# Evolving Open Quantum Systems

A quantum algorithm for evolving environment-interacting quantum dynamical systems

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# 1 Introduction

Quantum state systems are of great importance as they describe real-world systems' behavior such as and most commonly used for atomic system (or an ensemble of such) analysis, where we are usually interested in how the quantum state evolves in time and what dynamical properties we can extract out of this system in order to gain information and better understand the system. Our project discusses a particular type of quantum state system which interacts with the environment as it evolves in time, known as an **Open Quantum System**. The idea of simulating quantum systems with quantum algorithms was first proposed by Richard Feynman. Ever since then, extensive research has been done in developing quantum algorithms that can simulate the evolution of a quantum system. However, few studies have been done on open quantum systems despite their importance. This is due to the difficulty of simulating the environment interaction, as it is a non-unitary operation. Our project discusses the study done by Zixuan H., Rongxin X. and Sabre K. which uses the Sz- Nagy dilation theorem that can represent a non-unitary operation as a sequence of unitary quantum gates, which we then are able to implement into a quantum circuit to extract needed information about the quantum system we are measuring.

# 2 Theory

Our method starts with an initial density matrix state $\rho$ which describes the quantum system before any interaction expressed by a sum of different pure quantum states $|\phi_i\rangle$ weighted by the associated probabilities $p_i$:

$$\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i| \tag{1}$$

Note here the different $|\phi_i\rangle$'s are not necessarily orthogonal to each other

We will then evolve the state using Kraus operators $M_k$ in order to get the time evolved state $\rho(t)$:

$$\rho(t) = \sum_k \rho_k(t) = \sum_k \mathbf{M}_k \rho \mathbf{M}_k^\dagger \tag{2}$$

$\rho(t)$ carries all the information we need about the output which we can then extract it using quantum tomography of which an explanation will be provided in the appendix. However, we can use projective measurements, exploiting the positive semi-definiteness of $\rho(t)$ which greatly reduces resource costs. We also note that each quantum system has what is known as a master equation which describes the time evolution of the density matrix state.

$$\dot{\rho}(t) = L\rho(t) \tag{3}$$

Which is a differential equation of the density matrix which can be converted into eq. (2) by solving it. Most physical systems are sufficiently described by a Lindblad Master equation.

We want to evolve $|\phi_i\rangle$ to $|\phi_{ik}(t)\rangle$ through the use of Kraus operators.

$$|\phi_{ik}(t)\rangle = \mathbf{M}_k|\phi_i\rangle = (c_{ik1}, c_{ik2}, \ldots, c_{ikn})^T \tag{4}$$

We use Kraus operators to simulate the effect of the environment on the state as it maps two different Hilbert spaces to each other as stated by Kraus' Operator Theorem
However, Kraus operators are non-unitary and do not preserve the norm of the state vector as they map two different dimensional Hilbert spaces. Here Nagy's theorem comes into play as Kraus operators are known as contractions defined as operators that preserve the norm or contract it, $\frac{||Av||}{||v||} \leq 1$

Nagy's dilation theorem states:
*"For any contraction T on a Hilbert space H, there is a unitary operator U on a larger Hilbert space K for which H belongs to, such that if P is the orthogonal projection of K onto H, then $T^n = P\,U^n P$ for all $n > 0$. The operator U is called a dilation of T and is uniquely determined if U is minimal, i.e. K is the smallest closed subspace invariant under U and U* containing H.*

$$\mathbf{A}^n = \mathbf{P}_H \mathbf{U}_A^n \mathbf{P}_H, \quad n \leq N \tag{5}$$

For the purpose of creating a quantum circuit the Sz.-Nagy dilation theorem allows us to simulate the effect of any non-unitary matrix by a unitary quantum gate, because every operator on a finite-dimensional space is bounded and therefore can be made into a contraction which has a unitary dilation. U can have any dimension higher than H. However, Nagy's theorem ensures that K has a minimized dimension needed to satisfy (5).
Generally we want to simulate N Krauses being applied successively and we do so by turning them into N dilations, ($M_k \xrightarrow{dilation} U_{M_k}$), An example of a minimal unitary dilation of A with N = 1

$$\mathbf{U}_A = \begin{pmatrix} \mathbf{A} & \mathbf{D}_{A^\dagger} \\ \mathbf{D}_A & -\mathbf{A}^\dagger \end{pmatrix} \tag{6}$$

Where $D_A = \sqrt{I - A^\dagger A}$ is called the Defect operator of A.

This shows that if we have some $M_k$ with dimensions n, then its minimum 1 dilation $U_{m_k}$ is 2n, and since it is a unitary operator we can break it down into a sequence of two level elementary unitary gates (check appendix). So we can now construct a quantum circuit that takes some $\mathbf{v}_i$ initial state and we apply a set of elementary quantum gates which correspond to some Kraus operator by use of Sz Nagy's theorem, Which gives us our time-evolved density matrix state $|\phi_{ik}(t)\rangle$ which we use to construct;

$$\rho(t) = \sum_{ik} p_i \cdot |\phi_{ik}(t)\rangle\langle\phi_{ik}(t)| \tag{7}$$

We either use quantum tomography or use the simpler, more efficient method of quantum projective measurement, exploiting the positive-semi-definiteness of the states to measure the expectation value of a physical observable $< \mathbf{O} >$ This gives us the expectation value without actually determining the states as we only find $|c_{ikj}|^2$ which is the jth diagonal element in $|\phi_{ik}(t)\rangle\langle\phi_{ik}(t)|$, this saves a lot of computational resources.
$Tr(\mathbf{O}\rho(t))$ gives the expectation value of $\mathbf{O}$. However, $\mathbf{O}\rho(t)$ is not always positive-semi-definite (**because $|c_{ikj}|^2$ can give a negative value? need to confirm**) so additional processing must be done before the trace can be obtained from projective measurements on the output quantum state.

Our observable's norm is always bounded by the Hilbert-Schmidt norm

$$\|A\| \leq \|A\|_{\mathrm{HS}}^2 \stackrel{\mathrm{def}}{=} \sum_{i \in I} \|Ae_i\|_H^2, \tag{8}$$

Where $e_i$ is an orthonormal basis. Thus we define:

$$\tilde{O} = \frac{O + I\|O\|_{HS}}{2\|O\|_{HS}} \tag{9}$$

We get an $\tilde{\mathbf{O}}$ which is a positive-semi-definite contraction which we can get its expectation value from:

$$\langle \hat{O} \rangle = \mathrm{Tr}(\hat{O}\rho(t)) = \mathrm{Tr}(\mathrm{L}\mathrm{L}^\dagger \rho(t)) = \mathrm{Tr}(\mathrm{L}^\dagger \rho(t)\mathrm{L}) = \sum_i \mathrm{Tr}(\mathrm{L}^\dagger (p_i \cdot |\phi_{ik}(t)\rangle\langle\phi_{ik}(t)|)\mathrm{L}) \tag{10}$$

Where we used Cholesky Decomposition, $\tilde{\mathbf{O}} = \mathbf{L}\mathbf{L}^\dagger$, where $\mathbf{L}$ is a lower triangular matrix. We can then get our original observable back though this equation:

$$\langle O \rangle = \mathrm{Tr}(O\rho(t)) = \mathrm{Tr}((2\|O\|_{HS}\hat{O} - I)\|O\|_{HS}\rho(t)) = 2\|O\|_{HS}\mathrm{Tr}(\hat{O}\rho(t)) - \|O\|_{HS} \tag{11}$$

Thusly, we obtained our desired expectation value from the system interacting with the environment.

We will now discuss how this method compares with other methods utilizing different theorems such as the Stinespring Dilation Theorem to attain the evolution of an open quantum system.

# 3 Efficiency & Complexity Analysis

We discuss the complexity of our method in terms of number of used gates and processes.

Generally, the number of two-level unitary gates needed to decompose a unitary gate is equal to the number of non-zero elements in the lower-triangular part of the gate. For our unitary operator $U_A$, we refer to eq. (5), $A$ and $-A^\dagger$ have $\frac{n^2-n}{2}$ non-zero elements each, $D_A$ has $n^2$ elements, giving us a total of $2n^2 - n$ elements which correspond to gates, which matches nicely with the classical complexity of computing $|\phi_{ik}(t)\rangle$, the maximum number of Kraus operators is equal to $n^2$ and we can say that number of pure states is comparable to n. When we sum over 'k' for the Kraus operators and 'i' for the pure states, we get a complexity of $2n^5 - n^4$ which is of order $O(n^5)$, moderately less complex than methods implementing the Stinespring Dilation theorem $O(n^6)$, We also note that conventional computation methods would require us to compute unitary transformations with $n^3$ dimensions, while our method only requires unitary transformation with 2n dimensions as mentioned before. The most important advantage over most methods in quantum computation is we can break the entire quantum operation which is of $O(n^5)$ into $n^3$ parallel processes of $O(n^2)$. Which greatly cuts down the computation time and is very convenient because all current quantum computing platforms have a limit on the maximum circuit depth due to gate errors, so we can simulate more complicated open quantum systems.

We also mentioned before that we do not need to use quantum tomography as we can instead use projective measurements because our density matrix state is positive semi-definite we need not the off-diagonal elements thus saving resources. However, if we are to want to find the state in a different basis, we would need to use to know the off-diagonal elements of the state matrix in order to apply a basis transformation

$$T|\phi_{ik}(t)\rangle = TM_k\mathbf{v_i} \xrightarrow{Dilation} \begin{pmatrix} \mathbf{T} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} U_{M_k}(v_i^T, 0, ..., 0)^T \tag{12}$$

This T transformation adds another $\frac{n^2-n}{2}$ making the complexity $\frac{5n^2-3n}{2}$ for our total operation. The quantum algorithm takes advantage of the unitarity of T and outperforms the classical computation of the basis transformation ($2n^2 - n \to 4n^2 - 2n$)

So far, no assumptions have been about the form of $M_k$, Using the traditional qubit system, computing one $M_k$ is of $O(n^2)$, so 'q' qubits give us a complexity of $O(4^q)$, thus M has to be exponential in q if it is general. However, in many practical scenarios, $M_k$ is known to be sparse which is to say its matrix form doesn't have entirely arbitrary terms (ie: not a full matrix), this makes the complexity polynomial in q, where it also allows $M_k$ to mediate $l > n$ the transition of quantum states. We also mention that an ancillary qubit is needed for simple state evolution with a two-fold dimensional increase in the Hilbert space, while for Observable evaluation we would need a three-fold dimensional increase in the Hilbert space and two ancillary qubits.

# 4 Practical Applications: Amplitude Damping Quantum Channel

To demonstrate the power of this method. We used the Amplitude Damping Quantum Channel which models the spontaneous emission of a two level atom, which is a highly environment affected system. We write the Lindblad equation for this model as follows:

$$\dot{\rho}(t) = \gamma(\sigma^+\rho(t)\sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho(t)\}) \tag{13}$$

Where $\gamma$ is the spontaneous emission rate, $\sigma^+ = |0\rangle\langle 1|$ is the Pauli raising operator and $\sigma^- = |1\rangle\langle 0| = (\sigma^+)^\dagger$ is the Pauli lowering operator, Which are operators associated with the two level quantum system where the raising operator raises the ground state $|0\rangle$ to the excited state $|1\rangle$ and the lowering obviously does the opposite for the excited state. In the operator sum representation:

$$\rho(t) = \mathbf{M}_0\rho\mathbf{M}_0^\dagger + \mathbf{M}_1\rho\mathbf{M}_1^\dagger \tag{14}$$

$$\mathbf{M}_0 = \frac{1+\sqrt{e^{-\gamma t}}}{2}\mathbf{I} + \frac{1-\sqrt{e^{-\gamma t}}}{2}\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{e^{-\gamma t}} \end{pmatrix} \tag{15}$$

$$\mathbf{M}_1 = \sqrt{1-e^{-\gamma t}}\,\sigma^+ = \begin{pmatrix} 0 & \sqrt{1-e^{-\gamma t}} \\ 0 & 0 \end{pmatrix} \tag{16}$$

We then proceed with the operator dilation process for $M_0$ and $M_1$ to construct $U_{M_0}$ and $U_{M_1}$ as in eq. (6) where :

$$D_{M_0} = D_{M_0^\dagger} = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{1-e^{-\gamma t}} \end{pmatrix}, \qquad U_{M_0} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{e^{-\gamma t}} & 0 & \sqrt{1-e^{-\gamma t}} \\ 0 & 0 & -1 & 0 \\ 0 & \sqrt{1-e^{-\gamma t}} & 0 & -\sqrt{e^{-\gamma t}} \end{pmatrix} \tag{17}$$

$$D_{M_1} = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{e^{-\gamma t}} \end{pmatrix}, \qquad D_{M_1^\dagger} = \begin{pmatrix} \sqrt{e^{-\gamma t}} & 0 \\ 0 & 1 \end{pmatrix}, \qquad U_{M_1} = \begin{pmatrix} 0 & \sqrt{1-e^{-\gamma t}} & \sqrt{e^{-\gamma t}} & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & \sqrt{e^{-\gamma t}} & -\sqrt{1-e^{-\gamma t}} & 0 \end{pmatrix} \tag{18}$$

The simulation of the dilation and the calculation of the density matrix at future time steps for an initial mixed state density matrix $\rho = \frac{1}{2}(|1\rangle\langle 1| + |+\rangle\langle +|)$is provided in the jupyter file.

# 5 References

(1) Hu, Z., Xia, R. Kais, S. A quantum algorithm for evolving open quantum dynamics on quantum computing devices. Sci Rep 10, 3301 (2020). https://doi.org/10.1038/s41598-020-60321-x