# Simulating Thermal Lindbladian Dynamics and Single Qubit General Dynamical Maps

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We implement and analyze a quantum simulation framework for open system dynamics, which enables the simulation of general (not necessarily completely positive) qubit dynamical maps using only one ancilla qubit. As a first step, we simulate the forward evolution of a single qubit under a thermal Lindblad master equation using IBM's Qiskit simulator. Although we successfully constructed the required unitaries for simulating the reverse evolution, limitations in initializing arbitrary density matrices and hardware constraints prevented its full implementation. Our results validate the forward protocol and lay the groundwork for future experiments on quantum error mitigation via time-reversed dynamics.

## I. INTRODUCTION

Simulating the dynamics of open quantum systems remains one of the key challenges in the development of practical quantum technologies. Unlike closed quantum systems, open systems interact with an external environment, leading to dissipative and often non-unitary evolution. In many scenarios, such dynamics can be accurately modeled by completely positive trace-preserving (CPTP) maps, or more specifically, via the Lindblad master equation in the Markovian regime. However, recent studies have emphasized the need for frameworks that extend beyond the CP-divisible paradigm, especially in contexts involving memory effects, initial system-environment correlations, or when considering inverse dynamics.

In their work, Rossini et al. [1] introduce a powerful simulation protocol capable of implementing general qubit dynamical maps that are Hermiticity-preserving and trace-preserving, but not necessarily completely positive. Such maps arise naturally as the inverses of CPTP maps or as intermediate propagators in non-Markovian time-local master equations with temporarily negative decay rates. Crucially, the authors show that any such general map can be decomposed as a weighted difference of two CPTP maps. This insight enables a novel error mitigation protocol—one that effectively reverses dissipative dynamics, thus recovering the original quantum state. The details of the method are provided in Sec II.

The aim of our project is to reproduce and expand upon the forward and backward simulation protocols presented, focusing specifically on the problem of error mitigation via time-reversal of a thermal Lindblad evolution. This involves simulating the evolution of a qubit coupled to a thermal reservoir under a standard Lindbladian generator, and subsequently attempting to reverse the evolution to recover the initial state. While the full implementation of the inverse dynamics is still ongoing, this report documents our current progress: the successful simulation of the forward thermal Lindblad evolution on IBM Quantum simulators.

## II. METHOD

We consider the general form of the time-local master equation

$$\frac{d}{dt}\rho_t = \mathcal{L}_t(\rho_t) = -i[H_t, \rho_t] + \sum_k \Gamma_{k,t}(L_k \rho_t L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho_t\}) \tag{1}$$

Given this form, there is a map $\Sigma_t$ such that $\rho_t = \Sigma_t(\rho_0)$. In general, we cannot assume the map $\Sigma_t$ to be completely positive (CP) due to the possibility of weights $\Gamma_{t,k}$ being negative. Moreover, trotterization of the map introduces intermediate maps $\Sigma_{\Delta t}$ that can be non-CP even though the initial map at the first time step is CP. Therefore, these types of maps are referred to as general dynamical maps [1].

For a Lindbladian with Hamiltonian $H$, Lindblad operators $\{L_k\}$ and weights $\Gamma_{k,t}$, we can construct the Liouville superoperator matrix as

$$\Sigma_{\Delta t} = \exp(\mathcal{L}\Delta t) \tag{2}$$

where the Lindladian is defined as

$$\mathcal{L} = -iI \otimes H + iH^T \otimes I + \sum_k \Gamma_{k,t}(L_k^* \otimes L_k - \frac{1}{2} I \otimes L_k^\dagger L_k - \frac{1}{2}(L_k^\dagger L_k)^T \otimes I) \tag{3}$$

### A. Decompose the General Dynamical Map

A general dynamical map $\Sigma$ can be decomposed into two CP maps [1],

$$\Sigma = \Sigma_+ - \Sigma_- \tag{4}$$

To achieve this, we first compute the Choi matrix for the general dynamical map,

$$C(\Sigma) = \sum_{i,j=1}^{d} |i\rangle\langle j| \otimes \Sigma(|i\rangle\langle j|) \tag{5}$$

Since $C(\Sigma)$ is diagonalizable, we can find its eigenvalues $\lambda_i$ and eigenvectors $v_i$ and construct the following

$$C_\pm(\Sigma) = \sum_i \max(0, \pm\lambda_i) v_i v_i^\dagger \tag{6}$$

This is essentially decomposing the Choi matrix into a positive and negative eigen-space such that $C(\Sigma) = C_+(\Sigma) - C_-(\Sigma)$. The map associated with the Choi matrix is defined as $\Sigma_\pm(\rho) = \mathrm{Tr}_t[C_\pm(\Sigma)(\rho^T \otimes I)]$. However, as we will see, we do not need to retrieve the map since we will be working with the Choi matrix. Moreover, it is worth noting that for a Choi matrix that has all positive eigenvalues, the map is CPTP and does not need to be decomposed.

### B. From CPTP Map to Extremal Map

For a CPTP map $\Lambda$, it can be written as a convex sum of two extremal maps [1],

$$\Lambda = \frac{1}{2}\Lambda_1 + \frac{1}{2}\Lambda_2 \tag{7}$$

To get the extremal maps, working with the Choi matrix is more efficient. In particular, we want to find $C(\hat{\Lambda}_{1,2})$ such that

$$C(\hat{\Lambda}) = \frac{1}{2}C(\hat{\Lambda}_1) + \frac{1}{2}C(\hat{\Lambda}_2) \tag{8}$$

where $\hat{\Lambda}$ is the adjoint of $\Lambda$. The Choi matrix of such maps is related by a unitary transformation

$$U_{adj} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

such that $C(\hat{\Lambda}) = \overline{U_{adj} C(\Lambda) U_{adj}}$. For a single qubit system, the Choi matrix as defined in Equation (5) is the block matrix

$$C(\hat{\Lambda}) = \begin{pmatrix} \hat{\Lambda}(E_{00}) & \hat{\Lambda}(E_{01}) \\ \hat{\Lambda}(E_{10}) & \hat{\Lambda}(E_{11}) \end{pmatrix} \equiv \begin{pmatrix} A & C \\ C^\dagger & B \end{pmatrix} \tag{9}$$

and since we know that $\Lambda$ is CPTP then $A \geq 0$, $B = I - A$, and $C = \sqrt{A} R \sqrt{I - A}$. From here, we can decompose the matrix $R$ with singular value decomposition as

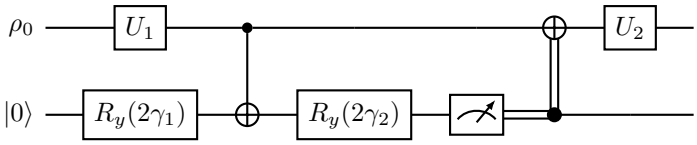
$$\begin{aligned} R &= V \begin{pmatrix} \cos\theta_1 & 0 \\ 0 & \cos\theta_2 \end{pmatrix} W^\dagger \\ &= \frac{1}{2} V \begin{pmatrix} e^{i\theta_1} & 0 \\ 0 & e^{i\theta_2} \end{pmatrix} W^\dagger + \frac{1}{2} V \begin{pmatrix} e^{-i\theta_1} & 0 \\ 0 & e^{-i\theta_2} \end{pmatrix} W^\dagger \\ &= \frac{1}{2}U_1 + \frac{1}{2}U_2 \end{aligned} \tag{10}$$

Thus, putting Equation (9) and (10) we arrive at

$$C(\hat{\Lambda}) = \frac{1}{2} \begin{pmatrix} A & \sqrt{A}U_1\sqrt{I-A} \\ \sqrt{I-A}U_1^\dagger\sqrt{A} & I - A \end{pmatrix} + \frac{1}{2} \begin{pmatrix} A & \sqrt{A}U_2\sqrt{I-A} \\ \sqrt{I-A}U_2^\dagger\sqrt{A} & I - A \end{pmatrix} \tag{11}$$

### C. Building the Quantum Circuit

At this point we have decomposed the general dynamical map into CPTP maps and rewritten the CPTP maps as convex sum of two extremal maps. The final step is to represent the action of the extremal map with a quantum circuit [2].




The circuit shown above describes the action of an extremal map on some initial state $\rho_0$ with only unitaries, rotations, and CNOT gates which can be obtained from the extremal map $\Lambda_{1,2}$. The map has a superoperator matrix of the form

$$\Lambda \to \mathbb{T} = \begin{pmatrix} 1 & 0 \\ t & T \end{pmatrix} \tag{12}$$

where $t$ is known as the shift vector and $T$ is the distortion matrix [2]. By performing the singular value decomposition on the distortion matrix ($T = R_1 T' R_2^\dagger$), we get a new shift vector and distortion matrix of the form

$$t' = R_2^\dagger t = (0, 0, \sin\mu \sin\nu)^T \tag{13}$$

$$T' = \mathrm{diag}(\cos\nu, \cos\mu, \cos\mu\cos\nu)^T \tag{14}$$

From this we can compute the rotation angles where $2\gamma_1 = \beta - \alpha + \pi/2$, $2\gamma_2 = \beta + \alpha - \pi/2$, $\alpha = (\mu + \nu)/2$, and $\beta = (\mu - \nu)/2$. Unitaries $U_1$ and $U_2$ are obtained from $R_1$ and $R_2^\dagger$. Notice that $R$ is a 3x3 rotation matrix while $U$ is a 2x2 rotation on a Bloch sphere. To transform $R \to U$, we first consider the general form of a rotation on a Bloch sphere

$$U = \exp\left(-i\theta\hat{n} \cdot \frac{1}{2}\vec{\sigma}\right) \tag{15}$$

where $\hat{n}$ is the axis of rotation obtained by solving $(R - I)\hat{n} = 0$, $\theta$ is the angle of rotation obtained by solving $\mathrm{Tr}(R) = 1 + 2\cos\theta$, and $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$.

## III. RESULTS AND DISCUSSION

## RESULTS AND DISCUSSION

To experimentally validate the forward evolution of a thermal Lindblad process, we simulated the dissipative dynamics of a single qubit coupled to a thermal reservoir using Qiskit. The evolution is governed by the master equation:

$$\dot{\rho} = -i\omega\left[\frac{\sigma_z}{2}, \rho\right] + \gamma\left(e^{\beta\omega}\mathcal{D}[\sigma_-](\rho) + \mathcal{D}[\sigma_+](\rho)\right), \tag{16}$$

where the dissipator is defined as $\mathcal{D}[L](\rho) = L\rho L^\dagger - \frac{1}{2}\{L^\dagger L, \rho\}$. For our simulations, we set $\beta = \omega = \gamma = 1$.

Figure 1 shows the evolution of the excited state population $\mathrm{Tr}[\sigma_+\sigma_-\rho(t)]$ for three representative initial states: the ground state $|0\rangle$, the excited state $|1\rangle$, and the superposition state $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. The results reveal the expected behavior:

- The excited state population decreases monotonically for $|1\rangle$, indicating dissipation to the environment.
- For $|0\rangle$, the population increases as the qubit thermally excites.
- The superposition state $|+\rangle$ trends toward equilibration, reflecting decoherence and partial thermalization.

These results confirm that our implementation of the forward thermal Lindbladian evolution behaves as theoretically expected. This serves as a benchmark for future experiments involving the time-reversed dynamics, where the goal is to recover the initial state using the simulation framework for general dynamical maps.

In addition, this step allows us to quantify state degradation under realistic hardware noise, laying the groundwork for a meaningful comparison with the subsequent recovery protocol. All circuits were executed using `AerSimulator()` from qiskit. Future experiments will include executions on real devices. The code used is available at Jain-Naman/OQS

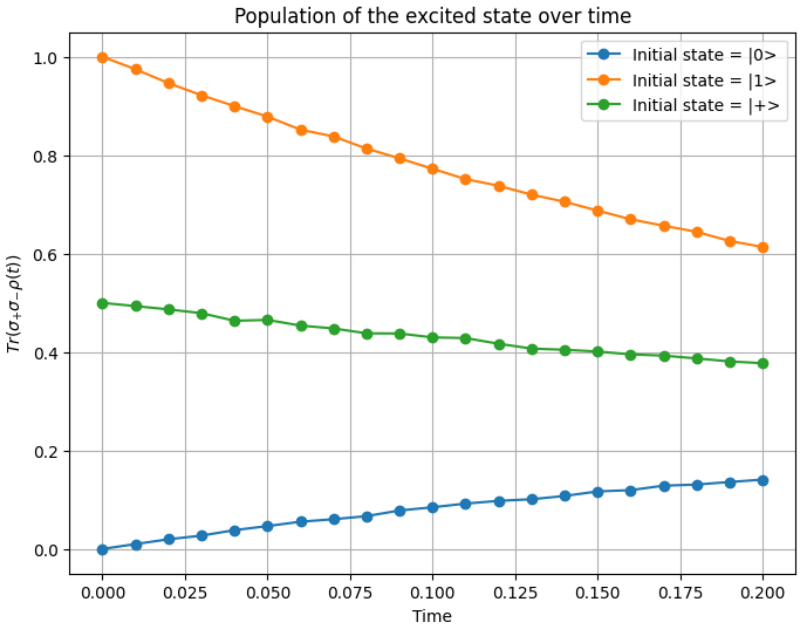



Figure 1. Evolution of the excited state population, $\mathrm{Tr}[\sigma_+\sigma_-\rho(t)]$, for three initial states ($|0\rangle$, $|1\rangle$, and $|+\rangle$) under thermal Lindbladian dynamics Eq. 16. The forward evolution was simulated using Qiskit, with parameters $\beta = \omega = \gamma = 1$, over a time window $t \in [0, 0.2]$. The excited state population decreases for $|1\rangle$, increases for $|0\rangle$, and stabilizes for $|+\rangle$, consistent with thermal relaxation.

### A. Limitations and Future Work

While we successfully implemented the forward evolution under the thermal Lindblad master equation, we were unable to simulate the reverse evolution. Although the necessary unitary operators for the extremal CPTP maps were constructed correctly and verified, a key bottleneck was the inability to initialize the quantum circuit with a density matrix corresponding to the system state at an intermediate time—specifically, at $t = 0.2$. Since IBM's native API does not directly support initializing arbitrary mixed states, we had no way to faithfully test the reversal protocol under realistic conditions.

Additionally, attempts to execute our circuits on real hardware were hindered by the following error: `Dynamic circuits used in a V2 Estimator job. -- V2 Estimator does not support dynamic circuits. Remove control flow operations or convert the job to use V2 Sampler instead.` While resolving this issue is technically feasible, it would require substantial refactoring of our current implementation, particularly to replace or re-encode the logic within the circuit. Due to time constraints, we deferred this effort and conducted all simulations using simulators. In future work, we plan to address this limitation by exploring alternative initialization strategies (such as state purification or custom state preparation circuits), and resume testing on real quantum hardware.

## IV. CONCLUSION

In this project, we explored a novel approach for simulating general (not necessarily completely positive) dynamical maps, as proposed by Rossini et al., with the goal of implementing a practical error mitigation scheme on NISQ-era quantum devices. The central idea is the decomposition of any trace-preserving, Hermiticity-preserving map into a weighted difference of two completely positive trace-preserving (CPTP) maps. This enables a simulation framework that requires only a single additional ancilla qubit and allows for simulating dynamics from any arbitrary time $t$, rather than being restricted to starting at $t = 0$. This feature is particularly useful for capturing time-reversed or non-Markovian behaviors.

As a first step, we successfully demonstrated the forward evolution of a single qubit under a thermal Lindblad master equation using the IBM Qiskit simulator. The excited state populations evolved as expected for various initial states, confirming the correct implementation of the Lindbladian dynamics and establishing a solid benchmark for future comparison.

However, due to practical constraints, we were unable to implement and test the reverse evolution. The main challenge was the inability to initialize the quantum circuit with a mixed state corresponding to the system's intermediate evolution at $t = 0.2$, which is required for validating the recovery protocol.

## WORK DISTRIBUTION

The work for this project was distributed across both team members to efficiently cover both the theoretical and practical components, including simulation, circuit construction, and documentation. Below is a breakdown of major responsibilities and tasks:

**Naman Jain -**

1. **Theoretical Modeling**
   - Construction of unitary operators from CP maps
   - Understanding the high-level logic
2. **Code Integration and Workflow Management**
   - Integration of independently developed modules (state evolution, Kraus extraction, circuit preparation) into a coherent simulation pipeline.
   - Reproducible scripts to run forward evolution from initial states and log results.
3. **Debugging, Documentation and Visualization**
   - Maintaining a clean, well-documented GitHub repository.
   - Figures to illustrate state evolution
   - debugging the code
4. **Auxiliary Tools and Testing**
   - Development of auxiliary Python functions to verify trace preservation, CP conditions, and Kraus completeness of the decomposed maps.
   - Scripts were created to visualize the action of maps on Bloch vectors and verify correctness of decomposition numerically.

**King Lin -**

1. **Theoretical Modeling and Decomposition**
   - Deriving the decomposition of general dynamical maps into weighted differences of CPTP maps and further into extremal maps using results from [3].
2. **Quantum Circuit Construction**
   - Construction of circuits for forward Lindblad evolution using Qiskit, including implementation of thermal dissipation.
3. **Auxiliary Tools and Testing**
   - Development of auxiliary Python functions to verify trace preservation, CP conditions, and Kraus completeness of the decomposed maps.
4. **Simulation and Hardware Configuration**
   - Setting up simulations using IBM's Qiskit framework
   - Exploration of real-device runs was attempted, but limited by unsupported features of Qiskit SDK.

Collaborative effort to write and edit the final report.

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[2] 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. **111**, 130504 (2013).

[3] C. King and M. Ruskai, Minimal entropy of states emerging from noisy quantum channels, IEEE Transactions on Information Theory **47**, 192 (2001).