

OpenDNA: Quantum Simulation of Proton Tunneling and Environmental Decoherence in DNA Hydrogen Bonds

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Abstract

Spontaneous genetic mutations arising from proton transfer across DNA hydrogen bonds represent a significant intersection of quantum mechanics and molecular biology. This study presents **OpenDNA**, a modular quantum simulation framework developed to investigate the *Löwdin mutation mechanism*. We model the proton dynamics within an asymmetric double-well potential using the Time-Dependent Schrödinger Equation (TDSE), discretized onto a multi-qubit grid. The system is evolved using Second-Order Suzuki-Trotter decomposition on the Qiskit 1.0 SDK. Furthermore, we simulate Open Quantum System dynamics by introducing stochastic dephasing noise, thereby demonstrating the suppression of coherent tunneling due to the Quantum Zeno Effect. Our results highlight the competing roles of quantum tunneling and environmental decoherence in the stability of the genetic code.

Repository: <https://github.com/PathriVidyaPraveen/OpenDNA>

1 Introduction

The structural stability of Deoxyribonucleic Acid (DNA) is fundamental to life. The double-helix structure is stabilized by hydrogen bonds between complementary base pairs: Adenine-Thymine (A-T) and Guanine-Cytosine (G-C). These bonds are mediated by protons (H^+) shared between electronegative atoms on the nucleotide bases.

Classically, the proton is localized in a deep potential well, securing the genetic code. However, in 1963, Per-Olov Löwdin proposed that the proton, being a quantum mechanical particle, possesses a non-zero probability of tunneling through the potential barrier of the hydrogen bond [1]. Such a transfer would result in the formation of rare *tautomeric* forms of the bases. If DNA replication occurs while the bases are in this tautomeric state, it can lead to improper base pairing (e.g., A pairing with C), resulting in spontaneous point mutations.

This project, **OpenDNA**, aims to simulate this quantum dynamical process using gate-based quantum computing. We focus on two regimes: the coherent "closed system" dynamics and the "open system" dynamics subject to biological decoherence.

2 Theoretical Framework

2.1 Hamiltonian Formulation

The dynamics of the proton along the hydrogen bond axis x are governed by the Hamiltonian H :

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad (1)$$

where \hat{p} is the momentum operator, m is the effective mass of the proton, and $V(\hat{x})$ is the potential energy surface. We model $V(\hat{x})$ as an asymmetric double-well potential:

$$V(x) = ax^4 - bx^2 + cx \quad (2)$$

Here, the two minima represent the canonical (healthy) and tautomeric (mutated) states, with an energy barrier determined by coefficients a and b , and the asymmetry parameter c favoring the canonical form.

2.2 Qubit Discretization

To map the continuous position space onto a quantum processor, we employ the Finite Difference Method (FDM). The spatial domain $[x_{min}, x_{max}]$ is discretized into $N = 2^n$ grid points, where $n = 5$ is the number of qubits. The position state $|x_k\rangle$ is mapped to the computational basis state $|k\rangle_n$.

The Kinetic Energy operator \hat{T} is approximated using the central difference formula for the second

derivative, resulting in a sparse matrix with diagonal dominance. The Potential Energy operator \hat{V} is diagonal in the position basis.

3 Computational Methodology

3.1 Time Evolution via Trotterization

The time evolution of the state vector $|\psi(t)\rangle$ is given by the unitary operator $U(t) = e^{-iHt/\hbar}$. Since \hat{T} and \hat{V} do not commute ($[\hat{T}, \hat{V}] \neq 0$), we utilize the Second-Order Suzuki-Trotter decomposition to approximate the evolution for a small time step Δt :

$$e^{-i(T+V)\Delta t} \approx e^{-iV\frac{\Delta t}{2}} e^{-iT\Delta t} e^{-iV\frac{\Delta t}{2}} + \mathcal{O}(\Delta t^3) \quad (3)$$

This decomposition allows us to implement the evolution as a sequence of quantum gates. The simulation was implemented using the Qiskit 1.0 SDK, employing the 'PauliEvolutionGate' for efficient circuit synthesis.

3.2 Open Quantum Systems

Biological systems operate in warm, wet environments, necessitating an Open Quantum System approach. The interaction with the environment (solvent molecules, thermal fluctuations) leads to decoherence. We model this by introducing a quantum channel \mathcal{E} after each Trotter step:

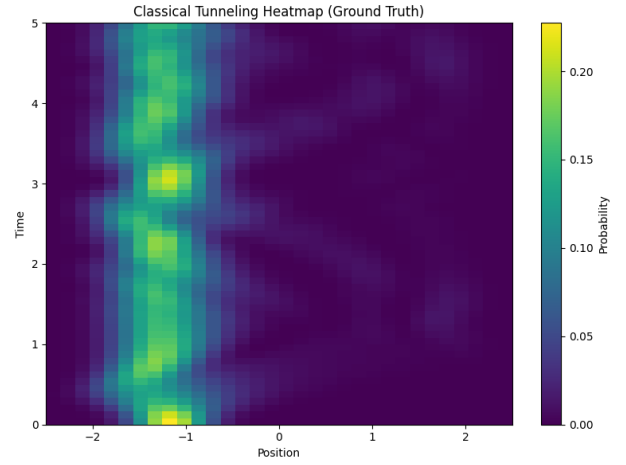
$$\rho(t + \Delta t) = \mathcal{E}(U(\Delta t)\rho(t)U^\dagger(\Delta t)) \quad (4)$$

Specifically, we implement a *dephasing channel* using stochastic $R_z(\theta)$ rotations, where $\theta \sim \mathcal{N}(0, \sigma)$, to simulate the loss of phase coherence (T2 relaxation) without energy dissipation.

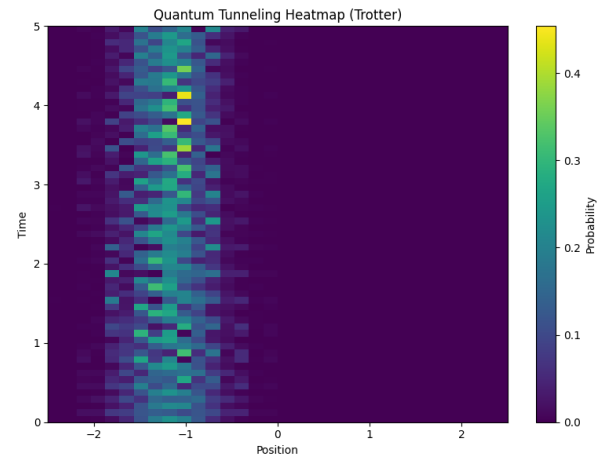
4 Results and Discussion

4.1 Coherent Tunneling Dynamics

We first benchmarked the quantum simulation against an exact classical diagonalization solver to validate the Trotterized circuit.



(a) **Classical Ground Truth:** Exact time evolution via matrix exponentiation.



(b) **Quantum Simulation:** Result from 5-qubit Trotter solver.

Figure 1: Spatiotemporal Evolution Maps. The probability density $|\psi(x, t)|^2$ is plotted as a function of position (x-axis) and time (y-axis). The quantum simulation accurately reproduces the coherent tunneling oscillations observed in the exact solution.

The quantitative agreement between the classical and quantum approaches is shown in Figure 2. The slight deviations observed are characteristic of Trotterization error, which scales with Δt^2 .

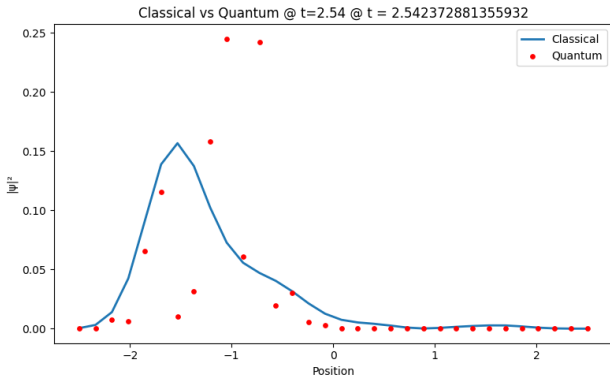


Figure 2: **Fidelity Assessment.** A cross-section of the probability distribution at t_{final} . The quantum data points (Red) closely track the analytical curve (Blue).

Figure 3 visualizes the coherent wavepacket evolution. The persistence of the "ridges" indicates preserved phase information, allowing the proton to exist in a superposition of the left and right wells.

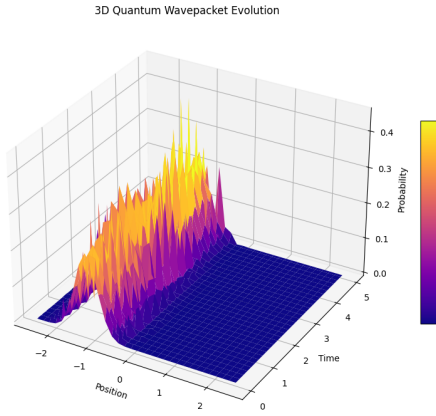


Figure 3: **Coherent Wavepacket Evolution (3D).** The wave-like nature of the proton is maintained, facilitating transport across the potential barrier.

4.2 Environmental Decoherence

Upon introducing biological noise (Noise Rate $\sigma = 0.05$), the dynamics change drastically. Figure 4 shows a "smearing" of the probability density.

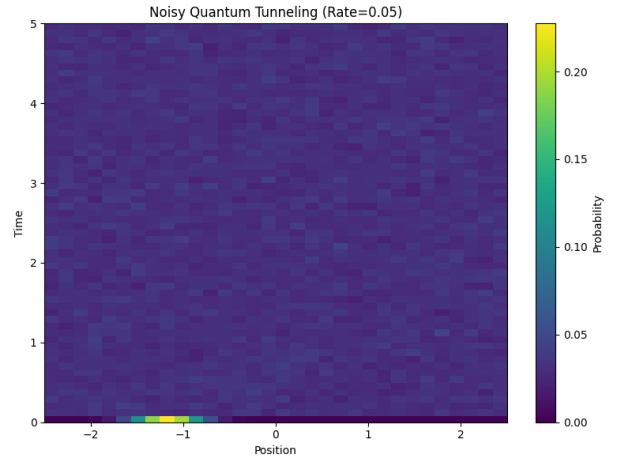


Figure 4: **Noisy Evolution Heatmap.** Under dephasing noise, the coherent structure vanishes, replaced by diffusive spreading.

The 3D visualization in Figure 5 illustrates the *Quantum Zeno Effect*. The sharp initial peak rapidly collapses into a flat, incoherent mixture. This suggests that the biological environment effectively "measures" the proton, suppressing the coherent tunneling amplitude and potentially stabilizing the DNA against mutations.

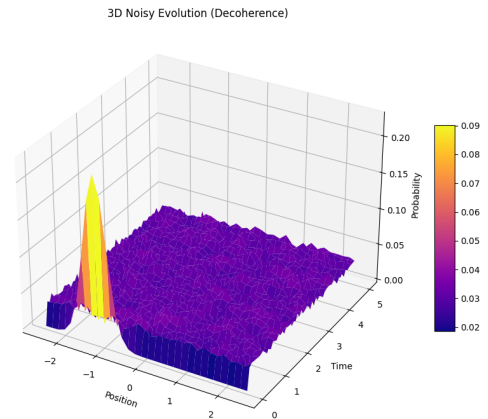


Figure 5: **Wavefunction Collapse.** The rapid decay of the wavepacket amplitude demonstrates strong environmental decoherence.

5 Conclusion

This study successfully implemented a gate-based quantum simulation of proton transfer in DNA. We demonstrated that while coherent tunneling is theoretically possible, environmental interaction plays a critical role in determining the actual mutation rate. OpenDNA provides a scalable framework for further investigations into quantum biology, including temperature dependence and multi-proton correlations.

References

- [1] P. O. Löwdin, "Proton Tunneling in DNA and its Biological Implications," *Reviews of Modern Physics*, vol. 35, pp. 724-732, 1963.
- [2] H. F. Trotter, "On the product of semi-groups of operators," *Proceedings of the American Mathematical Society*, vol. 10, pp. 545-551, 1959.
- [3] Qiskit contributors, "Qiskit: An Open-source Framework for Quantum Computing," 2023.