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

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Abstract

Call a spectrum of Hamiltonian sparse if each eigenvalue can be quickly restored with accuracy ε from its rough approximation in within ε_1 by means of some classical algorithm. It is shown how a behavior of system with sparse spectrum up to time $T = \frac{1-\rho}{14\varepsilon}$ can be predicted with fidelity ρ on quantum computer in time $t = \frac{4}{(1-\rho)\varepsilon_1}$ plus the time of classical algorithm. The quantum knowledge of Hamiltonian H eigenvalues is considered as a wizard Hamiltonian W_H which action on any eigenvector of H gives the corresponding eigenvalue. Speedup of evolution for systems with sparse spectrum is possible because for such systems wizard Hamiltonians can be quickly simulated on a quantum computer. This simulation, generalizing Shor trick, is a part of presented algorithm. In general case the action of wizard Hamiltonian cannot be simulated in time smaller than the dimension of main space which is exponential of the size of quantum system. For an arbitrary system (even for classical) its behavior cannot be predicted on quantum computer even for one step ahead. This method can be used also for restoration of a state of an arbitrary primary system in time instant -T in the past with the same fidelity which requires the same time.

1 Introduction and background

A behavior of typical quantum system cannot be analyzed at hand or by classical computer because huge dimension of its Hamiltonian makes it impossible to solve Shröedinger equation even numerically. 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 a behavior of other more simple primary system with some profit in time. In the particular case where the primary system is a classical computer with oracle this is a 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 [Sh]), Grover search algorithm (look at [Gr]).

In general case the problem of prediction has the following form: given a low of evolution for some system (classical or quantum) is there a device (wizard) of not exponential size which

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can predict the behavior of this system? To predict the behavior means that given a time instant, wizard returns a state of initial system in this instant earlier than this state appears in its natural evolution. Note that in general case of quantum evolution a wizard may use quantumly not only Hamiltonian (like in case of quantum computations with oracle) but some hidden information about primary system. What kind of such information may be useful for prediction? This is the information about eigenvalues of primary Hamiltonian. This article analyses the possibility of quantum predictions in terms of spectrum of primary system.

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

2 Definitions

Let H be some Hamiltonian which induces unitary transformations U in some N dimensional space Y of states of n qubits by the usual rule in quantum mechanics: $U(\tau) = \exp(-iH\tau/h)$, $N = 2^n$. 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 may of course choose another value for τ but this would only involve the change in time scale without any subsequences for the algorithm complexity. Call a system primary if its evolution is determined by unitary transformation U.

We assume that the complexity of computation is the number of U applications. Time of all other transformations we use here is assumed to be negligible comparatively with the time of computation. Quantum Fourier transform (QFT) requires the time of order n^2 (look at [Sh]). Here we shall use this transform for $\log_2(M)$ gubits in the following form:

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

Let eigenvalues of H have the form $-2\pi\omega_k h$, $k = 0, 1, \ldots, N-1$, when frequencies ω_k are 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 other unit τ for 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 in within 1/N given eigenvector Φ_k of H. Introduce the following notations. Every frequency ω_k has binary notation $0.\epsilon_1\epsilon_2...$ Let $p \leq n$ be some integer, $M = 2^p$. Denote the string of ones and zeroes $\epsilon_1\epsilon_2...\epsilon_p$ by $\vec{\epsilon}_k^p$. ϵ_k^p may be considered as integer if we cancel all first zeroes. And vise versa, every integer l less than M can be written in form $\vec{\epsilon}_k^p$ if we add suitable number of zeroes in front. Then the number $\tilde{\omega}_k^M = 0.\bar{\epsilon}_k^p$ will be approximation of w_k in within 1/M. We shall define this number $0.\bar{\epsilon}_k^p$ from [0,1) by $(0.l)_p$. Wizard action in these notations will be

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

where \oplus is the biwise addition modulo 2.

At last introduce auxiliary transformations WH and U_{seq}^p . Let the memory is divided into the main part x of n qubits and ancilla a of $p \leq n$ qubits: $|x, a\rangle$, $M = 2^p$. Put:

1). WH $|x,a\rangle = \frac{1}{\sqrt{M}} \sum_{s=0}^{M-1} (-1)^{a \cdot s} |x,s\rangle$. This is Walsh - Hadamard transform applied to ancilla where \cdot denotes dot product modulo 2.

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

Walsh-Hadamard 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} (conditional application of U) depending on U: $U_{cond}|x,\alpha\rangle \longrightarrow |x',\alpha\rangle$, where x' = x if $\alpha = 0$ and x' = Ux if $\alpha = 1$, α is one qubit register. An application of U_{cond} cannot be reduced to the simple using 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 4.5.

3 Wizard transformation

3.1 How wizard predicts evolution

Assume temporarily that we have exact equations $\omega_k = \tilde{\omega}_k^N$. Given a wizard transformation W_U how can we predict evolution of initial system? Let $|\xi\rangle$ denote initial state as a contents of n qubits main register. Let

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

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

Now apply the wizard 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 the number t we can turn each state in the first register by angle determined by the second register and t: $2\pi\omega_k t$. This gives the state

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

At last apply wizard again obtaining

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

and now cancellation ancilla gives exactly the state $U^t |\xi\rangle$ which is the state in time instant t of initial system. Thus given a wizard we can predict the behavior of initial system provided the action of wizard takes smaller time than t/2.

3.2 Simulation a wizard

In this subsection I describe the procedure of simulation a wizard action on zero ancilla. The particular case p = n of this procedure was proposed in other purpose in the paper [AL].

We start from the state of the form (1) with ancilla attached initialized by zeroes. Wizard action on the initial state with zero ancilla is defined by the following:

$$QFT_M U_{seq}^p WH |\xi, 0^p\rangle.$$
⁽²⁾

Why this procedure must work? Let us again assume temporarily that $\omega_k = \tilde{\omega}_k^M$ exactly. Then we have WH $|\xi, 0^p\rangle = \chi_0 = \frac{1}{\sqrt{M}} \sum_{k=0}^{N-1} \sum_{s=0}^{M-1} x_k |\Phi_k, s\rangle$. Application of U_{sec}^p gives: $\chi_1 = U_{sec}^p \chi_0 = \frac{1}{\sqrt{M}} \sum_{k=0}^{N-1} \sum_{s=0}^{M-1} x_k \exp(2\pi i \omega_k s) |\Phi_k, s\rangle$. Now QFT $_M \chi_1 = \sum_{k=0}^{N-1} x_k |\Phi_k, \bar{\epsilon}_k^p\rangle$. This is just the wizard action. But in general case the result of QFT transform has not so simple form. It means that we cannot merely clean ancilla by repetition of wizard action in predicting algorithm even if we have a wizard action on all words. Hence the precision of a wizard simulation by (2) must be elaborated in more details.

3.3 Accuracy of a wizard simulation

Let $\{\tilde{\omega}_{k,i}\}$ be some set of integers. Denote $L_{\varepsilon}(\tilde{\omega}_{k,i}) = \{i : |(0.\tilde{\omega}_{k,i})_p - \omega_k| \le \varepsilon$ or $|(0.\tilde{\omega}_{k,i})_p - \omega_k - 1| \le \varepsilon\}$. 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 $\sum_{k=0}^{N-1} \sum_{i \in L_{\varepsilon}(\tilde{\omega}_{k,i})} |\lambda_{i,k}|^2 \ge 1 - \delta$ for any ξ . Thus, δ is an error probability from the quantum superposition, and ε is a precision of eigenvalues approximations.

Lemma 1 The transformation QFT_M U_{seq}^p WH belongs to the type $W_{\frac{1}{K},\frac{K}{M}}$ for any $K \in \{1, 2, \ldots, M\}$.

Proof Denote $\operatorname{QFT}_M \operatorname{U}_{seq}^p \operatorname{WH} |\xi, 0^p\rangle$ by $\chi_{p,2}$. Then we have

$$\chi_{p,2} = \frac{1}{M} \sum_{k=0}^{N-1} \sum_{l=0}^{M-1} x_k H_{l,k} |\Phi_k, l\rangle$$
(3)

where $H_{l,k} = \sum_{s=0}^{M-1} \exp(2\pi i s(\omega_k - (0.l)_p))$. Put $\Delta = \omega_k - (0.l)_p$. Then by summing the progression we obtain

$$H_{l,k} = \frac{1 - \exp(2\pi i M\Delta)}{1 - \exp(2\pi i \Delta)}.$$
(4)

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

$$\sum_{k=0}^{N-1} \sum_{K=K_0}^{M-K_0} |x_k|^2 \frac{1}{M^2} |H_{l,k}(K)|^2 \le 4 \sum_{k=0}^{N-1} \sum_{K=K_0}^{M-K_0} |x_k|^2 / \pi^2 K^2 \le \frac{4}{\pi^2} \sum_{K=K_0}^{M-K_0} \frac{1}{K^2} \le \frac{1}{K_0}$$

This is exactly what is needed. Lemma 1 is proved.

What would happen if we apply other sequence of transformations QFT_M^{-1} $(U_{seq}^p)^{-1}$ WH instead of $QFT_M U_{seq}^p$ WH for revealing frequencies?

Lemma 2 Let for some state χ

$$\chi_2 = \operatorname{QFT}_M \operatorname{U}_{seq}^p \operatorname{WH} |\chi, 0^p\rangle = \sum_k \sum_{l=0}^{M-1} y_{k,l} |\Phi_k, l\rangle$$

$$\chi'_2 = \operatorname{QFT}_M^{-1} (\operatorname{U}_{seq}^p)^{-1} \operatorname{WH} |\chi, 0^p\rangle = \sum_k \sum_{l=0}^{M-1} y'_{k,l} |\Phi_k, l\rangle$$

Put $\delta_{k,l} = \tilde{\omega}_k^N - (0.l)_p, \ \Delta = \omega_k - (0.l)_p, \ \chi_2'' = \sum_k \sum_{l=0}^{M-1} y'_{k,l} \exp(2\pi i (M-1)\delta_{k,l}) |\Phi_k, l\rangle.$ Let $M/N < \epsilon$. Then $\|\chi_2'' - \chi_2\| < 7\epsilon$

Proof

We have $y_{k,l} = x_k H_{k,l}$ (look at (3),(4)), where $H_{k,l} = H_{k,l}(\Delta)$. Then $y'_{k,l} = x_k H_{k,l}(-\Delta)$. Now $H_{k,l}(\Delta) = H_{k,l}(-\Delta) \exp(2\pi i (M-1)\Delta)$, $|\delta_{k,l} - \Delta| \le 1/N$, $2\pi (M-1) |\delta_{k,l} - \Delta| \le 7M/N$ and Lemma 2 follows.

3.4 Complexity of a wizard

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 general case the following theorem takes place.

Theorem 1 It is impossible to simulate a wizard action with precision up to O(1/N) using less than $\Omega(N)$ conditional application of initial transformation U_{cond} .

Proof

A lower bound for the time of quantum computation of the PARITY function is N/2 by the results [FGGS] and [BBCMW]. These constructions can be extended to the case when we can use more general oracle U_{cond} instead of U when evaluating PARITY. Assuming that a wizard action can be simulated using less than $\Omega(N)$ application of U_{cond} , 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 accuracy) which leads to the contradiction. Theorem 1 is proved.

Call a unitary transformation U classical if it maps basic states to basic states. One can ask is there any way to predict a behavior of classical system on a quantum computer? This statement is independent of a form of spectrum. It turns that in general case a behavior of the bulk of classical systems in a short time frame is impossible on quantum computer even on one step ahead (look at [Oz]). Here short time means approximately $O(N^{1/7})$, where N - the number of all states.

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

4 Prediction of the evolution of the systems with sparse spectrum

4.1 Case of precise eigenvalues

What would happen if we use less number of qubits p < n instead of n in the ancilla? Simulation of the wizard will be shorter, but it will be simulated with the corresponding loss in precision and we obtain no prediction.

Nevertheless, if the spectrum is sparse then prediction is possible. Indeed, suppose that we have classical algorithm h enhancing the accuracy of eigenvalues approximation.

Namely, let p < n, $M = 2^p$ and let $h : \{0, 1\}^p \longrightarrow \{0, 1\}^n$ be integer function mapping rough frequency approximation up to 1/M to the more precise approximation up to 1/N.

Given the initial state ξ and time instant t we shall now describe the procedure of quick finding $U^t\xi$. The idea is simple: Repeat the procedure from above with only p ancillary qubits instead of n, and enhance accuracy by h.

At first we assume for the simplicity that we have exact equalities $\omega_k = \tilde{\omega}_k^M$. Here is the detailed description of the algorithm.

First we apply Walsh-Hadamard transform to the ancilla and obtain

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

Then we apply U_{seq}^p . Since $s \leq p$ this operation requires p conditional applications of U. This gives the state

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

Now application of QFT_M to the second register yields:

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

where $0.\tilde{w}_k$ is approximation of eigenvalue ω_k in within 1/M.

This is the point when we will use that the spectrum is sparse. Add one more register with n qubits initialized by zeroes: $\sum_{k=0}^{N-1} x_k |\Phi_k, \tilde{\omega}_k, 0^n\rangle$. Apply the unitary version of the algorithm h enhancing accuracy to two ancillary registers: $|a,b\rangle \longrightarrow |a,b \oplus h(a)\rangle$. This gives the state $\sum_{k=0}^{N-1} x_k |\Phi_k, \tilde{\omega}_k, h(\tilde{\omega}_k)\rangle$. Now we 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. Now apply 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_{seq}^{p} and Walsh-Hadamard transform to the ancilla. The result will be:

 $\sum_{k=0}^{N-1} x_k \exp(2\pi i \omega_k t) |\Phi_k, 0^p\rangle.$ The wanted state is in the main register now.

Note that all the work with enhancing an accuracy here is not mandatory because $\omega_k = \tilde{\omega}_k^M$ exactly. Why this scheme doesn't work for the case when $\tilde{\omega}_k^M$ are only approximations of the true eigenvalues ω_k ? The point is that χ_2 will not have so simple form and in addition multiplication frequencies by t will cause big error for t = O(N). Thus for the general case more refined algorithm is needed.

4.2 General case

We have numbers n and p. Choose some $q: p \leq q < n$ and put $L = 2^q$. Without loss in generality we can extend h to the mapping $h: \{0,1\}^q \longrightarrow \{0,1\}^n$ so that if $\tilde{\omega}_k^L = (0.x)_q$ then $\tilde{\omega}_k^N = (0.h(x))_n$.

Our initial state has the form

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

1. Apply $QFT_L U_{seq}^q WH$ to the initial state to get $\chi_{q,2}$.

2. Add one more register with n qubits initialized by zeroes:

 $\sum_{k} \sum_{l=0}^{L-1} y_{k,l} |\Phi_k, l, 0^p\rangle$ 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. 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 given time instant. 4. Put $\delta_{k,l}^* = (0.h(l))_n - (0.l)_q.$ Turn every state of the form $|\Phi_k, l, h(l)\rangle$ to the angle

 $-2\pi(L-1)\delta_{k,l}^*$. Denote the result by χ_5 .

5. Now apply unitary version of h which cleans up n last ancillary qubits and then discard them: T 1

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

6. Apply to χ_6 the transformation WH U_{sec}^q QFT_L, then observe and discard ancilla.

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

Lemma 3 Denote the result of algorithm 1-6 by $U_{q,t}$. For any $\delta > 0$ for any p, q, n, t altering so that $q = p + c, L = 2^q, t: 0 < t \le CN$, where $c = \log_2(\frac{4}{\delta}), p \ge c, C = \frac{\delta}{14}$ we shall have

$$\left\| \mathbf{U}_{q,t} - \mathbf{U}^t \right\| < \delta$$

Proof

Introduce the simplifying notations:

$$\chi = \sum_{k} \sum_{l=0}^{L-1} y_{k,l} \exp(2\pi i \omega_k t) |\Phi_k, l, h(l)\rangle, \quad \tilde{\chi} = \text{QFT}_L^{-1} (\mathbf{U}_{seq}^q)^{-1} \text{ WH} \exp(2\pi i \omega_k t) \sum_{k} x_k |\Phi_k, 0^q\rangle,$$
$$\chi' = \sum_{k} \sum_{l=0}^{L-1} y_{k,l} \exp(2\pi i \omega_k t) \exp(-2\pi i (L-1) \delta_{k,l}^*) |\Phi_k, l\rangle.$$

By Lemma 1 $\|\chi_4 - \chi\| < \frac{\delta}{2}$. The passages $\chi_4 \longrightarrow \chi_6$ and $\chi \longrightarrow \chi'$ are fulfilled by the same unitary transformation, which preserves lengths. Consequently, $\|\chi_6 - \chi'\| < \frac{\delta}{2}$. By Lemma 2 $\|\tilde{\chi} - \chi'\| < \frac{\delta}{2}$. Then triangle inequality gives $\|\chi_6 - \tilde{\chi}\| < \delta$. The passages $\chi_6 \longrightarrow U_{q,t}$ and $\tilde{\chi} \longrightarrow U_{q,t}$ U^t are fulfilled by the same unitary transformation WH U_{sec}^q QFT_L. Hence $||U^t - U_{q,t}|| < \delta$. Lemma 3 is proved.

By Lemma 3 this algorithm gives the prediction of state in time instant O(N) in time O(M) if classical algorithm enhancing accuracy obtain eigenvalues in negligible time. Thus if it is possible to enhance accuracy of eigenvalues from ϵ_1 to ϵ the speedup will be $\frac{\epsilon_1(1-\rho)}{56\epsilon}$, where ρ is a fidelity, $0 < \rho < 1$. The result can be formulated as

Theorem 2 Given a Hamiltonian of system with sparse spectrum and algorithm enhancing the accuracy of eigenvalues from ε_1 to ε and a fidelity ρ , a state of the system in the time instant $\frac{1-\rho}{14\varepsilon}$ can be obtained in time $\frac{4}{(1-\rho)\varepsilon_1}$ with this fidelity.

4.3 Generalizations

4.3.1 Sparse areas of spectrum

A spectrum of real system like molecule typically contains strips where spectrum is continuos separated by gaps where energy levels are absent at all. Let w be the maximal width of strips and g be the minimal width of gapes.

Regard the times of evolution less than 1/w (here we assume the system of units where Plank constant is unit). For these times the width of strips is negligible and we can assume that $\varepsilon_1 = 1/g$ in Theorem 2. So in this situation $\varepsilon = w$ and we obtain the following generalization of Theorem 2.

If t = o(1/w) we can predict the state U(t) of primary system in time $t_{pre} = O(t\frac{w}{q})$.

Yet more generalization can be obtained if we consider the spectrum which is not sparse at all but has sparse areas. Here if the initial state of primary system is concentrated in sparse area, the prediction is possible with such probability which is equal to the degree of concentration.

4.3.2 Travelling in a time: predictions and restoration of a history

A wizard transformation may be used not only for predictions a future but for restoration of a history as well. If we replace the time t by -t in predicting procedure then we obtain the state of primary system in time instant -t which means the restoration of a history. Perform procedure from the section 4.2 with -t instead of t, where 0 < t < CN. This makes possible to obtain the state of primary system in time of order -N in the past. Thus we conclude the following generalization of Theorem 2.

Theorem 3 Given a Hamiltonian of some system, its states in time instant $T = \frac{1-\rho}{14\varepsilon}$ in future as well as in time instant -T in the past can be obtained in time $\frac{4}{(1-\rho)\varepsilon_1}$ with fidelity ρ provided each eigenvalue can be quickly calculated with precision up to ε given its approximation with accuracy ε_1 .

Note that for restoration of a history we don't need a sparse spectrum, may be $\varepsilon_1 = \varepsilon$. This is surprising because the algorithm uses only operator U when the natural way to obtain a state from the past is to use an inverse transformation U⁻¹ and there is no evident way to simulate the action of the inverse transformation by means of U.

4.4 Examples

4.4.1 Shor factoring algorithm

Formula (2) for a wizard simulation can be considered as a natural generalization for the quantum part of Shor factoring algorithm ([Sh]). Let a unitary operator U in (2) has the form $U|x\rangle \longrightarrow |ax \pmod{q}\rangle$, where ax is a multiplication of integers, (a,q) = 1. Then eigenvectors of U have the form $\frac{1}{\sqrt{r}} \sum_{j=0}^{r-1} \exp(-2\pi i k j/r) |a^j \pmod{q}\rangle$ and its eigenvalues are $\exp(2\pi i j/r)$ where r is a period of a (minimal integer such that $a^r \equiv 1 \pmod{q}$). If we apply an operator (2)

with this U to zero initial state and observe the second register then by Lemma 1 we obtain an approximation of a number j/r up to O(1/N) with high probability. Using this procedure sequentially we can restore the value r of a period. This procedure was used for factoring by Shor.

Here we use a wizard simulation (2) as a technical element of the algorithm 4.2. Alternatively, one can try to use Kitaev's method instead of QFT in (2). Namely, consider one controlling qubit and use Hadamard transform after conditional application of U and repeat this with numerous controlling qubits. Then by some auxiliary transformation it is possible to extract eigenvalues in ancillary register (look at [Ki] for details). But then we must get rid of revealed eigenvalues like in the point 6 of the algorithm and it faces a little difficulty when using Hadamard transform instead of QFT in (2), because we have not U_{cond}^{-1} and must always manage with only U_{cond} .

4.4.2 Grover search algorithm

Consider Grover algorithm for the fast quantum search: $U(t)|\tilde{0}\rangle = (I_{\tilde{0}}I_a)^t|\tilde{0}\rangle$, where I_b denotes inversion of the state b: $I_b|b\rangle = -|b\rangle$, $I_b|s\rangle = |s\rangle$ for $\langle b|s\rangle = 0$. It was shown in [Gr2] that if $|\langle \tilde{0}|a\rangle| = O(1/\sqrt{N})$ then $U(t_1) \approx |a\rangle$ for $t_1 = O(\sqrt{N})$ independently of $\tilde{0}$, where N is the dimension of main space. What will happen if we apply Theorem 2 for U as a primary evolution? The problem in fact will be two dimensional and the minimal gap between eigenvalues will be of order $1/\sqrt{N}$. Hence, by Theorem 2 we can predict the states U(t) for t = O(N) in time of order \sqrt{N} . As for $t = O(\sqrt{N})$ we obtain no additional speedup.

4.5 About practical implementations

The two main components of the algorithm are conditional iterations of a primary transformation U and QFT.

The main difficulty for the practical implementation of this method is in conditional iterations of U. Given only a primary device realizing U one cannot immediately fulfil this iterations because it requires quantum control on the number of iterations. The solution may be following. Decomposition of a primary device into elementary parts that can be included to the quantumly controlled circuit and realize the conditional iterations of U for all parts simultaneously. All controlling qubits should be used in entangled state as a Shröedinger cat. Given a quantum gate array computing U we can easily construct a new gate array computing U_{cond} . To put it otherwise a conditional application of U is possible through the control on microscopic level (this bears a resemblance with the control in living cells).

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 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 $x = 0, \frac{1}{M}, \frac{2}{M}, \ldots, \frac{M-1}{M}$. 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 Plank constant h is one. This integral sum will be just the sum in the definition of QFT where x plays a role of s/M and $p/2\pi$ plays a role of l.

Then the main algorithm acquires the following general form.

a). Primary evolution quantumly controlled by a magnitude containing in the properly prepared ancillary register.

b). Simple actions depending on the canonically conjugate magnitude.

c). Repetition of a).

Procedure of such a kind can predict a behavior of a primary system with sparse spectrum and restore the state of arbitrary system in the past. This scheme seems to be very simple and would be interesting to find its natural physical analog. The good starting point here may be the comparison between spectral features of the known systems and their functions and complexity.

5 Conclusion

Formulate again the main result: the method is presented which makes possible to obtain states of a primary quantum system earlier than they appear naturally in its evolution provided the spectrum of system is sparse. This speedup will be the more if the gaps between continuous strips of spectrum increase comparatively to the width of strips. This method can be applied also for restoration of states of the arbitrary primary system in the past. This method yields a speedup and it can make possible to fit into the time when coherent states exist and thus fight decoherence in quantum computations.

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