Markovian quantum simulation of Fenna-Matthew-Olson (FMO) complex using one-parameter semigroup of generators

M.Mahdian* and H.Davoodi Yeganeh†

Faculty of Physics, Theoretical and astrophysics department, University of Tabriz, 51665-163 Tabriz, Iran

Abstract

The application of the theory of open quantum systems in biological processes such as photosynthetic complexes, has recently received renewed attention. In this paper, a quantum algorithm is presented for simulation of arbitrary Markovian dynamics of the FMO complex exist in photosynthesis using a 'universal set' of one-parameter semigroup of generators. We investigate the detailed constitution of each generator that obtain from spectral decomposition of the Gorini-Kossakowski-Sudarshan (GKS) matrix by using of linear combination and unitary conjugation. Also, we design a quantum circuit for implementing of these generators.

Keyword FMO complex, Linear combination, Unitary conjugation, GKS matrix

*mahdian@tabrizu.ac.ir
†h.yeganeh@tabrizu.ac.ir
1 Introduction

In recent years, the study of biological systems in which quantum dynamics are visible and the theory of open quantum system is applied to describe these dynamics have attracted much attention [1]. One of these biological systems in plants is a group of prokaryotes like green sulfur bacteria that utilize photosynthesis as a process to produce energetic chemical compounds by free solar energy. Harvesting of light energy and its conversion to cellular energy currently is mainly done in photosystem complexes present in all photosynthetic organisms [2]. Photosystem is mainly constructed of two linked sections: an antenna unit includes several proteins referred as light-harvesting complexes (LHCs) which absorb light and conduct it to the reaction center (RC). Both the LHCs and RC consists of many pigment molecules that increases accessible spectrum for the photosynthesis process. After absorbing a photon, the FMO antennae complex transfers it to the RC and acts like a quantum wire between the antenna and RC [3]. The FMO complex structure is relatively simple, consisting of three monomers. Each monomer environment includes seven bacterial proteins or molecules called bacteriochlorophyll (BChl). The key process in photosynthesis is the interaction of light with the electronic degrees of freedom of the pigment molecules which are quantum mechanical in nature also long-lived quantum coherence among the electronic excited states of the multiple pigments in FMO complex has been shown by 2D electronic spectroscopy [4, 5, 6, 7, 8]. After the pigment molecule absorbs the light energy, it goes from a ground state to an excited state and also behaves like two-level system. Several researchers have studied the electronic excitation transfer by diverse methods such as Forster theory in weak molecular interaction limit or by Redfield master equations derived from Markov approximation in weak coupling regime between molecules and environment [3, 9, 10, 11]. Effective dynamics in the FMO complex is modeled by a Hamiltonian which describes the coherent exchange of excitations between sites and local Lindblad terms that take into account the dissipation and dephasing caused by the surrounding environment [12].

Classical computers fail to efficiently simulate quantum systems with complex many-body interactions due to the exponential growth of variables for characterizing these systems. Quantum simulation was proposed to solve such an exponential explosion problem using a controllable quantum system as originally conjectured by Feynman [13, 14, 15]. The dynamical evolution of closed systems is described by unitary transformation and can be simulated
directly with quantum simulator. In the real world, all quantum systems are invariably in contact with an environment and are an open quantum system. Therefore, the dynamic evolution of these systems in the presence of decoherence and dissipation are non-unitary operations. Generally, dynamics of open quantum system is very complex and often used to describe the dynamics of proximity like the Born and Markov approximations are used [16]. A lot of analytical and numerical methods have been employed to simulate the dynamics of open quantum systems like composition framework for the combination and transformation of semigroup generators, simulation of Markovian quantum dynamics by logic network and in particular simulation of arbitrary quantum channels [17, 18, 19, 20, 21, 22]. However, in these methods there exists no universal set of non-unitary processes through which all such processes can be simulated via sequential simulations from the universal set, but they are applicable in many problems. Rayn et al. introduce efficient method to simulate Markovian open quantum system, described by a one-parameter semigroup of quantum channels, which can be through sequential simulations of processes from the universal set. They use linear combination and unitary conjugation to simulate Markovian open quantum systems [23].

The simulation dynamics of light-harvesting complexes is highly regarded and a large number of various experimental and analytically studies has been conducted on them. Finding spectral density by molecular dynamics and numerical method has been studied in [24, 25, 26]. The system dynamics simulation have been done with different platforms for implementing quantum simulators, such as two-dimensional electronic spectroscopy [27], superconducting qubits [28] and nuclear magnetic resonance [29, 30]. In this paper, we use a linear combination and unitary conjugation to simulate Markovian non-unitary processes in photosynthetic FMO complex. Also, we consider of constructing efficient quantum circuits based on quantum gate model for the quantum dynamic simulation subject to dissipation and dephasing environment.

The remainder of the paper is organized as follows. In Sec.2 we give a brief description of effective dynamics FMO complex. We descrip method to universal simulation of Markovian open quantum systems. in Sec.3. In Section 4 calculations to simulate the non-Unitarian processes in photosynthetic FMO complex will be study. We finally express our results in Sec.5.
2 FMO complex

The FMO complex is generally constituted of multiple chromophores which transform photons into excations and transport to a RC. As already mentioned that efficient dynamics FMO complex express by combining Hamiltonian which describe the coherent exchange of excitations between sites, and local Lindblad terms that take into account the dephasing and dissipation caused by the external environment as non-unitary evolution [12]. For expressing the dynamics of the non-unitary part assumed that the system is susceptible simultaneously to two distinct types of noise processes, a dissipative process and dephasing process. Dissipative processes pass on excitation energy with rate $\Gamma_j$ to the environment and dephasing process destroys the phase coherence with rate $\gamma_j$ of site $j^{th}$. We approached the Markovian master equation for FMO complex, dissipative and dephasing processes are captured with local terms, respectively, by the Lindblad super-operators as:

$$\mathcal{L}_{\text{diss}}(\rho) = \sum_{j=1}^{7} \Gamma_j (-\sigma_j^+ \sigma_j^- \rho - \rho \sigma_j^+ \sigma_j^- + 2 \sigma_j^- \rho \sigma_j^+), \quad (1)$$

$$\mathcal{L}_{\text{deph}}(\rho) = \sum_{j=1}^{7} \gamma_j (-\sigma_j^+ \sigma_j^- \rho - \rho \sigma_j^+ \sigma_j^- + 2 \sigma_j^- \rho \sigma_j^+ \sigma_j^-). \quad (2)$$

Where $\sigma_j^+ = |j\rangle \langle 0|$ and $\sigma_j^- = |0\rangle \langle j|$ are raising and lowering operators for site $j$ respectively and $|j\rangle = |g_1\rangle \otimes ... \otimes |e_j\rangle \otimes ... \otimes |g_7\rangle$ denote one excitation in the site $j$. That mean’s $|j\rangle$ are basis of single excitation space. Finally, the total transfer of excitation is measured by the population in the sink.

3 Simulation of non-unitary dynamics of FMO complex

Assume that we have quantum system coupled to a environment with the Hilbert space $\mathcal{H}_S \cong \mathbb{C}^d$ and a state of this system can be describe by density matrix $\rho \in \mathcal{M}_d(\mathbb{C})$. The density matrix evolves according to a quantum Markovian master equation

$$\frac{d}{dt} \rho(t) = \mathcal{L} \rho(t), \quad (3)$$
where $\mathcal{L}$ is the generator of one parameter semigroup of quantum channels $\{T(t)\}$ [16]. At time $t > t_0$, the state of the quantum system obtained from $\rho(t) = T(t - t_0)\rho(t_0)$. In this case we almost can write $\mathcal{L}\rho(t)$ follow as:

$$
\mathcal{L}(\rho) = i[\rho, H] + \sum_{l,k} A_{l,k}(F_l \rho F_k^\dagger - \frac{1}{2}\{F_k^\dagger F_l, \rho\}),
$$

(4)

where $H$ is Hermitian operator ($H \in \mathcal{M}_d(\mathbb{C})$), $A_{l,k}$'s are element’s matrix $A \in \mathcal{M}_{d^2-1}(\mathbb{C})$ and $\{F_i\}$ is basis for the space of traceless matrix’s in $\mathcal{M}_d(\mathbb{C})$. Eq. (4) is known as the Gorini, Kossakowski, Sudarshan and Lindblad (GKSL) form of the quantum Markov master equation and $A$ is the GKS matrix. By diagonalisation of the GKS matrix $A$, we obtain Lindblad master equation as

$$
\mathcal{L}(\rho) = i[\rho, H] + \sum_{k=1}^n \gamma_k (L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\}),
$$

(5)

where $n$ is the number of non-zero eigenvalues of $A$.

We begin by transforming Lindblad master equation into the GKS form. After obtaining the GKS matrix $A$, we decompose $A$ into the linear combination of rank 1 generators through the spectral decomposition. Then each constituent generator $\vec{a}_k \vec{a}_k^\dagger$ decomposed into the unitary conjugation of a semigroup from the universal set. See reference [18, 23] for details and proof of Theorem.

### 3.1 Dissipative processes

For the dissipative process we have

$$
\mathcal{L}_{\text{diss}}(\rho) = \sum_{j=1}^7 \Gamma_j (-\sigma_j^+\sigma_j^- \rho - \rho\sigma_j^+\sigma_j^- + 2\sigma_j^-\rho\sigma_j^+),
$$

(6)

We use the fact of $\{F_k\}$ is basis for the space of traceless matrix’s in $\mathcal{M}_8(\mathbb{C})$ and $\{iF_k\}$ is a basis for $su(8)$, has the following form:

$$
\{F_i\}_{i=1}^7 \equiv d^l, \quad d^l = \frac{1}{\sqrt{l(l+1)}}[\sum_{j=1}^l |j\rangle\langle j| - l(l+1)|l+1\rangle\langle l+1|],
$$

(7)

$$
\{F_i\}_{i=8}^{35} \equiv \{\sigma^{jk}_x\}_{j<k \leq 8}, \quad \sigma^{jk}_x = \frac{1}{\sqrt{2}}(|j\rangle\langle k| + |k\rangle\langle j|),
$$

(8)
In our problem, we find, after simplifying:

transformation is the phase transformation. If

where \( \hat{a} \) set. In general form, we can write

decomposed into the unitary conjugation of a semigroup from the universal set. Now we can write

\[\vec{\alpha} = (a_1, \ldots, a_{35})^T\] by \( a_i = \frac{\pi}{2}, \quad i = 1, \ldots, 34 \) and \( a_{35} = \frac{3\pi}{2} \) for \( k = 1, 2, \ldots, 7 \). So we can implement

\[
\vec{a}_k \hat{a}_k^\dagger = G_{U(k)}[A^{(k)}(\theta_k, \hat{a}_k^R, \hat{a}_k^I)]G_{U(k)}^T,
\]

Now we can write \( \sigma_j^+ \) and \( \sigma_j^- \) as below

\[
\sigma_j^+ = \frac{1}{\sqrt{2}} (F_{j+7} - iF_{j+35}) \quad \text{and} \quad \sigma_j^- = \frac{1}{\sqrt{2}} (F_{j+7} + iF_{j+35}).
\]

So by putting up in Eq.(6) GKS matrix can be obtained and nonvanishing elements of GKS matrix \( A \) are

\[
\begin{array}{cccc}
  a_{8,8} = \Gamma_1 & a_{36,36} = \Gamma_1 & a_{8,36} = -i\Gamma_1 & a_{36,8} = i\Gamma_1 \\
  a_{9,9} = \Gamma_2 & a_{37,37} = \Gamma_2 & a_{9,37} = -i\Gamma_2 & a_{37,9} = i\Gamma_2 \\
  a_{10,10} = \Gamma_3 & a_{38,38} = \Gamma_3 & a_{10,38} = -i\Gamma_3 & a_{38,10} = i\Gamma_3 \\
  a_{11,11} = \Gamma_4 & a_{39,39} = \Gamma_4 & a_{11,39} = -i\Gamma_4 & a_{39,11} = i\Gamma_4 \\
  a_{12,12} = \Gamma_5 & a_{40,40} = \Gamma_5 & a_{12,40} = -i\Gamma_5 & a_{40,12} = i\Gamma_5 \\
  a_{13,13} = \Gamma_6 & a_{41,41} = \Gamma_6 & a_{13,46} = -i\Gamma_6 & a_{46,13} = i\Gamma_5 \\
  a_{14,14} = \Gamma_7 & a_{42,42} = \Gamma_7 & a_{14,42} = -i\Gamma_7 & a_{42,14} = i\Gamma_7 \\
\end{array}
\]

Now, we decompose the matrix’s \( A \) as:

\[
A = \sum_{k=1}^{7} \lambda_k \vec{a}_k \hat{a}_k^\dagger,
\]

where \( \lambda_k = 2\Gamma_k \) and \( a_k \)s have non-vanishing elements \( a_{k+7} = -i\frac{1}{\sqrt{2}} \) and \( a_{k+35} = \frac{1}{\sqrt{2}} \). Now, each generator \( \vec{a}_k \hat{a}_k^\dagger \) of the linear combination should decomposed into the unitary conjugation of a semigroup from the universal set. In general form, we can write

\[
e^{i\psi_k} \vec{a}_k = \cos(\theta_k) \hat{a}_k^R + i \sin(\theta_k) \hat{a}_k^I,
\]

where \( \hat{a}_k^R \) and \( \hat{a}_k^I \) are real and imaginary part of \( a_k \), respectively and \( \psi \) is the phase transformation. If \( \hat{a}_k^R \hat{a}_k^R = 0 \) and \(|\hat{a}_k^R| = |\hat{a}_k^I| = 1\) then the phase transformation is \( \psi = 0 \) and \( \theta_k \in [0, \pi/4] \).

In our problem, we find, after simplifying: \( \psi_k = 0 \), \( \theta_k = \pi/4 \), \( \vec{a}_k^R = 0 \) and \( \vec{a}_k^I = (a_1, \ldots, a_{35})^T \) by \( a_i = \pi/2, \quad i = 1, 2, \ldots, 34 \) and \( a_{35} = 3\pi/2 \) for \( k = 1, 2, \ldots, 7 \). So we can implement

\[
\vec{a}_k \hat{a}_k^\dagger = G_{U(k)}[A^{(k)}(\theta_k, \vec{a}_k^R, \vec{a}_k^I)]G_{U(k)}^T,
\]
where \( A^{(k)}(\theta_k, \alpha^R_k, \alpha^I_k) \) represents an element of the universal set of semigroup generators and \( G_{U^{(k)}} = \text{Int}(U^{(k)}) \) by considering \( U^{(k)} = U_k \) that \( U_n \) is single unitary operation \( R_y(-\frac{\pi}{2}) \) and \( U_{lm} \) is two qubit gate. Furthermore if \( L_k \) is generator of a Markovian semigroup, we can simulate any channel \( T_k(t) = \exp(tL_k) \) from the semigroup generated by \( \alpha^R_k \alpha^I_k \),

\[
T_k(t)(\rho) = U^{(k)^\dagger}(T_{A^{(k)}}(t)[U^{(k)}\rho U^{(k)^\dagger}]U^{(k)},
\]

where \( T_{A^{(k)}}(t) = \exp(tL_{A^{(k)}}) \).

We drive this equation’s for semigroup generated by \( \alpha^R_1 \alpha^I_1 \) directly. For \( \alpha^I_1 \) we obtain \( \alpha^R_1 = |36\rangle, \alpha^I_1 = -|8\rangle \).

The next step is finding \( \tilde{\alpha}^R_1 \) and \( \tilde{\alpha}^I_1 \), for this work we use of map \( f : su(8) \rightarrow \mathbb{R}^{63} \) that define as \( f(iF) = |j\rangle \). If define \( \tilde{A}^{R} \equiv f^{-1}(\hat{a}^R_1) \), we have

\[
\hat{A}^{R}_1 = iF_{36},
\]

by using of the matrix \( U^{(1)}_1 \), the matrix \( \tilde{A}^{R}_1 \) can be diagonalized as

\[
U^{(1)}_1 = \begin{pmatrix}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

\[
\tilde{A}^{R}_{d,1} \equiv U^{(1)}_1 \hat{A}^{R}_1 U^{(1)^\dagger}_1 = iF_1.
\]

For imaginary part

\[
\hat{A}^{I}_1 = -iF_8,
\]

and

\[
\hat{A}^{I}_1 \equiv U^{(1)}_1 \hat{A}^{I}_1 U^{(1)^\dagger}_1 = -iF_{36} \equiv \tilde{A}^{I}_1,
\]

we need not to find \( U^{(2)}_2 \) because of \( A^{I}_1 \) is desired form. So

\[
f(\tilde{A}^{R}_{d,1}) = |1\rangle, \quad f(\tilde{A}^{I}_1) = -|36\rangle.
\]
If we define \( \tilde{a}_1^R = f(\tilde{A}_1^R) \) and \( \tilde{a}_1^I = f(\tilde{A}_1^I) \) we haven’t second unitary transformation because \( \tilde{a}_1^R \) and \( \tilde{a}_1^I \) have desired form. So by defining \( U^{(1)} = U_1^{(1)\dagger} \) and \( G_{U^{(1)}} = Int(U^{(1)}) \), we can implement

\[
\tilde{a}_1\tilde{a}_1^\dagger = G_{U^{(1)}}[A^{(1)}(\theta_1, \tilde{a}_1^R, \tilde{a}_1^I)]G_{U^{(1)}}^T,
\]

where \( A^{(1)}(\theta_1, \tilde{a}_1^R, \tilde{a}_1^I) \) is an element of the universal set of semigroup generators, by \( \theta_1 = \pi/4 \), \( \tilde{a}_1^R = 0 \), \( \tilde{a}_1^I = (a_1, \ldots, a_{35}) \) by \( a_i = \pi/2 \), \( i = 1, 2, \ldots, 34 \) and \( a_{35} = 3\pi/2 \). Furthermore if \( \mathcal{L}_1 \) is generator of a Markovian semigroup we can simulate any channel \( T_1(t) = \exp(t\mathcal{L}_1) \) from the semigroup generated by \( \tilde{a}_1\tilde{a}_1^\dagger \),

\[
T_1(t)(\rho) = U^{(1)\dagger}(T_A^{(1)}(t)[U^{(1)}\rho U^{(1)\dagger}])U^{(1)},
\]

where \( T_A^{(1)}(t) = \exp(t\mathcal{L}_A^{(1)}) \).

Now we are designing the quantum circuit for implement of \( U_1^{(i)} \). At first we obtain quantum circuit for implement \( U_1^{(1)} \) and for other \( U_1^{(i)} \) similarly circuit can be designed. By finding action of unitary operation \( U_1^{(1)} \) on the \( |q_1, q_2, q_3\rangle \) where three qubits space bases, we obtain below conditions.

1. If second qubit was in state \( |1\rangle \), state of qubit’s first and third gets be NOT.

2. If first and second qubit was in state \( |0\rangle \), state of third qubit will be rotation.

3. If first qubit were in state \( |1\rangle \) and second qubit in state \( |0\rangle \), state of third qubit will be flip.

Given the above conditions we need two CNOT gate, a single qubit gate \( (R_y(-\pi/2)) \) and a X gate. Quantum circuit for implement of \( U_1^{(1)} \) shown in Fig.1

---

![Figure 1: Quantum circuit for implement of \( U_1^{(1)\text{dissipative}} \)](image-url)
3.2 Dephasing process

Similarly, in the previous section we obtain GKS matrix for this process and decompose it. So we have

\[ A = \sum_{k=1}^{7} \lambda_k \vec{a}_k \vec{a}_k^\dagger, \quad (23) \]

with \( \lambda_k = 4\gamma_k \) for \( k = 2, 3, \ldots, 7 \) and \( \lambda_1 = 4\sqrt{2}\gamma_1 \). \( \vec{a}_1 \) have nonvanishing elements \( a_{10} = \frac{-i(1+\sqrt{2})}{\sqrt{4+2\sqrt{2}}} \), \( a_{38} = \frac{1}{\sqrt{4+2\sqrt{2}}} \). Nonvanishing elements of \( \vec{a}_2 \) are \( a_{16} = \frac{1}{\sqrt{2}}(-2i) \), \( a_{47} = \frac{1}{\sqrt{2}} \) and for \( \vec{a}_3 \): \( a_{12} = \frac{1}{\sqrt{5}}(-2i) \), \( a_{40} = \frac{1}{\sqrt{5}} \). As the same way nonvanishing elements of \( \vec{a}_4, \vec{a}_5, \vec{a}_6, \vec{a}_7 \) are \( \psi_k = \frac{\pi}{2} \) for \( k = 1, 2, 3 \) and equal with zero for \( k = 4, \ldots, 7 \). \( \theta_1 = \arccos(\frac{1+\sqrt{2}}{\sqrt{4+2\sqrt{2}}} \), \( \theta_2 = \theta_3 = \arccos(\frac{2}{\sqrt{5}}) \) and \( \theta_k = \frac{\pi}{4} \) for \( k = 4, \ldots, 7 \).

Furthermore we can obtain \( \vec{a}_{1,7}^R = 0 \) and \( \vec{a}_{1,7}^I = (a_1, \ldots, a_{35})^T \) by \( a_i = \frac{\pi}{2}, \ i = 1, 2, \ldots, 34 \) and \( a_{35} = \frac{3\pi}{2} \) for \( \vec{a}_{2,3} \) can be written \( \vec{a}_{2,3}^R = 0, \ \vec{a}_{2,3}^I = \pi \), and for \( \vec{a}_{4,5,6} \) we obtain \( \vec{a}_{4,5,6}^R = \vec{a}_{4,5,6}^I = \pi \).

Now we consider semigroup generated by \( \vec{a}_1 \vec{a}_1^\dagger \) and decompose it into the unitary conjugation of a semigroup from the universal set. we begin by \( \hat{a}_1^R = |10\rangle, \ \hat{a}_1^I = |38\rangle \). So

\[ f^{-1}(\hat{a}_1^R) = f^{-1}(|10\rangle) = iF_{10} = \hat{A}_1^R, \]

now by using of \( U_1^{(1)} \) we can diagnose the matrix \( \hat{A}_1^R \).

\[ U_1^{(1)} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (24) \]

Then we’ll have

\[ U_1^{(1)} \hat{A}_1^R U_1^{(1)\dagger} = iF_1 = \hat{A}_d^R. \]
for an imaginary part

\[ f^{-1}(\hat{a}_1^I) = f^{-1}(|38\rangle) = iF_{38} = \hat{A}_1^R, \]

and

\[ U_1^{(1)} \hat{A}_1^I U_1^{(1)\dagger} = iF_{36} = \widetilde{A}_1^I, \]

because \( \hat{A}_1^I \) is desired form, no need to find a matrix \( U_2^{(1)} \). If we define \( \tilde{a}_1^R \equiv f(\hat{A}_1^R) = |1\rangle \) and \( \tilde{a}_1^I \equiv f(\hat{a}_1^I) = |36\rangle \). We need not to second unitary transformation because \( \tilde{a}_1^R \) and \( \tilde{a}_1^I \) are have the desired form. By consider 

\[ U^{(1)} = U_1^{(1)\dagger} \text{ and } G_{U^{(1)}} = \text{Int}(U^{(1)}) \text{ similar to the previous one} \]

\[ \tilde{a}_1 \tilde{a}_1^\dagger = G_{U^{(1)}}[A^{(1)}(\theta_1, \tilde{a}_1^R, \tilde{a}_1^I)]G_{U^{(1)}}^T, \]

where \( A^{(1)}(\theta_1, \tilde{a}_1^R, \tilde{a}_1^I) \) an element of the universal set of semigroup generators, by \( \theta_1 = \text{arccos}(\frac{1+\sqrt{2}}{\sqrt{4+2\sqrt{2}}} \). \( \tilde{a}_1^R = 0 \) and \( \tilde{a}_1^I = (a_1, \ldots, a_{35})^T \) by \( a_i = \pi/2, \ i = 1, 2, \ldots, 34 \) and \( a_{35} = 3\pi/2 \). Furthermore if \( L_1 \) is generator of a Markovian semigroup we can simulate any channel 

\[ T_1(t) = \text{exp}(tL\tilde{a}_1\tilde{a}_1^\dagger), \]

where \( T_1^{(1)}(t) = \text{exp}(tL_{A^{(1)}}) \).

Note in any case must be calculated \( U_1^{(1)} \) and \( U_i^{(2)} \) for \( i = 2, \ldots, 6 \) except in case \( \tilde{a}_{1,7} \) that their calculation is straightforward.

Now we design quantum circuit to implement of \( U_1^{(1)} \). We drive below conditions by finding action of \( U_1^{(1)} \) on three qubits space bases.

1. If first and second qubit was in state \( |0\rangle \) and \( |1\rangle \), state of qubit third will be rotation.

2. If first qubit was in state \( |1\rangle \) and second qubit in state \( |0\rangle \), state of qubit third will be flip.

3. If second qubit was in state \( |1\rangle \), state of qubit’s first and third gets be NOT.

4. For state \( |001\rangle \) does not exist output.

Furthermore via two CNOT gate and single qubit gate \( R_y(-\frac{\pi}{2}) \) and a one gate \( X \), unitary operation \( U_1^{(1)} \) can be implement.

Quantum circuit of \( U_1^{(1)} \) shown in Fig.2. For other \( U_i^{(1)} \) quantum circuit can be design analogous \( U_1^{(1)} \).
4 Conclusion

In this paper, we have investigated universal simulation of Markovian dynamics of FMO complex. At first we have transformed Lindblad master equation into the GKS form for non-Unitarian processes in FMO complex. Next decomposed GKS matrix into the linear combination of rank 1 generators through the spectral decomposition. Then each constituent generator $\hat{a}_k \hat{a}_k^\dagger$ decomposed into the unitary conjugation of a semigroup from the universal set. Finally, the quantum circuit had designed for implementing unitary matrix’s that applied for simulation of the structure generators.

References

[1] N. Lambert, Y.-N. Chen, Y.-C. Cheng, C.-M. Li, G.-Y. Chen, and F. Nori, “Quantum biology,” Nature Physics, vol. 9, no. 1, p. 10, 2013.

[2] O. Sinanoğlu, Modern Quantum Chemistry: Action of light and organic crystals. Academic Press, 1965.

[3] M. Grover and R. Silbey, “Exciton migration in molecular crystals,” J. Chem. Phys., vol. 54, no. 11, pp. 4843–4851, 1971.

[4] D. Jonas, “Two-dimensional femtosecond spectroscopy,” Annual review of physical chemistry, vol. 54, pp. 425–63, 02 2003.

[5] S. Mukamel, “Multidimensional femtosecond correlation spectroscopies of electronic and vibrational excitations,” Annual review of physical chemistry, vol. 51, pp. 691–729, 02 2000.
[6] M. Khalil, N. Demirdöven, and A. Tokmakoff, “Coherent 2d ir spectroscopy: Molecular structure and dynamics in solution,” Journal of Physical Chemistry A - J PHYS CHEM A, vol. 107, 06 2003.

[7] P. Tian, D. Keusters, Y. Suzaki, and W. S Warren, “Femtosecond phase-coherent two-dimensional spectroscopy,” Science (New York, N.Y.), vol. 300, pp. 1553–5, 07 2003.

[8] T. Brixner, T. Mancal, I. V Stiopkin, and G. R Fleming, “Phase-stabilized two-dimensional electronic spectroscopy,” The Journal of chemical physics, vol. 121, pp. 4221–36, 10 2004.

[9] M. Yang and G. R. Fleming, “Influence of phonons on exciton transfer dynamics: comparison of the redfield, förster, and modified redfield equations,” J. Chem. Phys., vol. 282, no. 1, pp. 163–180, 2002.

[10] V. I. Novoderezhkin, M. A. Palacios, H. Van Amerongen, and R. Van Grondelle, “Energy-transfer dynamics in the lhcii complex of higher plants: modified redfield approach,” J. Phys. Chem. B, vol. 108, no. 29, pp. 10363–10375, 2004.

[11] S. Jang, M. D. Newton, and R. J. Silbey, “Multichromophoric förster resonance energy transfer,” Phys. Rev. Lett., vol. 92, no. 21, p. 218301, 2004.

[12] F. Caruso, A. W. Chin, A. Datta, S. F. Huelga, and M. B. Plenio, “Highly efficient energy excitation transfer in light-harvesting complexes: The fundamental role of noise-assisted transport,” J. Phys. Chem. B, vol. 131, no. 10, p. 09B612, 2009.

[13] R. P. Feynman, “Simulating physics with computers,” Int. J. Theor. Phys., vol. 21, no. 6-7, pp. 467–488, 1982.

[14] A. Trabesinger, “Quantum simulation.,” Nature Physics., vol. 8, no. 263, p. 00, 2012.

[15] I. M. Georgescu, S. Ashhab, and F. Nori, “Quantum simulation,” Rev. Mod. Phys., vol. 86, pp. 153–185, Mar 2014.

[16] H.-P. Breuer, F. Petruccione, et al., The theory of open quantum systems. Oxford University Press on Demand, 2002.
[17] M. Hillery, M. Ziman, and V. Bužek, “Implementation of quantum maps by programmable quantum processors,” *Phys. Rev. A*, vol. 66, no. 4, p. 042302, 2002.

[18] D. Bacon, A. M. Childs, I. L. Chuang, J. Kempe, D. W. Leung, and X. Zhou, “Universal simulation of markovian quantum dynamics,” *Phys. Rev. A*, vol. 64, no. 6, p. 062302, 2001.

[19] M. Ziman, P. Štelmachovič, and V. Bužek, “Description of quantum dynamics of open systems based on collision-like models,” *J. Open Syst. Inform. Dynam.*, vol. 12, no. 1, pp. 81–91, 2005.

[20] M. Koniorczyk, V. Buzek, P. Adam, and A. Laszlo, “Simulation of markovian quantum dynamics on quantum logic networks,” *arXiv preprint quant-ph/0205008*, 2002.

[21] M. Koniorczyk, V. Bužek, and P. Adam, “Simulation of generators of markovian dynamics on programmable quantum processors,” *J. Eur. Phys. D*, vol. 37, no. 2, pp. 275–281, 2006.

[22] D.-S. Wang, D. W. Berry, M. C. de Oliveira, and B. C. Sanders, “Solovay-kitaev decomposition strategy for single-qubit channels,” *Phys. Rev. Lett.*, vol. 111, no. 13, p. 130504, 2013.

[23] R. Sweke, I. Sinayskiy, D. Bernard, and F. Petruccione, “Universal simulation of markovian open quantum systems,” *Phys. Rev. A*, vol. 91, p. 062308, Jun 2015.

[24] X. Wang, G. Ritschel, S. Wüster, and A. Eisfeld, “Open quantum system parameters for light harvesting complexes from molecular dynamics,” *J. Phys. Chem. B*, vol. 17, no. 38, pp. 25629–25641, 2015.

[25] J. Moix, J. Wu, P. Huo, D. Coker, and J. Cao, “Efficient energy transfer in light-harvesting systems, iii: The influence of the eighth bacteriochlorophyll on the dynamics and efficiency in fmo,” *The Journal of Physical Chemistry Letters*, vol. 2, no. 24, pp. 3045–3052, 2011.

[26] M. B. A. M. Mahdian and F. Marahem, “Chain mapping approach of hamiltonian for fmo complex using associated, generalized and exceptional jacobi polynomials,” *International Journal of Modern Physics B*, vol. 30, no. 1650107, p. 16, 2016.
[27] S.-H. Yeh and S. Kais, “Simulated two-dimensional electronic spectroscopy of the eight-bacteriochlorophyll fmo complex,” *J. Phys. Chem.*, vol. 141, no. 23, p. 12B645_1, 2014.

[28] S. Mostame, J. Huh, C. Kreisbeck, A. J. Kerman, T. Fujita, A. Eisfeld, and A. Aspuru-Guzik, “Emulation of complex open quantum systems using superconducting qubits,” *J. Quantum Inf. Process.*, vol. 16, no. 2, p. 44, 2017.

[29] Q. A. T. X. N. L. D. R. Y.-C. C. F. N. F.-G. D. Bi-Xue Wang, Ming-Jie Tao and G.-L. Long, “Efficient quantum simulation of photosynthetic light harvesting,” *npj Quantum Information*, vol. 4, no. 52, 2018.

[30] H. Y. M. Mahdian, “Quantum simulation of fenna-matthew-olson(fmo) complex on a nuclear magnetic resonance(nmr) quantum computer,” *arXiv:1901.03118*. 