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How behavior of systems with sparse spectrum can be predicted on a quantum computer

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Call a spectrum of Hamiltonian H sparse if each eigenvalue can be quickly restored within ε from its rough approximation within ε_1 by means of some classical algorithm. It is shown how a behavior of system with sparse spectrum up to time $T = (1-\rho)/14\varepsilon$ can be predicted on a quantum computer with the time complexity $t = 4/(1-\rho)\varepsilon_1$ plus the time of classical algorithm, where ρ is the fidelity. The quantum knowledge of Hamiltonian eigenvalues is considered as the new Hamiltonian W_H whose action on each eigenvector of H gives the corresponding eigenvalue. Speedup of an evolution for systems with the sparse spectrum is possible because for such systems the Hamiltonian W_H can be quickly simulated on the quantum computer. For an arbitrary system (even in the classical case) its behavior cannot be predicted on a quantum computer even for one step ahead. By this method we can also restore the history with the same efficiency.

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1. Introduction and background. A typical quantum system cannot be analyzed at hand or by a classical computer because the dimension of its Hamiltonian is huge. Nevertheless one can expect that this analysis would be easier in the framework of quantum computing. The idea of this approach is to force one quantum system to simulate the behavior of the other more simple primary system with some time saving. In the particular case where the primary system is the classical computer with oracle this is the problem of quantum speedup for classical computations: given a classical algorithm with oracle, is there a quantum algorithm computing the same function faster using the same oracle quantumly? Examples: Shor factoring algorithm (look at [1]), Grover search algorithm (look at [2]).

The general form of the problem of prediction is as follows. Given a law of evolution for some system (classical or quantum) is there a device (wizard) of the polynomial size which can predict the behavior of this system? To predict the behavior means that the wizard returns states of initial system earlier than these states appear in the natural evolution. We note that in the general case of quantum evolution the wizard can use quantumly not only the Hamiltonian (like in the case of quantum computations with oracle) but some hidden information about the primary system. What kind of such information may be useful for the prediction? This is the information about the eigenvalues of the primary Hamiltonian. We analyse the possibility of quantum predictions in terms of the spectrum of the primary system.

The first general quantum method of finding eigenvalues was presented by Abrams and Lloyd in the work [3]. Their method uses Quantum Fourier transform (QFT) and requires of the order N implementations of the initial Hamiltonian where N is the dimension of the main space. That method generalizes the Shor factoring algorithm. Thus, their algorithm requires the exponential time and it cannot be used for the quantum speedup. However, for the systems whose spectrum is sparse the idea of this approach with QFT can be used for predictions. We proceed with the exact definitions.

2. Definitions. Let H be a Hamiltonian which induces the unitary transformations U in the N dimensional space Y of states of n qubits by the usual quantum rule, $U(\tau) = \exp(-iH\tau/h)$, $N = 2^n$. In order to apply notions from the algorithm theory, such as complexity, etc., we assume that the time of Hamiltonian action is always $\tau = 1$. We can choose another value for τ but this choice would only involve the change in time scale without any subsequences for the algorithm complexity. The system which evolution is determined by the unitary transformation U is called the primary system.

We assume that the complexity of computation is the number of U applications. The time of all other transformations we use here is assumed to be negligible comparatively with the time of computation. Quantum Fourier transform requires the time of the order n^2 (look at [1]).

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Here we shall use this transform for $\log_2(M)$ gubits in the following form:

$$\mathrm{QFT}_M: \quad |s\rangle \longrightarrow \frac{1}{\sqrt{M}} \sum_{l=0}^{M-1} \exp(-2\pi i s l/M)|l\rangle.$$

Let eigenvalues of H have the form $-2\pi\omega_k h$, $k = 0, 1, \ldots, N-1$, where the frequencies ω_k are the real numbers from the segment $[0, 1)$. Then the eigenvalues of U will be $\exp(2\pi i \omega_k)$. This is not loss in generality because we always can choose another unit τ for the Hamiltonian action time. Let us give the precise definitions of the "knowledge of eigenvalues" of H. It means that there exists another Hamiltonian W_H called a wizard for H which acts in N^2 dimensional Hilbert space and returns an approximation of frequencies ω_k within $1/N$ given the eigenvector Φ_k of H. How frequencies can be represented in a quantum memory? Every frequency ω_k has the binary notation $0.\epsilon_1\epsilon_2\ldots$. Let $p \leq n$ be an integer, $M = 2^p$. We denote the string of ones and zeroes $\epsilon_1\epsilon_2\ldots e_p$ by $\bar{\epsilon}_k^p$. ϵ_k^p may be considered as an integer if we cancel all first zeroes. And vise versa, every integer $l < M$ can be written in the form $\bar{\epsilon}_k^p$ if we add the corresponding string of zeroes in front. Then the number $\tilde{\omega}_k^M = 0.\bar{\epsilon}_k^p$ approximates w_k within $1/M$. We define this number $0.\bar{\epsilon}_k^p \in [0, 1)$ by $(0.l)_p$. The simulation in these notations has the form

$$W_U|\Phi_k, b\rangle \longrightarrow |\Phi_k, b \bigoplus \bar{\epsilon}_k^p\rangle$$

where $\bigoplus$ is the biwise addition modulo 2.

At last we introduce auxiliary transformations Walsh–Hadamard (WH) and U_{seq}^p. Let the memory be divided into the main part x of n qubits and the ancilla a of $p \leq n$ qubits: $|x, a\rangle$, $M = 2^p$. We set

1). $\mathrm{WH}|x, a\rangle = \frac{1}{\sqrt{M}} \sum\limits_{s=0}^{M-1} (-1)^{a\cdot s}|x, s\rangle$. It is the WH transformation applied to the ancilla where $\cdot$ denotes the dot product modulo 2.

2). $U_{\mathrm{seq}}^p|x, a\rangle = |U^a x, a\rangle$. This is the result of a sequential applications of U to the main register.

The WH transform can be fulfilled in a standard model of quantum computer. To fulfill U_{seq}^p it would suffice to use the following oracle U_{cond} (the conditional application of U) depending on U: $U_{\mathrm{cond}}|x, \alpha\rangle \longrightarrow |x', \alpha\rangle$, where $x' = x$ if $\alpha = 0$ and $x' = Ux$ if $\alpha = 1$, α is one qubit register. The application of U_{cond} cannot be reduced to the simple application of U as an oracle because a conditional application of U is quantumly controlled by the second register. One proposal about its practical implementation can be found in the section 4.1.

3. Simulating transformation. *3.1. How to predict evolution.* Given a simulating (wizard) transformation how can we predict the evolution of primary system? Assume temporarily that the binary notations can represent our frequencies exactly. Let $|\xi\rangle$ denote the initial state of the main register. Let

$$\xi = \sum_{k=0}^{N-1} x_k|\Phi_k \tag{1}$$

be an expansion of our state in basis of eigenvectors of U. Add n qubits ancillary register initialized by zeroes and obtain the state $|\xi, 0^n\rangle$.

We then apply the transformation W_U to the main register ($p = n$). It gives the state

$$\xi' = \sum_{k=0}^{N-1} x_k|\Phi_k, \bar{\epsilon}_k^p\rangle.$$

Given a number t we can turn each state in the first register by the angle determined by the second register and the value t, $2\pi\omega_k t$. This gives the state

$$\xi'' = \sum_{k=0}^{N-1} x_k \exp(2\pi i\omega_k t)|\Phi_k, \bar{\epsilon}_k^p\rangle.$$

We then apply the transformation W_U again and obtain

$$\xi''' = \sum_{k=0}^{N-1} x_k \exp(2\pi i\omega_k t)|\Phi_k, 0^n\rangle.$$

Now the cancellation of ancilla gives exactly the state $U^t|\xi\rangle$ which is the state in time instant t of the initial system. Therefore given the transformation W_U we can predict the behavior of initial system provided the action of this transformation takes the time smaller than $t/2$.

3.2. Approximate simulation. In this subsection we describe the procedure of simulation the predicting operator on zero ancilla. The particular case $p = n$ of this procedure was proposed in the other purpose in the paper [3].

We start from the state of the form (1) with the ancilla initialized by zeroes. The action of the operator W_H on the initial state with zero ancilla is defined as follows

$$\mathrm{QFT}_M\ U_{seq}^p\ \mathrm{WH}\ |\xi, 0^p\rangle. \tag{2}$$

Why this procedure must work? Let us assume temporarily that the frequencies have an exact representation by their binary notation. Then an application of the first operator in the definition (2) gives

$$\chi_0 = \frac{1}{\sqrt{M}} \sum_{k=0}^{N-1} \sum_{s=0}^{M-1} x_k|\Phi_k, s\rangle.$$

The second operator gives:

$$\chi_1 = U^p_{\sec}\chi_0 = \frac{1}{\sqrt{M}}\sum_{k=0}^{N-1}\sum_{s=0}^{M-1} x_k \exp(2\pi i\omega_k s)|\Phi_k, s\rangle.$$

The third operator results in the target state

$$\sum_{k=0}^{N-1} x_k|\Phi_k, \bar{\epsilon}^p_k\rangle.$$

In the general case the same idea works but with the slight corrections resulting from an inaccuracy of frequencies. We shall see below how to manage with this error.

3.3. Accuracy of finding the frequencies. The feasibility of the simulation procedure results from the precise estimation of the inaccuracy in determining frequencies. The proof of this fact can replace Shor's substantiation of the factoring algorithm. The idea is similar to uncertainty principle. Let ε and δ be the respectival errors in a frequency binary approximation and in a probability of finding the right frequency by the observation of the corresponding ancilla. Then their product $\varepsilon\delta$ cannot be smaller than $1/M$. Slightly thinking we agree that this formulation would be very natural. To formulate it carefully we need a definition of the wide class of transformations with this property. Let $\{\tilde{\omega}_{k,i}\}$ be some set of integers. We denote $L_\varepsilon(\tilde{\omega}_{k,i}) = \{i : |(0.\tilde{\omega}_{k,i})_p - \omega_k| \leq \varepsilon$ or $|(0.\tilde{\omega}_{k,i})_p - \omega_k - 1| \leq \varepsilon\}$. Let ξ be a state of the form (1).

Definition. *A transformation W of the form*

$$W: |\xi, 0^p\rangle \longrightarrow \sum_{k=0}^{N-1}\sum_{i=0}^{M-1}\lambda_{i,k}|\Phi_k, \tilde{\omega}_{k,i}\rangle$$

is called a transformation of $W_{\delta,\varepsilon}$ type if $\sum\limits_{k=0}^{N-1}\sum\limits_{i\in L_\varepsilon(\tilde{\omega}_{k,i})}|\lambda_{i,k}|^2 \geq 1-\delta$ *for any ξ.*

Lemma 1. *The operator W_H belongs to the set $W_{1/K,K/M}$ for any $K \in \{1, 2, \ldots, M\}$.*

Consider a result of action of the operator W_H:

$$\chi_{p,2} = \frac{1}{M}\sum_{k=0}^{N-1}\sum_{l=0}^{M-1} x_k H_{l,k}|\Phi_k, l\rangle,$$

$$H_{l,k} = \sum_{s=0}^{M-1}\exp(2\pi i s(\omega_k - (0.l)_p)).$$

Put $\Delta = \omega_k - (0.l)_p$. By the summing of this progression we then obtain

$$H_{l,k} = \frac{1-\exp(2\pi i M\Delta)}{1-\exp(2\pi i\Delta)}. \tag{3}$$

Let $\Delta = K/M + \delta$, $K = K(l)$, where $0 \leq \delta < 1/M$, K is integer. Then each $H_{l,k}$ depends on K : $H_{l,k} = H_{l,k}(K)$. We fix some value for K: K_0. It means that the accuracy of eigenvalues approximations will be K_0/M. We estimate the sum of squared amplitudes for the states $|\Phi_k, l\rangle$ for which $K : K_0 \leq K \leq M - K_0$. The module of denominator in (4) is separated from zero by $\min\{\pi K/M, \pi(M-K)/M\}$. We then have

$$\sum_{k=0}^{N-1}\sum_{K=K_0}^{M-K_0}|x_k|^2\frac{1}{M^2}|H_{l,k}(K)|^2 \leq$$

$$\leq 4\sum_{k=0}^{N-1}\sum_{K=K_0}^{M-K_0}|x_k|^2/\pi^2K^2 \leq \frac{4}{\pi^2}\sum_{K=K_0}^{M-K_0}\frac{1}{K^2} \leq \frac{1}{K_0}.$$

Lemma 1 is proved.

What would happen if we apply another operator $\mathrm{QFT}^{-1}_M\ (U^p_{seq})^{-1}$ WH instead of (2) for revealing frequencies? Then the difference will be only in the simple factors of the basic states. This method is useful for a cleaning ancilla.

Lemma 2. *Let χ be a state and the application of (2) give $\chi_2 = \sum\limits_k\sum\limits_{l=0}^{M-1} y_{k,l}|\Phi_k, l\rangle$ and $\chi'_2 = \mathrm{QFT}^{-1}_M\ (U^p_{\mathrm{seq}})^{-1}$ $\mathrm{WH}|\chi, 0^p\rangle = \sum\limits_k\sum\limits_{l=0}^{M-1} y'_{k,l}|\Phi_k, l\rangle$. Put $\delta_{k,l} = \tilde{\omega}^N_k - (0.l)_p$, $\Delta = \omega_k - (0.l)_p$, $\chi''_2 = \sum\limits_k\sum\limits_{l=0}^{M-1} y'_{k,l}\exp(2\pi i(M-1)\delta_{k,l})|\Phi_k, l\rangle$. Let $M/N < \epsilon$. Then $\|\chi''_2 - \chi_2\| < 7\epsilon$.*

We have $y_{k,l} = x_k H_{k,l}$ (look at (3)), where $H_{k,l} = H_{k,l}(\Delta)$. Then $y'_{k,l} = x_k H_{k,l}(-\Delta)$. Now $H_{k,l}(\Delta) = H_{k,l}(-\Delta)\exp(2\pi i(M-1)\Delta)$, $|\delta_{k,l} - \Delta| \leq 1/N$, $2\pi(M-1)|\delta_{k,l} - \Delta| \leq 7M/N$ and Lemma 2 follows.

3.4. Complexity of the method for finding frequencies. It is readily seen that the above procedure for $p = n$ requires N applications of the initial transformation U, hence it cannot be used on purpose to predict its evolution. It turns that in the general case it is impossible to simulate an action of the operator W_H with a precision up to $O(1/N)$ using less than $\Omega(N)$ conditional application of the initial transformation U_{cond}. It follows from the lower bounds for quantum complexity of parity function as $N/2$ (look at [4, 5]). We assume that an action of the operator W_H can be simulated using less than $\Omega(N)$ applications of U_{cond}. Then in view of the previous subsection we would be able to compute the function parity on a quantum computer in time less than $N/2$ (adding appropriate constant to the number n in order to enhance an accuracy) that leads to the contradiction.

We note that the behavior of the bulk of classical systems in general case in a short time frame is impredictable on quantum computer even on one step ahead (look at [6]), where a short time means approximately $O(N^{1/7})$, where N is the number of all states.

But for one class of systems the quantum prediction is possible. This is the class of systems with a sparse spectrum.

4. Prediction of the evolution of the systems with a sparse spectrum. What would happen if we use less number of qubits $p < n$ instead of n in the ancilla? Simulation of the operator W_H wizard will be shorter, but it will be simulated with the corresponding loss in the precision and we obtain no prediction.

Nevertheless, if the spectrum is sparse then the prediction is possible. Indeed, suppose that we are given a classical algorithm h enhancing the accuracy of the eigenvalues approximation. Let $p < n$, $M = 2^p$ and let $h: \{0,1\}^p \longrightarrow \{0,1\}^n$ be an integer function mapping a rough frequency approximation up to $1/M$ to the more precise approximation up to $1/N$. The idea of the prediction is as follows. We repeat the procedure from above with p ancillary qubits only instead of n, and then enhance accuracy by application of the function h.

We assume for the simplicity that the frequencies binary representation is exact. Our algorithm then has the following form.

First we apply the WH transform to the ancilla and obtain the state

$$\chi_0 = \frac{1}{\sqrt{M}} \sum_{k=0}^{N-1} \sum_{s=0}^{M-1} x_k |\Phi_k, s\rangle.$$

Then we apply the operator U^p_{seq}. This operation requires p conditional applications of U and results in the state

$$\chi_1 = \frac{1}{\sqrt{M}} \sum_{k=0}^{N-1} \sum_{s=0}^{M-1} \exp(2\pi i \omega_k s) x_k |\Phi_k, s\rangle.$$

Now application of Fourier transform to the second register gives the state

$$\chi_2 = \sum_{k=0}^{N-1} x_k |\phi_k, \tilde{\omega}_k\rangle.$$

This is the point when we use the sparse spectrum. We add an ancillary register with n qubits initialized by zeroes: $\sum\limits_{k=0}^{N-1} x_k |\Phi_k, \tilde{\omega}_k, 0^n\rangle$. We apply the unitary version of the algorithm h enhancing accuracy to two ancillary registers: $|a, b\rangle \longrightarrow |a, b \bigoplus h(a)\rangle$. It gives the state $\sum\limits_{k=0}^{N-1} x_k |\Phi_k, \tilde{\omega}_k, h(\tilde{\omega}_k)\rangle$. We then turn every state of the form $|\Phi_k, \tilde{\omega}_k, l\rangle$ to the angle $2\pi \cdot 0.l \cdot t$ and obtain the state

$$\sum_{k=0}^{N-1} x_k \exp(2\pi i \cdot 0.l \cdot t) |\Phi_k, \tilde{\omega}_k, l\rangle.$$

Here t is a given time instant. We apply the unitary version of h which cleans up n last ancillary qubits and then discard them:

$$\sum_{k=0}^{N-1} x_k \exp(2\pi \omega_k t) |\Phi_k, \tilde{\omega}_k\rangle,$$

and again QFT_M to the p ancillary qubits:

$$\frac{1}{\sqrt{M}} \sum_{k=0}^{N-1} \sum_{s=0}^{M-1} x_k \exp(2\pi i \omega_k t) \exp(-2\pi i \tilde{\omega}_k s) |\Phi_k, s\rangle,$$

then again U^p_{seq} and the WH transform to the ancilla. The result has the following form

$$\sum_{k=0}^{N-1} x_k \exp(2\pi i \omega_k t) |\Phi_k, 0^p\rangle.$$

The target state is in the main register now.

Why this scheme does not work for the case when the binary notations from ancilla are the approximations of the true eigenvalues ω_k? The reason is the same as above. To make a necessary corrections we need only to apply multipliers arose in Lemma 2. The resulting algorithm looks more complicated but factually differs only in the point 4 where we correct undesirable phase shifts. Its scheme is as follows.

We are given the numbers n and p. We choose some $q: \ p \le q < n$ and put $L = 2^q$. Our initial state has the form $\xi = \sum\limits_{k=0}^{N-1} x_k |\Phi_k, 0^q\rangle$:

1. We apply the operator (2) to the initial state.
2. We add one more register with n qubits initialized by zeroes: $\sum\limits_k \sum\limits_{l=0}^{L-1} y_{k,l} |\Phi_k, l, 0^p\rangle$ and apply the unitary version of the algorithm h enhancing accuracy to two ancillary registers:

$$\chi_3 = \sum_k \sum_{l=0}^{L-1} y_{k,l} |\Phi_k, l, h(l)\rangle.$$

3. We turn every state of the form $|\Phi_k, l, h(l)\rangle$ to the angle $2\pi \cdot 0.h(l) \cdot t$ and obtain the state

$$\chi_4 = \sum_k \sum_{l=0}^{L-1} y_{k,l} \exp(2\pi i \cdot 0.h(l) \cdot t) |\Phi_k, l, h(l)\rangle.$$

Here t is the given time instant.

4. We put $\delta^*_{k,l} = (0.h(l))_n - (0.l)_q$. We turn every state of the form $|\Phi_k, l, h(l)\rangle$ to the angle $-2\pi(L-1)\delta^*_{k,l}$. The result is denoted by χ_5.

5. We apply the unitary version of h which cleans up n last ancillary qubits and then discard them:

$$\chi_6 = \sum_k \sum_{l=0}^{L-1} y_{k,l} \exp(2\pi i \cdot 0.h(l) \cdot t) \times \\ \times \exp(-2\pi i (L-1)\delta^*_{k,l}) |\Phi_k, l\rangle.$$

6. We apply to χ_6 the transformation WH U^q_{sec} QFT_L, then observe and discard the ancilla.

The time of this algorithm is $2L + 2t_{\text{QFT}_L} + 2t_h + w$ where t_{QFT_L} is the time of the Fourier transform, t_h is the time of enhancing accuracy and w is the time of rotations.

Let $\delta > 0$ be some number, $q = p + c, L = 2^q$, $t:\ 0 < t \le CN$, where $c = \log_2(4/\delta)$, $p \ge c$, $C = \delta/14$. Then a straightforward calculation based on Lemmas 1 and 2 gives the estimation of difference between the result of this algorithm and the ideal state as δ.

This result can be formulated in the following convenient form:

Given a Hamiltonian of system with the sparse spectrum and an algorithm enhancing the accuracy of eigenvalues from ε_1 to ε and a fidelity ρ, a state of the system in the time instant $(1-\rho)/14\varepsilon$ can be obtained in the time $4/(1-\rho)\varepsilon_1$ with this fidelity.

4.1. Generalizations, examples and practical implementation. We note that the spectrums of real systems like moleculae typically contain strips where the spectrum is continuos separated by gaps where the energy levels are absent at all. Let w be the maximal width of strips and g be the minimal width of gapes.

Considering the evolution in the time frame less than $1/w$ (here we assume the system of units where the Plank constant is the unit) we obtain the following generalization of the result from the previous section.

If $t = o(1/w)$ we can compute the state $U(t)$ of primary system in the time $t_{pre} = O(tw/g)$.

The more general result can be obtained if we consider the spectrum which is not sparse but has sparse areas.

The operator H_W can be used not only for the predictions of a future but for the restoration of a history as well. *The states of primary system in the time instant $T = (1-\rho)/14\varepsilon$ in future and in the time instant $-T$ in the past can be obtained in the time $4/(1-\rho)\varepsilon_1$ with the fidelity ρ provided each eigenvalue can be quickly calculated with the precision up to ε given its approximation with the accuracy ε_1.*

Formula (2) can be considered as a natural generalization for the quantum part of the Shor factoring algorithm [1]. Our approach is applicable for the factoring problem if U has the form $U|x\rangle \longrightarrow |ax \pmod q\rangle$, where ax is a multiplication of integers, $(a,q) = 1$ with the eigenvectors of U of the form

$$\frac{1}{\sqrt{r}} \sum_{j=0}^{r-1} \exp(-2\pi i k j/r) |a^j \pmod q\rangle$$

with the eigenvalues $\exp(2\pi i j/r)$ where r is the period of a (the minimal integer such that $a^r \equiv 1 \pmod q$).

The main difficulty for the practical implementation of this method is contained in the conditional iterations of U. This scheme can be reformulated by means of analogous quantum computing if we consider QFT on an ancillary register as a passage to the canonically conjugate magnitude. Say, if we use a value of coordinates in operations with a register then canonically conjugate will be the corresponding impulse. The passage from the coordinate representation of a wave function to the impulse representation in one-dimensional case can be defined as

$$\phi(p) = \int_{-\infty}^{+\infty} \exp(-ipx/h)\psi(x)dx$$

where a probability to obtain the impulse in a segment $(p, p+dp)$ is $|\phi(p)|^2 dp/2\pi h$. Assume that we have one particle which can be located in M points of the form $x = 0, 1/M, 2/M, \dots, (M-1)/M$. Then the coordinate quantum space for one particle will be M dimensional. Consider the corresponding integral sum for $\phi(p)$ in the system of units where the Plank constant h is equals one. This integral sum will be just the sum in the definition of QFT where x plays the role of s/M and $p/2\pi$ plays the role of l.

Then the main algorithm acquires the following general form:

a) the primary evolution quantumly controlled by a magnitude containing in the properly prepared ancillary register;

b) the simple actions depending on the canonically conjugate magnitude;

c) the repetition of a).

Such a procedure can predict the behavior of primary system with sparse spectrum and restore the state of arbitrary system in the past.

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