THEORETICAL INVESTIGATION OF ELECTRONIC EXCITATION TRANSFER BETWEEN CHLOROPHYLLS IN LIGHT-HARVESTING ANTENNA OF PHOTOSYSTEM II USING QUANTUM COMPUTERS

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The excitation energy transfer between chlorophylls in major and minor antenna complexes of photosystem II (PSII) was investigated using quantum Fourier transforms. These transforms have an important role in the efficiency of quantum algorithms of quantum computers. The equation $2^N$ was used to make the connection between excitation energy transfers using quantum Fourier transform, where $n$ is the number of qubits required for simulation of transfers and $N$ is the number of chlorophylls in the antenna complexes.

Keywords: major and minor antenna of photosystem-II light-harvesting complex II (PSII-LHII) supercomplex; quantum Fourier transform; quantum gates.

INTRODUCTION

In higher plants, photosystem II-light-harvesting complex II (PSII-LHII) in the thylakoid membranes is a supercomplex containing PSII surrounded by the light harvesting complex which includes the major LHII proteins and three minor monomeric LHC proteins, CP29, CP26 and CP24. The supercomplex collects light energy, converts it into electro-chemical energy and drives electron transfer from water to plastoquinone. The reaction center (RC) is at the center of this complex.

The major LHII proteins are composed of three chlorophyll a/b binding proteins including LHII Type I, II and III, encoded by Lhcb1, Lhcb2 and Lhcb3 genes, respectively. The X-ray crystal structure of the major antenna LHII proteins in spinach (higher plants) at 2.72 Å resolution revealed that these proteins form trimers. Each monomer LHII polypeptide has been identified as 14 chlorophylls, 2 luteins and one neoxantin. These 14 chlorophylls (8 Chla and 6 Chlb) are vertically oriented into two layers lying close to the stromal or luminal surface. The eight chlorophylls (5 Chla and 3 Chlb) are located in the layer close to the stromal surface. The remaining six chlorophylls (3 Chla and 3 Chlb), which form two separate clusters including 4 chlorophylls (3 Chlb and 1 Chla) and a Chla-Chla dimer, are located in the layer close to the luminal surface.

The minor antennae CP29, CP26 and CP24 in green plants lie at the interface between the core antenna and the major antenna (LHII) of PSII-LHII supercomplex. These minor complexes, which together bind about 15% of total PSII chlorophyll, appear to be involved in the dissipation of the chlorophyll excitation energy required to stop overexcitation and photoinhibition of PSII. Since at the level of single atoms and photons, quantum effects are significant, classical computation essentially becomes insufficient. New methods of computation, for example, quantum computations, have become possible. The basic concepts of quantum mechanics computation were formulated more than 20 years ago.

The quantum Fourier transform

In mathematics and computer science, the transformation of a problem into some other with a known solution is a highly efficiently way of solving this problem. One such transformation is the discrete Fourier transform which can be computed much faster on a quantum computer than on a conventional computer. In the usual mathematical notation, for the discrete classical Fourier transform of $N$ inputs of complex numbers, $x_j (j = 0, 1, 2, ..., N-1)$, outputs $y_k (k = 0, 1, 2, ..., N-1)$ can be defined as:

\[ y_k = \sum_{j=0}^{N-1} x_j \cdot e^{-2\pi i jk/N} \]
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\[ y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j e^{2\pi i j k/N} \]  

(1)

Correspondingly, the discrete quantum Fourier transform on an
arthonormal basis |0\rangle, …, |N − 1\rangle is a unitary transformation which
is defined by

\[ |j\rangle \rightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i j k/N} |k\rangle \]  

(2)

It suffices to take \( N = 2^n \), with \( n \) as an integer, and the basis
|0\rangle, …, |2^n − 1\rangle is the computational basis for an \( n \)-qubit quantum
computer. It is preferable to write the state |j\rangle using the binary re-
presentation \( j = j_1 j_2 \ldots j_n \). More formally

\[ j = j_1 2^{n-1} + j_2 2^{n-2} + \ldots + j_n 2^0 \]  

(3)

For simplicity, the quantum Fourier transform can be rewritten
as the following useful product representation:

\[ |j, j_2, \ldots, j_n\rangle \rightarrow \frac{1}{\sqrt{2^n}} \left( |0\rangle + e^{2\pi i j_1 2^{n-1}} |1\rangle \right) \ldots \left( |0\rangle + e^{2\pi i j_n 2^0} |1\rangle \right) \]  

(4)

where \( j_1, j_2, \ldots, j_n \rightarrow \frac{j_1}{2} + \frac{j_2}{4} + \ldots + \frac{j_n}{2^{n-1}} \)

and \( j_l (l = 1, 2, \ldots, n) \) is equal to 0 or 1.

As explained later this representation allows construction of an
efficient quantum circuit for the Fourier transform.¹⁴

Quantum gates

The internal state of the quantum computer is changed by quantum
gates. A quantum gate is a sequence of unitary operations, the so-called
quantum algorithm. In the first step, we introduce the Hadamard, ro-
tational and swap gates which are useful in quantum algorithms. The
Fourier transformations can be performed very efficiently by these gates.

The Hadamard gate which sets one qubit in superposition is a
single-qubit gate defined by:

\[ H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \]  

(6)

A symbolic representation of the Hadamard gate is given in
Figure 1a.

\[ R_k \]  

(7)

A symbolic representation of \( R_k \) is given in Figure 1b. This gate
is depends on whether qubit \( k \) is 0 or 1.

The swap gate interchanges two qubit and a graphical represen-
tation of this gate is shown in Figure 1c.

Efficient circuits for the quantum Fourier transform

To construct the quantum circuit that performs QFT on an \( n \)-
qubit quantum computer, a specific sequence of the \( H \) and \( R_k \) gates
is applied. The efficient circuit for the quantum Fourier transform is
shown in Figure 2. The blocks labeled H perform a Hadamard trans-
form, and the other blocks perform a controlled phase shift by the
angle indicated. The series of swap gates that interchange the output
qubits is not shown in the circuit. Consider what happens when the state
\( |j_1, j_2, \ldots, j_n\rangle \) is input. The Hadamard gate which sets the first qubit
in superposition is applied in the first step.

\[ \frac{1}{\sqrt{2}} \left( |0\rangle + e^{2\pi i j_1} |1\rangle \right) |j_2, \ldots, j_n\rangle \]  

(8)

where \( e^{2\pi i j_1} = +1 \) when \( j_1 = 0 \), and is –1 otherwise. In the se-
cond step, a unitary controlled-\( R_k \) gate is applied and produces the
state

\[ \frac{1}{\sqrt{2}} \left( |0\rangle + e^{2\pi i j_k 2^k} |1\rangle \right) |j_2, \ldots, j_n\rangle \]  

(9)

"Figure 1. Graphical representation of some of the basic gates used in quantum
computation; (a) Hadamard gate; (b) rotational (\( R_k \)) gate; (c) swap gate"

"Figure 2. Efficient circuit for the quantum Fourier transform. This circuit is
easily derived from the product representation (4) for the quantum Fourier
transform. Not shown are swap gates at the end of the circuit which reverse
the order of the qubits in the output"

We carry on applying the controlled-\( R_k \), \( R_k \) through \( R_k \) gates, each
of which adds an extra qubit to the phase of co-efficient of the first
|1\rangle. Finally, this gives the state:

\[ \frac{1}{\sqrt{2}} \left( |0\rangle + e^{2\pi i j_k 2^k} |1\rangle \right) |j_2, \ldots, j_n\rangle \]  

(10)

Next, a similar procedure is carried out on the second qubit. The
Hadamard gate is applied to the second qubit:

\[ \frac{1}{\sqrt{2}} \left( |0\rangle + e^{2\pi i j_2 2^1} |1\rangle \right) |j_3, \ldots, j_n\rangle \]  

(11)

and the controlled-\( R_k \) through \( R_k \) gates yield the state:

\[ \frac{1}{\sqrt{2}} \left( |0\rangle + e^{2\pi i j_2 2^1} |1\rangle \right) |j_3, \ldots, j_n\rangle \]  

(12)

Continuing in this manner for each qubit gives the final state:

\[ \frac{1}{\sqrt{2}} \left( |0\rangle + e^{2\pi i j_2 2^1} |1\rangle \right) \ldots \left( |0\rangle + e^{2\pi i j_n 2^0} |1\rangle \right) \]  

(13)

The relationship between quantum computers and light
harvesting complexes of PSII

Excitation transition resulting from photon absorption in each
of light harvesting complexes of major (LHCII) and minor antennas
(CP29, CP29 and CP24) of PSII, could be simulated with quantum
computers. The relationship between quantum computers and the
light harvesting complexes is established with QFT.
The relationship between electron excitation transfer in a LHCII monomer and QFT

LHCII is a major antenna and has an important role in effective absorption of light energy. The configuration and number of chlorophyll are different in both luminal and stromal near-to-surface layers of membrane. Since the number of chlorophylls is an important parameter in determination of qubits in QFT, simulation of excitation transfer between chlorophylls in these two surfaces is studied individually with QFT.

In order to determine the relationship between the number of chlorophylls with QFT, the \(2^n = N\) equation is used. In this equation, \(n\) represents the number of required qubits for simulation of transfers with QFT and \(N\) represents the number of chlorophylls and also indicates the number of states or the number of the computational basic set.

The total number of chlorophylls in the monomer luminal surface is six molecules. These chlorophylls are configured in two individual clusters with 2 and 4 molecules of chlorophylls, respectively. Since the number of chlorophylls is different in this surface, these two clusters are simulated with QFT individually.

The relationship between binary cluster of luminal surface of LHCII monomer and QFT

In the binary cluster of the luminal surface, by substituting the number of chlorophylls (\(N = 2\)) using the equation \(2^n = N\) we obtain the number of qubits (\(n\)) which is equal to 1. The transfer energy between chlorophylls of the binary cluster of LHCII luminal monomer surface can then be simulated with a single-qubit Fourier transform. In order to achieve this, the equations outlined in the section above are rewritten and executive quantum circuits of these transforms drawn.

Rewriting equations for single-qubit Fourier transform

For single-qubit Fourier transform, basic set includes two members \(|0\rangle, |1\rangle\), thus the state used is \(|j\rangle = |j\rangle\), which by substituting in Equation 2 gives Equation 14:

\[
|j\rangle \rightarrow \frac{1}{\sqrt{2}} \left[ (|0\rangle + e^{2\pi ij/2} |1\rangle) \right] \quad (14)
\]

\(j/2 = 0.j\), is replaced and Equation 14 becomes Equation 15:

\[
|j\rangle \rightarrow \frac{1}{\sqrt{2}} \left[ (|0\rangle + e^{2\pi 0.1j} |1\rangle) \right] \quad (15)
\]

Equation 15 is now executing a single-qubit Fourier transform.

Drawing executive quantum circuits of single-qubit Fourier transform

The executive circuit diagram of the single-qubit Fourier transform is shown in Figure 3. A two-member basis set \(|0\rangle, |1\rangle\) is the input and \(\frac{1}{\sqrt{2}} \left[ (|0\rangle + e^{2\pi 0.1j} |1\rangle) \right]\) is the output. This circuit has only one Hadamard gate. Table 1 shows the output of single-qubit Fourier transform for the states \(|0\rangle\) and \(|1\rangle\).

Table 1. Representations of single-qubit Fourier transform

| \(|j\rangle\) | Output of first qubit |
|---|---|
| \(|0\rangle\) | \(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\) |
| \(|1\rangle\) | \(\frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi 0.1j} |1\rangle)\) |

Matrix representation of single-qubit Fourier transforms

Fourier transforms can be shown in matrix notation. The number of columns and rows of the matrix is given by \(2^n\), where \(n\) represents number of qubits. Representing the operator of Fourier transform as \(F\), the \(2 \times 2\) matrix elements \(F\) can be rewritten as follows:

\[
\langle j | F | j \rangle = \frac{1}{\sqrt{N}} e^{2\pi ij/N} 
\]

Therefore, the single-qubit Fourier transform matrix \(F\) can be written as:

\[
F = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} 
\]

The relationship between quartet cluster of luminal surface of LHCII monomer and QFT

In this cluster, by substituting the number of chlorophylls (\(N = 4\)) in the equation \(2^n = N\), we then obtain the number of qubits (\(n\)) which is equal to 2. Energy transfer between chlorophylls of the quartet cluster of the LHCII monomer luminal surface can be simulated with a two-qubit Fourier transform. In order to achieve this, the equations outlined in the section above are rewritten and executive quantum circuits of these transforms then drawn.

Rewriting equations for two-qubit Fourier transform

For two-qubit Fourier transform, the basic set includes four members \(|00\rangle, |01\rangle, |10\rangle, |11\rangle\), where state used is \(|j\rangle = |j_1j_2\rangle\), which by substituting in Equation 3, gives \(j = 2j_1 + j_2\). Table 2 shows all states \(|j\rangle\). The state \(|j\rangle\) in terms of qubits \(|0\rangle\) and \(|1\rangle\) can thus be expressed as:

\[
|j\rangle \rightarrow \frac{1}{2} \left[ (|0\rangle + e^{2\pi 0.1j} |1\rangle) (|0\rangle + e^{2\pi 0.1j} |1\rangle) \right] 
\]

Substituting Equation 3 into Equation 18 and comparing the results with Equation 5 gives the state vector of the system in the form of Equation 19:

\[
|j\rangle \rightarrow \frac{1}{2} \left[ (|00\rangle + e^{2\pi j_1} |11\rangle) (|00\rangle + e^{2\pi j_2} |11\rangle) \right] 
\]

Equation 19 is executing two-qubit Fourier transform.

Table 2. States of \(j\) for quartet cluster of luminal surface of LHCII monomer

| \(j_1\) | \(j_2\) | \(j = 2j_1 + j_2\) | \(|j\rangle = |j_1j_2\rangle\) |
|---|---|---|---|
| 0 | 0 | 0 | \(|0\rangle = |00\rangle\) |
| 0 | 1 | 1 | \(|1\rangle = |01\rangle\) |
| 1 | 0 | 2 | \(|2\rangle = |10\rangle\) |
| 1 | 1 | 3 | \(|3\rangle = |11\rangle\) |
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The circuit that represents two-qubit Fourier transform is shown in Figure 4.

\[ F = \frac{1}{\sqrt{4}} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & e^{2\pi i/4} & e^{2\pi i/4} & e^{2\pi i/4} \\ 1 & e^{2\pi i/4} & e^{2\pi i/4} & e^{2\pi i/4} \\ 1 & e^{2\pi i/4} & e^{2\pi i/4} & e^{2\pi i/4} \end{bmatrix} \]

The matrix elements may be written out explicitly, using powers of \( \omega \) as shown in Equation 24:

\[ F = \frac{1}{\sqrt{4}} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & -1 & \omega^3 \\ 1 & -1 & 1 & -1 \\ 1 & -\omega & -1 & \omega^2 \end{bmatrix} \]

where \( \omega = e^{2\pi i/4} \).

Investigation of excitation energy transfer between chlorophylls of stromal surface of a LHCII monomer using QFT

The total number of chlorophylls in the stromal surface of the LHCII monomer is equal to eight molecules, which are configured in an octet cluster. Substitution of \( N = 8 \) in the equation \( 2^n = N \) gives a value of \( n \) of 3. Thus transfer energy among chlorophylls of octet cluster of the LHCII monomer stromal surface can be simulated with a three-qubit Fourier transform. In order to achieve this, the equations outlined in the section above are rewritten and executive quantum circuits of this transform then drawn.

Rewriting equations for three-qubit transform for three-qubit Fourier transform

The basic set includes eight members \( \{|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle\} \) thus state used is \( |j\rangle = |j_1 j_2 j_3\rangle \) which by substituting in Equation 3, gives \( j = 4j_1 + 2j_2 + j_3 \). Table 4 shows the all states \(|j\rangle\). The state \(|j\rangle\) in terms of qubits \(|0\rangle\) and \(|1\rangle\) can be expressed as:

\[ |j\rangle \rightarrow \frac{1}{2^{3/2}} \left[ (|0\rangle + e^{2\pi i/4} |1\rangle)(|0\rangle + e^{2\pi i/4} |1\rangle) \right] \]

\[ (|0\rangle + e^{2\pi i/4} |1\rangle) \]

Table 4. States of \( j \) for octet cluster of steromal surface of monomer LHCII

| \( j_1 \) | \( j_2 \) | \( j_3 \) | \( j = 4j_1 + 2j_2 + j_3 \) | \( |j\rangle = |j_1 j_2 j_3\rangle \) |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 000 |
| 0 | 0 | 1 | 1 | 001 |
| 0 | 1 | 0 | 2 | 010 |
| 0 | 1 | 1 | 3 | 011 |
| 1 | 0 | 0 | 4 | 100 |
| 1 | 0 | 1 | 5 | 101 |
| 1 | 1 | 0 | 6 | 110 |
| 1 | 1 | 1 | 7 | 111 |

Substituting Equation 3 into Equation 25 and comparing the results with Equation 5 gives the state vector of the system as shown in Equation 26:

\[ |j\rangle \rightarrow \frac{1}{2^{3/2}} \left[ (|0\rangle + e^{2\pi i/4} |1\rangle)(|0\rangle + e^{2\pi i/4} |1\rangle) \right] \]

\[ (|0\rangle + e^{2\pi i/4} |1\rangle) \]
Equation 26 is executing three-qubit Fourier transform.

Drawing executive quantum circuits of three-qubit Fourier transform

The circuit that represents three-qubit Fourier transform is shown in Figure 5.

To construct the quantum circuit that performs three-qubit QFT, a specific sequence of the Hadamard and $R_2$ rotation gates is applied. The input state is the computational base state $|j_1j_2j_3\rangle$. For the first sequence, the Hadamard, $R_2$, and $R_3$ rotation gates are applied on the first qubit. For the second sequence, the Hadamard and $R_2$ rotation gates are applied on the second qubit. For the third sequence, the Hadamard gate is applied on the third qubit. Applying the Hadamard gate to the first qubit produces the state:

$$|j_1j_2j_3\rangle\rightarrow\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_1/2}|1\rangle)|j_2j_3\rangle$$ (27)

Applying the $R_2$ and $R_3$ rotation gates produce the state:

$$\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_2/4}|1\rangle)|j_3\rangle=\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/8}|1\rangle)|j_1j_2\rangle$$ (28)

Applying the Hadamard gate and then $R_2$ rotation gate to the second qubit produce the state:

$$\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_2/8}|1\rangle)(|0\rangle+e^{2\pi i j_3/16}|1\rangle)|j_3\rangle=\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_2/8}|1\rangle)\left(|0\rangle+e^{2\pi i j_3/16}|1\rangle\right)|j_3\rangle$$ (29)

Applying the Hadamard gate to the third qubit produces:

$$\frac{1}{\sqrt{2^3}}\left[\left(|0\rangle+e^{2\pi i j_2/4}\right)\left(|0\rangle+e^{2\pi i j_3/8}\right)\left(|0\rangle+e^{2\pi i j_3/16}\right)\right]\left(|0\rangle+e^{2\pi i j_2/8}\right)$$ (30)

Comparing Fourier transform represented as output Equation 26 with circuit output Equation 30 shows that the position of qubits in these equations is inverted. One swap gate omitted from Figure 5 is then used to reverse the order of the qubits.

Table 5 shows the output of three-qubit Fourier transform for the eight states $|000\rangle$, $|001\rangle$, $|010\rangle$, $|100\rangle$, $|011\rangle$, $|101\rangle$, $|110\rangle$, and $|111\rangle$.

Matrix representation of three-qubit Fourier transform

The three-qubit Fourier transform operator $F$ can be written as an 8x8 matrix which has the following form:

$$F=\frac{1}{\sqrt{8}}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ e^{2\pi i 8/8} & e^{4\pi i 8/8} & e^{6\pi i 8/8} & e^{8\pi i 8/8} & e^{10\pi i 8/8} & e^{12\pi i 8/8} & e^{14\pi i 8/8} & e^{16\pi i 8/8} \\ e^{6\pi i 8/8} & e^{8\pi i 8/8} & e^{10\pi i 8/8} & e^{12\pi i 8/8} & e^{14\pi i 8/8} & e^{16\pi i 8/8} & e^{18\pi i 8/8} & e^{20\pi i 8/8} \\ e^{12\pi i 8/8} & e^{8\pi i 8/8} & e^{14\pi i 8/8} & e^{20\pi i 8/8} & e^{22\pi i 8/8} & e^{24\pi i 8/8} & e^{26\pi i 8/8} & e^{28\pi i 8/8} \\ e^{12\pi i 8/8} & e^{14\pi i 8/8} & e^{20\pi i 8/8} & e^{22\pi i 8/8} & e^{24\pi i 8/8} & e^{26\pi i 8/8} & e^{28\pi i 8/8} & e^{30\pi i 8/8} \\ e^{14\pi i 8/8} & e^{20\pi i 8/8} & e^{26\pi i 8/8} & e^{30\pi i 8/8} & e^{32\pi i 8/8} & e^{34\pi i 8/8} & e^{36\pi i 8/8} & e^{38\pi i 8/8} \\ e^{16\pi i 8/8} & e^{22\pi i 8/8} & e^{28\pi i 8/8} & e^{34\pi i 8/8} & e^{36\pi i 8/8} & e^{38\pi i 8/8} & e^{40\pi i 8/8} & e^{42\pi i 8/8} \\ e^{20\pi i 8/8} & e^{26\pi i 8/8} & e^{32\pi i 8/8} & e^{38\pi i 8/8} & e^{40\pi i 8/8} & e^{42\pi i 8/8} & e^{44\pi i 8/8} & e^{46\pi i 8/8} \end{bmatrix}$$ (31)

The matrix elements may be written out explicitly, using powers of $i\pi$ as shown in Equation 32:

| Table 5. Representations of three-qubit Fourier transform |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $|j\rangle$     | $|j_1j_2j_3\rangle$ Output of first qubit | Output of second qubit | Output of third qubit |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| $|0\rangle$     | $|000\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ |
| $|1\rangle$     | $|001\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_1/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ |
| $|2\rangle$     | $|010\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_2/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/4}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/4}|1\rangle)$ |
| $|3\rangle$     | $|011\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/4}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ |
| $|4\rangle$     | $|100\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_2|1\rangle})$ | $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ |
| $|5\rangle$     | $|101\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_2/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/4}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/4}|1\rangle)$ |
| $|6\rangle$     | $|110\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ |
| $|7\rangle$     | $|111\rangle$    | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ | $\frac{1}{\sqrt{2}}(|0\rangle+e^{2\pi i j_3/2}|1\rangle)$ |
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Table 6. Representation of relationship among the number of qubits and chlorophylls with number of gates in the major and minor complexes of PSII

<table>
<thead>
<tr>
<th>Minor antenna</th>
<th>LHCII</th>
<th>Major antenna</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>Sterolal surface</td>
<td>Lumenal surface</td>
</tr>
<tr>
<td>CP24</td>
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<td>8</td>
</tr>
<tr>
<td>CP26</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>CP29</td>
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</tbody>
</table>

\[ F = \frac{1}{\sqrt{N}} \left[ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \right] \]

\[ \omega^* = e^{2\pi i/8}. \]

The relationship between electron excitation transfer in minor antenna monomers CP24, CP26, CP29 with QFT

Minor antenna of Photosystem II consists of 3 monomers CP29, CP26 and CP24 whose number of chlorophylls is 8, 9 and 10 molecules, respectively. Substitution of \( N = 8, 9, \) and 10 in the equation \( 2^n = N \) gives \( n \) values of 3, 3.17, and 3.32, respectively. For good approximation, excitation transfer among chlorophylls can be simulated in each of the monomers CP24, CP26 and CP29 with a three-qubit Fourier transform. Likewise, the executive quantum circuits and matrix representation could be applied for simulation of electron excitation transfer in minor antenna monomers CP24, CP26, CP29 using three-qubit Fourier transform (Table 6).

CONCLUSIONS

Quantum computers exist in nature. Photosynthesis is one example in which a quantum computer component may play a role in the classical world of complex biological systems. Biological systems represent an untapped resource for thinking about the design and operation of quantum computers and expanding our current conception of what defines a ‘quantum computer’ in nature.

In this report excitation energy transfer among chlorophylls of light-harvesting major complexes (LHCII) and light-harvesting minor complexes (CP24, CP26 and CP29) of Photosystem II was studied for the first time using quantum computers. The results have shown that excitation energy transfer among chlorophylls of these antenna systems can be simulated with quantum Fourier transform.

In order to establish a relationship between excitation energy transfer resulting from photon absorption by chlorophyll molecules of minor and major antenna with quantum Fourier transforms, equation \( 2^n = N \) has been used. In this equation, \( n \) represents the number of required qubits for the simulation with QFT and \( N \) shows the number of states created with \( n \)-qubit Fourier transform which is equal to the number of chlorophylls in the studied antenna system.

Since the number of chlorophylls is a major factor for the determination of the number of required qubits in the simulation with QFT, transfer in each complex was studied individually.

The electron excitation transfer in binary and quartet clusters of the luminal surface of the LHCII monomer was simulated using single and two-qubit Fourier transforms, respectively. The three-qubit Fourier transform was applied to simulate the electron excitation transfer in the octet cluster of the luminal surface of the LHCII monomer and CP26, CP24, and CP29 monomers. Table 6 provides a brief summary of our results. Simulator quantum circuits of these transforms in each part have been drawn using Hadamard, \( R_\theta \) rotation and swap quantum gates.

REFERENCES