Implementation of Quantum Fourier Transform and Simulation of Wave Functions by Fixed Interaction

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Abstract

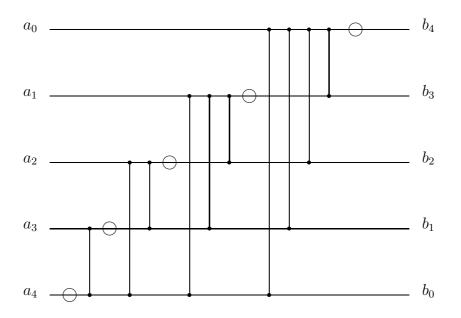
We study a quantum computer with fixed and permanent interaction of diagonal type between qubits. It is controlled only by one-qubit quick transformations. It is shown how to implement Quantum Fourier Transform and to solve Shroedinger equations with linear and quadratic potentials by a quantum computer of such type. The method is adaptable to the wide range of interactions of diagonal form between qubits and to the case when different pairs of qubits interact variously.

1 Introduction

The main difficulty in practical implementation of quantum computing is to fulfill two qubits transformations playing a crucial role in quantum algorithms. To perform such transformations specially we must in fact artificially and exactly control the degree of their entanglement that is determined by overlapping of their spatial wave functions. However to distinguish different qubits the share of overlapping amplitudes must be much less than the overall amount of amplitude and thus in the same degree one-qubits transformations are easier to fulfill than two qubits transformations. While we perform a transformation with one pair of qubits a physical interaction between other pairs of qubits cannot be stopped. This permanent interaction existing in all real systems requires special and nontrivial methods of correcting. These difficulties complicate a straightforward implementation of quantum algorithms. Here we shall study a nonstandard model of quantum computer possessing formally more narrow possibilities but which may be more feasible. It is controlled by only one-qubit transformations whereas two qubits interactions are fixed and determined by the spatial disposition of qubits, they go permanently in course of computation. To show the possibilities of such model we shall at first study how to implement Quantum Fourier Transform (QFT) by such quantum computer assuming that the potential of two qubits interaction has a diagonal form and decreases as Yukawa potential. Then it will be shown how this method can be generalized to wide range of interactions of diagonal form. By means of properly chosen one-qubit transformations this method can be easily adopted to the case when different pairs of qubits interact differently. At last this approach will be applied to the solution of Shoedinger equation for linear and quadratic potentials.

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Quantum Fourier Transform (QFT) is a key subroutine in quantum computing. It is used in variety of algorithms (look at [Sh, AL, Oz]) as a main step generating interference of amplitudes which makes quantum computations so powerful. A simple quantum gate array implementing the reversal for QFT is shown at the picture 1. It was proposed in several works and was used by Shor for fast factoring (see [Sh]). Let us agree to represent an integer of the form $a = a_0 + a_0 2 + \ldots + a_{l-1} 2^{l-1}$ by the basic state $|a_0 \ a_1 \ \ldots \ a_{l-1} \ \rangle = |a\rangle$ forming a basis for input states of a gate array and dispose all a_j from top to bottom. The same agreement will be for output only binary figures b_j for an integer $b = b_0 + b_0 2 + \ldots + b_{l-1} 2^{l-1}$ will be written in reverse order - from bottom to top.



Picture 1. Gate array for QFT⁻¹ with one and two qubits control. Circles denote Hadamard gates, two qubits gates has the form (1)

This array fulfills QFT⁻¹ in $O(l^2)$ steps whereas its matrix is $N=l^2$ dimensioned.

However, a direct implementation of this scheme requires a control over two qubits transformations and thus it does not fit into our model of quantum computer. In this paper it is shown how QFT and its reversal can be implemented by means of fixed Hamiltonian of two particles interaction of the form

where all $\rho = \rho_0 \frac{e^{-br}}{r}$; b = const; r is a distance between the particles and $\rho_1 + \rho_4 \neq \rho_2 + \rho_3$. Dispose our l qubits on one line with equal intervals. We shall consider a case when interaction

between jth and kth qubits will have Hamiltonian $H_{j,k}$ of the forms (1).

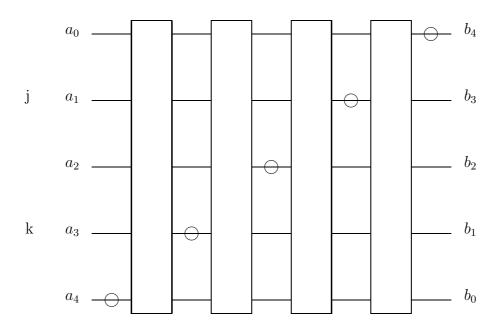
This type of Hamiltonians appears for example in Ising model for particles with spin 1/2. The required decrease of interaction with the distance could be obtained by placing each particle in the appropriate potential hole. Choosing appropriate unit of the length we can make b = 1. At first we shall study fixed interaction of the form (1, A) and then extend our results to (1, B).

2 Implementation of QFT in within phase shifts

We assume that QFT and its reversal have the form ¹:

QFT:
$$|a\rangle \longrightarrow \frac{1}{\sqrt{N}} \sum_{b=0}^{N-1} e^{-\frac{2\pi i \ ab}{N}} |b\rangle, \qquad \text{QFT}^{-1}: |a\rangle \longrightarrow \frac{1}{\sqrt{N}} \sum_{b=0}^{N-1} e^{\frac{2\pi i \ ab}{N}} |b\rangle.$$
 (2)

The reversal transformation for QFT can be fulfilled by the following gate array.



Picture 2. Frameboxes denote fix interaction of the form (1, A), circles denote Hadamard gates.

Here by a framebox we denote a unitary transformation of the form $U=e^{-i\tilde{H}}$ where $\tilde{H}=\sum\limits_{l>j>k\geq 0}\tilde{H}_{j,k}$, and each of $\tilde{H}_{j,k}$ has the form (1,A) with $\rho_0=\pi,\ r=j-k$. If we choose a unit of time so that Plank constant multiplied by ρ_0 equals π and a unit of length so that

 $^{^{1}}$ This agreement corresponds to the definition of ordinary Fourier transform. Typically in quantum computing literature it is assumed a reversal definition.

r=j-k then U will be exactly the transformation of state vector induced by the considered Hamiltonian in the unit time frame. We assume here that the time of all one-qubit gates action is negligible so that two qubits interaction cannot corrupt phases while these gates act. This gate array may be obtained from the previous by insertion of "missing" gates corresponding to interactions existing physically in the system with constant Hamiltonian. To prove that this gate array fulfils QFT⁻¹ we follow the method of amplitudes counting proposed in the paper [Sh]. Given a basic input state $|a\rangle$ consider the corresponding output state. It is a linear combination of basic states $|b\rangle$ with some amplitudes. All modules of these amplitudes equal $1/\sqrt{L}$ and we should only count the phases. For the simplicity we introduce the notation $a'_j = a_{l-1-j}, \ j=0,1,\ldots,l-1$. In the process of the gate array application values of qubits with numbers j and $k \leq j$ pass through the gates on the picture 2 from left to right. Following this passage we separate the following four types of segments: interacting of a'_j with itself and a'_k with itself by Hadamard gates, interacting of a'_j with a'_k (j>k), interacting of a'_j with b_k for j>k, and interacting of b_j with b_k (j>k). The times of these actions are: zero, k, j-k and l-1-j correspondingly. Summing the deposits of all these actions we obtain the resulting phase

$$\pi \sum_{l>j>k\geq 0} \frac{a'_j a_k k}{2^{j-k}(j-k)} + \pi \sum_{l>j>k\geq 0} \frac{a'_j b_k (j-k)}{2^{j-k}(j-k)} + \pi \sum_{l>j\geq 0} a'_j b_j + \pi \sum_{l>j>k\geq 0} \frac{b_j b_k (l-j-1)}{2^{j-k}(j-k)}.$$
 (3)

Denote the first and last summands by A and B correspondingly. Their deposits correspond to the actions of diagonal Hamiltonians on $|a\rangle$ and $|b\rangle$ correspondingly. Leave this deposit so far - till the next section. Take up a part of sum formed by the second and third summands. After the replacement j by l-1-j this part acquires the form

$$\pi \sum_{l-1>k+j\geq 0} \frac{a_j b_k 2^{j+k}}{2^{l-1}} + \pi \sum_{l-1\geq j\geq 0} a_{l-1-j} b_k = 2\pi \sum_{l>k+j\geq 0} \frac{a_j b_k 2^{j+k}}{2^l} = 2\pi S + 2\pi \sum_{l>k,j\geq 0} \frac{a_j b_k 2^{j+k}}{2^l} = 2\pi S + 2\pi \frac{a_j b_k 2^{j+k}}{2^l} = 2\pi$$

for some integer S. The first summand here does not change the phase and we obtain all what is required for QFT⁻¹ but deposits of A and B.

3 Correcting of phase shifts

To cope with the deposit of diagonal summands A and B to the phase we present one trick. At first consider only a summand A. It consists of addends of the form $A_{j,k} = c_{j,k}a'_ja'_k$, where $c_{j,k}$ depends only on j and k but not on a. Declare jth and kth qubits separated. We shall apply one qubit gate NOT several times to all qubits but separated ones to suppress all two qubits interactions excluding interaction between separated qubits.

At first consider a pair of not separated qubits with numbers p, q, q > p. Their permanent interaction in time frame Δt gives the addend $d_{p,q}\Delta t$ $a'_p a'_q$ to the phase where a real number $d_{p,q}$ depends only on how fast does interaction decrease and not on a'_p, a'_q . For example for a decreasing of Yukawa type we have $d_{p,q} = e^{-|q-p|}/|q-p|$. Now invert one of these qubits,

no matter which, say qth by NOT gate. Its state will be $1 - a'_q$. Then the second Δt period of permanent interaction gives the addend $d_{p,q}\Delta t$ $a'_p(1-a'_q)$ to the phase. At last restore the contents of qth qubit by the second application of NOT. The resulting phase shift of this four steps transformation will be $d_{p,q}\Delta t$ a'_p and it depends on the contents of pth qubit only. Now we can compensate this phase shift by a simple one-qubit transformation. If we consider a pair of qubits with numbers p,q where one, say pth is separated and other is not, then we can compensate their interaction by the same way using one-qubits operations: two NOTs for q and one phase shift for pth.

Now we should so modify this method that compensate all influence of not separated qubits simultaneously. For each not separated qubit number p consider the Poisson random process \mathcal{A}_p generating time instants $0 < t_1^p < t_2^p < \ldots < t_{m_p}^p < 1$ with some fixed density $\lambda \gg 1$. Let all \mathcal{A}_p are independent. Now fulfil transformations NOT on each pth qubit in instants t_m^p sequentially. In instant 1 fulfil NOT on pth qubit if and only if m_p is odd. Thus after this procedure each qubit restores its initial value. Count the phase shift generated by this procedure. Interaction between separated qubits will be unchanged. Fix some not separated qubit number p and count its deposit to phase. It consists of two summands: the first comes from interaction with separated and the second - from interaction with not separated qubits. Count them sequentially.

- 1. In view of big density λ of Poisson process \mathcal{A}_p about half of time our pth qubit will be in state a'_p and the rest half in $1 a'_p$. Its interaction with a separated qubit, say jth brings the deposit $\frac{1}{2}d_{p,j}a'_pa'_j + \frac{1}{2}d_{p,j}(1 a'_p)a'_j$ that is $\frac{1}{2}d_{p,j}a'_j$.
- 2. Consider a different not separated qubit number $q \neq p$. In view of independence of time instants when NOTs are fulfilled on pth and qth qubits and big density λ these qubits will be in each of states $(a'_p, \ a'_q), \ (a'_p, \ 1 a'_q), \ (1 a'_p, \ a'_q), \ (1 a'_p, \ 1 a'_q)$ approximately a quarter of time. The resulting deposit will be $\frac{1}{4}d_{p,q}[a'_pa'_q + a'_p(1 a'_q) + (1 a'_p)a'_q + (1 a'_p)(1 a'_q)] = \frac{1}{4}d_{p,q}$.

A total phase shift issued from the presence of not separated qubits in our procedure now is obtained by summing values from items 1 and 2 for all $p \notin \{j, k\}$. It is

$$\frac{1}{2} \left[\sum_{p \notin \{j,k\}} d_{p,j} a'_j + \sum_{p \notin \{j,k\}} d_{p,k} a'_k \right] + \frac{1}{4} \sum_{p,q \notin \{j,k\}} d_{p,q}.$$

This shift can be compensated by one-qubit operations because the first two summands depend linearly on the qubits values and the second does not depend on qubits values at all. Thus we obtain a gate with permanent two qubits interaction and one-qubit operations fulfilling phase shift to $d_{j,k}a'_ja'_k$. If we take time frame Δt instead of unit time in this procedure we obtain the phase shift to $\Delta t \ d_{j,k}a'_ja'_k$. If we want to obtain the shift to $-\Delta t \ d_{j,k}a'_ja'_k$ we should at first apply NOT to the jth qubit, then apply the above procedure, then again apply NOT to jth qubit and at last add $-\Delta t \ d_{j,k}a'_k$ by one-qubit operation. So we are able to make any addition of the form $c \cdot a'_ja'_k$ to the phase for real c independently of its sign. An appropriate combinations of such gates gives us a phase shifts to

$$\sum_{j,k} c_{j,k} a_j' a_k' \tag{5}$$

for any $c_{j,k}$. Placing such gates before and after QFT⁻¹ procedure from the previous section we compensate summands A and B in the phase and thus obtain a gate implementing QFT⁻¹.

Errors arising in this method issue from the possible imperfection of Poisson processes generating instants for the qubits inversions and interactions continuing in course of these inversions. It can be minimized by increasing of density λ and by decreasing of the time needed for NOT operation in comparison with typical time of two qubits operation defined by the interaction $d_{i,k}$.

4 Possibility to use interactions of the different types

Up to now we considered Hamiltonian of two qubits interaction given by (1, A) with decreasing of Yukawa type. Now we are going to extend our technique at first to Hamiltonians of the form (1, A) for arbitrary degree of decreasing, then to Hamiltonians of the form (1, B) for arbitrary decreasing (even for different degrees of decreasing for different pairs of qubits), at last - to the interactions which can be diagonalized by one-qubit transformations. Namely, we shall prove that it is possible to generate a phase shift of the form (5) and of the form

$$\sum_{l>j>k\geq 0} c_{j,k} a_j' b_k \tag{6}$$

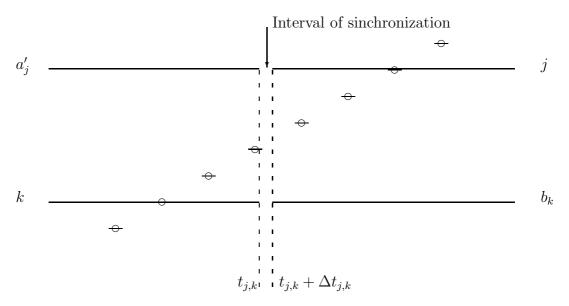
for any $c_{j,k}$.

Consider an interaction of the form (1, A) for arbitrary degree of decreasing. Generating of quadratic phase shifts of the form (5) remains unchanged. The only thing we should do is to generate QFT⁻¹ in within quadratic phase shift. To do it we start with a gate array represented at the picture 2 but now a time interval ΔT between nearest Hadamard gates will not equal 1 - it will be determined a bit later. Given a number j let t_j be instant of the corresponding Hadamard transformation. We shall obtain the required gate array inserting sequential NOT operations on each qubit. Construct a list of Poisson random processes \mathcal{A}_p $p=0,1,\ldots,l-1$ corresponding to qubits and generating time instances for NOT operations on them. But now these processes will not be completely independent. At first require that a number of these NOT operations on jth qubit preceding t_j is even. It will guarantee that a value of jth qubit before Hadamard transform will be a'_j . Then require that jth and kth processes generate the same time instances in the time frame $(t_{j,k}, t_{j,k} + \Delta t_{j,k})$ corresponding to each pair of qubits jth and kth, j > k (qubits are numerated from bottom to top). Call these time frames (j, k)th interval of synchronization. They will have the following properties:

- a) they will not overlap for different pairs, and
- b) each time frame $(t_{j,k}, t_{j,k} + \Delta t_{j,k})$ lies between the instances of kth and jth Hadamard gates,
- c) $\Delta t_{i,k} \gg 1/\lambda$ for a density λ of processes \mathcal{A}_p .

Appropriately choosing λ we can satisfy c). Consider subdivision of intervals between nearest Hadamard gates to equal halves and agree that the points of division belong to the left of

possible time frames. Agree that (j,k)th interval of synchronization lies in the same half as $t = (t_j + t_k)/2$. Then only r < 2l such intervals will lie in the same half and to make them not overlapping we only should divide each half to r segments which lengths will be completely determined when we choose the values of $\Delta t_{j,k}$, associate each interval with some segment and then assume that each of these r intervals belongs to the corresponding segment. Thus we ensure conditions a) and b). Now to determine a gate array (look at the picture 3) we need only values $\Delta t_{j,k}$.



Picture 3. Gate array implementing QFT⁻¹. It consists of one-qubit gates and different fixed permanent interactions of diagonal form

At first consider the case when numbers of NOT operators preceding the first NOT in synchronized interval have the same oddity for jth and kth qubits. Count a phase shift generated by this gate array omitting linear summands like $c_j a'_j$ or $d_k b_k$ which can be easily compensated by the appropriate one-qubit gates: $\Delta t_{j,k} \frac{1}{2}((1-a'_j)(1-b_k)+a'_j b_k)+S_{lin}+S_{negl}$. S_{lin} consists of linear summands, S_{negl} issues from interaction outside synchronized intervals and for high density λ it consists of mutually canceling additions like above. In the case of different oddities we obtain a similar expression. In all cases we can choose such values for all $\Delta t_{j,k}$ (they will depend on pairs j, k) that our gate array fulfils QFT⁻¹ in within linear phase shift and it takes a time $O(l^2)$. Composing it with gates for appropriate linear phase shifts before and after this gate array we obtain a required implementation of QFT⁻¹ in time $O(l^2)$.

Given interaction of the form (1, A) where ρ is negative we can reduce this case to the considered one by inverting one of interacting gates and adding linear shift. It is straightforwardly seen that it results in the only change in our constructions as adding linear shift to the phase. By the same manner we can implement the direct transformation QFT given a gate array implementing its reversal and complexity of the gate array will be about the same.

Given interactions of the form (1, B) its application in time frame 1 gives phase shift to

 $\rho_1(1-a_j')(1-b_k) + \rho_2(1-a_j')b_k + \rho_3a_j'(1-b_k) + \rho_4a_j'b_k$ that may be reduced by the linear phase shift to the above case because $\rho_1 + \rho_4 \neq \rho_2 + \rho_3$.

At last this technique may be straightforwardly generalized to interactions with Hamiltonians that may be diagonalized by one-qubits transformations. Note that this class of interactions is not yet the most general at all, say a model of quantum computations with CNOT gates cannot be immediately reduced to it.

5 Simulation physics by means of fixed interaction

Now we take up an important idea dating back to Feynman ([Fe]): to simulate physics by quantum computers. A sketch of such simulating method referring to Coppersmith-Deutsch-Shor scheme (see picture 1) for QFT^{-1} was proposed by Zalka ([Za]) and Wiesner ([Wi]). The method of QFT implementation presented above gives an easy way for simulation in case of linear and quadratic potentials by means of constant and permanent interaction between qubits. Hamiltonians with quadratic potentials serve as a good approximation for description of such important physical objects as free particle, ensembles of linear harmonic oscillators, free fields, complex molecules. Such Hamiltonian for s_1 particles has the form

$$H = \sum_{k=1}^{s} \frac{p_k^2}{2m_k} + \frac{1}{2} \sum_{j,k=1}^{s} v_{j,k} q_j q_k, \tag{7}$$

where $s = 3s_1$ is the total number of spatial coordinates q_k determining a spatial state of system, p_k are impulses and $v_{j,k}$ are constants. We now take up a case k = 1 because the general case may be considered similarly.

At first we remind the main ideas of simulation physics by a quantum computer. We have to approximate an action of operator e^{-iHt} on a wavefunction ψ_0 where $H=H_p+H_q$, $H_p=\frac{p^2}{2m}$, $H_q=V(q), \ p=\frac{1}{i}\frac{\partial}{\partial q}$ and potential V(q) is a real quadratic function. Without loss of generality we can take t=1. To have a useful approximation we must deal with coordinate or impulse basis in the space of state vectors and in both cases Hamiltonian will not be diagonal. In order to reduce the problem to the simple diagonal case choose a small time interval Δt and represent our evolutionary operator approximately by

$$e^{-iH} \approx (e^{-iH_q\Delta t} e^{-iH_p\Delta t})^{1/\Delta t}.$$
 (8)

Choosing, say coordinate basis we have a diagonal operator H_q . Using Fourier transform FT: $f \longrightarrow \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ipq} f(q) dq$ and its property to replace derivative $\partial/\partial q$ by factor ip we can represent an action of impulse part of operator as $e^{-iH_p} = \mathrm{FT}^{-1} \ e^{-ip^2\Delta t/2m}$ FT where the medium operator has a diagonal form. If we can implement FT and phase shift on $-p^2/2m$ then the sequential application of such operators from (8) gives the required approximation.

Assume that a wave function $\psi(q)$ is defined on a segment (-A,A) and its impulse representation FT ψ is defined on a segment (-B,B). Choosing a small values Δq and Δp we can approximate it by $\sum_{a=0}^{2A/\Delta q} \psi(q_a) \delta_a$ where $\delta_a(q)$ takes a value 1 on a segment $(q_a, q_a + \Delta q)$ and

zero for other q. Then we can approximate FT by a linear operator whose action on δ_a gives $\frac{1}{\sqrt{2\pi}}\Delta q\sum_{b=0}^{2B/\Delta p}e^{-ip_bq_a}\sigma_b(p)$ where $\sigma_b(p)$ is one step impulse function analogous to δ_a . Introducing new one step functions for coordinate and impulse by $d_a(q) = \delta_a(q-A)$, $s_b(p) = \sigma_b(p-B)$ we rewrite FT in the form

$$d_a \longrightarrow \frac{1}{\sqrt{2\pi}} \Delta q \sum_{b=0}^{2B/\Delta p} e^{-i ba\Delta q \Delta p} s_b \tag{9}$$

that looks similar to QFT.

Assume that the physical space is grained in coordinate and impulse representations with the sizes of grains Δq and Δp . Then our particle may exist only in points of the form q_a or may have impulse only of the form p_b . We associate a position q_a ; $a=0,1,\ldots,N=2^l$ with the basic state $|a\rangle$ of l qubits quantum system. For the simplicity choose such units for the length that $\Delta q = \Delta p = \sqrt{2\pi}/\sqrt{N}$ and let $A=B=\sqrt{\pi N/2}$. Then (9) corresponds to QFT of the form (2) and phase shift to $-p^2\Delta t/2m$ from (8) corresponds to phase shift to $-\pi b^2\Delta t/mN$. We can implement the both operations by means of fixed interactions because the last has the form from above. At last the first operator in (8) can be implemented by the same way in the case under consideration.

If we simulate a system with s_1 particles then we should get s_1 copies of quantum register for one particle and fulfill the procedure described above for this joint quantum memory.

6 Advantages of quantum simulation of wave functions

A proposed way of quantum solution of Shroedinger equation as well as implementation of QFT preserves all advantages of known quantum tricks (look at [Sh, Za, Wi]). Namely, given constant interactions between qubits our method of implementation of QFT requires the time $O(l^2)$. If we restrict ourselves by approximate version of QFT (it may be obtained by omitting exponentially small phase shifts) then the correspondent modification of our method takes the time O(l) where a constant depends on the chosen accuracy.

As for the simulation of wave function the main advantage of quantum method are displayed for the case when a simulated system contains many particles. Let we have a system of s one-dimensional particles. Its wave function in a fixed time instant has the form $\psi(x_1, x_2, \ldots, x_s)$ where x_j denotes a coordinate for jth particle. To store the approximation of this function with grain ϵ and arguments bounded by b we need of order N^s bits where $N = b/\epsilon$. At the same time quantum method of simulation requires of order $\log N$ qubits for each particle and all memory will be of order $s \log N$ qubits that is logarithm of classical size. But the proposed method shows advantages even in case of one particle. Limit the time frame of the required simulation for the simplicity by 1, a coordinate and impulse - by B. To use the formula (8) we must have only $\Delta t \longrightarrow 0$. Then the total time of quantum simulation has an order $\log^2(1/\epsilon)\frac{1}{\Delta t}$ whereas an approximate solution of Shroedinger equation on a classical computer requires scanning of all massive of wave function values that is $1/\epsilon$ in each of $1/\Delta t$ passes. Hence quantum methods of simulation give almost exponential time and space saving as compared with classical methods.

7 Conclusion

We considered a model of quantum computer controlled only by one-qubit impulses whereas interaction between qubits is fixed and remains unchanged in course of computation. Advantage of this model is taken of the simplicity of control. It was found a simple way to implement Quantum Fourier Transform by such quantum computer. This method makes possible to solve Shroedinger equation for linear and quadratic potentials and thus in principle such type of computer can simulate systems of harmonic oscillators, free fields and particles and molecules consisting of many atoms.

Further investigations can go to several directions. The first is: to clarify possibilities of such simple model of quantum computer, say to find an effective implementation of Grover search algorithm ([Gr]) in the framework of this model (preliminary step in this direction was made in [FG] but it is not a complete feasible solution). Would be important to extend the results to not diagonal Hamiltonians. At last it may be interesting to reformulate some areas of quantum mechanics in terms of qubit representation of wave function that we used for quantum computing. For example such reformulation assumes the existence of spatial grain and traditional difficulty of field theory issuing from the divergence of rows for high frequencies would be removed. This reformulation also can turn to be more economical than the conventional because the time and space resources required to describe a many particles system grows much slower than for conventional case when the number of particles increases.

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