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Search via Quantum Walk

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1. Introduction

For an unsorted database, it takes long time to find a special element. If the number of elements in the database increases, the searching time is proportional to the size of the database N. It is expected that there is no efficient search algorithm in the classical realm. The conceive of quantum computer may bring us the hope of improving the solution to the searching problems, just as to some other intractable problems such as factoring large numbers and discrete logarithm. The first quantum algorithm for searching an unsorted database is discovered by Grover, which is named as Grover algorithm (Grover (1997)). Grover algorithm can search the unsorted database with a quadratic speed up, soon after that it is proved to be the fastest speed up with the quantum computer. Although unlike some other quantum algorithms that make exponentially speed up upon the corresponding classical algorithms, it can not prevent us to treat Grover algorithm as an elegant harvest of the quantum computer since for very large unsorted database the quadratic speed up is not a trivial achievement. Suppose a classical search needs 10^6 steps, and 1 step costs 8.64 seconds, then the total calculation spends 100days. While the corresponding quantum search needs 10^3 steps, and thus the total calculation spends only 0.1 day!

Besides Grover algorithm, quantum walk is another approach to achieve quadratic speed up. Furthermore, quantum walk is soon generalized to other searching problems such as element distinctness, substructure finding etc. These problems can not be solved by Grover algorithm efficiently. This is far from ending. As we know, quantum computer is still a beautiful dream, which drives many people to double the effort to find the search algorithm based on conventional quantum computer or quantum walk. Some people may suspect that the decoherence can shatter the dream of building a quantum computer. But such pessimism would be taken away considering quantum walk may play an important role in many natural processes, such as photosynthesis. It is not surprising at all that someday the dream will come true.

In this chapter we will focus on the search algorithm based on quantum walk. The structure of this chapter is as follows, section 2 is the introduction of the quantum walk, including the coined and continuous quantum walk; section 3 is the search algorithm via quantum walk, for the general searching and the special searching problems; section 4 is focused on the physical implementation of quantum-walk-based search algorithm using an NMR quantum computer; in section 5 we will introduce the application of quantum walk in nature such as photosynthesis, in which the high efficiency of the energy transfer is still an enigma. And finally section 6 is the conclusion and proposals for the further study.

2. Quantum walk

Random walk is known as the Markovian chain which has been applied on the algorithms generally, it was quantized after the concept of quantum computer is formed. In this section we shall introduce the concept of quantum walk developed from the classical random walk and then the two forms of quantum walk - coined and continuous quantum walk.

2.1 Classical random walk

In principle, the random walk can be defined on arbitrary graph. Without loss of generality, we could focus on the random walk on one dimensional lattice. Suppose there are N lattice points arrayed on a line, each labeled by an integer, negative or positive, such as in Fig. 1, the lattices are labeled form -9 to 9 . At any time we can be at only one lattice point. Then we start at lattice 0 for example, we flip a coin to decide if we go to the left lattice or the right lattice, if the coin is up, we go to left, otherwise we go to right, then we flip the coin again to decide the next left or right. So at each step we flip a coin to decide which direction to go. After T steps, we can calculate the possibility on each lattice, for example we can see the Fig. 2. For this case we set the probability going to each direction to be 0.5. Of course, we can also set the probability different if necessary.
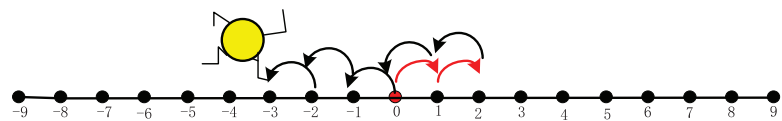

Fig. 1. In the case of the one dimensional lattice, a walker just has two direction to choose. In classical random walk, going to left or right may be decided by flipping a coin with two sides. This picture is from (Kendon et al. (2007)).

i T	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$		$\frac{1}{2}$				
2				$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$			
3			$\frac{1}{8}$		$\frac{3}{8}$		$\frac{3}{8}$		$\frac{1}{8}$		
4		$\frac{1}{16}$		$\frac{1}{4}$		$\frac{3}{8}$		$\frac{1}{4}$		$\frac{1}{16}$	
5	$\frac{1}{32}$		$\frac{5}{32}$		$\frac{5}{16}$		$\frac{5}{16}$		$\frac{5}{32}$		$\frac{1}{32}$

Fig. 2. In this table T is the number of steps of the classical random walk in one dimensional lattice, i is the number that labels the position of the lattice. From this table we can know that after T steps, the walker will be at the center (or the start place) with the maximum probability (Kempe (2003)).

From a formal derivation we can get the probability distribution of the walker on each lattice. For details we can consult the book of 'A modern Course in Statistical Physics' (Reichl (1998)).

According to probability theory, the probability distribution of the random walker on the position after a time long enough is

$$\rho(x, T) = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{x^2}{2T}\right) \tag{1}$$

where x is the position on one dimensional lattice, T is the step number.

Fig. 3 is the probability density of the distribution as the function of the position and the step number. Fig. 4 shows the results after some typical steps. It is not difficult to conclude that after many steps, the probability of the position of the random walker become flat on the lattice, tending to a Gauss distribution. The average position is 0 and the covariance of the position is

$$\sigma^2 = T \tag{2}$$

So statistically the walker's departure from the center is proportional to the square root of the step number.
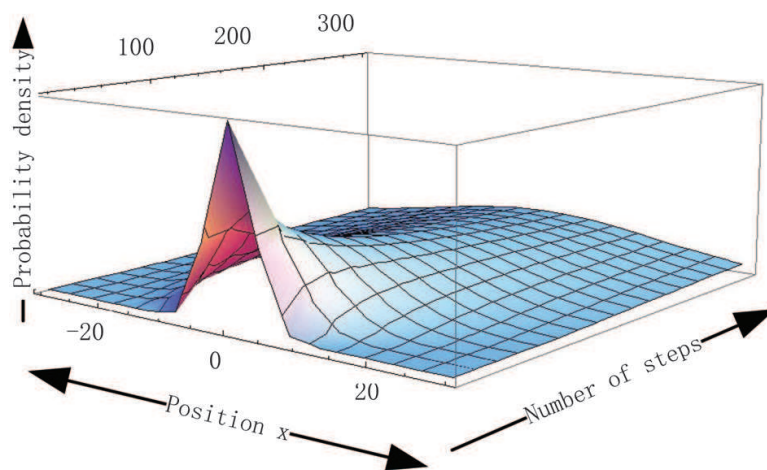

Fig. 3. The probability distribution of the classical random walk as a function of the position and number of step, which shows we know that as the number of steps increases, the walker will diffuse to all the lattice points. This character is used by many computer algorithms.

2.2 Coined quantum walk

Classical random walk has been applied to many fields such as Brownian motion, randomized algorithm etc.. But we still look forward to the quantization of the random walk to get more powerful applications, mainly attributed to the superposition principle of quantum realm. This was done by Y. Aharonov, L. Davidovich, and N. Zagury in 1993 (Aharonov et al. (1993)). For an intuitional view, the quantum walk can be regarded as the quantization of the classical random walk. However, in the classical random walk, the walker can go to only one lattice at a time. In contrast, the quantum walker can turn to both sides until it is measured, which is showed in Fig. 5.

Formally, we should define the quantum walk in Hilbert space. For simplicity we focus on the one dimensional lattice.
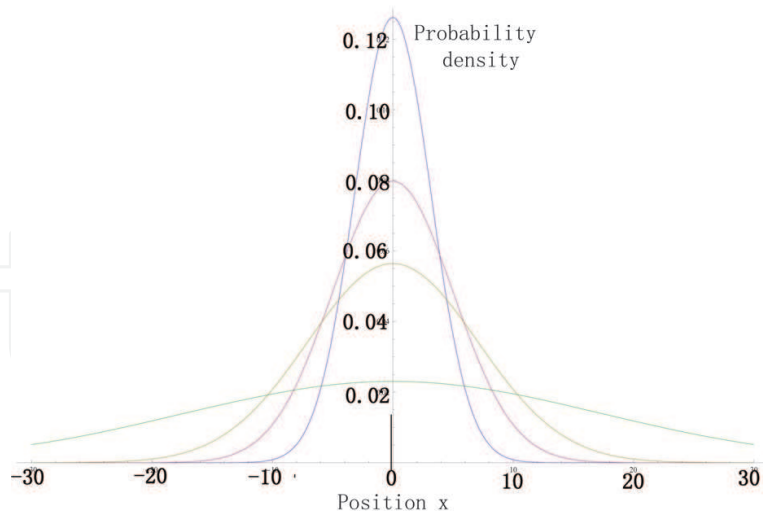
Fig. 4. Probability distribution of the classical random walk after some special steps.(green: T=300; yellow: T=50; red: T=25; blue: T=10).
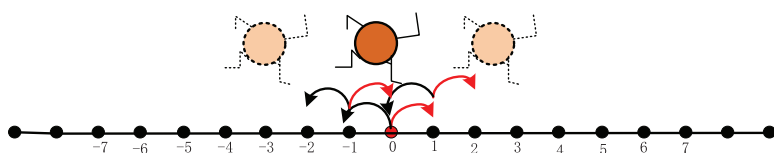

Fig. 5. The illustration of quantum walk in an intuitionistic way. Here the walker can go left and right simultaneously, which is one of the most amazing properties of quantum mechanics, first illustrated by Feynman with the tool of path integral. This picture comes from (Kendon et al. (2007)).

In the coined quantum walk, we should define two Hilbert space:

$$H = H_c \otimes H_p \tag{3}$$

where H_c is the coin Hilbert space and H_p is the position space, having the following forms:

$$H_p = \{|x\rangle\,; x \in \mathbb{Z}\}\,, H_c = \{|+1\rangle\,, |-1\rangle\} \tag{4}$$

where the integer x is the position. In the coin space +1 means go to right and -1 means go to left. In quantum walk, the walking process can be realized by the shift operator:

$$S = |+1\rangle\,\langle +1| \otimes \sum_x |x+1\rangle\,\langle x| + |-1\rangle\,\langle -1| \otimes \sum_x |x-1\rangle\,\langle x| \tag{5}$$

And the coin operator is :

$$C = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{6}$$

The S and C operator are all unitary and hermitian, so for each step the evolution of the coin and space is also unitary as follows :

$$U = S(C \otimes I) \tag{7}$$

The state of the quantum coin can be a superposition of up and down, which is different from the classical case. As a result, the initial condition in quantum walk can be supposed as

$$|\Psi_{in}\rangle = (\alpha\,|+1\rangle + \beta\,|-1\rangle) \otimes |x\rangle \qquad (8)$$

After T steps, the final state before measurement is:

$$U^T\,|\Psi_{in}\rangle \qquad (9)$$

Then we can perform the measurement of the position of the walker and get the position distribution according to the quantum mechanical rule.

As an example, we can set two quantum register: the coin register and the position register. The coin register has two possible state |+1> or |-1>, and the position register can be the state |x>, where x is an integer.

The walking process is to flip the coin first and then shift, and we can set the coin operator as:

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad (10)$$

Flipping leads to the following changes of the states:

$|+1> \rightarrow (|+1> +|-1>)/\sqrt{2}, |-1> \rightarrow (|+1> -|-1>)/\sqrt{2}$

Shift is :

$|+1>|x> \rightarrow |+1>|x+1>, |-1>|x> \rightarrow |-1>|x-1>$

We can also understand why the quantum walk is different from the classical random walk with the help of path integral method as illustrated in Fig. 6 (Pérez Delgado (2007)).

In Fig. 6, the dotted line is all the possible paths and the real line is one of them. The classical walker can only select one of the paths to walk, while the quantum walker can walk in all possible paths simultaneously, with the probability amplitude of every path interfering to each other.

If the initial state of the coin is |-1>, then we can get the possibility distribution as Fig. 7 shows.

Otherwise if we set the initial state of the coin to $\frac{1}{\sqrt{2}}(|+1\rangle + i\,|-1\rangle)$, then the possibility distribution is as Fig. 8 shows. This is very different from classical random walk whose possibility distribution is independent of the initial conditions.

Another difference of quantum walk from classical random walk is the diffusion rate of the walker from the center. As we know from section 2.1, the deviation of the walker is proportional to the root of the step number N, but in quantum walk, the deviation of the walker is proportional to N, which get a quadric speed up(for a detail see the Fig. 9).

2.3 Continuous time quantum walk

Continuous time quantum walk is introduced by Edward Farhi and Sam Gutmann in 1998 (Farhi & Gutmann (1998)). In contrast with the coined quantum walk, the continuous quantum walk does not need a coin, and is often defined with the tool of graphs.
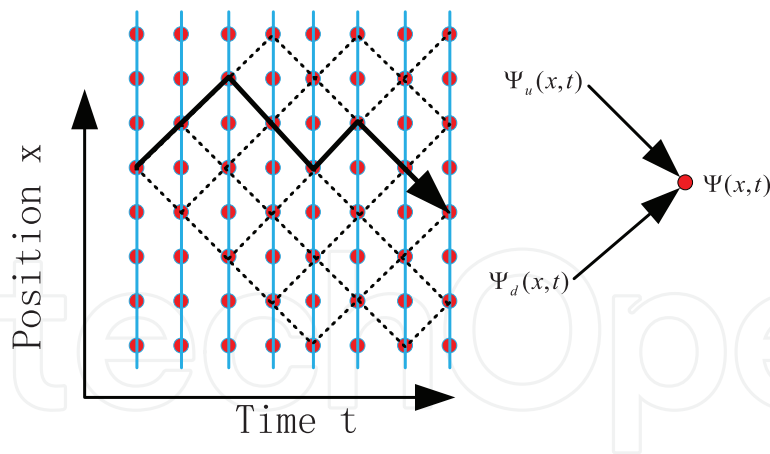
Fig. 6. Illustration of the quantum walk with the tool of path integral (Pérez Delgado (2007)). The red point stands for the lattice and the dotted line is all the possible path. In classical random walk, the walker can only choose one of the paths (the real line) with a probability, but in quantum walk one can walk in all possible paths simultaneously. The probability amplitude of every path can then interfere to each other if allowed.
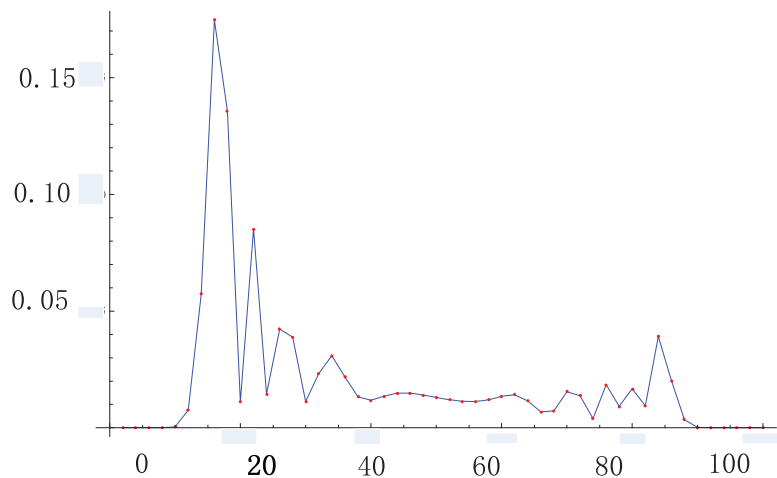

Fig. 7. Probability distribution of quantum walk with the initial state |-1> of the coin. The walker starts at the position x=50 and the number of steps is 50.

It is convenient to illustrate the continuous time quantum starting from the classical random walk on a graph. The process can be described by a matrix M, which transforms the probability distribution on the vertex of graph:

$$p_i^{t+1} = \sum_j M_{ij} p_j^t \tag{11}$$

where M_{ij} is the matrix element of M, the probability at the i th vertex at time t.
The next step is to make the transform process continuous, which requires to jump to only the neighbor vertex. Then we should use the infinitesimal generator matrix H to describe the walk process, i.e.

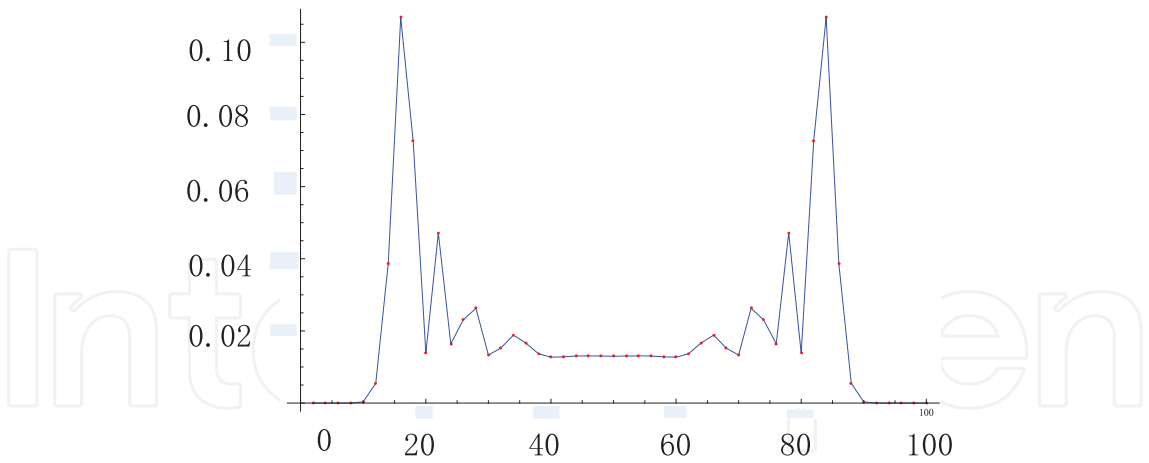$$\frac{dp_i(t)}{dt} = -\sum_j H_{ij} p_j(t) \tag{12}$$

Fig. 8. Probability distribution of quantum walk with another initial state of the coin of
$\frac{1}{\sqrt{2}}(|+1\rangle + i|-1\rangle)$. The walker starts at x=50. By comparing Fig. 7 and Fig. 8 we can easily
find that the probability distribution of quantum walk depends on the initial state of the coin,
which is different from the classical random walk, whose probability distribution is
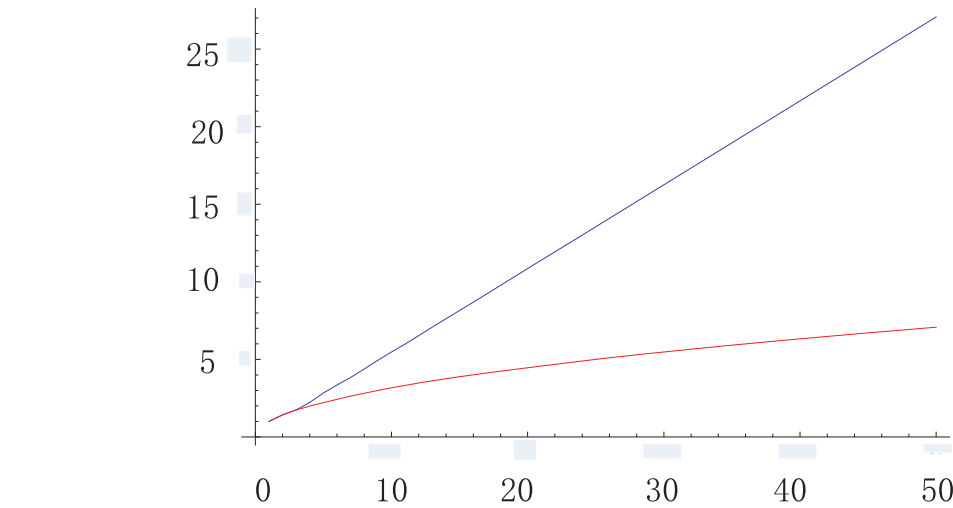independent of the initial state of the coin.

Fig. 9. The diffusion rate of the walker from the center, which is characterized by the
deviation of the walker's position from the center (i.e. the start place of the walker). The
horizontal axis represents the number of the steps T and the vertical axis represents the
deviation of the position. In this picture the blue line is the case of quantum walk and the red
line is the case of the classical random walk. It can be concluded that the diffusion rate of the
quantum walk is quadratic speed up upon the classical random walk.

Solving the equation we get:

$$p(t) = \exp(-Ht)p(0) \tag{13}$$

where p is the vector of probability distribution.

Equation (12) has the similiar form with the Schrödinger equation, so the classical random
walk is quantized in a continuous form.

3. Search algorithm via quantum walk

In section 2.2 we have know that in one dimensional lattice the walker departs from the center quadratically faster than classical random walk, however it is not a search. Search is the reverse process: starting in a uniform superposition of all the databases and returning to the marked item. So it is not difficult to understand why the quantum walk based search algorithm is quadratic speed up upon the classical search algorithm. Generally coined quantum walk can make quantum walk faster than the continuous time quantum walk(Ambainis (2005)).

Quantum walk can also be simulated by quantum circuit(Douglas & Wang (2009)), thus we can realized the quantum based search algorithm by the quantum computer in principle. This makes quantum walk not only a conceived tool for algorithm, but also useful for the computation theory to explore more efficient algorithms for intractable problems. For a review of the algorithm application of quantum walk we can see the article of Andris Ambainis and Vivien M Kendon (Ambainis (2003); Kendon (2006))

3.1 Searching on graphs

In this subsection we will focus on the search on graphs. Searching on graphs is to find a marked vertex of the graph. Sometimes one is also interested in finding a marked edge or even a marked subgraph, which is generalized from the search of vertex.

Searching on the graph can be done by coined quantum walk (Shenvi et al. (2003)) or continuous time quantum walk (Childs & Goldstone (2004)), we will focus on the coined quantum walk based search algorithm most of the time. Hitherto the quantum walk is all defined on highly symmetric graphs such as hypercube.

In section 2.2 we have introduced the coined quantum walk on one dimensional lattice just for illustration. In order to interpret the search algorithm via quantum walk it is necessary to get the definition of quantum walk on graph. This will be showed with the example of hypercube of dimension n. The first quantum walk based search algorithm is discovered by Neil Shenvi, Julia Kempe, and K. Birgitta Whaley (Shenvi et al. (2003)), which is called SKW algorithm. As an example we will illustrate the SKW algorithm without loss of generality.

The only difference between the quantum walk on higher dimensional graph and that on a line is the dimension of the Hilbert space of coin and position. In graph the position is replaced by the vertex and the dimension of the coin Hilbert space is the degree of the graph. For an n dimensional hypercube, the degree of every vertex is n and the number of the total nodes is $N = 2^n$, thus the Hilbert space of the vertex and coin is:

$$H = H_v \otimes H_c \tag{14}$$

where H_v is the vertex space and H_c is the coin space respectively which have the form:

$$H_v = \{|x\rangle : x \in \mathbb{Z}_N\} \tag{15}$$

$$H_c = \{|c\rangle : c \in \mathbb{Z}_d\} \tag{16}$$

where N is the number of the total nodes and d is the degree of every vertex.

Then we can define the coin operator and the shift operator on the Hilbert space of the coin and vertex in the following forms (Shenvi et al. (2003)):

$$S = \sum_{d=0}^{n-1} \sum_{\vec{x}} |d, \vec{x} \oplus \vec{e}_d\rangle \langle d, \vec{x}| \tag{17}$$

$$C = C_0 \otimes I \qquad (18)$$

where $\vec{e}_d$ is the d th basis vector on the hypercube. C_0 is an $n \times n$ unitary operator acting on the coin space and I is an identity operator. To implement the search algorithm it is natural to apply a marked coin operator. In the SKW algorithm for instance the marked coin operator is as follows:

$$C' = C_0 \otimes I + (C_1 - C_0) \otimes \left| \vec{0} \right\rangle \left\langle \vec{0} \right| \qquad (19)$$

The marked coin can be any $n \times n$ unitary operator, for detail information we can see the literature (Shenvi et al. (2003)).

The more generalized searching target on the graph can be an edge or even a subgraph (Hilley et al. (2009)). Element distinctness is another algorithm that can be viewed as a quantum walk based search (Ambainis (2007))

3.2 Searching the exits

Another algorithm of search using quantum walk is found by Andrew M. Childs et al in 2003, which is the first quantum walk based algorithm. This algorithm uses the exponential speed up of hitting time of quantum walk upon classical random walk (Childs et al. (2003)). Contrast of the unsorted database, the algorithm found by Andrew M. Childs et al. is based on a particular sort of network (Fig. 10). Suppose that we are at the entrance of the network, our task is to find another exit as fast as possible. For classical case the best strategy may be to choose a direction randomly, i.e. the classical random walk. It still takes the time increasing exponentially with the wide of the network. One may be lost in the middle of the network. In quantum walk, however, one can choose all the possible paths simultaneously and reach the exit with the time increasing polynomially with the wide of the network, which makes an exponential speed up.
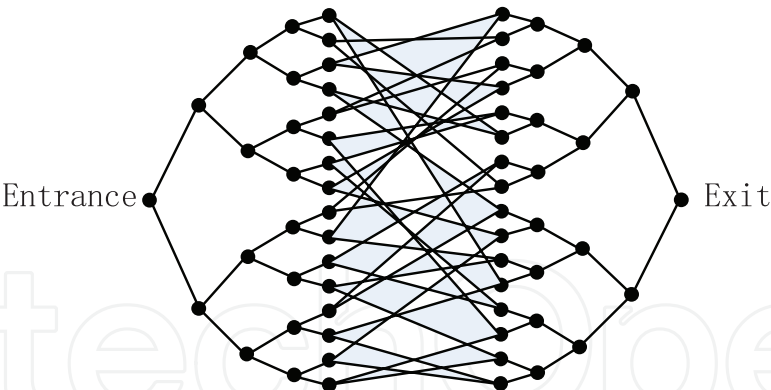

Fig. 10. The network of the first algorithm found by Andrew M. Childs et al. that is based on quantum walk (Childs et al. (2003)).

4. Physical implementation of quantum walk based search

4.1 Introduction to the SKW algorithm

The quantum random walk search algorithm proposed by Shenvi, Kempe and Whaley (SKW algorithm, Shenvi et al. (2003)) is one of the novel algorithms which exhibits the superiority of quantum computation. It belongs to the discrete-time quantum random walk model. Similar to Grover's quantum search algorithm, the SKW algorithm performs an oracle search on a

database of N items with $O(\sqrt{N})$ calls, where N is the size of the search space. Whereas, when the diffusion step of Grover algorithm cannot be implemented efficiently, this algorithm may be still available, which is a significant advantage comparing to the Grover algorithm. Afterwards various optimizations of the SKW algorithm have been brought up to reduce the complexity (Ambainis (2005); Chandrashekar (2008); Reitzner et al. (2009); Tulsi (2008)).

The original problem can be described as follows: given a function $f(x)$, $f(x) = 1$ if $x = a$, otherwise $f(x) = 0$. The goal is to find a, where $0 \leqslant a \leqslant 2^n - 1$. It is equivalent to search for a single marked node among the $N = 2^n$ nodes on the n-cube.

The coined quantum walk model requires a flipping coin and defines a two-step procedure consisting of a coin-flip step and coin-controlled walk step. The two steps can be expressed as $U = SC$, where C denotes a unitary operation corresponding to flipping the quantum coin (coin-flip step) and S is a permutation matrix which performs a controlled shift based on the state of the coin space (coin-controlled walk step). Specially, in the SKW algorithm, an oracle is needed to realize the searching procedure. The oracle acts by applying a marking coin C_1 to the marked node and the original coin C_0 to the unmarked nodes, which is defined as a new coin operator C'. After applying $U' = SC'$ for $t_f = \frac{\pi}{2}\sqrt{2^n}$ times, we gain the marked node with probability $\frac{1}{2} - O(1/n)$ by measurement.

A simple case for $n = 2$ is considered. We need three qubits to demonstrate the algorithm, with one coin qubit (labeled by qubit 0) and two database qubits (labeled by qubit 1 and 2). The target node is one of the four computational bases $|00\rangle_{12}, |01\rangle_{12}, |10\rangle_{12}, |11\rangle_{12}$, named by 1-out-of-4 algorithm. The network is shown in Fig.11. Now we describe the searching process in details. Suppose the initial state is a pure state $|000\rangle$.
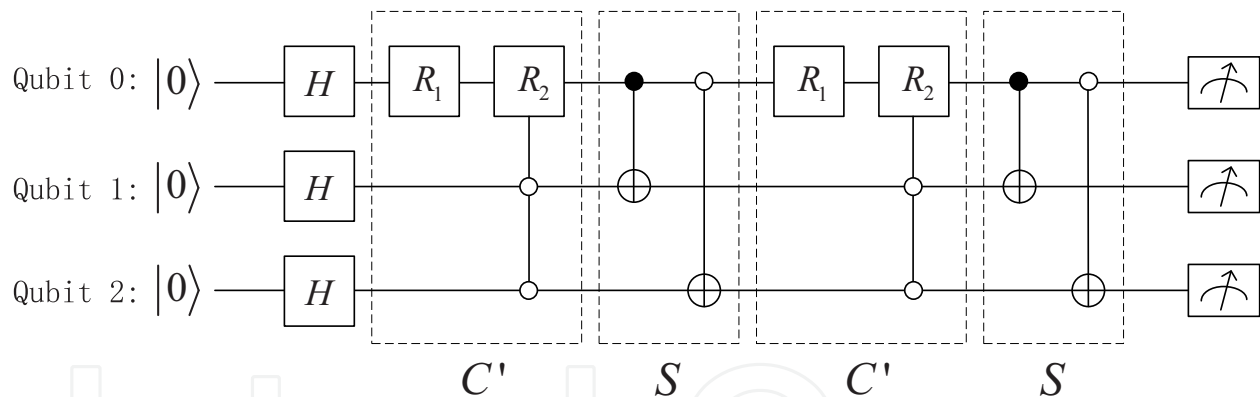

Fig. 11. Quantum network for the algorithm of 1-out-of-4 searching, with the target state being $|00\rangle_{12}$. Qubit 0 is the coin qubit, while qubit 1 and 2 are database qubits. The Hadamard gates are applied to produce an equal superposition over all the computational bases. The solid circle represents 1-control gate whereas the open circle represents the opposite. The purpose of oracle C' is to implement $C_1 = R_x^0(\pi/2)$ (rotating qubit 0 around the x axis by angle $\pi/2$) when the database is $|00\rangle_{12}$ and $C_0 = R_x^0(3\pi/2)$ otherwise. It is equivalent to be replaced by $R_1 = R_x^0(3\pi/2)$ and $R_2 = R_x^0(-\pi)$. The two controlled-not gates are inverting qubit 1 if qubit 0 is $|1\rangle_0$ and inverting qubit 2 if qubit 0 is $|0\rangle_0$, respectively. The measurement requires all the populations' reconstruction. Similar circuits can be obtained in a straightforward manner for other target states. For instance, if the goal is $|10\rangle_{12}$, we need only change the controlled condition of the three-body-interaction gate to state $|10\rangle_{12}$.

(I) Applying a Hadamard operation to every qubit to prepare the state

$$|\psi_i\rangle = \frac{|0\rangle_0 + |1\rangle_0}{\sqrt{2}} \otimes \frac{|0\rangle_1 + |1\rangle_1}{\sqrt{2}} \otimes \frac{|0\rangle_2 + |1\rangle_2}{\sqrt{2}}, \tag{20}$$

which is exactly an equal superposition over all the computational bases.

(II) Perform the oracle C' on the coin qubit depending on the state of database qubits, namely, $C_1 = R_x^0(\pi/2) = e^{-i\pi\sigma_x/4}$ if the database qubits are on the target state $|\tau\sigma\rangle_{12}$, and $C_0 = R_x^0(3\pi/2) = e^{-i3\pi\sigma_x/4}$ otherwise. Therefore, the whole coin operation is

$$C' = C_0 \otimes (E_{12} - |\tau\sigma\rangle_{12} {}_{12}\langle\tau\sigma|) + C_1 \otimes |\tau\sigma\rangle_{12} {}_{12}\langle\tau\sigma| \qquad (21)$$

where E_{12} is the identity operator. Then the database qubits undergo the shift operation S conditioned on the state of coin qubit:

$$|0\rangle_0 |00\rangle_{12} \Longleftrightarrow |0\rangle_0 |01\rangle_{12}$$
$$|0\rangle_0 |10\rangle_{12} \Longleftrightarrow |0\rangle_0 |11\rangle_{12}$$
$$|1\rangle_0 |00\rangle_{12} \Longleftrightarrow |1\rangle_0 |01\rangle_{12}$$
$$|1\rangle_0 |01\rangle_{12} \Longleftrightarrow |1\rangle_0 |11\rangle_{12} \qquad (22)$$

(III) Repeat step (II) twice to implement the quantum walk, which will reach the final state

$$\left|\psi_f\right\rangle = (SC')^2 |\psi_i\rangle \qquad (23)$$

(IV) Measure all the populations of the database qubits. For example, in the case of finding $|00\rangle_{12}$, we can obtain that the probabilities of $|00\rangle_{12}$, $|01\rangle_{12}$, $|10\rangle_{12}$, $|11\rangle_{12}$ are 0.5, 0.25, 0.25, 0, respectively.

For other target states, with the controlled condition changed to the target node similar networks can be given easily. The results have an analogy with the aforementioned one.

4.2 NMR experimental implementation

Now we turn to our NMR quantum computer to implement the SKW algorithm. The three qubits are represented by the three ^{1}H spins in a sample of 1-Bromo-2,3-Dichlorobenzene oriented in liquid-crystal solvent (ZLI-1132). The molecular structure is shown in Fig.12(a). The system Hamiltonian can be described as

$$\mathcal{H} = \sum_{j=1}^{3} 2\pi\nu_j I_z^j + \sum_{j,k,j<k\leqslant 3} 2\pi J_{jk}(I_x^j I_x^k + I_y^j I_y^k + I_z^j I_z^k)$$
$$+ \sum_{j,k,j<k\leqslant 3} 2\pi D_{jk}\left(2I_z^j I_z^k - I_x^j I_x^k - I_y^j I_y^k\right) \qquad (24)$$

where ν_j is the resonance frequency of the jth spin, D_{jk} and J_{jk} are the dipolar coupling strengths and scalar coupling strengths between spins j and k, respectively. All the sums are restricted to the spins within one molecule. All experiments were carried out on a Bruker Avance 500 MHz spectrometer at room temperature. The spectrum of the thermal equilibrium state $\rho_{th} = \sum_{i=1}^{3} \sigma_z^i$ followed by a $\pi/2$ hard pulse is shown in Fig.12(b). With some initially guessed parameters assuming the molecular geometry, we iteratively fit the calculated and observed spectra through the parameters' perturbation (Suryaprakash (2000)). The values of parameters are listed in Table.1(a).

Since the system Hamiltonian has nondiagonal elements, the eigenstates are not Zeeman product states any more but linear combinations of them. To simplify the measurement of
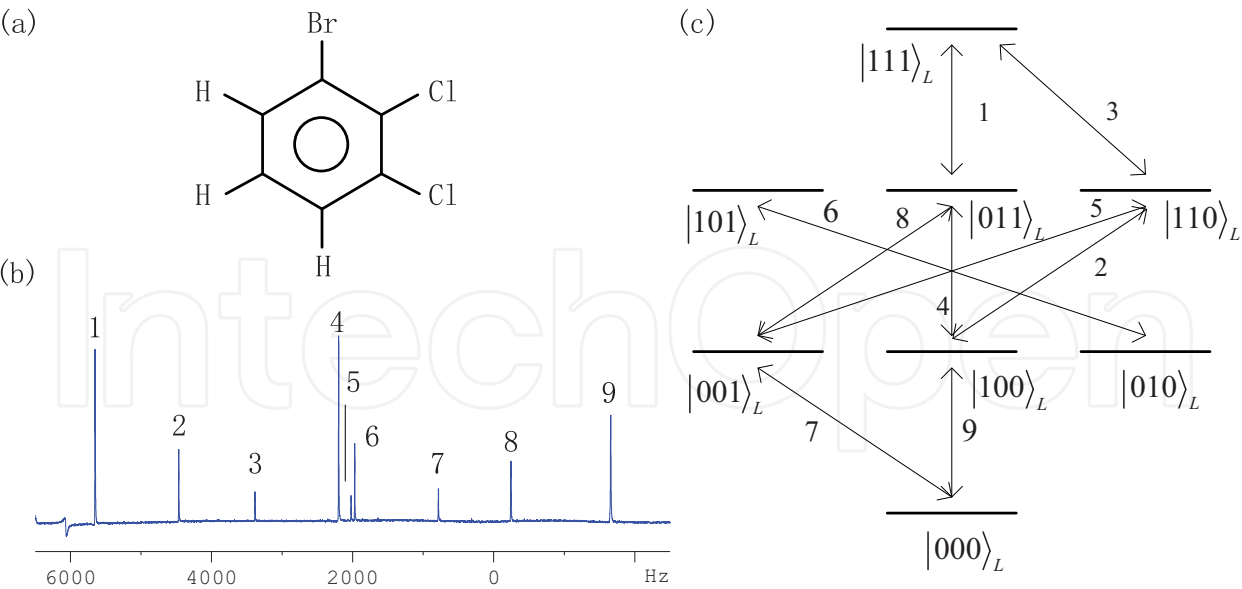
Fig. 12. (a) Molecular structure of 1-Bromo-2,3-Dichlorobenzene in which the three protons form a 3-qubit system. (b) Spectrum of the thermal equilibrium state followed by a $\pi/2$ hard pulse. All the observable transitions are labeled according to the descending orders of the frequencies. (c) Diagram of corresponding transitions in the eigenbasis.

(a)

	H_1	H_2	H_3
H_1	1945.5	−1633.3	−1341.7
H_2	8	2094.8	−339.35
H_3	8	1.4	2147.2

(b)

spin 1 No.9	$UR_y^1(\pi/2)$	$UR_y^1(\pi/2)R_y^2(\pi)$	$UR_y^1(\pi/2)R_y^3(\pi)$	$UR_y^1(\pi/2)R_y^{2,3}(\pi)$
	$P(1)-P(5)$	$P(3)-P(7)$	$P(2)-P(6)$	$P(4)-P(8)$
spin 2 No.8	$UR_y^2(\pi/2)$	$UR_y^2(\pi/2)R_y^1(\pi)$	$UR_y^2(\pi/2)R_y^3(\pi)$	$UR_y^2(\pi/2)R_y^{1,3}(\pi)$
	$P(2)-P(4)$	$P(6)-P(8)$	$P(1)-P(3)$	$P(5)-P(7)$
spin 3 No.7	$UR_y^3(\pi/2)$	$UR_y^3(\pi/2)R_y^1(\pi)$	$UR_y^3(\pi/2)R_y^2(\pi)$	$UR_y^3(\pi/2)R_y^{1,2}(\pi)$
	$P(1)-P(2)$	$P(5)-P(6)$	$P(3)-P(4)$	$P(7)-P(8)$

Table 1. (a) The parameters for fitting the spectrum of 1-Bromo-2,3-Dichlorobenzene (Hertz). The diagonal elements are chemical shifts of the three protons, the upper-right off-diagonal elements are dipolar coupling strengths, and the lower-left ones are scalar coupling strengths. (b) The read-out pulses and corresponding values of $P(i) - P(j)$. The results are shown on the transitions of No.9, 8 and 7.

populations (marked from $P(1)$ to $P(8)$), we found a feasible unitary matrix U to realize the transformation between the computational basis and eigenbasis, which satisfies

$$H_L = U H_S U^\dagger, \tag{25}$$

where H_S is the system Hamiltonian and H_L is a diagonal Hamiltonian (i.e., the Hamiltonian in the eigenbasis). With adding the pulse of implementing transformation matrix U after the original readout pulses in liquid NMR and combining with the normalization $\sum_{i=1}^{8} P(i) = 1$, we can obtain all eight population values straightforwardly. Table. 1 (b) shows all the available values of $P(i) - P(j)$ through different read-out pulses (for more explanations and details see Lu et al. (2010).

The experiment was divided into three steps: the psesudo-pure state preparation, quantum random walk searching process, and population measurement. Starting from the thermal equilibrium state, firstly we need to create the PPS $\rho_{000} = \frac{1-\epsilon}{8}\mathbf{1} + \epsilon |000\rangle \langle 000|$, where ϵ represents the polarization of the system and $\mathbf{1}$ is the identity matrix. We used shape pulses based on GRadient Ascent Pulse Engineering (GRAPE) algorithm (Baugh et al. (2007); Khaneja et al. (2005); Ryan et al. (2008)) and gradient pulses to realize the PPS preparation, with the numerical simulated fidelity 0.977.

The quantum random walk searching process contains two parts actually: The preparation of initial state $|+\rangle^{\otimes 3}$ ($|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$) and two iterations of unitary evolution. We packed them together and calculated one GRAPE pulse of 20ms and 250 segments whose fidelity is higher than 0.990. The reading-out operators listed in Table.1(b) are also performed when generating the GRAPE pulses of 20ms with the fidelity 0.990. The probabilities of gaining $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$ are 0.513, 0.232, 0.197, and 0.058, respectively, which demonstrates that we have completed searching $|00\rangle$ based on the SKW algorithm.

Besides $|00\rangle$, we altered the target states to $|01\rangle$, $|10\rangle$ and $|11\rangle$. The experimental results are plotted in Fig. 13. It can be seen the experimental and theoretical results are mostly consistent with little error. The slight difference between theory and experiment may be attributed to decoherence, the RF field inhomogeneity and imperfect implementation of GRAPE pulses.

In summary, we experimentally implemented a search algorithm based on the quantum random walk (the SKW algorithm) in the case of 1-out-of-4. This algorithm performs an oracle search on a database of N items with $O(\sqrt{N})$ calls, with a speedup similar to the Grover search algorithm. The experiment was carried out on an NMR quantum information processor with strongly dipolar coupled spins. We used GRAPE pulses to realize high-fidelity unitary operations and provided an effective way to measure the populations of the density matrix. The experimental results agree well with the theoretical expectations, which exhibits the superiority of the algorithm.

5. Quantum walk based search in nature

One of the astonishing phenomena of nature is the photosynthesis, which supplies all the chemical energy of our earth and acts as an important form of energy storage. However the high efficiency of the energy transfer in photosynthesis is still an enigma, the method of quantum walk has been introduced to try to explain the process of energy transfer (Mohseni et al. (2008); Rebentrost (2009)) since the quantum walk can increase the search efficiency with exponentially speed up in the case of the uncharted network (Childs et al. (2003)). Also in some literature the search process in photosynthesis from the pigment antenna to the reaction center is compared with the Grover type search, it is more natural to use the algorithm of section 3.2 to explain the high efficiency of the energy transfer process.
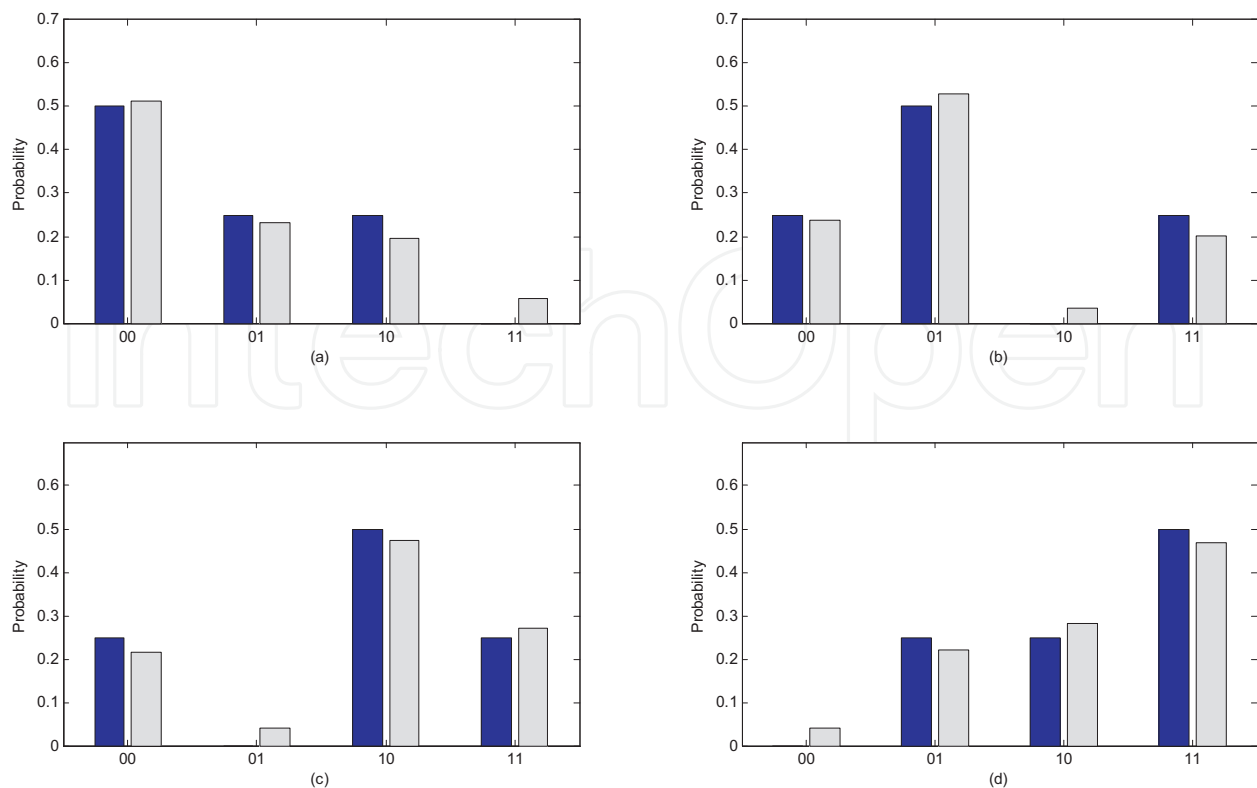
Fig. 13. Experimental results of the SKW algorithm. (a), (b), (c), (d) correspond to the cases of finding $|00\rangle_{12}$, $|01\rangle_{12}$, $|10\rangle_{12}$ and $|11\rangle_{12}$. The blue (dark) bars represent the theoretical prediction and the gray (light) bars represent the experimental analog, respectively.

5.1 Photosynthesis and quantum walk

In photosynthesis the energy is absorbed by pigments and then transferred to the reaction center where the energy is converted to the chemical energy and starts the electron transfer process. The most model of the energy transfer from the antennas to the reaction center is illustrated in the Fig. 14 (Blankenship (2002)). In the past the popular view is the excitons from the antennas hop to the reaction center, which is analogical to the classical random walk. However this is challenged by recent experiments and theory model, in which the quantum coherence is applying to the energy transfer process in order to explain the high efficiency in photosynthesis.

The first wavelike energy transfer through quantum coherence is found in FMO protein complex of purple bacteria at the temperature of 77K (Engel et al. (2007)) and soon the long lived quantum coherence in photosynthetic complexes is observed at physiological temperature (Panitchayangkoon et al. (2010)).

The theory model of the energy transfer in photosynthesis is using the quantum walk (Mohseni et al. (2008); Rebentrost (2009)), at most of the time the array of the pigment can be treated as a graph network of quantum walk (Fig. 15), in the figure the red sites is just as the exits of the Fig. 10 and the gray sites act as the entrance.

Another astonishing result is the assist of the environment to the quantum walk transport in photosynthetic energy transfer, if we know that environment is the main source of the decoherence of quantum systems and the decoherence is the main obstacle to build a quantum computer that surpass the classical computer. In contrast the interaction of the free Hamiltonian of the protein complex with the thermal fluctuations in the environment leads to an increase of the energy transfer efficiency from about 70% to 99% (Mohseni et al. (2008)).
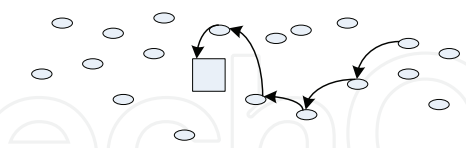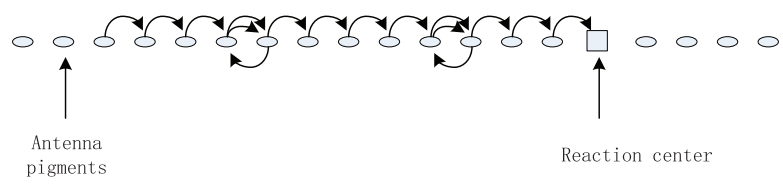
Fig. 14. Antenna organization models. The circle represents the antennas and the rectangle acts as the reaction center. The top schematic is the one dimensional array and the bottom schematic is the three dimensional array model. Of course the three dimensional model is more close to the actual case. The schematics come from the book written by Robert E. Blankenship. (Blankenship (2002)).
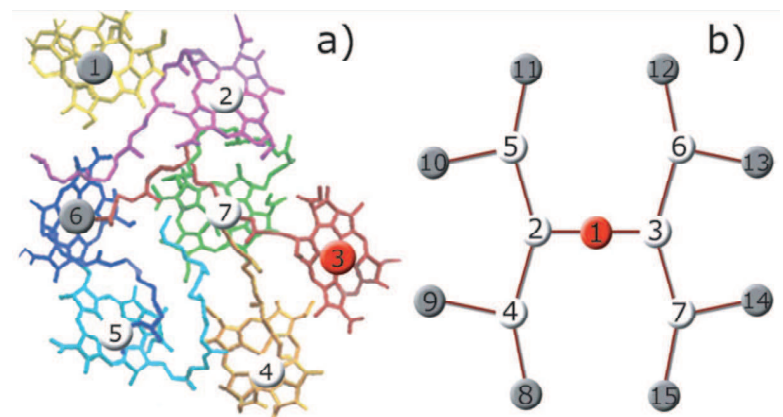

Fig. 15. a) chlorophyll molecules Fenna-Matthews-Olson (FMO) protein complex, this is investigated widely for its simple structure compared with the chlorophyll molecules in higher plant and algae. b) artificial systems described by a tight-binding Hamiltonian. Here is a four generation binary tree. In particular, an exponential speed up in reaching certain target sites (red) in these structures has been proposed in the context of quantum walk algorithms. (The gray sites represent initial states for the quantum transport.) (Rebentrost (2009)).

5.2 Biomimetic application in solar energy

Energy is a crucial problem for human since the fossil fuels are being exhausted. A commonly accepted alternative energy consuming way is to use the solar energy directly, since it can be got continuously. However the efficiency of utilizing the solar energy now is still very low. On the other hand the efficiency of the energy transfer in the photosynthesis is very high: more than 90% sometimes upon to 99%. If the energy transfer efficiency in the solar cell achieve to the same as in photosynthesis then the conversion efficiency of solar cell will double up. This will give an exciting perspective to the future of the energy utilization if we can understand the principle of the energy transfer in photosynthesis. Hitherto many groups have committed to build an artificial photosynthesis system, but so far no results successful enough have been obtained. Although many of them claim to solve the puzzler of the energy in the earth, from

a scientific view we cannot conclude when we can see the hydrogen emerge from the water extensively under the shine of the sun.

It is not necessary to list the benefit of the solar energy since there are so many eyes searching them. The only task for us is to make the principle of the photosynthesis clear so we can utilize it as we will do.

6. Conclusions and future directions

Quantum walk is another approach to design a quantum algorithm surpassing the classical algorithms, hitherto many scientists have made commitment to build a quantum computer. Apart from the search problem, there are many problems that can not be solved by classical computer efficiently, but can be solved by quantum algorithms in a relative short time. Quantum walk is not just the artificial tool for the search algorithm, but is also likely to be the tool for nature. All of these are instilling confidence for us to solve the intractable problems we have met.

However, the main obstacle of the quantum walk based algorithms including the search algorithm is the physical implementation since the decoherence occurs almost everywhere and every time. Thus in the future an important investigation is overcoming the decoherence or realizing the coherent manipulation of the quantum bits and quantum systems for relative long time in particular case. There are many physical systems proposed to implement the quantum computer and the quantum walk, but which is the practical one is still unknown. Quantum walk has been realized in various physical systems, first in NMR based computer (Du et al. (2003))for continuous time quantum walk and then coined quantum walk (Ryan et al. (2005)). Other successful physical systems include waveguide lattices (Perets et al. (2008)), trapped ions (Schmitz et al. (2009); Zähringer et al. (2010)), photon systems (Broome et al. (2010); Schreiber et al. (2010)) and optical lattices (Karski et al. (2009)). But the number of steps is still very small. Maybe the photons in waveguide lattice is a particular system since more than one hundred steps can be performed in it for the continuous quantum walk, though it is not convenient to modulate the walker. Anyway it is a great progress to realize the quantum walk in physical systems, based on which various search algorithms may be carried out.

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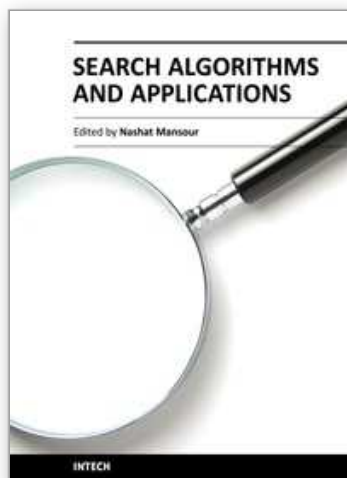
Search Algorithms and Applications

Edited by Prof. Nashat Mansour

Search algorithms aim to find solutions or objects with specified properties and constraints in a large solution search space or among a collection of objects. A solution can be a set of value assignments to variables that will satisfy the constraints or a sub-structure of a given discrete structure. In addition, there are search algorithms, mostly probabilistic, that are designed for the prospective quantum computer. This book demonstrates the wide applicability of search algorithms for the purpose of developing useful and practical solutions to problems that arise in a variety of problem domains. Although it is targeted to a wide group of readers: researchers, graduate students, and practitioners, it does not offer an exhaustive coverage of search algorithms and applications. The chapters are organized into three parts: Population-based and quantum search algorithms, Search algorithms for image and video processing, and Search algorithms for engineering applications.

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