi_1\varphi_2 \ldots \varphi_m 0000$ differs from the true phase φ by a value that can be characterised by the parameter δ, lying in range 0–1:

$$\varphi = \tilde{\varphi} + 2^{-m}\delta, \quad 0 \leqslant \delta < 1. \tag{5}$$

The conditional probability P_k of correct measurement of the state of each significant bit (provided that the previous bits were measured correctly) was found in [6]. This probability is determined by the δ value in correspondence with the expression [16]

$$P_k = \cos^2(\pi 2^{k-m-1}\delta). \tag{6}$$

Therefore, to obtain a correct sequence of bits even for an ideal quantum processor, one must measure repeatedly the state of each bit. In addition, the error in implementing quantum gates leads to additional errors, as can be seen in Fig. 5.

When carrying out a quantum measurement, the IBM processor makes it possible to perform no less than 1024 repeated measurements to collect statistics. This number of measurements is sufficient to correct efficiently errors according to the following rule: if the measured probability of obtaining '1' exceeds 50%, the measurement result is taken to be '1'.

The probability of finding the correct result for a smaller number of repeated measurements was estimated numerically. The accuracy of single measurement was estimated by plotting 10^4 random 25-bit sequences, for each bit of which the probability of obtaining the specified value corresponded to the experimental results presented in Fig. 5. The error with respect to the true value, $|\varphi - \tilde{\varphi}|$, was calculated for each sequence. The distribution of the number of sequences over the error value in binary notation is shown in Fig. 6a. It can

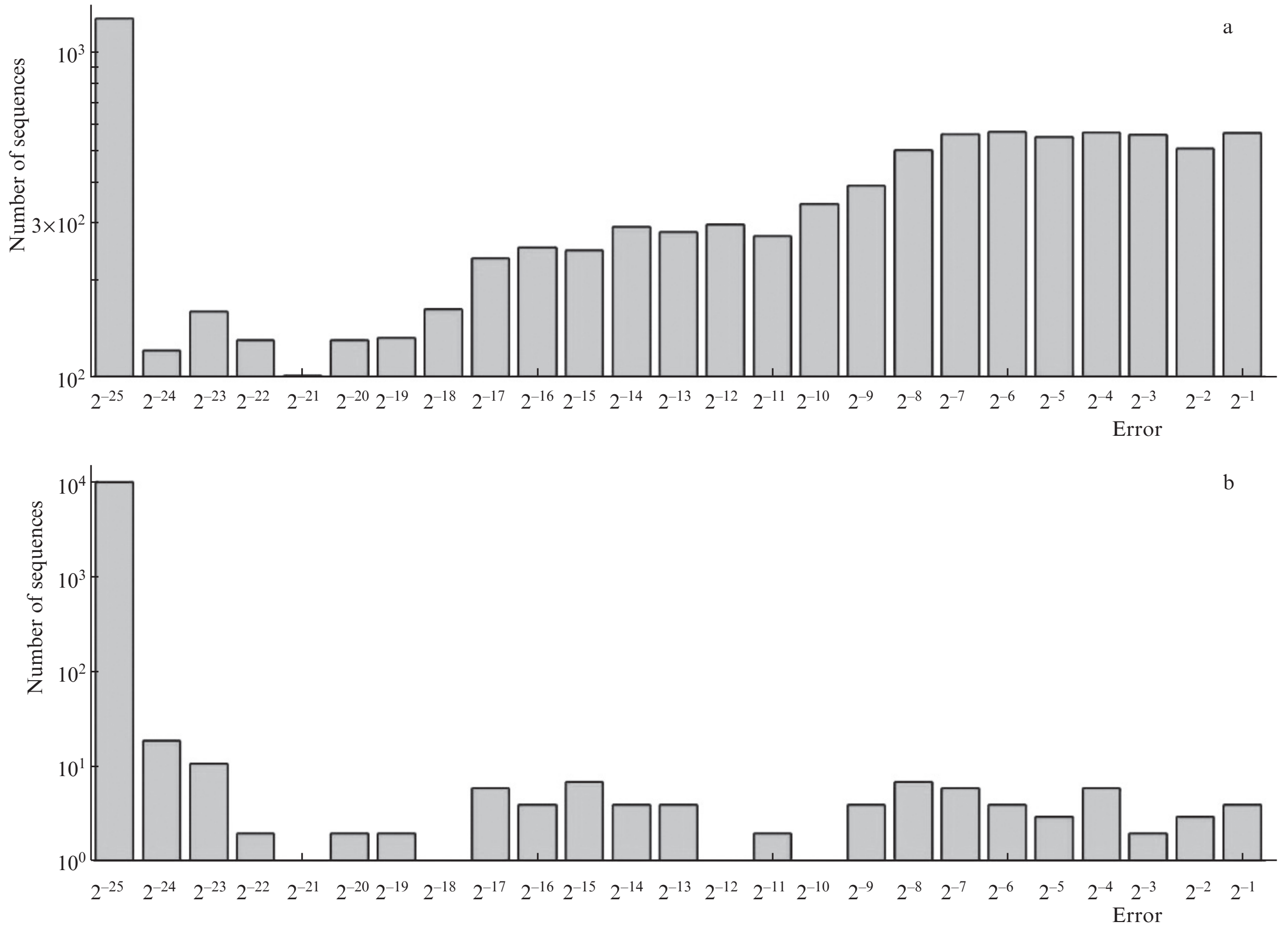

Figure 6. Error distributions of the number of generated bit sequences for (a) a single measurement and (b) in case of averaging over nine measurements with subsequent choice of the more likely value for each bit. The left columns correspond to exact coincidence of the sequence with the true value (the error is below 2^{-25}).

be seen that the probability of exact coincidence (corresponding to an error less than 2^{-25}, the left column of the histogram) is equal to ~12%, which is close to the product of the probabilities presented in Fig. 5 for an experimental sequence of bits.

If, instead of one bit sequence, nine sequences with the same probability of obtaining the specified value of each bit are generated and then the final sequence is chosen based on the largest number of coincidences of values of each bit among all nine sequences, the probability of finding the correct phase increases significantly, as can be seen in Fig. 6b. The results of estimating the accuracy of measured phase values for different numbers of repeated measurements are listed in Table 1. It can be seen that, even at nine repeated measurements, the probability of obtaining the exact bit sequence exceeds 98.8%, and the probability of obtaining an error less than 10^{-6} exceeds 99%.

Table 1. Probability *P* of obtaining the specified accuracy of measured phase value at a specified number of iterations.

Number of repetitions	Maximum error in measuring phase		
	$\leqslant 2^{-25}$	$\leqslant 10^{-6}$	$\leqslant 10^{-3}$
1	0.1235	0.1782	0.4411
3	0.6037	0.6607	0.8112
5	0.8720	0.8972	0.9419
7	0.9589	0.9684	0.9839
9	0.9881	0.9917	0.9957

5. Conclusions

The results of iterative quantum phase estimation based on the Kitaev algorithm and using an IBM processor ibmqx2 are presented. It is shown that, applying the classical error correction, one can obtain a correct sequence of 25 significant bits, despite the limited accuracy of two-qubit gates. The numerical estimation of the probability of finding the correct result showed that a correct sequence of bits can also be obtained at a number of measurements much smaller than the number of measurements performed on the IBM processor.

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