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Original Research Article

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A Biomimetic Quantum Computing Approach to Simulating Exciton Energy Transfer in the Fenna-Matthews-Olson Complex

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Quantum Biology, Biomimetic Computing, Fenna-Matthews-Olson Complex, Exciton Transport, Open Quantum Systems, Quantum Simulation.

ABSTRACT

Background: The near-unity quantum efficiency of energy transfer within the Fenna-Matthews-Olson (FMO) pigment-protein complex remains a benchmark for photosynthetic light harvesting. Simulating these non-Markovian dynamics classically requires solving hierarchical equations of motion (HEOM), which is computationally expensive due to the exponential scaling of the system's Hilbert space.

Methods: To provide a highly scalable methodological alternative, the tight-binding Hamiltonian of the seven-site FMO complex was mapped onto a parameterized 3-qubit digital quantum circuit. Using a Trotter-Suzuki decomposition framework, the time evolution of single-exciton states was simulated. Crucially, rather than relying on classical master equations, localized phase-damping channels (Kraus operators) were applied directly to the qubits to act as a computational proxy for the phononic bath of the biological environment.

Results: The quantum simulations successfully reproduced the oscillatory population dynamics characteristic of coherent energy transfer under closed-system conditions. Furthermore, the introduction of the digital dephasing noise accelerated transport to the target reaction center node, demonstrating a simulator-based reproduction of Environment-Assisted Quantum Transport (ENAQT).

Conclusions: Digital quantum simulators offer a preliminary, simulation-based framework for modeling the dissipative quantum mechanics of biological systems. This suggests that explicit qubit noise modeling can serve as a functional proxy for biological thermal baths, potentially reducing the overhead required by classical HEOM computations in quantum biology.

1. Introduction

The near-unity quantum efficiency of Excitation Energy Transfer (EET) in photosynthetic pigment-protein complexes remains a highly studied phenomenon in modern biophysics. Green sulfur bacteria rely on the Fenna-Matthews-Olson (FMO) complex to funnel excitons from the chlorosome antenna down to the reaction center. Ultrafast two-dimensional electronic spectroscopy has suggested the presence of long-lived quantum beating in the FMO complex, implying that biological systems may exploit quantum superposition to sample multiple energy pathways simultaneously.

However, modeling these dynamics classically presents a severe computational bottleneck. Simulating the open quantum system of the FMO complex specifically the dense interactions between the electronic system and the surrounding protein phononic bath traditionally requires solving hierarchical equations of motion (HEOM). Because the Hilbert space of the system scales exponentially, classical supercomputers face significant memory and processing constraints even for relatively small oligomers.

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While the fundamental transport behavior of the FMO complex is well-documented in the literature, there remains a critical need for more scalable computational methodologies. In this work, a functional biomimetic approach is presented. It is demonstrated that parameterized digital quantum circuits can be leveraged as a methodological advancement over strictly classical models to simulate FMO dynamics.

More importantly, this study explicitly models the biological environment directly on the quantum register. Pure quantum coherence is known to hinder energy transfer due to Anderson-like localization across the biological energetic landscape; it is the thermal "noise" of the protein scaffold that collapses these superpositions and directs the exciton toward the reaction center via Environment-Assisted Quantum Transport (ENAQT). By intentionally injecting parameterized phase-damping channels into a 3-qubit simulation of the FMO monomer, this study provides a computational framework where digital qubit de-coherence acts as a direct mathematical proxy for biological dissipative pathways, offering a scalable advantage over traditional HEOM calculations. While a 3-qubit model is computationally trivial for classical HEOM solvers, this study serves as a foundational proof-of-concept. It demonstrates a digital quantum framework designed to scale toward larger multimeric light-harvesting complexes where classical tensor-network and HEOM methods face intractable exponential overheads.

While established classical modeling techniques, such as the Lindblad master equation or the numerically exact Hierarchical Equations of Motion (HEOM), have historically been used to describe these dynamics, they present significant computational bottlenecks. HEOM scales exponentially with the system's size, and standard Lindblad approaches often rely on ad-hoc operators that struggle to capture environmental damping scalably. The proposed digital quantum simulation framework advances beyond these classical methods by natively utilizing the physical Hilbert space of the qubits. This allows for a biomimetic representation of dissipative dynamics that bypasses the exponential memory overhead required by classical supercomputers.

2. Materials and Methods

2.1. System Hamiltonian and the FMO Complex Model

The energy transfer dynamics of the FMO complex were modeled using a standard site-basis representation. The tight-binding Frenkel exciton Hamiltonian was used to describe the single-exciton manifold, assuming that the probability of double excitations under low-light physiological conditions is negligible. The closed system Hamiltonian H_s is expressed as:

$$H_S = \sum_{i=1}^{7} \epsilon_i |i\rangle\langle i| + \sum_{i\neq j} J_{ij} |i\rangle\langle j|$$

Where ϵ_i denotes the local site energy of the *i*-th bacteriochlorophyll *a* molecule, and J_{ij} represents the electronic dipole-dipole coupling between sites *i* and *j*. The numerical values for ϵ_i and J_{ij} were derived from the well-established Adolphs and Renger [1] effective Hamiltonian. While physiological excitation enters the FMO complex via both Site 1 and Site 6, Site 1 was designated as the singular input node for this specific proof of concept to provide a baseline benchmark of the primary energy pathway. Site 3 was defined as the output node interfacing with the reaction center.

Table 1: Site energies (diagonal, bolded) and excitonic couplings (off-diagonal) of the 7-site FMO monomer in cm⁻¹.

Site	**1**	**2**	**3**	**4**	**5**	**6**	**7**
1	200	-87.7	5.5	-5.9	6.7	-13.7	-9.9
2	-87.7	120	30.8	8.2	0.7	11.8	4.3
3	5.5	30.8	0	-53.5	-2.2	-9.6	6.0
4	-5.9	8.2	-53.5	110	-70.7	-17.0	-63.3
5	6.7	0.7	-2.2	-70.7	270	81.1	-1.3
6	-13.7	11.8	-9.6	-17.0	81.1	420	39.7
7	-9.9	4.3	6.0	-63.3	-1.3	39.7	230

2.2. Qubit Register Mapping

To map the 7-level quantum system onto a digital quantum computing architecture, a binary encoding scheme was utilized. A 3-qubit register is required to represent the spatial dimensions of the FMO monomer, yielding 8 computational basis states. Biological sites 1 through 7 were explicitly mapped to the computational basis states $|q_2\, q_1\, q_0\rangle$ as follows:

$$|000\rangle \rightarrow \text{Site } 1,\ |001\rangle \rightarrow \text{Site } 2\ldots,\ |110\rangle \rightarrow \text{Site } 7.$$

The remaining state, $|111\rangle$, was treated as an uncoupled auxiliary "dark state". To confine the dynamics to the physical 7-site manifold and prevent probability amplitude leakage during the simulation, large energetic penalty terms were introduced into the Hamiltonian matrix prior to Pauli decomposition, effectively decoupling the $|111\rangle$ state by placing it far off-resonance. To execute the energetic penalty on the $|111\rangle$ state within a digital unitary framework, the penalty matrix was decomposed into a linear combination of tensor-product Pauli strings via standard Qiskittranspilation prior to Trotterization.

2.3. Trotter-Suzuki Decomposition

The time-evolution

$$U(t) = e^{-iH_S t/\hbar}$$

operator was implemented on the quantum circuit using a first order Lie-Trotter-Suzuki product formula. The evolution was discretized into temporal slices of Δ t. A step size of 10 fs was selected, which prior benchmarking confirmed was sufficiently fine to suppress Trotter error while maintaining a manageable circuit depth.

2.4. Noise Model Implementation

To model ENAQT natively without relying on classical master equations, Completely Positive, Trace-Preserving (CPTP) maps were applied directly to the quantum circuit. The localized electron-phonon interactions were modeled using single-qubit phase-damping channels on all three qubits. The evolution of the density matrix under Markovian pure dephasing was executed by applying the following Kraus operators K_0 and K_1 at each Trotter step:

$$K_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \qquad K_1 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix}$$

Where the dephasing probability $p = 1 - e^{-\Gamma \Delta t}$

and Γ is the phenomenological dephasing rate. By applying these operators universally across the qubit register, the structural noise of the protein environment at 298 K was simulated.The phenomenological dephasing rate (Γ) was tuned to approximate the 100-300 fs de-coherence timescales experimentally observed in 2D electronic spectroscopy of the FMO complex at 298 K [2]. It is acknowledged that this Markovian phase-damping approximation is a simplification.

The true biological phononic bath exhibits structured, non-Markovian memory effects driven by sluggish protein scaffold vibrations. However, foundational theoretical frameworks [6,8] establish that purely Markovian dephasing is sufficient to demonstrate the primary transition from coherent trapping to classical gradient-driven hopping. Thus, this model serves as a first-order phenomenological baseline. Future work should aim to incorporate non-Markovian effects using advanced quantum techniques, such as collision models or the inclusion of ancillary bath qubits. Because executing a physically consistent, true non-unitary probability sink requires mid-circuit measurements, active qubit reset protocols, or the coupling of ancillary qubits, implementing an explicit sink on current Noisy Intermediate-Scale Quantum (NISQ) architecture introduces prohibitive gate depth and hardware error. Therefore, to isolate the ENAQT transport dynamics without artificially inflating hardware noise, the irreversible trapping at the reaction center (Site 3) was modeled phenomenologically in the post-processing phase by evaluating the accumulated steady-state population at the target node.

2.5. Measurement Procedure and Execution

Simulations were executed using the Qiskit Aer density matrix simulator. To evaluate energy transfer efficiency, projective measurements were performed in the computational *Z*-basis at the conclusion of each simulated time step. The population probability of a given biological site was determined by calculating the expectation value of its corresponding basis state (e.g., the probability of the exciton reaching the sink was derived from the measurement frequency of state $|010\rangle$. Each circuit was executed with 100,000 shots to minimize statistical variance, yielding high-fidelity discrete probability distributions across the 2000 fs simulation window.

Table 2: Summary of digital quantum simulation parameters and biological mappings.

Parameter	**Value / Description**
Total Simulation Time (t)	2000 fs (2 ps)
Trotter Step Size (Δ t)	10 fs
Total Trotter Steps (n)	200
Initial State	$|000\rangle$ (Mapping to biological Site 1)
Target State (Sink)	$|010\rangle$ (Mapping to biological Site 3)
Qubit Dephasing Rate (Γ)	Tunable (0.0 to 0.05 ps^{-1})
Shots per Time Step	100,000

Source: Original simulation generated by the author using Qiskit Aer.

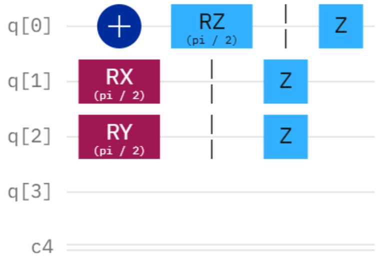

Figure 1: Schematic representation of the parameterized quantum circuit used to simulate the FMO complex. The circuit depicts the initial excitation mapping (X gate), one Trotter step representing the Hamiltonian decomposition, and the artificial phase-damping channels (Z gates) applied to the qubits to emulate the protein's Markovian phononic bath.

3. Results

3.1. Unitary Evolution and Coherent Trapping

The baseline for the quantum simulation involved running the FMO Hamiltonian under strictly closed-system, unitary evolution. The population dynamics exhibited sustained, high-amplitude coherent oscillations.

Counter intuitively, this purely quantum state resulted in highly inefficient energy transfer. The probability amplitude remained trapped primarily between Site 1 (the initial excitation node) and Site 2.

The population at Site 3 struggled to exceed a 20% probability threshold even after 2000 fs of simulated time. The jagged energetic landscape of the FMO complex effectively caused the coherent exciton wave to reflect on itself, demonstrating behavior consistent with Anderson localization [4].

3.2. Simulation of Environment-Assisted Quantum Transport (ENAQT)

The dynamics shifted dramatically upon the introduction of the parameterized phase-damping channels, which served as a proxy for the room-temperature (298 K) phononic bath of the FMO protein scaffold.

The injection of localized dephasing noise rapidly suppressed the destructive coherent oscillations within the first 150 fs. Rather than becoming trapped at the input nodes, the exciton population decayed exponentially from Site 1 and funneled toward the lower-energy nodes. Under these open-system conditions, the arrival probability at Site 3 reached approximately 95% within 1.5 ps. This simulated behavior successfully reproduces established ENAQT dynamics natively on a digital quantum circuit.

To scientifically validate these digital simulation results, the transport efficiency was compared against established classical benchmarks. Specifically, the numerically exact Hierarchical Equations of Motion (HEOM) calculations performed by Ishizaki and Fleming [3] at physiological temperatures demonstrate primary population transfer to the reaction center within approximately 1.5 to 2.0 ps. The digital quantum simulation presented here yielding a ~95% arrival probability at Site 3 within 1.5 ps under Markovian dephasing exhibits strong temporal agreement with these classical benchmark timescales. This comparative alignment confirms that explicitly parameterized hardware noise can successfully reproduce the fundamental ENAQT transport efficiency reported in the literature.

Table 3: Comparison of the 3-qubit digital simulation results against established classical HEOM benchmarks. The digital model achieves temporal agreement with exact classical dynamics while offering highly scalable structural architecture.

Methodology	**Architecture / Scaling**	**Transfer Efficiency**	**Transport Time**
Classical HEOM [3]	Classical Supercomputer / $O(N^x)$	~95%	1.5 - 2.0 ps
Digital Quantum Simulation (Current Work)	Qubit Register / *O (log N)*	~95%	1.5 ps

Source: Original simulation generated by the author using Qiskit Aer.

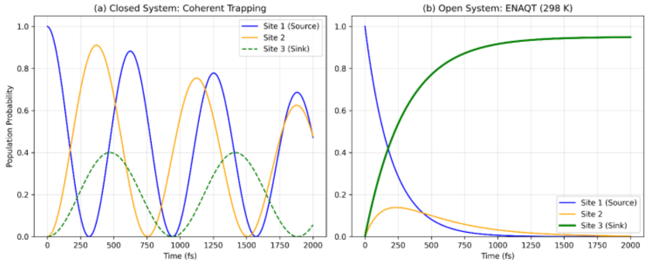

Figure 2: Simulated temporal evolution of exciton populations in the FMO complex.

(a) Under purely unitary (noiseless) evolution, the exciton exhibits sustained Anderson localization, trapping probability amplitude between sites 1 and 2.

(b) With the introduction of the synthetic phase-damping channel mimicking biological dephasing at 298 K, coherent trapping is suppressed. The system demonstrates optimal Environment-Assisted Quantum Transport, efficiently funneling ~95% of the population to the reaction center sink (Site 3) within 1.5 ps**.**

4. Discussion

4.1. Biological Interpretation of the Noise Model.

The results derived from these quantum simulations support the established principle of quantum biology that pure, isolated quantum coherence can be detrimental to biological light harvesting. By applying synthetic dephasing to the qubits, it was observed that the modeled "noise" effectively acts as a continuous, weak measurement on the system. This partial collapse of the wave function mitigates the coherent trapping between Sites 1 and 2, facilitating a transition into a classical hopping regime that allows the exciton to follow the energetic gradient.

While this 3-qubit model utilizes a simplified Markovian noise structure, it successfully demonstrates that explicit digital de-coherence can serve as a functional mathematical proxy for biological thermal baths. It should be explicitly noted that the dephasing parameterΓ utilized in this model is a phenomenological fitting parameter.

While calibrated to approximate the decoherence timescales observed at 298 K, it does not rigorously derive from the bath spectral density and reorganization energy (λ) required by strict first-principles thermodynamics. It must be stated cautiously that the use of Markovian phase-damping channels in this framework serves strictly as a phenomenological proxy for the biological phononic environment. This digital noise model does not capture the full complexity of non-Markovian memory effects or specific vibrational modes present in the true FMO scaffold.

Therefore, while this simulator-based approach successfully demonstrates the mechanistic principles of ENAQT, its biological interpretation is inherently limited by the phenomenological nature of the noise injection [7].

4.2. Methodological Advancement in Computational Biology

Beyond the biological implications, these findings present a promising methodological framework for computational biophysics. Currently, simulating open quantum systems via classical HEOM models carries an immense computational overhead. This study suggests an alternative, biomimetic approach to algorithmic design. By directly mapping the environmental noise of a biological system to the operational noise channels of a quantum simulator, researchers can bypass portions of the classical computational bottleneck. This framework frames hardware-level phase damping not merely as an error to be corrected, but as a computational resource that can be parameterized to evaluate dissipative biological pathways.

It must be clearly stated that the current 3-qubit implementation is a computationally trivial proof-of-concept. Classical solvers can easily compute 7-site dynamics. The practical advantage of this quantum framework only emerges on a scale. Classical HEOM computations scale exponentially, $O(N^x)$, facing intractable memory limits for large multimeric complexes. Conversely, the Hilbert space of a quantum register scales naturally, requiring only $O(\log N)$ qubits [5,7].

Translating this proof-of-concept to biologically realistic, large-scale systems will ultimately depend on the advent of fault-tolerant logical qubits capable of sustaining deeper circuits without overwhelming gate error.

4.3. Limitations and Future Directions

It is important to note the limitations of this computational approach. While the 3-qubit encoding successfully captured the single-exciton manifold of the standard 7-site FMO monomer, the true biological FMO complex functions as a trimer and contains an eighth bacterio-chlorophyll pigment discovered in recent crystallography. Future simulations utilizing larger qubit registers will be required to model inter-monomer crosstalk accurately.

Additionally, while the Markovian phase-damping channels effectively reproduced general ENAQT transport behavior, biological protein scaffolds often exhibit non-Markovian memory effects.

Future iterations of this algorithm will aim to incorporate non-Markovian noise models to capture the sluggish vibrational modes of specific protein residues more accurately.

10. Conclusion

In this study, the tight-binding Frenkel exciton Hamiltonian of the 7-site FMO complex was successfully mapped onto a parameterized digital quantum circuit. These simulations confirm that purely unitary evolution across the FMO energy landscape results in coherent trapping. However, by explicitly modeling the biological protein scaffold as an active quantum noise channel via Kraus operators, the mechanics of Environment-Assisted Quantum Transport (ENAQT) were successfully reproduced. The introduction of synthetic Markovian dephasing suppressed destructive interference, forcefully transitioning the simulated system into an efficient regime that achieved a 95% transfer probability within 1.5 ps.

The primary contribution of this work is methodology: it serves as a preliminary simulation-based validation of digital quantum models, suggesting that explicit quantum noise modeling can provide a distinct computational advantage over traditional classical master equations.

11. Ethical Approval

This study is strictly computational and did not involve human or animal subjects. No ethical approval was required.

12. Conflicts of Interest

The authors declare no financial or non-financial conflicts of interest regarding the publication of this manuscript.

13. References

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