Theoretical framework for environment assisted quantum transport and it’s application to chemical complexes

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Environment assisted quantum transport (ENAQT) has been found to increase efficiency of energy transfer in open quantum systems. Chemical complexes like the photosynthetic Fenna-Mathews-Olson (FMO) complex exhibit such phenomenon. ENAQT in the FMO complex has been simulated on analog quantum simulators. However, digital quantum simulators are universal models for quantum simulation and offer greater flexibility over analog simulations. Here we develop the theoretical framework for digital quantum simulation of ENAQT in open quantum systems with tunable bath coupling. The main challenge in developing theoretical models for digital quantum simulation is that the solutions to the quantum master equation are unknown. We give an exact analytical solution for the Lindblad master equation for ENAQT and develop time evolution operators and evolution equation to solve the system. We apply the evolution equation to give a theoretical model for digital quantum simulation of the FMO complex and reproduce the high efficiency and temperature dependence of the dynamics in the complex.

I. INTRODUCTION

Quantum simulators are devices that can turn the exponential scaling of resources needed to simulate and understand properties of complex quantum systems on classical computers into a favourable polynomial overhead. Original proposal for quantum computers by Feynman [1] was to simulate complex quantum systems such as many body quantum systems in low temperature physics and lattice gauge theories. An algorithm by Shor to solve the discrete logarithm problem on a quantum computer [2] highlighted the broader application of quantum computers. However, a full scale quantum computer with millions of qubits is far from being realised [3]. Ongoing experimental research is geared towards making quantum simulators with small number of qubits [4] as first practical applications of a quantum computer. Quantum simulators can be analog or digital. Analog simulations use continuous time evolution models such as the Lindblad master equation [5]. Digital simulations are done using quantum gates for simulating discrete time evolution operators. Compared to analog quantum simulators, digital quantum simulations offer universality and flexibility [5]. One of the major challenges in building a quantum simulator has been the presence of noise due to environment. However, recently a number of studies have remarkably shown that noise can facilitate transmission of energy in quantum simulators through a process called environment assisted quantum transport(ENAQT) [6]. ENAQT is being studied [7] to understand the role of noise in building quantum simulators for various applications.

One of the important application of quantum simulators in near-term is to understand the dynamics in chemical systems. Chemical complexes have been found to show a variety of quantum effects [8] such as ENAQT. The Fenna-Mathews-Olson (FMO) protein complex is the one of most widely studied photosynthetic systems. It transfers the excitation energy from light harvesting antenna to the reaction centre in the photosynthetic complex of certain bacteria [9]. FMO complex has been studied for decades to understand the underlying mechanism of high efficiency excitation energy transfer(EET) [10] in photosynthetic complexes [11–19]. The phenomenon of delocalized exciton states has been observed via electronic spectroscopy in light-harvesting complexes [14] and the FMO protein complex [20]. A combination of quantum and classical effects have been observed to facilitate the transfer of excitation energy through the complex [20]. Engel et al. [15] found direct evidence for quantum coherence in the FMO complex and Mohseni et al. [21] gave a continuous time quantum walk model with environment assisted transport(ENAQT) to successfully explain the high efficiency. Quantum walks provide models for quantum simulation [22]. Quantum simulations of FMO complex have been done to understand simulations of open quantum systems [23] and other systems in quantum chemistry [24]. It is also being studied to develop efficient artificial light-harvesting systems [25]. Analog quantum simulations of FMO complex have been done on NMR quantum computer [26], superconducting qubits [27], superconducting circuits [28, 29] and ultracold atoms [30]. In [31, 32], Mahdian et al. described a setup for digitally simulating the FMO complex. But their study does not include quantum jumps and the interplay of quantum and classical effects which are the salient features of the environment assisted quantum walk. These previous studies led us to explore and characterize the theoretical model with a general framework for digital quantum simulation of the dynamics in chemical complexes along with FMO complex as a specific example.

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In this work, we develop a theoretical framework for digital simulation of environment assisted energy transfer in open quantum systems. Developing theoretical model for digital quantum simulation of open quantum systems proves to be challenging as one needs to solve the Lindblad master equation for which solution is otherwise not known. We give an exact analytical solution for the Lindblad Master Equation for this model and develop time evolution operators and evolution equation to solve the system. We apply the evolution equation to model environment assisted energy transfer in the FMO Complex and reproduce the high efficiency and temperature dependence of the dynamics in the complex. We use the quantum walk master equation of ENAQT to understand environment assisted energy transport. We abstract out the processes contributing to ENAQT and model them into an open quantum system. The key results of this paper are: evolution operators which capture the interplay of quantum and classical effects, and an evolution equation to solve the master equation with tunable bath coupling. We systematically find a discrete time dynamical model for environment assisted transport in a toy system with one quantum jump and then generalise it to model multiple quantum jumps. We give evolution operators for the system by combining unitary quantum evolution and Kraus operators (which model quantum jumps). Then we develop the density matrix evolution equation using these operators and prove that this equation is the discrete time solution of the Master equation. We show that the different terms in the equation uniquely capture decoherence and interplay of quantum jumps and unitary quantum evolution that cannot be captured by separately simulating the unitary and non unitary parts. Thus we obtain a general model for environment assisted transport in open quantum systems. We apply this model to simulate the dynamics of the FMO complex. The operators are made so as to characterize the delocalised exciton transfer. At the end, we generalise the evolution equation to model variable bath coupling due to dependence on the environment temperature. We demonstrate that calculations done using this model agree with theoretical and experimental evidences of the FMO complex dynamics.

This article is organised as follows. In Sec. II, the basic description of ENAQT is given. Sec. III describes master equation and it’s solution for ENAQT. In Sec. IV, the solution of the master equation is applied to simulate ENAQT in the FMO complex. The general model for variable bath coupling is presented in Sec. IV C. Some concluding remarks are given in Sec. V.

II. ENVIRONMENT ASSISTED QUANTUM TRANSPORT

Hamiltonians describing the dynamics of the quantum systems typically possess energy mismatches, that can hinder transmission of excitation due to Anderson localization [33]. However, quantum systems are also generally subjected to relatively high levels of environment-induced noise and decoherence. A certain degree of noise can cause transfer of excitation through classical processes, which can overcome localization. The interplay between the coherent dynamics of the system and the incoherent action of the environment can result in greater transport efficiency than coherent dynamics on its own [34]. This phenomenon is called ENAQT and is achieved through a combination of dephasing-relaxation noise and coherent dynamics. The Hamiltonian of the system due to pure quantum interactions is given by,

$$H = \sum_m \varepsilon_m |m\rangle \langle m| + \sum_{n<m} V_{mn} \left( |m\rangle \langle n| + |n\rangle \langle m| \right)$$  \hspace{1cm} (1)

where $\varepsilon_m$ are the energies of the states and $V_{mn}$ denotes the coupling leading to coherence between different states. The main effects of the environment, dephasing and relaxation lead to quantum jumps between states. Quantum jumps are represented by the following phonon bath Hamiltonian,

$$H_p = \sum_{m,n} q_{mn} |m\rangle \langle n|$$  \hspace{1cm} (2)

where $q_{mn}$ are the couplings due to the phonon bath. This leads to the Lindblad master equation,

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[H,\rho] + \mathcal{L}(\rho),$$

$$\mathcal{L}(\rho) = \sum_{m,n} \gamma_{mn} \left( L_{mn} \rho L_{mn}^\dagger - \frac{1}{2} L_{mn}^\dagger L_{mn} \rho - \frac{1}{2} \rho L_{mn} L_{mn}^\dagger \right)$$  \hspace{1cm} (3)

where $L_{mn} = |m\rangle \langle n|$ and $\gamma_{mn}$ is obtained from $q_{mn}$.

The dynamics of ENAQT depend on quantum coherence, described by the system Hamiltonian and on the environment induced quantum jumps between different states. Quantum coherence causes a speedup in transfer of energy from initial state to the final state. The quantum jumps give directionality to the walk and transfer the population density from initial state towards the final state. The environment causes decoherence of the states. These effects together cause a transfer of excitation energy in quantum systems. The overall dynamics due to environment are non unitary and trace preserving.

III. SOLUTION OF MASTER EQUATION FOR ENVIRONMENT ASSISTED QUANTUM TRANSPORT

A. Open quantum systems

We can represent a system in interaction with the environment as an open quantum system, where the environment is modelled by a phonon bath. An open quantum
system can be represented as a larger closed system with Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$, where $\mathcal{H}_B$ is the phonon bath Hilbert space [35]. Assuming the initial state is represented by the separable density matrix $\rho = \rho_S \otimes |0\rangle_B \langle 0|_B$, the evolution of the total system is,

$$\rho(t) = U_{SB}(\rho_S \otimes |0\rangle_B \langle 0|_B) U_{SB}^\dagger.$$  

A partial trace over B gives the evolution of the system $S$,

$$\rho_S(t) = Tr_B(\rho(t)) = \sum_k \langle k| U_{SB}(\rho_S \otimes |0\rangle_B \langle 0|_B) U_{SB}^\dagger |k\rangle \langle k| = \sum_k \langle k| U_{SB} |0\rangle_S \rho_S(0) \langle 0|_B U_{SB}^\dagger |k\rangle \langle k|$$

which in the form of Kraus operators $M_k$ will be,

$$\rho_S(t) = M(\rho_S(0)) = \sum_k M_k \rho_S(0) M_k^\dagger$$  \hspace{1cm} (4)

where

$$M_k = \langle k| U_{SB} |0\rangle = Tr_B(|0\rangle \langle k| U_{SB}).$$  \hspace{1cm} (5)

Here $|k\rangle$ is an orthonormal basis for $\mathcal{H}_B$ and $\sum_k M_k^\dagger M_k = \mathbb{1}$. This can be used to obtain operators for effects of environment on the system by introducing a bath to describe the dynamics and then tracing it out.

B. Numerical solution and it’s drawbacks

The conventional way of digital simulation of open quantum systems is to simulate quantum and classical dynamics separately in the following manner.

Pure quantum evolution under the Hamiltonian $H_S$ is given by,

$$\rho(t + \partial t) = U \rho(t) U^\dagger$$  \hspace{1cm} (6)

and the evolution of the system due to effects of the bath can be described using Kraus operators,

$$\rho_S(t) = M(\rho_S(0)).$$  \hspace{1cm} (7)

To get a system + environment evolution, we can combine Eq.6 and Eq.7 in the following manner to have trace preserving evolution,

$$\rho(t + \partial t) = (1 - \eta) U \rho(t) U^\dagger + \eta M(\rho_S(t))$$

where $\eta \in [0,1]$. This will lead to the following master equation,

$$\frac{\partial \rho(t)}{\partial t} = -(1 - \eta) \frac{i}{\hbar} [H_S, \rho(t)] + \eta L(\rho(t)).$$

We can note that the no value of $\eta$ can reproduce the actual master equation. This shows that separately simulating quantum and classical dynamics cannot capture the the interplay of quantum and classical effects in environment assisted quantum transport. One needs to solve the master equation to digitally simulate the environment assisted quantum dynamics.

C. Analytical solution

In this section we develop a model to digitally simulate ENAQT in open quantum systems by solving the Lindblad master equation. The model is a discrete time evolution equation of an open quantum system with energy transfer dynamics. We use the following methodology for developing the solution:

**Methodology:** To model both quantum and classical effects we introduce evolution operators which are a combination of Kraus operators and unitary quantum evolution. Using these operators, we derive the evolution equation for density matrix. We develop the general model by first taking a toy system and step by step adding different processes to it, to arrive at the final picture. We consider a system with one quantum jump and find a model for this toy system using the following procedure: We write an evolution for system + bath which appropriately captures the quantum jump. We trace out the bath from the evolution and find the Kraus operators for quantum jump in the system. Then, we introduce unitary quantum evolution to this system in addition to the quantum jump. Thus, the new evolution operators are obtained by appropriately combining Kraus operators and unitary quantum evolution operator. We use these operators to write the discrete time evolution equation for this setup, which appropriately captures the interplay of quantum and classical effects.

Next, we add another quantum jump to the system to generalise the toy model to simulate multiple quantum jumps. Again, we draw a parallel from the first case and follow the above procedure to develop a model for this setup. We write the evolution operators and arrive at the dynamical equation for this setup. This gives a general model for simulating ENAQT in open quantum systems with unitary quantum evolution and multiple environment induced quantum jumps.

1. Toy Model: Single quantum jump

Consider a 2 level system with states given by $|0\rangle_S$ and $|1\rangle_S$. Say the bath B induces a quantum jump from $|0\rangle_S$ to $|1\rangle_S$ with probability $p_{0\rightarrow 1}$. The system + bath evolution can be formalised as follows,

$$|0\rangle_S |0\rangle_B \rightarrow \sqrt{1 - p_{0\rightarrow 1}}|0\rangle_S |0\rangle_B + \sqrt{p_{0\rightarrow 1}}|1\rangle_S |1\rangle_B$$

$$|1\rangle_S |0\rangle_B \rightarrow |1\rangle_S |0\rangle_B.$$
The operators can be combined with unitary quantum evolution in their usual meaning, first term represents the quantum evolution and the second operator captures the decoherence due to the bath and contribute to the normalisation terms. The first term and the last term are due to the quantum jump. Correspondence of the different terms to the Lindblad equation given above can be seen here. $U$ and $U^\dagger$ capture the quantum coherence.

2. General Model: Multiple quantum jumps

We can generalise the previous setup by including another quantum jump from $|1\rangle_S$ to $|0\rangle_S$ with probability $p_{1\rightarrow 0}$. Then the system + bath evolution is given by,

\[
|0\rangle_S|0\rangle_B \rightarrow \sqrt{1 - p_{0\rightarrow 1}}|0\rangle_S|0\rangle_B + \sqrt{p_{0\rightarrow 1}}|1\rangle_S|1\rangle_B;
|1\rangle_S|0\rangle_B \rightarrow \sqrt{1 - p_{1\rightarrow 0}}|1\rangle_S|0\rangle_B + \sqrt{p_{1\rightarrow 0}}|0\rangle_S|1\rangle_B
\]

and the corresponding Kraus operators for the system, after tracing out the bath are:

\[
M_{00} = \sqrt{1 - p_{0\rightarrow 1}}|0\rangle\langle 0|, \quad M_{01} = \sqrt{p_{0\rightarrow 1}}|1\rangle\langle 0|;
M_{10} = \sqrt{p_{1\rightarrow 0}}|0\rangle\langle 1|.
\]

Adding quantum evolution to Kraus operators when the system is also subject to free Hamiltonian $H_S$, similar to the previous case leads to the following evolution operators:

\[
M'_{00} = M_{00} U, \quad M'_{01} = M_{01},
M'_{11} = M_{11} U, \quad M'_{10} = M_{10}.
\]

Drawing parallel from Eq.(13), the discrete time dynamical equation is given by:

\[
\rho(t + \Delta t) = (1 - p_{0\rightarrow 1})|0\rangle\langle 0|U\rho(t)U^\dagger|0\rangle\langle 0| + \sqrt{1 - p_{0\rightarrow 1}}|0\rangle\langle 0|U\rho(t)U^\dagger|1\rangle\langle 1|
+ \sqrt{1 - p_{1\rightarrow 0}}|1\rangle\langle 1|U\rho(t)U^\dagger|0\rangle\langle 0| + (p_{0\rightarrow 1})|1\rangle\langle 0|\rho(t)|0\rangle\langle 1|
+ (p_{1\rightarrow 0})|0\rangle\langle 1|\rho(t)|1\rangle\langle 0|.
\]

The second and the third terms of the preceding equation capture the decoherence due to the bath and contribute to the normalisation terms. The first term and the last term are due to the quantum jump.

Substituting Eq.(8) in Eq.(12),

\[
\rho(t + \Delta t) = (1 - p_{0\rightarrow 1})|0\rangle\langle 0|U\rho(t)U^\dagger|0\rangle\langle 0| + \sqrt{1 - p_{0\rightarrow 1}}|0\rangle\langle 0|U\rho(t)U^\dagger|1\rangle\langle 1|
+ \sqrt{1 - p_{0\rightarrow 1}}|1\rangle\langle 1|U\rho(t)U^\dagger|0\rangle\langle 0| + (p_{0\rightarrow 1})|1\rangle\langle 0|\rho(t)|0\rangle\langle 1|
+ (p_{1\rightarrow 0})|0\rangle\langle 1|\rho(t)|1\rangle\langle 0|.
\]

The Kraus operators for quantum jumps on the system, obtained from tracing out the bath are,

\[
M_0 = \begin{pmatrix} \sqrt{1 - p_{0\rightarrow 1}} & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad M_1 = \begin{pmatrix} 0 & 1 \\ \sqrt{p_{0\rightarrow 1}} & 0 \end{pmatrix}.
\]

The operators can also be written as,

\[
M_0 = \sqrt{1 - p_{0\rightarrow 1}}|0\rangle\langle 0| + |1\rangle\langle 1| \quad \text{and} \quad M_1 = \sqrt{p_{0\rightarrow 1}}|1\rangle\langle 0|.
\]

Now, introduce quantum evolution to the system. The Lindblad equation, with the system being subject to free Hamiltonian $H_S$ is,

\[
\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_S, \rho(t)] + L(\rho(t))
\]

where $L(\rho(t))$ is due to the effect of quantum jumps, where

\[
L(\rho(t)) = \sum_k [L_k \rho L_k^\dagger - \frac{1}{2}L_k L_k^\dagger \rho - \frac{1}{2} \rho L_k L_k^\dagger].
\]

Here $L_k$ are quantum jump operators. The terms carry their usual meaning, first term represents the quantum jumps and the other two terms are normalisation terms for the case when the jump does not happen. The Kraus operators can be combined with unitary quantum evolution as follows to solve this master equation,

\[
M'_0 = M_0 U \quad M'_1 = M_1
\]

where $U = e^{-\frac{\Delta t}{\hbar}H_S}$. It can be verified that $M'_0 M'_0 + M'_1 M'_1 = 1$. These evolution operators, Eq.(11), where $M'_0$ has unitary quantum evolution and $M'_1$ does not, will be useful to capture the appropriate dynamics, as will be proved in the following section. The operators can be interpreted as follows. Two processes are happening in the system at any time $t$: coherent evolution and quantum jumps. From a state, the population density can move out of the state via these two processes. From the total population, some goes out via quantum jumps. And from the population remaining after the quantum jumps, some goes out via quantum coherence. The second operator $M'_1$ depicts the moving out through quantum jumps. $M_0$ in the first operator capture's the population that remains after the quantum jump. From this remaining population, some moves out via quantum coherence as captured by $U$ in $M'_0 = M_0 U$.

Thus, the discrete time density matrix evolution equation obtained from these operators is given by,

\[
\rho(t + \Delta t) = M'_0 (\sqrt{\Delta t}) \rho(t) M'_0^\dagger (\sqrt{\Delta t}) + M'_1 (\sqrt{\Delta t}) \rho(t) M'_1^\dagger (\sqrt{\Delta t}).
\]
Substituting Eq. (15) in Eq. (16), we arrive at the general model for simulating quantum jumps and unitary quantum evolution,

\[
\rho(t + \Delta t) = M_{00}'(\sqrt{\Delta t})\rho(t)M_{00}'(\sqrt{\Delta t}) \\
+ M_{01}'(\sqrt{\Delta t})\rho(t)M_{10}'(\sqrt{\Delta t}) \\
+ M_{11}'(\sqrt{\Delta t})\rho(t)M_{11}'(\sqrt{\Delta t}) \\
+ M_{01}'(\sqrt{\Delta t})\rho(t)M_{01}'(\sqrt{\Delta t}) \\
+ M_{10}'(\sqrt{\Delta t})\rho(t)M_{10}'(\sqrt{\Delta t}).
\]  

(17)

The second and third terms above are the crucial features of this dynamical equation. These asymmetric terms with \(M_{00}'\) and \(M_{11}'\) representing decoherence make this equation conceptually different from the evolution equation obtained from Kraus operators (Eq. 4),

\[
\rho_S(t) = \sum_k M_k \rho_S(0) M_k^\dagger.
\]

This evolution equation does not have asymmetric terms of the form \(M_k \rho_S(0) M_k^\dagger\), which are present in the above equation (Eq. 17). We had arrived at Eq. (17) by drawing a parallel (Eq. 16) from the case with single quantum jumps (Eq. 13). Now we can see that this parallelism gave us insight to add these asymmetric terms to Eq. (15), which would have been hard to see directly from the evolution equation for Kraus operators (Eq. 4). This shows that the methodology used in developing the model is effective to flesh out the finer details of the theoretical framework. Eq. (15) can be applied to digitally simulate any open quantum system with environment assisted evolution. It is the discrete time solution of the Lindblad master equation.

**D. Proof of correctness**

The equivalence of the dynamical equations, Eq. (12) and (15) to the Lindblad formalism, Eq. (9) is proven in this section. Considering the case with single quantum jump, the following derivation shows that Eq. (12) is the discrete time solution to Lindblad master equation governing the system.

The master equation is in continuous time formalism. For continuous time limit of the discrete dynamics substituting \(\Delta t \to \partial t\) in Eq. (12),

\[
\rho(t + \partial t) = M_0'(\sqrt{\partial t})\rho(t)M_0'(\sqrt{\partial t}) \\
+ M_1'(\sqrt{\partial t})\rho(t)M_1'(\sqrt{\partial t}).
\]

(18)

Using Eq. (11),

\[
M_0'(\sqrt{\partial t}) = M_0 U = M_0(\sqrt{\partial t})e^{-i\omega_m} \\
\approx M_0(\sqrt{\partial t})\left[1 - \frac{i\partial t}{\hbar}\right].
\]

(19)

Now, \(M_0 M_0^\dagger + M_1 M_1^\dagger = \mathbb{1}\) and \(M_0 = M_0^\dagger\), so \(M_0(\sqrt{\partial t})\) can be written as,

\[
M_0(\sqrt{\partial t}) \approx \sqrt{\mathbb{1} - M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t})} \\
\approx 1 - \frac{1}{2} M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t}).
\]

(20)

Substituting Eq. (20) in Eq. (19),

\[
M_0'(\sqrt{\partial t}) \approx M_0(\sqrt{\partial t})\left[1 - \frac{i\partial t}{\hbar}\right] \\
\approx \left[1 - \frac{1}{2} M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t})\right] \left[1 - \frac{i\partial t}{\hbar}\right].
\]

(21)

Considering terms only up to first order in \(\partial t\), we get,

\[
M_0'(\sqrt{\partial t}) \approx \left[1 - \frac{i\partial t}{\hbar}\right] - \frac{1}{2} M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t}) \\
M_0'(\sqrt{\partial t}) \approx \left[1 + \frac{i\partial t}{\hbar}\right] - \frac{1}{2} M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t}).
\]

(22)

Substituting \(M_0\), Eq. (22) and \(M_1\), Eq. (11) in Eq. (18),

\[
\rho(t + \partial t) \approx \left\{1 - \frac{i\partial t}{\hbar}\right\} - \frac{1}{2} M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t})^* \\
+ M_1(\sqrt{\partial t})\rho(t)M_1'(\sqrt{\partial t}).
\]

(23)

Considering terms only up to first order in \(\partial t\) and rearranging the terms,

\[
\rho(t + \partial t) = \rho(t) - \frac{i\partial t}{\hbar}[H, \rho(t)] \\
+ M_1(\sqrt{\partial t})\rho(t)M_1'(\sqrt{\partial t}) \\
- \frac{1}{2} M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t})\rho(t) \\
- \frac{1}{2} \rho(t)M_1(\sqrt{\partial t})M_1'(\sqrt{\partial t}).
\]

(24)

We can see that the evolution operators, Eq. (11) helped us get the quantum jump and the normalisation terms correctly. Padding \(M_1\) as well with unitary quantum evolution \(U\) would lead to extra unwanted terms.

Set \(M_1(\sqrt{\partial t}) = L_1 \sqrt{\partial t}\),

\[
\rho(t + \partial t) = \rho(t) + \partial t \left[ - \frac{i}{\hbar}[H, \rho(t)] + L_1 \rho(t)L_1^\dagger \\
- \frac{1}{2} L_1 L_1^\dagger \rho(t) - \frac{1}{2} \rho(t)L_1 L_1^\dagger \right].
\]

(25)

We obtain the Lindblad equation,

\[
\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_S, \rho(t)] + L(\rho(t)) \\
\left(L(\rho(t)) = L_1 \rho(t)L_1^\dagger - \frac{1}{2} L_1 L_1^\dagger \rho(t) - \frac{1}{2} \rho(t)L_1 L_1^\dagger \right).
\]

We started from the dynamical equation, Eq. (12) and arrived at the Lindblad master equation, Eq. (9). Thus,
for the case with single quantum jump, we showed that the dynamical model is the solution for its Lindblad equation in the Markov approximation. A similar proof for the more general case with multiple quantum jumps, Eq.(17) can be worked out.

Thus, Eqs.(15) and (17) can be used to describe the complete dynamics of environment assisted quantum walk in general open quantum systems. In the next section, we apply this model to simulate the FMO complex.

IV. SIMULATING THE FMO COMPLEX

A. Energy transfer in FMO complex

FMO complex is the quantum transport channel for excitation energy transfer in green sulphur bacteria. The complex contains chromophores, which act as sites for excitons and are held by a protein scaffold at the right distances and orientations for efficient energy transfer. The sites show quantum coherence. The Hamiltonian [21] for the multi chromophoric system is given by,

$$H_c = \sum_{m=1}^{N_c} \varepsilon_m a_m^{\dagger} a_m + \sum_{n<m}^{N_c} V_{mn}(a_m^{\dagger} a_n + a_n^{\dagger} a_m).$$  \hspace{1cm} (26)

$N_c = 7$ is the number of chromophores in FMO complex. The $a_m^{\dagger}$ and $a_m$ are the creation and annihilation operators for an electron-hole pair (exciton) at chromophore $m$ and $\varepsilon_m$ are the site energies. $V_{mn}$ are Coulomb couplings of the transition densities of the chromophores. At any time there is one exciton in the complex. Initial excitation occurs at site 1 or 6 and is transported to the sink at sites 3 and 4. The structure of the FMO complex [36] is shown in Fig. 1. The channel is subjected to noise by the environment. The phonon bath (protein scaffold) induces quantum jumps, decoherence and dephasing of excitons without changing the number of excitations. The phonon coupling Hamiltonian is,

$$H_p = \sum_{m,n}^{N_c} q_{mn} a_m^{\dagger} a_m a_n^{\dagger} a_n.$$

Damping of the excitation due to the radiation field is given by the Hamiltonian,

$$H_r = \sum_{m}^{N_c} q_m (a_m^{\dagger} + a_m).$$

Lamb shifts due to phonon and photon bath coupling contribute negligibly to the dynamics[37], so are excluded from the equations. The Lindblad master equation in the Born-Markov and secular approximations is given by,

$$\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_c, \rho(t)] + L_p(\rho(t)) + L_r(\rho(t)).$$  \hspace{1cm} (27)

The respective Lindblad superoperators $L_p$ and $L_r$ are given by,

$$L_k(\rho(t)) = \sum_{\omega}^{k} \Gamma^k(\omega) \left[ A_m^k(\omega) \rho A_n^{k\dagger}(\omega) - \frac{1}{2} A_m^k(\omega) A_n^{k\dagger}(\omega) \rho - \frac{1}{2} \rho A_m^k(\omega) A_n^{k\dagger}(\omega) \right]$$

Here $(k = p, r)$, $A_m^k(\omega) = \sum_{\omega_1-\omega_2=\omega} c_m(\omega_1) c_{m}(\omega_2) |M_{\omega_1}\rangle |M_{\omega_2}\rangle$, $c_{m}(\omega) = (M_{\omega}|M_{\omega}\rangle)$ is the exciton with frequency $\Omega_{\omega}$ and $\langle M_{\omega_1}|M_{\omega_2}\rangle = \sum_{m} c_m(\omega_{\omega_1}) c_{m}(\omega_{\omega_2})$. The exciton states and their energies are the eigenvectors and eigenvalues, obtained by diagonalizing Hamiltonian $H_c$ (given in Eq.(26)). Excitons are delocalised over sites and the $A_m^k(\omega)$ represent delocalised exciton transport. The system Hamiltonian delocalises the excitons over sites due to coherence and phonon bath induces relaxation of these delocalised excitons. To delocalise over different sites and the quantum jumps act between these delocalised exciton states rather than between different sites. The equation has both quantum and classical effects and captures their interplay which leads to greater transport efficiency. Quantum coherence causes excitons to delocalise over different sites and the quantum jumps act between these delocalised exciton states rather than between different sites. The equation has both quantum and classical effects and captures their interplay which leads to greater transport efficiency. Quantum coherence causes a speedup in transport and jumps give directionality to the walk and cause the transfer of exciton from initial sites towards the sink. $\Gamma^p(\omega)$ are the rates for quantum jumps [20] given by,

$$\Gamma^p(\omega) = 2\pi J(\omega)(1 + n(\omega))$$  \hspace{1cm} (29)
where $J(\omega)$ is Ohmic spectral density and $n(\omega) = 1/\exp(h\omega/kT) - 1$. The rate of quantum jumps increases with temperature. This can be understood in terms of spontaneous and induced relaxations caused by the environment. As the temperature increases, the probability of induced relaxation increases, which cause more quantum jumps and thus the phonon coupling is higher.

Damping is of the order of 1 ns$^{-1}$ [38] and the transfer time for excitation across the complex is $\sim 4$ ps [37]. Since the damping contribution is negligible for the duration of the quantum walk, it is neglected in the analysis. Overall, the dynamics are given by,

$$\frac{\partial \rho(t)}{\partial t} \approx -\frac{i}{\hbar}[H_c, \rho(t)] + L_p(\rho(t)).$$ \hspace{1cm} (30)

The above is similar to the ENAQT quantum walk described in Eq. (3). Thus, the dynamics in the FMO complex are described by the master equation for ENAQT. We can treat the multichromophoric system in the FMO complex as an open quantum system. In the next section, we give the theoretical framework for digital quantum simulation of the dynamics of the FMO complex using the general solution, Eq.(17) of the master equation developed in Sec.III C.

### B. Theoretical model for simulating FMO complex

The quantum jumps, analogous to Lindblad operators, Eq.(28) show delocalised exciton transport and can be represented as follows. Say, the system is in the exciton state $|M\rangle$. If the probability of quantum jump to state $|N\rangle$ in time $\sqrt{\Delta t}$ is $\gamma_{M\rightarrow N}$ (obtained from $T^k(\omega)$), for any $|N\rangle \neq |M\rangle$, then the Kraus operators for quantum jumps from $|M\rangle$ are given by:

$$M_{MN} = \sqrt{\gamma_{M\rightarrow N}}|N\rangle\langle M|$$

$$M_{MM} = \left(1 - \sum_{N \neq M} \gamma_{M\rightarrow N}|M\rangle\langle M|\right).$$ \hspace{1cm} (31)

Similar operators can be given for jumps from all such $|M\rangle$. Using the general model (Eq.15,17), the dynamical equation for the FMO complex is given by ($U = \exp(-\frac{iH_c\Delta t}{\hbar})$),

$$\rho(t + \Delta t) = \sum_M \left[M_{MM}U\rho(t)U^\dagger M_{MM}^\dagger + \sum_{N \neq M} \left(M_{MN}\rho(t)M_{NM}^\dagger + M_{MM}U\rho(t)U^\dagger M_{NN}^\dagger\right)\right].$$ \hspace{1cm} (32)

As proven in Sec.III D, this equation is the solution for the Lindblad equation for ENAQT in FMO complex. It should be noted that the last term in this equation is the decoherence term and the first and second terms are due to the quantum jumps. The evolution is trace preserving($\sum_{i,j} M_{ij}^\dagger M_{ij} = 1$). This is the theoretical model for digital quantum simulation of the FMO complex.

### C. Model for tunable bath coupling

The dynamics of the FMO complex are temperature dependent. The phonon couplings vary with temperature, Eq.(29). The coupling strength increases as the temperature increases. The dynamics in the FMO complex have been observed at ambient temperatures. For lower temperatures, the coupling strength is a fraction of the maximum coupling constants. We can denote this fraction as $\chi \in [0,1]$. The coupling strength dependent master equation can be written as,

$$\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_c, \rho(t)] + \chi L_p(\rho(t))$$ \hspace{1cm} (33)

This can be modified to be written as,

$$= -(1-\chi)\frac{i}{\hbar}[H_c, \rho(t)] + \chi \left[\frac{i}{\hbar}[H_c, \rho(t)] + L_p(\rho(t))\right].$$ \hspace{1cm} (34)

For $\chi = 1$ this reduces to the normal master equation for the quantum walk at ambient temperatures. For other values of $\chi$, it captures the dynamics at different temperatures. This can be digitally simulated by the following dynamical equation,

$$\rho_\chi(t + \Delta t) = (1 - \chi)U\rho(t)U^\dagger + \chi\rho(t + \Delta t)$$ \hspace{1cm} (35)

where $\rho(t + \Delta t)$ is given by Eq.(32). Eq. (35) describes the complete evolution of density matrix in the FMO complex. It captures the classical and quantum effects contributing to the transfer of energy through the complex and models the temperature dependence of the dynamics. $\chi$ can be used to study variation of the dynamics with respect to other variables as well, not just temperature. Using Eq.(17) instead of Eq.(32) for $\rho(t + \Delta t)$, Eq.(35) can be directly applied to any other open quantum system. Thus we obtain the discrete time dynamical equation for digital quantum simulation of environment assisted quantum walk with variable bath coupling.

### D. Numerical simulation

Equations (32) and (35) represent evolution of the density matrix in the FMO complex. To verify the effectiveness of these models, we simulate them numerically and present the results. Evolution of population densities at different sites is calculated using Eq.(32). The step size ($\Delta t$) is chosen to be 100 fs, as observed coherence time is $\sim 300$ fs and exciton relaxation time is $\sim 100$ fs [15]. The values of the system Hamiltonian and the jump rates are taken from [20] and [37, 39].
FIG. 2. Time evolution of the population at each site in the FMO complex calculated using Eq. (32). Initial Excitation at site 1, efficiency achieved = 96.5%.

FIG. 3. Time evolution of the population at each site in the FMO complex calculated using Eq. (32). Initial Excitation at site 6, efficiency achieved = 96.6%.

1. Result: High efficiency of energy transfer

In Figures 2, 3 we show the evolution of population densities when the initial excitation is at site 1 (Fig. 2) and site 6 (Fig. 3). The efficiency attained (sum of population on site 3 and site 4) is \(\sim 97\) percent. It is in agreement with theoretical evidence presented in [21], by using master equation model, Eq. (27). It can also be seen from the graphs that transfer happens faster if the initial excitation is at site 6, as observed experimentally in [37].

2. Result: Dependence on environment temperature

In Figures 4 and 5 we show the results of simulations with different phonon couplings, Eq. (35). For \(\chi = 0.42\) the evolution of population densities at different sites are shown when the initial excitation at site 1 (Fig. 4) and site 6 (Fig. 5). These graphs are plotted for the first 1 ps of the walk only to zoom into the initial dynamics. In Fig. 4 it can be seen that there is an initial oscillation of population between site 1 and 2. This is due to the high coupling between these two sites which causes the exciton over site 1 to delocalise to site 2. Slowly this oscillation dies, as quantum jumps cause the population to move towards the sink at sites 3 and 4, whose population starts rising. There is some population at site 7 as well, which serves as the connecting link between different sites (as can be seen in Fig. 1). As compared to Fig. 2, there is an enhanced effect of quantum dynamics (coherence between site 1 and 2) visible in Fig. 4. This is expected since the strength of the bath coupling is lower for \(\chi = 0.42\), leading to suppression of environment induced quantum jumps. Similar dynamics can be seen in Fig. 5 where there is an initial oscillation of population between site 6 and site 5. This population is slowly transported towards the sink at site 3 and 4.

Figures 4 and 5 represent the dynamics in the FMO complex at 77K. These results can be matched with the dynamics obtained in previous theoretical study [40]. We can see that the results of calculations done using the discrete time evolution model of Eqs. (32) and (35) match with theoretical [21, 40] and experimental studies [37] done on the FMO complex.
Thus, the discrete time evolution equation, together with a rather straightforward way of varying the coupling strength of environment provides a valuable method to digitally simulate environment assisted transport in open quantum systems.

V. CONCLUDING REMARKS

We have developed a theoretical framework for digital quantum simulation of the environment assisted quantum transport (ENAQT) in open quantum systems in the discrete-time density matrix evolution formalism. We modelled ENAQT into an open quantum systems and developed a methodology to solve the Lindblad master equation for ENAQT. We have obtained evolution operators, Eq.(15) to capture the interplay of quantum coherence and quantum jumps. Using the obtained evolution equation, Eq.(17) and the operators, we have proved its equivalence to the Lindblad master equation. We have shown that our approach is an improvement over the conventional numerical solution in which the quantum and classical effects are simulated separately. We applied the general solution of ENAQT master equation to simulate the FMO complex using delocalised exciton transport. Then, we generalised it to capture temperature dependence as variable strength of phonon coupling. We have demonstrated that calculations done on our model are in good agreement with experimental and theoretical evidence. Our model can be used to simulate the FMO complex dynamics for different temperatures and conditions.

Open quantum system are generally described using master equations for which solutions are otherwise not known. The solution of the master equation we developed can have great scope for applications to digital quantum simulation of ENAQT. The model can be used to understand noise assisted transport (NAT) in quantum simulators. It could help in developing systems with tunable level of noise. It can also be applied to study artificial photovoltaic quantum systems and quantum communication channels to achieve desired efficiency and other properties. The methodology developed to solve the Lindblad equation for ENAQT can be valuable in developing solution of master equation for other processes. It could be used to model multiple noise effects in complex systems with diverse sources of environmental interactions. Modelling effects such as depolarization and damping in open quantum systems, can be subjects for further research work. This can help in further developing the theory of digital quantum simulations. Another interesting line of work can be exploring the experimental implications of our work on developing quantum simulators. In particular, developing quantum gates to simulate the asymmetric terms in the evolution equation, Eq.(17) is a challenge to be overcome to develop quantum circuits for our model.

ACKNOWLEDGMENTS

CMC would like to thank Department of Science and Technology, Government of India for the Ramnathan Fellowship grant No.:SB/S2/RJN-192/2014. We also acknowledge the support from Interdisciplinary Cyber Physical Systems (ICPS) programme of the Department of Science and Technology, India, Grant No.:DST/ICPS/QuST/Theme-1/2019/1 and US Army ITC-PAC contract no. FA520919PA139.

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