Report-2: IBM Q Experience as a versatile experimental testbed for simulating open quantum systems

Mainak Roy and Jessica John Britto Indian Institute of Technology Kharagpur

December 16th, 2022

Concepts covered - Open Quantum Systems and Summary of the Paper

1 Introduction

1.1 Density Matrix

A density matrix is used for describing physical systems whose information is not completely known (such as the statistical mixtures) or for those systems which are entangled with another system. The density matrix does not uniquely describe a physical system. It is a generalized version of statevectors that are used for describing the pure states. It is hermitian, positive semi-definite; its trace is one. A density matrix represents a pure state if it can be expressed as the outer product of the state vector of the pure state with itself, be a rank-one projector, and if it is idempotent and the trace of the square of the density matrix must be one. The difference between probabilistic mixtures of quantum states and quantum superposition is that a system that is a mixture of quantum states with probabilities p_i is a mixed state, while a quantum superposition is a pure state which has probability amplitudes. In the geometric sense, a set of density operators is a convex set, and the pure states are the extremal points of the set. The mixed states are in the interior of the Bloch sphere, and points of unit distance represent pure states for a qubit quantum system.

The time-evolution of the density matrix is given by the von Neumann equation and is given by $i\hbar\frac{\partial\rho}{\partial t}=[H,\rho]$. For a time-independent Hamiltonian, the von Neumann equation can be solved to give the following result- $\rho(t)=e^{\frac{-iHt}{\hbar}}\rho(0)e^{\frac{iHt}{\hbar}}$. This equation is given by the Heisenberg model, which assumes that the density matrix describing the physical system does not change with time; however, the operators acting on it evolve with time. For a general Hamiltonian, it is given by $-\rho(t)=U(t)\rho(0)U(t)^{\dagger}$ where U(t) is a wavefunction propagator over some interval, and it is a unitary operator. The trace norm of a matrix is defined as $||A||_1=Tr(\sqrt{AA^{\dagger}})$. It is the sum of the singular values (which are the square roots of the eigenvalues of AA^{\dagger}) of A. For the case of the Hermitian matrix (such as ρ), the trace norm is the sum of the absolute value of the eigenvalues of the density matrix. Quantum state space is endowed with a metric structure and is given by $D[\rho,\sigma]=\frac{1}{2}||\rho-\sigma||_1$. D takes the values from 0 to 1 and is a measure of distinguishability between two density matrices. When D is 1, it implies that the two density matrices are orthogonally supported.

1.2 Positive and Completely Positive Maps

A map is a mathematical object that takes operators to operators, while a quantum channel is a type of map which takes states to states. A quantum channel need not be unitary in nature. A positive map takes positive elements to positive elements, and it is a monotone map. A linear map is Hermicity-preserving iff $\phi(A^{\dagger}) = [\phi(A)]^{\dagger}$, positive iff $\phi(M_n^+(C)) \subset M_n^+(C)$, trace-preserving iff $Tr\phi(A) = TrA$, unital iff $\phi(I_n) = I_n$. A positive and trace-preserving map has the following properties -

$$||\phi(X)||_1 \le ||X||_1$$
$$D[\phi(\rho), \phi(\sigma)] \le D[\rho, \sigma]$$

This implies that the distinguishability between two density matrices do not increase under the action of such a map. If two maps are positive, their combination need not be positive, but for two completely positive maps, their combination gives a completely positive map. CP maps are the most general representation of quantum evolutions. For example, if we consider a density matrix ρ and take its transpose, then its eigenvalues and determinants do not turn out to be positive upon doing the math. Another instance where the P-maps fail is the case of entangled systems. Let $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ be a two-qubit entangled system, then its density matrix is given by ρ -

$$\rho = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

When we take partial transpose over qubit-1, we get the following density matrix ρ^{T_2} -

$$\rho^{T_2} = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Clearly, not all of its eigenvalues are positive, hence, P-maps fail at this point. Therefore, we need a quantum channel to be a CP-map and a quantum channel must be unitary in nature. All CP-maps are a subset of P-maps. In general, when we extend P-map to a higher dimension, i.e from $\phi: H(A) \to H(B)$ to $Id \otimes \phi: C^{k \times k} \otimes H(A) \to C^{k \times k} \otimes H(B)$, therefore, ϕ is k-positive if $Id \otimes \phi$ else ϕ is CP if ϕ is k-positive for all k. If dim(H) = n, then ϕ is CP if and only if ϕ is n-positive. k-positivity means l-positivity if l < k. A CP-map can be represented by Kraus Operators.

2 Born-Markov Approximation and Lindblad Form

2.1 Born-Markov Master Equation

From the Born-Markov equation, we can trace out the bath degrees of freedom to get the Lindblad form. Consider a principal system S coupled with the environment B. Let the total Hamiltonian be $H(t) = H_s \otimes I_B + I_S \otimes H_B + \alpha H_{SB}$, where H_{SB} is the Hamiltonian for the system-bath in the interaction picture and hamiltonians of the system and bath are time-independent. The equation of motion of the total system is given by -

$$i\hbar \frac{d\rho_{SB}}{dt} = [H_s \otimes I_B + I_S \otimes H_B + \alpha H_{SB}, \rho_{SB}] - (1)$$

and we know the hamiltonian and density operator can be evolved in time in the following way -

$$H(t) = e^{i(H_S + H_B)/\hbar} H_{SB} e^{-i(H_S + H_B)/\hbar} - (2)$$

and

$$\rho(t) = e^{i(H_S + H_B)/\hbar} \rho_{SB} e^{-i(H_S + H_B)/\hbar} - (3)$$

and we get the following equation-

$$i\hbar \frac{d\rho(t)}{dt} = \alpha[H(t), \rho(t)] - (4)$$

Solving the equation, we get -

$$\rho(t) = \rho(0) - \frac{i}{\hbar} \alpha \int_{0}^{t} [H(t'), \rho(s)] dt' - (5)$$

Putting equation 5 in 4, we get-

$$i\hbar \frac{d\rho(t)}{dt} = \alpha[H(t), \rho(0)] - \alpha^2 \frac{i}{\hbar}[H(t), \int_0^t [H(t'), \rho(t')]dt'] - (6)$$

and from equation 3, we can find ρ_{SB} -

$$\rho(t) = e^{-i(H_S + H_B)/\hbar} \rho e^{i(H_S + H_B)/\hbar} - (7)$$

We can find the density matrix of the principle system S by taking trace of ρ_{SB} and its equation of motion can be written as-

$$i\hbar \frac{d\rho_S(t)}{dt} = \alpha t r_B[H(t), \rho(0)] - \alpha^2 \frac{i}{\hbar} t r_B[H(t), \int_0^t [H(t'), \rho(t')] dt'] - (8)$$

We know the H(t) can be expressed in terms of H_{SB} and on doing so, the first term of equation 8 gets cancelled, and we get the following-

$$i\hbar \frac{d\rho_S(t)}{dt} = -\alpha^2 \frac{i}{\hbar} tr_B[H(t), \int_0^t [H(t'), \rho(t')] dt'] - (9)$$

On integrating the above equation from t to t', we see that the difference between the density matrices at t = t and t' is in the order of square of α . For complete interaction between the system and the environment, we set α to 1, and taking to t to ∞ and $\rho = \rho_S \otimes \rho_B$, we get the following equation of motion for the principle system and this is called Born-Markov Master equation-

$$i\hbar \frac{d\rho_S(t)}{dt} = -\alpha^2 \frac{i}{\hbar} tr_B[H(t), \int_0^\infty [H(t'), \rho(t')] dt'] - (10)$$

In Born-Markov approximation, we consider there's a weak coupling between the system and the environment and the correlation between them is for a very short interval and this is called short memory effect.

3 Summary of the paper

The authors first give a brief overview of open quantum systems theory and a description of current advances in the field. They note that most experiments in this field utilize an analogue quantum simulator, which is a quantum system that follows similar dynamics to the system they desire to study. They then contrast this with the idea of a gate-based universal quantum computer that can simulate the dynamics of any system if programmed suitably.

The objective of this paper is to demonstrate that cloud-based quantum computers like the IBM Q Experience systems, which are relatively widely accessible to the general public, are a suitable testbed for future experiments in this field, compared to special analogue quantum simulators which are only available in labs and possibly quite expensive as well. Of course, there are issues to be taken into consideration, like errors during measurements or during circuit execution because of the circuit depth or gates used.

They implement several simulations of quantum channels and compare them with theoretical predictions, and they demonstrate an example of reservoir engineering, where the environment is carefully engineered so that the favored stationary state of the system is an entangled state instead of the loss of entanglement that usually occurs. They also explore Markovian and non-Markovian dynamics. Particularly, they demonstrate some recently discovered phenomena like essential and eternal non-Markovianity and implement a recently proposed non-Markovian witness. They also demonstrate the non-monotonic behavior of quantum channel capacity and extractable work with regard to quantum communication and quantum thermodynamics, respectively.

3.1Markovian reservoir engineering

Generally, the effect of the environment on a quantum system makes it lose quantum properties like coherence and entanglement. However, a carefully designed environment can give rise to interactions that drive the system to a stationary state exhibiting manifestly quantum properties.

In this example, they simulate a semigroup Markovian master equation

which has the Bell state $|\psi^{-}\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$ as its stationary state. The 4 Bell states can be identified as the eigenstates of the operators $\sigma_{x}^{(1)} \otimes \sigma_{x}^{(2)}$ and $\sigma_{z}^{(1)} \otimes \sigma_{z}^{(2)}$ as shown below:

Bell state	Eigenvalue wrt $\sigma_x^{(1)} \otimes \sigma_x^{(2)}$	Eigenvalue wrt $\sigma_z^{(1)} \otimes \sigma_z^{(2)}$
$ \phi^{+}\rangle = \frac{1}{\sqrt{2}} \left(00\rangle + 11\rangle \right)$	+1	+1
$ \phi^{-}\rangle = \frac{1}{\sqrt{2}} \left(00\rangle - 11\rangle \right)$	-1	+1
$ \psi^{+}\rangle = \frac{1}{\sqrt{2}} \left(01\rangle + 10\rangle \right)$	+1	-1
$ \psi^{-}\rangle = \frac{1}{\sqrt{2}} \left(01\rangle - 10\rangle \right)$	-1	-1

Now, they design two channels which they name the XX pump and the ZZ pump. The action of each is to pump states from the +1 eigenspace to the -1 eigenspace of the corresponding operator. From the table above, we can see that the only state belonging to the -1 eigenspace of both $\sigma_x^{(1)} \otimes \sigma_x^{(2)}$ and $\sigma_z^{(1)} \otimes \sigma_z^{(2)}$ is $|\psi^-\rangle$. So if we compose the two channels and apply them together, we should be able to pump everything to a single state, which is $|\psi^{-}\rangle$. Also, applying any one channel by itself will obviously pump states to a mixture of the states in the corresponding -1 eigenspace (which is $\{|\phi^-\rangle, |\psi^-\rangle\}$ for the XX pump and $\{|\psi^+\rangle, |\psi^-\rangle\}$ for the ZZ pump).

The form of the XX pump and ZZ pump are given as

$$\Phi_{xx}\rho_s = E_{1x}\rho_s E_{1x}^{\dagger} + E_{2x}\rho_s E_{2x}^{\dagger}$$

$$\Phi_{zz}\rho_s = E_{1z}\rho_s E_{1z}^{\dagger} + E_{2z}\rho_s E_{2z}^{\dagger}$$

with

$$E_{1z} = \sqrt{p} \mathbb{I}^{(1)} \otimes \sigma_x^{(2)} \frac{1}{2} (\mathbb{I} + \sigma_z^{(1)} \otimes \sigma_z^{(2)})$$

$$E_{1z} = \frac{1}{2} (\mathbb{I} - \sigma_z^{(1)} \otimes \sigma_z^{(2)}) + \frac{\sqrt{1-p}}{2} (\mathbb{I} + \sigma_z^{(1)} \otimes \sigma_z^{(2)})$$

and E_{1x} and E_{2x} are the same with the replacements $\sigma_z^{(2)} \to \sigma_x^{(2)}$ and $\sigma_z^{(1)} \otimes \sigma_z^{(2)} \to \sigma_x^{(1)} \otimes \sigma_x^{(2)}$.

The above maps are parametrized by a parameter p with $0 \le p \le 1$. For $p \ll 1$, the repeated application of Φ_{zz} generates a master equation of Lindblad form with Lindblad/jump operator $V = \frac{1}{2}\mathbb{I}^{(1)} \otimes \sigma_z^{(2)} \left(\mathbb{I} + \sigma_z^{(1)} \otimes \sigma_z^{(2)}\right)$. For p = 1, the map generates $|\psi^-\rangle$ always.

To experimentally simulate the above, the authors provide circuit implementations of each pump. Then they compare the theoretical and experimental results of applying each pump individually and their composition for different values of p.

3.2 Depolarising and Pauli channels

3.2.1 Pauli channel

The most general single-qubit open quantum system model is given by the time-dependent Pauli channel:

$$\frac{d\rho_s}{dt} = \frac{1}{2} \sum_i \gamma_i(t) \left[\sigma_i \rho_s(t) \sigma_i - \rho_s(t) \right]$$

where i = x, y, z.

The dynamics generated by the above master equation is generally not phase-covariant except if $\gamma_x(t) = \gamma_y(t)$. Also, since the decay rates may become negative, conditions for complete positivity must be imposed, which can be expressed as a set of inequalities.

The authors later use a specific form of the time dependent Pauli channel which gives rise to the phenomenon of eternal non-Markovianity: a situation where the dynamical map is non-CP-divisible for all times t. They then further use it to demonstrate a theoretical prediction, which is, the presence of oscillations in extractable work.

3.2.2 Depolarising channel

If we set $\gamma_i(t) = \gamma$ in the equation for the time-dependent Pauli channel, we get the master equation for the depolarising channel. The dynamical map of an open quantum system subject to depolarising noise is given by

$$\Phi_t \rho_s = \left[1 - \frac{3}{4}p(t)\right] + \frac{p(t)}{4} \sum_i \sigma_i \rho_s \sigma_i$$

where i = x, y, z and $p(t) = 1 - e^{\gamma t}$, with γ being the Markovian decay rate.

The depolarising channel is one of the most common models of qubit decoherence because of its symmetry properties. It can be described as, with probability 1-p the qubit stays the same, while with probability p it becomes maximally mixed. The mixing is described by a combination of σ_x for a bit flip error, σ_z for a phase flip error, and σ_y for both.

The authors experimentally simulate this channel for various initial states (though they only provide the plot for one specific example $|\psi\rangle = \cos\frac{\pi}{8}|0\rangle + \sin\frac{\pi}{8}e^{\frac{i\pi}{4}}|1\rangle$) and find the density matrix elements using quantum state tomography, and compare them with theoretical predictions for various values of p. They observe that the agreement between theory and experiment is independent of the intial state.

4 References

- 1. Open Quantum Systems with Qiskit
- 2. Density Matrix
- 3. Time-Dependent Solutions: Propagators and Representations
- 4. Nielsen and Chuang
- 5. CP and P maps
- 6. A simple derivation of the Lindblad equation