Beyond quantum nonlocality in continuous variable systems and thermalization of a qubit

By

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DECLARATION

I, hereby declare that the investigtion presented in the thesis has been carried out by me. The work is original and has not been submitted earlier as a whole or in part for a degree / diploma at this or any other Institution / University.

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List of Publications arising from the thesis

Journal

1. "Uncertainty principle as a postquantum nonlocality witness for the continuous-variable multimode scenario", Prathik Cherian J, Amit Mukherjee, Arup Roy, Some Sankar Bhattacharya, and Manik Banik, *Physical Review A* **99** 012105 (2019).

2. "On thermalization of two-level quantum systems", Prathik Cherian J, Sagnik Chakraborty, and Sibasish Ghosh, *Europhysics Letters* **126** 40003 (2019).

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Posters/Talks Presented in School/ Conferences:

1. "Qubit thermalisation in the presence of 2-qubit interaction" at International School & Conference in Quantum Information 2016, 9-18 February, 2016 at Institute of Physics, Bhubaneswar, India.

2. "Thermalisation of two-level quantum systems", at National Workshop on Quantum Information and Information Security 2018 5-11 October, 2018 at International Institute of Information and Technology, Hyderabad, India.

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Dedicated to my Amma

Contents

List of Figures

Chapter 4

Summary and Future Directions

In this thesis, firstly we studied postquantum nonlocality in continuous variable systems. We used the language of probabilistic measures to define continuous outcome correlations. We then developed a systematic approach through which the postquantum and nonlocal features of such correlations can be studied. We showed that the Robertson-Schrödinger uncertainty relation can be employed as a witness for postquantumness and that the Cavalcanti-Foster-Reid-Drummond (CFRD) Bell-type inequalities can be used to ascertain nonlocality of continuous outcome correlations. We have also given a class of m-mode postquantum nonlocal continuous outcome correlations.

As a future direction, it would be interesting to see whether for any postquantum nonlocal correlation some form(s) of uncertainty principle is violated. Another possible direction would be to construct *genuine* nonlocal inequality for m-mode scenario with continuous outcome, which can be used to certify the inbuilt genuineness of the correlation presented. It would also be of great interest to determine whether there exists some operational task that could detect postquantum nonlocality and potentially exploit it as a resource.

Secondly, we studied thermalization of a two-level quantum system. Specifically, we were able to derive a 2-qubit Hamiltonian that simulates the thermalization of a qubit interacting with a thermal reservoir described by the quantum optical master equation. We studied the conditions for the generic form of such a Hamiltonian to describe Markovian dynamics and the conditions for it to describe a thermalization process. We were also able to derive a class of Lindblad-type master equations that can describe Markovian as well as non-Markovian thermalization.

An obvious extension for this work would be to extend the analysis beyond single qubit and to look at multiple qubits as in the case of an n-qubit chain. It would also be intriguing to look at qubit thermalization scenarios that require more than a single-qubit ancilla. Another possible future direction would be to generalize the work to higher dimensions including infinite dimensions.

Although here we studied thermalization of a two-level quantum system, a similar study can, in principle, be carried out for the case of a single-mode quantized radiation field (i.e. a 1D quantum harmonic oscillator) in which, the two-mode interaction Hamiltonian (between the system mode and an ancilla mode) may typically be generated by a beam-splitter type Hamiltonian. In fact, there exists a Markovian master equation similar to the quantum optical master equation that describes thermalization of a quantum harmonic oscillator interacting with a heat bath. Starting from that master equation, with a similar approach it is possible to derive a two-mode Hamiltonian that simulates the reduced system dynamics and to derive the necessary condition for Markovianity as well.

From this perspective, one can now, in principle, put together the two seemingly disjoint studies in the thesis – namely, from the perspective of studying both static as well as dynamic quantum correlations in multi-mode quantum systems.

The infinite dimensional case would also be of extreme interest as it can help us better understand the thermalization of quantum harmonic oscillators. We expect that our work would help to better understand the process of thermalization in both Markovian as well as non-Markovian scenarios. We could also consider possible applications to study and design of quantum engines, refrigerators etc. It could in turn further develop our understanding of the foundations of quantum thermodynamics.

Synopsis

Introduction and Motivation

My Ph.D. thesis consists of two research works – one in the domain of non-locality for continuous variable quantum systems while the other is on thermalization for two-level quantum systems. Thus, although both of them fall under the field of Quantum Information, nevertheless, perspectives of these two works are different. Below, we will therefore, describe these works one by one.

Nonlocality is one of the most bizarre features of multipartite quantum systems established for the very first time in the seminal paper of J. S. Bell [1]. However, nonlocality is not a salient feature of quantum theory alone. In 1994, Popescu and Rohrlich designed a correlation, famously known as PR correlation, which satisfies the relativistic causality or more broadly no-signalling (NS) principle but at the same time depicts stronger nonlocal behavior as it achieves the algebraic maximum of the Bell type inequality– Clauser-Horne-Shimony-Holt (CHSH) inequality.

A great deal of research has been done on quantum and postquantum nonlocal correlations in discrete input-output scenario. But, these studies mainly consider finite-input finite-output correlations arising from finite dimensional quantum systems. Although nonlocal correlations have been studied for infinite dimensional continuous variable (CV) systems, those results are fundamentally not different from the finite input-output scenario as discrete binning of continuous outcomes has been considered there. In this regard, a notable work in the infinite dimensional CV systems is the CV Bell inequalities introduced by Cavalcanti, Foster, Reid, Drummond (CFRD) [2]. A natural area of interest in this context is the notion of postquantum nonlocal correlations. Very recently, A. Ketterer et al. have developed a formalism to address this question for generic NS black-box measurement devices with continuous outputs and they have also provided a class of postquantum nonlocal correlations when only two sites/modes are involved [3].

A relevant question in the continuous outcome scenario is: how to certify postquantum nonlocality of a given correlation? This question is addressed in the first part of the thesis. We develop a systematic approach to study postquantum nonlocal correlations for continuous outcome scenario in multimode systems [4]. We find that Robertson-Schrödinger (RS) uncertainty relation has a key role to play in this regard. We construct a class of continuous outcome postquantum nonlocal correlations for generic m-mode scenario. While the nonlocality of the proposed class of correlations is certified through violation of CFRD inequalities, postquantum nature is guaranteed by violation of RS uncertainty relation.

In the second part, we look into the thermalization of a two-level quantum system interacting with an environment (typically, a heat reservoir). Equilibriation of an open system into the Gibbs thermal state with temperature corresponding to the reservoir is called thermalization. The study of evolution of open systems towards equilibrium has always been a challenging problem in Statistical Mechanics. The difficulty lies in prescribing a form of interaction between the system and the environment at the microscopic level that will give rise to equilibration. We look at this thermodynamic problem from a quantum mechanical perspective.

There have been a number of models describing quantum thermalization. But none of them provide a Hamiltonian description at the microscopic level. My work was motivated by this problem. We are able to derive a 2-qubit unitary operator (and thus, a 2-qubit

Hamiltonian) that can simulate a thermalization process for a qubit interacting with a thermal bath. Here, the reduced dynamics of the unitary operation gives rise to the exact dynamics of the system qubit.

To completely characterize the joint Hamiltonian of the system and environment that results in equilibration of the system, is a formidable task. So, instead we ask the following question: whether for a given thermalization process of a system, there exists an ancilla in a specific state and a joint Hamiltonian of system-ancilla that gives rise to the exact process of equilibration on the system. In my work, we provide an affirmative answer to this question in the case of quantum optical master equation [6].

We work out a *thermalizing Hamiltonian* H_{th} for the quantum optical master equation [5] which simulates thermalization dynamics of the system qubit. We find that a single-qubit ancilla initialized in a thermal state is sufficient for such a dynamics to be mimicked. We also derive the necessary and sufficient conditions for such a Hamiltonian to lead to Markovian dynamics for the system evolution. Further, we derive the Lindblad type master equation for a system dynamics arising from the general form of our Hamiltonian.

Postquantum Nonlocality in Continuous Variable Systems

In the first part, we focus on our work done in [4] wherein we have shown that the Robertson-Schrödinger (RS) uncertainty relation can be used for certifying postquantum nature of correlations in multimode continuous-variable (CV) systems. The standard $m-n-k$ Bell scenario considers m space-like separated observers/sites denoted as $\mathcal{A}_i$, with $i \in \{1, 2, \ldots, m\}$, each observer performs one out of n possible local measurements denoted by X_i, with $X_i \in \{0, 1, \ldots, n-1\}$; and each measurement having k distinct outcomes denoted by A_i^j, with $j \in \{0, 1, \ldots, k-1\}$. Now, we consider that the outcomes are continuum instead of k distinct values. As pointed out by Ketterer et. al. in [3], it is convenient to adopt the language of probability measures while considering continuous outcomes.

A probability space consists of three elements: (i) a sample space (Ω), (ii) the Borel σ-algebra ($\mathcal{B}(\Omega)$) of events on Ω, and (iii) a valid Borel probability measure $\xi : \mathcal{B}(\Omega) \to [0, 1]$. In our case, the sample space would be $\Omega = \Omega_1 \times \Omega_2 \times \cdots \times \Omega_m$, with each $\Omega_i = \mathbb{R}$ being the outcome sample space of i^{th} site. The probability measure satisfies the normalization condition: $\xi(\mathbb{R} \times \mathbb{R} \cdots \times \mathbb{R}) = 1$, and also satisfies the additivity property: $\xi(\cup_i \omega_i) = \sum_i \xi(\omega_i)$, for all countable sequences $\{\omega_i\}_i$ of disjoint events $\omega_i \in \mathcal{B}(\Omega)$. The relation between a probability measure ξ and a probability density p is given by,

$$\xi(A_1 \times \cdots \times A_m) := \int_{A_1 \times \cdots \times A_m} d\xi(a'_1, \cdots, a'_m) = \int_{A_1} \cdots \int_{A_m} p(a'_1, \cdots, a'_m) da'_1 \cdots da'_m. \tag{1}$$

Here $A_1 \times \cdots \times A_m \in \mathcal{B}(\Omega)$, each $A_i \in \mathcal{B}(\mathbb{R})$, $p(a'_1, \cdots, a'_m)$ denotes the corresponding probability density to ξ. We will denote the set of all probability measures on $\mathcal{B}(\Omega)$ as $\mathcal{M}_{\mathbb{R}^m}$.

From now on we consider that one of two possible local measurements will be performed on each site, i.e., $X_i \in \{0, 1\}$, $\forall\, i$. In such a scenario, an m-mode Bell behavior is defined as the collection of joint conditional probability measures $\{\xi^{\mathcal{A}_1 \cdots \mathcal{A}_m}_{X_1 \cdots X_m} \mid X_1, \cdots, X_m = 0, 1\}$, where each $\xi^{\mathcal{A}_1 \cdots \mathcal{A}_m}_{X_1 \cdots X_m} \in \mathcal{M}_{\mathbb{R}^m}$. Whenever there is no confusion we will avoid the superscript notation denoting the modes. Collection of all m-mode Bell behavior will be denoted as $\mathcal{M}^{2^m}_{\mathbb{R}^m}$. Consider any arbitrary grouping of m modes into two disjoint (nonempty) sets $\mathcal{K}$, $\mathcal{K}^c$ with $\mathcal{K} \cup \mathcal{K}^c = \{\mathcal{A}_1, \cdots, \mathcal{A}_m\}$. NS condition puts the restrictions that measurement choice of one set does not determine the outcome probability of other set for any of the above groupings. In measure theoretic language these conditions read as:

$$\xi_{\{X_i\}_{i \in \mathcal{K}} \cup \{X_j\}_{j \in \mathcal{K}^c}} \left(\prod_{i \in \mathcal{K}} A_i \times \prod_{j \in \mathcal{K}^c} \mathbb{R}_j \right) = \xi_{\{X_i\}_{i \in \mathcal{K}} \cup \{X_j \oplus 1\}_{j \in \mathcal{K}^c}} \left(\prod_{i \in \mathcal{K}} A_i \times \prod_{j \in \mathcal{K}^c} \mathbb{R}_j \right) \tag{2}$$

for all $A_i \in \mathcal{B}(\mathbb{R})$, where $\oplus$ denotes sum modulo 2. The set of all no-signalling correlations $\mathcal{M}_{\mathrm{NS}}$ is naturally a strict subset of $\mathcal{M}^{2^m}_{\mathbb{R}^m}$. A behavior will be called quantum *iff* it can be obtained according to Born probability rule, i.e.: $\xi_{X_1 \cdots X_m}(A_1 \times \cdots \times A_m) =$

$\mathrm{Tr}\left[\otimes_{i=1}^{m} M_{X_i}(A_i)\rho\right]$, $\forall\ A_i \in \mathcal{B}(\mathbb{R})$; where ρ is a density operator acting on some tensor product Hilbert space $\otimes_{i=1}^{m}\mathcal{H}_i$, with $\mathcal{H}_i$ being the i^{th} site's Hilbert space (in this case infinite dimensional); and $M_{X_i}(A_i) : \mathcal{B}(\mathbb{R}) \mapsto \mathcal{L}_{+}(\mathcal{H}_i)$ are positive operator valued measures on $\mathcal{H}_i$. A behavior $\{\xi_{X_1\cdots X_m}\}_{X_i=0,1}$ will be called postquantum if $\{\xi_{X_1\cdots X_m}\}_{X_i=0,1} \in \mathcal{M}_{NS}$ but $\{\xi_{X_1\cdots X_m}\}_{X_i=0,1} \notin \mathcal{M}_Q$, the set of quantum behaviors. Local-realistic correlations are those where the outputs are locally generated from local inputs and some pre-established classical correlations encoded in some shared variable $\lambda \in \Lambda$. Such behaviors are of the form $\xi_{X_1\cdots X_m} = \int_{\Lambda} \delta_{a_1(X_1,\lambda),\cdots,a_m(X_m,\lambda)}\, d\eta(\lambda)$, where $\eta : \mathcal{B}(\Lambda) \to \mathbb{R}_{\geq 0}$ is a probability measure and $\delta_{a_1(x_1,\lambda),\cdots,a_m(X_m,\lambda)}$ is the CV local deterministic response function: $\delta_{a_1,\cdots,a_m}(A_1 \times \cdots \times A_m) := 1$ if $a_i \in A_i$ and 0, otherwise. Set of all local behaviors $\mathcal{M}_L$ is a strict subset of $\mathcal{M}_Q$ and behaviors not belonging to $\mathcal{M}_L$ manifest nonlocal feature.

In [2] Cavalcanti, Foster, Reid and Drummond (CFRD) derived a class of local realistic inequalities without any assumption on the number of measurement outcomes and therefore their inequalities are directly applicable to CV systems with no need of discrete binning of the outcomes. They have focused on the correlation functions of observables for m sites or observers, each equipped with n possible local measurement settings, and considered any real, complex, or vector function $F(\mathbf{X}^1, \mathbf{X}^2, \cdots)$ of the local observables. All such functions, in a local hidden variable (LHV) theory, are functions of hidden variables $\lambda \in \Lambda$. The average over the LHV ensemble $P(\lambda)$ is given by, $\langle F \rangle = \int_{\Lambda} P(\lambda) F(\mathbf{X}^1, \mathbf{X}^2, \cdots) d\lambda$. Using the fact that any function of random variables has non-negative variance, the class of CRFD local realistic inequalities read as: $|\langle F \rangle|^2 \leq \left\langle |F|^2 \right\rangle$. We use CFRD inequality to certify non-local feature of a given CV outcome correlation.

For an m-mode quantum state denoted by ρ, the non-commutativity of the canonical operators and the positive semi-definiteness of the state lfeads to the famous restriction – the RS uncertainty relation: $\mathbf{V} + \iota\mathbf{\Omega} \geq 0$, where $\mathbf{V}$ is a $2m \times 2m$ real symmetric matrix, namely, the covariance matrix (CM) and $\mathbf{\Omega}$ is the *symplectic form* and $\iota = \sqrt{-1}$. CM is calculated from the second moments of position ($\hat{q}_i$) and momentum ($\hat{p}_i$) operators.

Whether any given real symmetric matrix corresponds to a *bona fide* quantum CM can be verified by RS uncertainty relation.

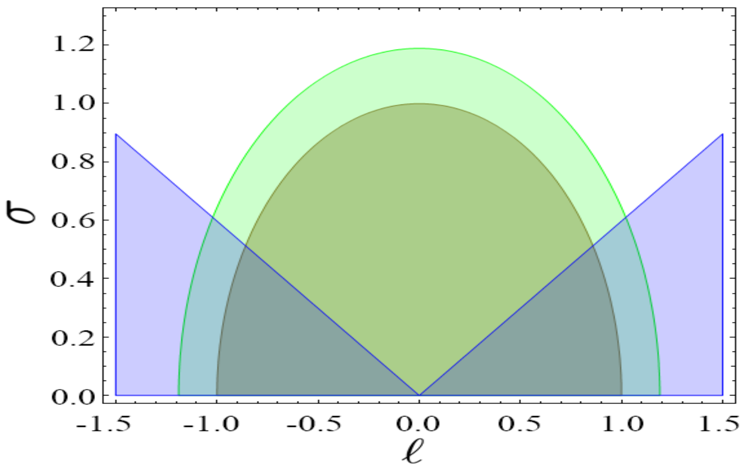

Figure 1: The blue region shows the CFRD violation. The smaller and larger half-circular regions denote RS uncertainty violations for $c = 0$ and $c = 1$ respectively.

First, we give an example in 3-mode case. Consider the following Bell behavior:

$$\xi_{111}^{\mathcal{A}_1\mathcal{A}_2\mathcal{A}_3} = \frac{1}{4}\left[\mathcal{N}_{(l,l,-l),\sigma} + \mathcal{N}_{(l,-l,l),\sigma} + \mathcal{N}_{(-l,l,l),\sigma} + \mathcal{N}_{(-l,-l,-l),\sigma})\right] \tag{3a}$$

$$\xi_{\text{rest}}^{\mathcal{A}_1\mathcal{A}_2\mathcal{A}_3} = \frac{1}{4}\left[\mathcal{N}_{(l,l,l),\sigma} + \mathcal{N}_{(l,-l,-l),\sigma} + \mathcal{N}_{(-l,l,-l),\sigma} + \mathcal{N}_{(-l,-l,l),\sigma}\right] \tag{3b}$$

where, rest $\in \{0,1\}^3 \setminus \{111\}$, with 0 and 1 denoting position and momentum measurements respectively. l is a real number while σ is a positive real number. $\mathcal{N}_{\mathbf{a},\sigma}$ is the normal (Gaussian) probability measure defined through (1) with probability density centered around $\mathbf{a} := (a_1, a_2, a_3)$ with width σ, *i.e.*, $p_{\mathbf{a},\sigma}(\mathbf{a}') = 1/(\sigma\sqrt{2\pi})^3 \exp\left[-\sum_{i=1}^{3}(a_i - a_i')^2/(2\sigma^2)\right]$. It is straightforward to show that the above behavior is indeed a NS behavior.

For the above correlation, the CFRD expression turns out to be $5l^6 \leq 2\left(l^2 + \sigma^2\right)^3$ whereas the RS relation is found to be $l^2+\sigma^2 < \sqrt{1+c^2}$ where c is a non-zero real number equalling the average of the non-product single mode joint distribution (with $c = 0$ being the case where the single mode joint distribution is taken as the product of the marginals). These are plotted in Fig. 1 and we can see the existence of postquantum nonlocal correlations.

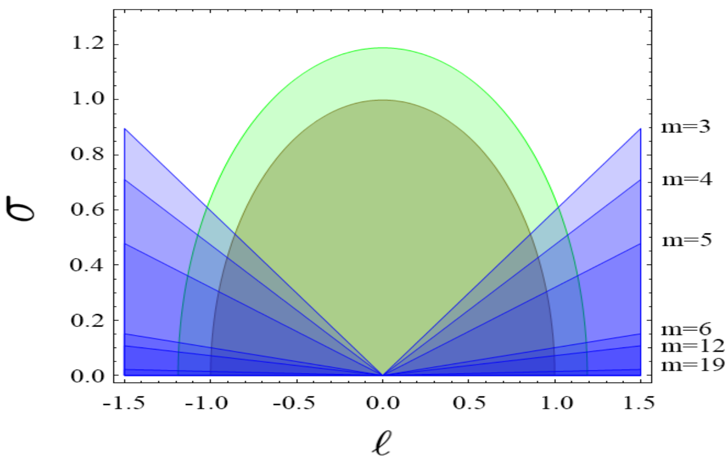

Figure 2: For different number of modes ($m = 3, 4, 5, 6, 12, 19$) the corresponding CFRD inequalities violation has been depicted by different shades of Blue regions as shown. The smaller and larger half-circular regions denote RS uncertainty violations for $c = 0$ and $c = 1$ as in Fig.1.

Consider now, an m-mode Bell behavior defined as,

$$\xi_{11\cdots1}^{\mathcal{A}_0\mathcal{A}_1\cdots\mathcal{A}_m} = \frac{1}{2^{m-1}} \sum_{\substack{i\in\mathbb{N}_o \\ i\leq m}} \sum_{\mathbf{P}_i\in\mathcal{P}_i} \mathcal{N}_{\mathbf{P}_i,\sigma} \,, \tag{4a}$$

$$\xi_{\text{rest}}^{\mathcal{A}_0\mathcal{A}_1\cdots\mathcal{A}_m} = \frac{1}{2^{m-1}} \sum_{\substack{i\in\mathbb{N}_e \\ i\leq m}} \sum_{\mathbf{P}_i\in\mathcal{P}_i} \mathcal{N}_{\mathbf{P}_i,\sigma} \,. \tag{4b}$$

Here, $\mathbb{N}_o$ and $\mathbb{N}_e$ denote the set of odd and even integers respectively. $\mathcal{N}_{\mathbf{a},\sigma}$ is the normal (Gaussian) probability measure defined through (1) with probability density centered around $\mathbf{a} \equiv (a_1, \cdots, a_m)$ with widths σ, *i.e.*, $p_{\mathbf{a},\sigma}(\mathbf{a}') = 1/(\sigma\sqrt{2\pi})^m \exp\left[-(\sum_{i=1}^m (a_i - a_i')^2)/(2\sigma^2)\right]$. The expression of m-mode CFRD inequality with this probability measure takes the following form:

When m is even, we get,

$$\left[\left(2^{m/2}\cos(\tfrac{m\pi}{4}) + (-1)^{\frac{m}{2}+1}2\right)^2 + 2^m \sin^2(\tfrac{m\pi}{4})\right] l^{2m} \leq 2^m \left(l^2 + \sigma^2\right)^m . \tag{5}$$

When m is even, we get,

$$\left[\left(2^{m/2}\sin(\tfrac{m\pi}{4}) + (-1)^{\frac{m-1}{2}+1}2\right)^2 + 2^m\cos^2(\tfrac{m\pi}{4})\right] l^{2m} \leq 2^m\left(l^2+\sigma^2\right)^m. \tag{6}$$

The RS uncertainly relation, calculated with single-mode product [non-product] joint distribution, will be violated by the probability measure (4) if $l^2+\sigma^2 < 1$ [$l^2+\sigma^2 < \sqrt{1+c^2}$]. The CFRD violation and the RS violation are plotted in Fig.2.

Thermalization of two-level systems

In the second part, we focus on our work [6] on thermalization of a qubit interacting with an environment (typically, a heat bath). We begin by choosing the following Markovian master equation (quantum optical master equation) which corresponds to a qubit interacting with a bosonic thermal bath under Markovian conditions [5].

$$\frac{d\rho(t)}{dt} = \gamma_0(N+1)\Big(\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho(t)\}\Big) + \gamma_0 N\Big(\sigma_+\rho(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho(t)\}\Big) \tag{7}$$

Here, $N = (\exp\frac{E(\omega)}{k_BT} - 1)^{-1}$ is the Planck distribution, k_B is the Boltzmann constant, T is temperature of the heat bath and $E(\omega) = \hbar\omega$ is the energy of the system at frequency ω. γ_0 is the spontaneous emission rate of the bath, and $\gamma = \gamma_0(2N+1)$ is the total emission rate (including thermally induced emission and absorption processes). Here the free evolution part of the dynamics is neglected since the point of interest is in the dissipative dynamics. This master equation can be readily solved.

Any single-qubit channel can be written as an affine transformation of the form $r_i(t) = \sum_{j=0}^{3} M_{ij}r_j(0) + C_i$ where $r_i(t)$ are the components of the Bloch vector $\bar{r}(t)$ for the solution. Hence, we can express our corresponding affine transformation as:

$$M = \begin{bmatrix} e^{-\gamma t/2} & 0 & 0 \\ 0 & e^{-\gamma t/2} & 0 \\ 0 & 0 & e^{-\gamma t} \end{bmatrix}, C = \begin{bmatrix} 0 \\ 0 \\ g(e^{-\gamma t} - 1) \end{bmatrix}. \tag{8}$$

In order to achieve a unitary dilation of any single-qubit channel (i.e., a unitary evolution of the tensor product of an arbitrary state of the qubit and a fixed state of ancilla system, followed by tracing out the ancilla system), one may use either a two, three, or a four dimensional ancilla system – depending upon whether there are respectively two, three, or four Kraus operators required for representing the channel action on any state of the susyem qubit. Interestingly, even if three or four Kraus operators are needed, it may still be possible – at least for certain types of qubit channels – to have a unitary dilation of the channel using a two dimensional ancilla (i.e., a qubit), prepared initially in some mixed state. The prescription for such a unitary was given by Narang and Arvind [7]. In particular, they used a single-qubit mixed state ancilla to parametrize the affine transformation of a single-qubit channel. We follow their technique to simulate our dynamical process for thermalization. To do so, we consider a single-qubit mixed state ancilla of the form $\rho_e = (1-\lambda)\frac{\mathbb{I}}{2} + \lambda|\phi\rangle\langle\phi|$. where $\frac{\mathbb{I}}{2}$ is the maximally mixed state and $|\phi\rangle$ is a general pure state given by, $|\phi\rangle = \cos\left(\frac{\xi}{2}\right)|0\rangle + e^{-i\eta}\sin\left(\frac{\xi}{2}\right)|1\rangle$. Note that the information regarding temperature will be included inside the λ parameter.

The *most general* two-qubit unitary U (upto a freedom of local unitary actions), is given in equation (9) below and it will result in the following affine transformation for the system qubit, as given in equations (10) and (11) below.

$$U = \begin{bmatrix} \cos\frac{\alpha+\delta}{2} & 0 & 0 & i\sin\frac{\alpha+\delta}{2} \\ 0 & e^{-i\beta}\cos\frac{\alpha-\delta}{2} & ie^{-i\beta}\sin\frac{\alpha-\delta}{2} & 0 \\ 0 & ie^{-i\beta}\sin\frac{\alpha-\delta}{2} & e^{-i\beta}\cos\frac{\alpha-\delta}{2} & 0 \\ i\sin\frac{\alpha+\delta}{2} & 0 & 0 & \cos\frac{\alpha+\delta}{2} \end{bmatrix} \tag{9}$$

$$C = \begin{bmatrix} -\lambda \sin\delta \sin\beta \sin\xi \cos\eta \\ -\lambda \sin\alpha \sin\beta \sin\xi \sin\eta \\ -\lambda \sin\alpha \sin\delta \cos\xi \end{bmatrix} \tag{10}$$

$$M = \begin{bmatrix} \cos\delta\cos\beta & \lambda\cos\delta\sin\beta\cos\xi & -\lambda\sin\delta\cos\beta\sin\eta\sin\xi \\ -\lambda\cos\alpha\sin\beta\cos\xi & \cos\alpha\cos\beta & \lambda\sin\alpha\cos\beta\cos\eta\sin\xi \\ -\lambda\cos\alpha\sin\delta\sin\eta\sin\xi & -\lambda\sin\alpha\cos\delta\sin\xi\cos\eta & \cos\alpha\cos\delta \end{bmatrix} \tag{11}$$

Comparing (8) with (10) and (11), we find the corresponding unitary operator. From the unitary, we derive the thermalizing Hamitonian $H_{th}(t)$ as,

$$H_{th}(t) = f(t)\Big(|\phi^+\rangle\langle\phi^+| - |\phi^-\rangle\langle\phi^-|\Big), \tag{12}$$

where, $|\phi^{\pm}\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$ and $f(t) = \frac{\gamma e^{-\gamma t/2}}{2\sqrt{1-e^{-\gamma t}}}$ —- (12′)

We can rewrite the Hamiltonian in the Pauli spin basis as $f(t)(\sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y)$. This represents a kind of spin exchange interaction similar to the double-quantum Hamiltonian used in NMR experiments and such Hamiltonians can in principle be realized [8]. In particular, $f(t)$ can be interpreted as a time-dependent coupling strength between the spins.

In general, for a 2-qubit Hamiltonian of the form (12), the necessary and sufficient condition for thermalization is found to be:

$$\lim_{t\to\infty} F(t) = (2n+1)\frac{\pi}{2} \tag{13}$$

where, $F(t) = \int_0^t f(\tau)d\tau$ and n is any integer.

In order to study the nature of system dynamics under such a Hamiltonian, we refer to [9] and find that the following conditions ensure Markovianity.

$$0 \leqslant F(t) \leqslant \frac{\pi}{2},\ \forall t \tag{14}$$

$$\frac{d}{dt}F(t) \geqslant 0,\ \forall t \tag{15}$$

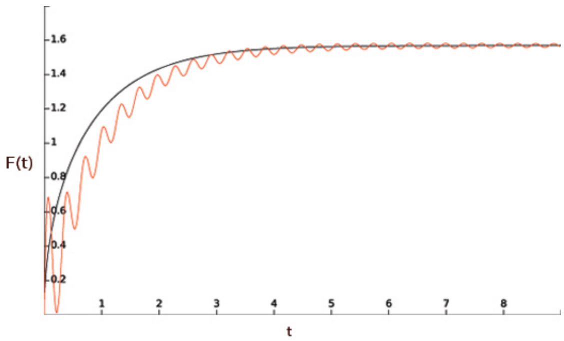

Figure 3: Red line is the F (t) corresponding to non-Markovian thermalizing Hamiltonian while the black corresponds to that of original Markovian form. Note that both converge to $\frac{\pi}{2}$ asymptotically and thus signify thermalization.

A simple example of $F(t)$ that is thermalizing but gives non-Markovian dynamics is:

$$F(t) = \frac{\sin(20t)}{1+10t} + (1-e^{-t})\frac{\pi}{2} \tag{16}$$

Fig.3 plots the original $F(t)$ from (12′) (black curve) and the one given in (16) (red curve).

We further derive the Lindblad-type master equations (with time-dependent coefficients) that refers to the system dynamics for thermalization under our specific form of Hamiltonian. For the derivation, we have used the prescription given in [10]. It is found to be of the following form,

$$\frac{d\rho(t)}{dt} = \gamma_1(t)\Big(\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho(t)\}\Big) + \gamma_2(t)\Big(\sigma_+\rho(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho(t)\}\Big) \quad (17)$$

where, $\gamma_1(t) = (1+g)f(t)\tan[F(t)], \gamma_2(t) = (1-g)f(t)\tan[F(t)]$. Here, $F(t) = \int_0^t f(\tau)d\tau$ and g is the parameter referring to the bath temperature used in defining the initial ancilla state as $\sigma_e(0) = \frac{1}{2}(\mathbb{I} + g\sigma_3)$.

This form of master equation is immediately reminiscent of the Lindblad (Markovian) form that we have used at the beginning in equation (7), hence we have a master equation that is Lindblad-type, but with time-dependent coefficients $\gamma_1(t)$ and $\gamma_2(t)$. It has been shown that the negativity of at least one of $\gamma_1(t)$ or $\gamma_2(t)$ signifies non-Markovianity [11]. For example, for $H(t)$, given in eqn. (12) with F(t) being given by eqn. (16), we find that the coefficients do indeed become negative and thus, signifying non-Markovianity.

The simulating Hamiltonian we derived can help us – in both Markovian as well as non-Markovian cases – to study the generic features of thermalization in open quantum systems and to further the understanding of fundamental dynamics leading to thermalization.

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Chapter 1

Introduction

The advent of quantum theory [1–4] in the twentieth century, forever altered the way we understand the world around us. Over the past century or so, it has gained the reputation as one of the most successful and yet, mysterious scientific theories. It is no surprise that it continues to fascinate and confound anyone trying to study it.

One of the key developments in quantum theory (and arguably, all of physics) was the seminal work produced by J.S. Bell [5]. Bell's work was a response to the famous Einstein-Podolsky-Rosen paper [6] that questioned the completeness of quantum theory. Bell was able to emphatically establish that quantum theory allows features of nonlocality. This piqued a lot of interest in the physics community and resulted in the production of many works that eventually lent itself to the creation of a new research field called quantum information theory.

Quantum information theory [7–10] is an attempt to both understand and use the properties of quantum systems such as nonlocality. Over the past couple of decades, quantum information theory has developed into a huge interdisciplinary field at the intersection of both, theoretical and experimental quantum physics, computer science, mathematics, quantum metrology and, more recently, quantum thermodynamics as well [11–17]. We have seen rapid and tremendous strides made in theoretical as well as experimental domains.

1.1 Study of Quantum Correlations

One of the most important fields of study in quantum information theory is that of quantum correlations [18–30]. This is largely an exercise in characterisation and quantification of various types of quantum correlations. We are also interested in exploiting these quantum correlations to gain operational advantages over tasks that employ classical resources. Quantum teleportation [31] is one famous example of such an operational task that gives an advantage by exploiting the quantum correlations shared between two spatially separated parties.

We are also interested in the comparison of correlations with classical systems and questions related to it such as, whether a given correlation can be achieved in classical scenarios or not. We are able to see that the purely quantum (non-classical) correlations can be used as a resource for various operational tasks that give an advantage or speed up over classical scenarios.

Broadly, one may look at quantum correlations in terms of kinematic and dynamic correlations. Kinematic correlations are those correlations that do not change in time (for example, measurement statistics obtained from spatially separated parties/observers) whereas dynamic correlations are those that continuously evolve in time (for example, the correlation between an open quantum system and its environment that evolves due to the system-environment interaction).

This Ph.D. thesis consists of two research works – one in the domain of nonlocality for continuous variable quantum systems[1] while the other is on thermalization for two-level quantum systems[2]. Although both of them fall under the general ambit of quantum information theory, nevertheless, perspectives of these two works are quite different.

[1]"Uncertainty principle as a postquantum nonlocality witness for the continuous-variable multimode scenario", Prathik Cherian J, Amit Mukherjee, Arup Roy, Some Sankar Bhattacharya, Manik Banik, Physical Review A 99 032130 (2019).

[2]"On thermalization of two-level quantum systems", Prathik Cherian J, Sagnik Chakraborty, Sibasish Ghosh, Europhysics Letters (EPL) 126, 40003 (2019).

Therefore, each of these works will be described as a separate chapter in the thesis. This thesis can be thought of as an undertaking in the vast domain of study of quantum correlations as explained below.

In the first part of the thesis, we endeavor to study kinematic (continuous outcome) correlations that are nonlocal and beyond quantum theory (i.e. *postquantum*). In particular, we are interested in understanding how we can establish both nonlocality and postquantumness of multimode systems when continuous outcome correlations are considered. This study can be of importance to uncover and understand the foundational principles of quantum theory.

In the second part of the thesis, we study the dynamics of correlations between a two-level quantum system and its environment. In particular, we are interested in those open system dynamics which result in thermalization of the system. For such dynamics, we can further study the classification of them being Markovian or non-Markovian. This study overall can lead us to understand the process of thermalization better and thus, enhance our understanding of a major area in quantum thermodynamics.

1.2 Outline of Thesis

In chapter 2, we develop a systematic approach to study postquantum nonlocal correlations for continuous variable multimode scenario. We show that the Robertson-Schrödinger inequality [32–35] plays a key role by certifying postquantum nature of the correlation while the continuous variable Bell-type inequalities introduced by Cavalcanti, Foster, Reid, and Drummond (CFRD) [36] certify nonlocality feature of the correlation. We also define a class of postquantum nonlocal continuous variable correlations in m-mode systems.

In chapter 3, we begin by considering the quantum optical master equation that describes the dynamics of thermalization for a two-level quantum system (qubit) interacting with a thermal reservoir [37]. We solve it and use the parametrization of 2-qubit unitaries done by G. Narang and Arvind [38] in order to find a 2-qubit unitary that can simulate the system dynamics. We then derive a 2-qubit thermalizing Hamiltonian that simulates the dynamics of a qubit interacting with a thermal reservoir. We further study the conditions for thermalization and Markovianity of such Hamiltonians. Lastly, we derive a class of Lindblad-type master equations that can describe both Markovian and non-Markovian thermalization dynamics based on the values of the dissipation parameters.

Finally, in chapter 4, we summarize the results obtained and discuss plausible future directions for the works discussed in the thesis.

Chapter 2

Postquantum Nonlocality in Continuous Variable Systems

2.1 Preliminaries

2.1.1 Bell Scenario

The classic $2-2-2$ Bell scenario involves two spatially separated parties (conventionally named as Alice and Bob), who each perform one of two possible measurements to obtain one of two possible discrete outcomes. Let Alice perform the measurement $x \in \{A_1, A_2\}$ to obtain the discrete outcome $a \in \{0, 1\}$ while Bob performs the measurement $y \in \{B_1, B_2\}$ to obtain the discrete outcome $b \in \{0, 1\}$. Then, the correlation is given by the probability distribution: $p(ab|xy)$.

An important physical principle in this context is the *no-signalling* principle which states that during measurement of an entangled state, an observer cannot communicate with another observer, by making measurements in a subsystem of the total system. In other words, measurement choice of Alice should not affect outcomes of Bob and vice versa. This is in accordance with principles of relativity and reiterates the fact that information cannot be transmitted instantaneously or above the speed of light.

In terms of the $2-2-2$ correlations $p(ab|xy)$, the no-signalling principle can be stated as follows.

Alice to Bob no-signalling:

$$\sum_a p(ab|xy) = \sum_a p(ab|x'y) = p(b|y), \quad \forall a, x, x', y. \tag{2.1}$$

Bob to Alice no-signalling:

$$\sum_b p(ab|xy) = \sum_b p(ab|xy') = p(a|x), \quad \forall b, x, y, y'. \tag{2.2}$$

Any valid physical correlation must satisfy the no-signalling principle.

We can easily generalize the $2-2-2$ scenario to the standard $m-n-k$ Bell scenario which considers m space-like separated observers/sites denoted as $\mathcal{A}_i$, with $i \in \{1, 2, ..., m\}$, each observer performs one out of n possible local measurements denoted by X_i, with $X_i \in \{0, 1, ..., n-1\}$; and each measurement having k distinct outcomes denoted by A_i^j, with $j \in \{0, 1, ..., k-1\}$.

A. Fine [39] showed that such a correlation is said to have a *local realistic* description if and only if,

$$p(ab|xy) = \sum_\lambda p_\lambda \, p(a|x, \lambda) p(b|y, \lambda). \tag{2.3}$$

where, λ is some variable shared by both Alice and Bob, and p_λ is its distribution. If such a factorization does not exist, then it is a *nonlocal* correlation. In other words, nonlocality means that local measurement choices can impact the correlation between different (spatially separated) parties.

J. S. Bell's success was in showing that quantum theory allowed for such nonlocal correlations [5]. It has also been shown that nonlocal correlations violate certain inequalities. One celebrated example is the Bell-CHSH inequality [40] for the $2-2-2$ scenario:

$$I_{CHSH} := \langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle \leq 2.$$

The algebraic maximum of the CHSH inequality is 4. But Cirel'son [41] showed that quantum theory allows for a maximum violation of $2\sqrt{2}$ i.e. for quantum theory,

$$I_{CHSH} \leq 2\sqrt{2}.$$

Incredibly, Popescu and Rohrlich [42] were able to design a correlation, famously known as PR box correlation, which satisfies the relativistic causality or more broadly, the no-signalling principle but at the same time depicts stronger than quantum nonlocal behavior as it achieves the algebraic maximum of the CHSH expression i.e. $I_{CHSH} = 4$. Thus, the PR box correlation is an example of a *postquantum nonlocal* correlation.

But what if we have continuous outcomes instead of discrete outcomes? Below, we explain the mathematical framework to tackle such a scenario.

2.1.2 Continuous Outcome Correlations

We consider that the outcomes are continuum instead of k distinct values. Ketterer et. al [43] pointed out that it is convenient to adopt the language of probability measures while considering continuous outcomes. We now discuss this mathematical framework for representing continuous variable correlations.

A probability space consists of three elements: (i) a sample space (Ω), (ii) the Borel σ-algebra ($\mathcal{B}(\Omega)$) of events on Ω, and (iii) a valid Borel probability measure $\xi : \mathcal{B}(\Omega) \to [0, 1]$. In our case, the sample space would be $\Omega = \Omega_1 \times \Omega_2 \times \cdots \times \Omega_m$, with each

$\Omega_i = \mathbb{R}$ being the outcome sample space of i^{th} site. The probability measure satisfies the normalization condition:

$$\xi(\mathbb{R} \times \mathbb{R} \cdots \times \mathbb{R}) = 1. \tag{2.4}$$

It also satisfies the additivity property:

$$\xi(\cup_i \omega_i) = \sum_i \xi(\omega_i), \tag{2.5}$$

for all countable sequences $\{\omega_i\}_i$ of disjoint events $\omega_i \in \mathcal{B}(\Omega)$.

The relation between a probability measure ξ and a probability density p is given by,

$$\begin{aligned} \xi(A_1 \times \cdots \times A_m) &:= \int_{A_1 \times \cdots \times A_m} d\xi(a'_1, \cdots, a'_m) \\ &= \int_{A_1} \cdots \int_{A_m} p(a'_1, \cdots, a'_m) da'_1 \cdots da'_m. \end{aligned} \tag{2.6}$$

Here $A_1 \times \cdots \times A_m \in \mathcal{B}(\Omega)$, each $A_i \in \mathcal{B}(\mathbb{R})$, $p(a'_1, \cdots, a'_m)$ denotes the probability density corresponding to ξ. We will denote the set of all probability measures on $\mathcal{B}(\Omega)$ as $\mathcal{M}_{\mathbb{R}^m}$.

Henceforth, we consider that the local measurements performed on each site will be one of two possible choices, i.e. $X_i \in \{0, 1\}\ \forall\ i$. In such a scenario, an m-mode Bell *behavior* is defined as the collection of joint conditional probability measures $\{\xi^{\mathcal{A}_1 \cdots \mathcal{A}_m}_{X_1 \cdots X_m} \mid X_1, \cdots, X_m = 0, 1\}$, where each $\xi^{\mathcal{A}_1 \cdots \mathcal{A}_m}_{X_1 \cdots X_m} \in \mathcal{M}_{\mathbb{R}^m}$. Collection of all m-mode Bell behavior will be denoted as $\mathcal{M}^{2^m}_{\mathbb{R}^m}$. Whenever there is no ambiguity, we will avoid the superscript notation denoting the modes.

Consider any arbitrary grouping of m modes into two disjoint (nonempty) sets $\mathcal{K}$, $\mathcal{K}^c$ with $\mathcal{K} \cup \mathcal{K}^c = \{\mathcal{A}_1, \cdots, \mathcal{A}_m\}$. The no-signalling (NS) condition puts the restriction that measurement choice of one set does not determine the outcome probability of other set for any of the above groupings. In measure theoretic language, these conditions read as:

$$\xi_{\{X_i\}_{i\in\mathcal{K}} \cup \{X_j\}_{j\in\mathcal{K}^c}} \left(\prod_{i\in\mathcal{K}} A_i \times \prod_{j\in\mathcal{K}^c} \mathbb{R}_j \right) = \xi_{\{X_i\}_{i\in\mathcal{K}} \cup \{X_j \oplus 1\}_{j\in\mathcal{K}^c}} \left(\prod_{i\in\mathcal{K}} A_i \times \prod_{j\in\mathcal{K}^c} \mathbb{R}_j \right), \tag{2.7}$$

for all $A_i \in \mathcal{B}(\mathbb{R})$, where $\oplus$ denotes modulo two sum. The set of all no-signalling correlations $\mathcal{M}_{\text{NS}}$ is naturally a strict subset of $\mathcal{M}^{2^m}_{\mathbb{R}^m}$.

A behavior will be called quantum *iff* it can be obtained according to Born probability rule, i.e.:

$$\xi_{X_1 \cdots X_m}(A_1 \times \cdots \times A_m) = \text{Tr}\left[\otimes_{i=1}^m M_{X_i}(A_i)\rho\right], \ \forall \ A_i \in \mathcal{B}(\mathbb{R}) \tag{2.8}$$

where, ρ is a density operator acting on some tensor product Hilbert space $\otimes_{i=1}^m \mathcal{H}_i$, with $\mathcal{H}_i$ being the i^{th} site's Hilbert space (in this case, infinite dimensional); and $M_{X_i}(A_i) : \mathcal{B}(\mathbb{R}) \mapsto \mathcal{L}_+(\mathcal{H}_i)$ are positive operator valued measures (POVMs) on $\mathcal{H}_i$. The set of all such quantum behaviors is denoted by $\mathcal{M}_Q$.

A behavior $\{\xi_{X_1 \cdots X_m}\}_{X_i=0,1}$ will be called postquantum if $\{\xi_{X_1 \cdots X_m}\}_{X_i=0,1} \in \mathcal{M}_{NS}$ but $\{\xi_{X_1 \cdots X_m}\}_{X_i=0,1} \notin \mathcal{M}_Q$. Local-realistic correlations are those where the outputs are locally generated from local inputs and some pre-established classical correlations encoded in some shared variable $\lambda \in \Lambda$. Such behaviors are of the form,

$$\xi_{X_1 \cdots X_m} = \int_\Lambda \delta_{a_1(X_1,\lambda),\cdots,a_m(X_m,\lambda)} \, d\eta(\lambda), \tag{2.9}$$

where $\eta : \mathcal{B}(\Lambda) \to \mathbb{R}_{\geq 0}$ is a probability measure and $\delta_{a_1(x_1,\lambda),\cdots,a_m(X_m,\lambda)}$ is the continuous variable local deterministic response function:

$$\delta_{a_1,\cdots,a_m}(A_1 \times \cdots \times A_m) : \begin{cases} 1, & \text{if } a_i \in A_i \ \ \forall i \\ 0, & \text{otherwise} \end{cases}$$

Set of all local behaviors $\mathcal{M}_L$ is a strict subset of $\mathcal{M}_Q$ and NS behaviors not belonging to $\mathcal{M}_L$ manifest nonlocal feature.

2.1.3 Continuous Variable Bell Inequalities

Initially, the study of Bell-type inequalities for continuous variable systems was based upon coarse graining of the continuous outcome spectrum into discrete domains [44–47]. One of the main motivations for studying continuous variable Bell scenario is to achieve better detection efficiency as the Homodyne detection method is a highly efficient detection technique [47–49].

Another way to increase the detection efficiency is to use the idea of continuous realizations of outcomes instead of discrete ones. The idea was initially motivated by the continuous variable version of Einstein-Podolsky-Rosen paradox [50]. In Ref. [36] Cavalcanti, Foster, Reid and Drummond (CFRD) derived a class of local realistic inequalities without any assumption on the number of measurement outcomes and therefore, their inequalities are directly applicable to continuous variable systems with no need of discrete binning of the outcomes or without having any restrictions on possible measurements.

CFRD focused on the correlation functions of observables for m sites or observers, each equipped with n possible local measurement settings, and considered any real, complex, or vector function $F(\mathbf{X}^1, \mathbf{X}^2, \cdots \mathbf{X}^m)$ of the local observables $\mathbf{X}^i = (X_1^i, X_2^i, \cdots X_n^i)$ at the i-th site. In a local hidden variable (LHV) theory, all such functions are functions of hidden variables $\lambda \in \Lambda$ where Λ is a parameter space.

The assumption of locality enters the reasoning by requiring that the local choice of observable does not affect the correlations between variables at different sites. Hence, for all terms in F, the averages are calculated over the same hidden variable ensemble $P(\lambda)$. The expression for the average over the LHV ensemble $P(\lambda)$ is given by,

$$\langle F \rangle = \int_\Lambda P(\lambda) F(\mathbf{X}^1(\lambda), \mathbf{X}^2(\lambda), \cdots \mathbf{X}^m(\lambda))) d\lambda. \tag{2.10}$$

It has been shown that deterministic LHV theories can be considered without any loss of generality [39]. The class of CRFD local realistic inequalities can now be defined using the fact that any function of random variables has non-negative variance. It reads as:

$$|\langle F\rangle|^2 \leq \left\langle |F|^2 \right\rangle. \tag{2.11}$$

For the two-site scenario, it was first shown that it is impossible to violate the CFRD inequality with quantum phase-space quadrature operators [51]. Subsequently, this result has been generalized to arbitrary quantum measurements [52]. However, it is possible to obtain violation of CFRD inequalities in quantum theory with higher number of modes, in particular, explicit violation has been shown for multipartite GHZ-like states [53]. We will use this particular class of inequalities to establish nonlocal feature of a continuous outcome correlation.

2.1.4 Robertson-Schrödinger Uncertainty Relation

A proper mathematical formulation of Heisenberg's preparation uncertainty relation was first introduced by Kennard [32]. Schrödinger re-derived this idea for two observables correlations in a more refined way [33] which was further extended for more than two observables by Robertson [34].

For an m-mode quantum state denoted by ρ, the non-commutativity of the canonical operators and the positive semi-definiteness of the state leads to the famous restriction – the Robertson-Schrödinger uncertainty relation [35]:

$$\mathbf{V} + \iota\mathbf{\Omega} \geq 0, \tag{2.12}$$

where $\mathbf{V}$ is a $2m \times 2m$ real symmetric matrix, namely, the covariance matrix (CM) and $\mathbf{\Omega}$ is known as the *symplectic form* and $\iota = \sqrt{-1}$. The covariance matrix is calculated from the second moments of position ($\hat{q}_i$) and momentum ($\hat{p}_i$) operators of i-th mode which we denote as elements of a vector $\hat{\alpha} = (\hat{q}_1, \hat{p}_1, \cdots \hat{q}_m, \hat{p}_m)^\intercal$. Then we have,

$$V_{ij} := \frac{1}{2} \left\langle \left\{ \Delta\hat{\alpha}_i, \Delta\hat{\alpha}_j \right\} \right\rangle_\rho \tag{2.13}$$

where $i, j = \{1, 2 \ldots 6\}$, $\Delta\hat{\alpha}_i := \hat{\alpha}_i - \langle\hat{\alpha}_i\rangle$, $\{., .\}$ denotes anti-commutator, $\langle . \rangle_\rho$ is the expectation value with respect to the state ρ and $\mathbf{\Omega}$ is defined as $2\iota\Omega_{ij} = [\hat{\alpha}_i, \hat{\alpha}_j]$. Whether any given real symmetric matrix corresponds to a *bona fide* quantum CM can be verified by the RS uncertainty relation. This criterion is necessary and sufficient for Gaussian states while for more general non-Gaussian states, it is only a necessary criterion.

The uncertainty relation given by (2.12) is just a natural consequence of the positive semi-definiteness of the density operator ρ ($\rho \geq 0$) and the non-zero commutation relation between position and momentum operators ($[\hat{q}_i, \hat{p}_i] = i$).

2.2 Robertson-Schrödinger Uncertainty Relation as Witness of Postquantumness

Nonlocality is one of the most bizarre features of multipartite quantum systems established for the very first time in the seminal paper of J. S. Bell [5]. Local outcomes of spatially separated quantum systems prepared in entangled states can produce correlations that can not have any *local realistic* description – manifesting the nonlocal phenomena. As previously mentioned, such nonlocal behavior can be witnessed through violation of some local realistic inequality known as Bell type inequality– Clauser-Horne-Shimony-Holt (CHSH) inequality is one such celebrated example [40].

However, as was mentioned previously, nonlocality is not a salient feature of quantum theory alone. This is evidenced by the existence of the PR box correlation [42] which achieves the algebraic maximum of the CHSH inequality which is beyond the quantum limit established by Cirel'son [41]. This observation raises a very important question: whether there exists some other fundamental principle(s) (apart from no-signalling) limiting the nonlocal strength of quantum theory.

In the last few years several information theoretic as well as physical principles, viz. non-trivial communication complexity [54], information causality [55], macroscopic locality [56], relativistic causality [57], local orthogonality [58] have been proposed that successfully explain the limited CHSH violation of quantum theory. These principles also identify a part of the boundary between the set of quantum correlations and the postquantum NS correlations [59, 60]. Furthermore, applicability of these principles have also been proved useful in the more general $m - n - k$ scenarios to witness postquantum correlations [61–66]. In a different approach, it has been shown that the limited CHSH nonlocality of quantum theory can be connected to other fundamental features of the theory: Heisenberg's uncertainty principle [67, 68], Bohr's complementarity principle [69, 70] and preparation contextuality [71]. These connections not only hold true in quantum theory but are also plausible in a larger class of theories.

A great deal of research has been done on quantum and postquantum nonlocal correlations in discrete input-output scenario [72–75]. In the quantum domain, these studies mainly consider finite input-finite output correlations arising from finite dimensional quantum systems. Although nonlocal correlations have been studied for infinite dimensional continuous variable (CV) systems [44–46, 52, 76, 77], those results are fundamentally not different from the finite input-output scenario as discrete binning of continuous outcomes has been considered there. In this regard, a notable exception is the CV Bell inequalities introduced by Cavalcanti, Foster, Reid, Drummond (CFRD) [36]. There the authors derived a class of nonlinear Bell inequalities that apply for continuous outcome spectrum without any need for discrete binning of the outcomes. A natural question of interest in this context will be the notion of CV postquantum nonlocal correlations. Very recently, Ketterer et al. have developed a formalism to address this question for generic NS black-box measurement devices with continuous outputs and they have also provided a class of postquantum nonlocal correlations when only two sites/modes are involved [43]. Black-box devices are those for which we make no assumptions on the inner mechanisms which led to the experimental result and the only information we can gather from many repetitions of sequential or simultaneous experiments is the probability distribution of the outputs conditioned on the inputs. They are usefully employed in describing device independent scenarios.

A relevant question in the continuous outcome scenario is: how to certify postquantum nonlocality of a given correlation? The authors in Ref. [43] have used the fact that for 2-mode scenario there is no quantum violation of the CFRD inequality [51], i.e. CFRD violation works at the same time as nonlocality witness as well as postquantumness witness. However, this is a very specific feature of 2-mode case that does not hold for higher number of modes in general [53]. On the other hand, the principle based methods [55, 56, 58] that have been proved to be useful for studying postquantum correlations in the discrete outcomes scenario are yet to be generalized for continuous outcome spectrum.

Apart from the aforementioned foundational aspect of postquantum nonlocality in CV scenario, there are motivations to explore it even from the perspective of applications. In the case of quantum information processing tasks, one of the most important notions is the device independent (DI) scenario. In DI protocols, the experimenters do not possess the exact working knowledge of the apparatus and can only acquire the input-output statistics from the apparatus. In discrete variable scenario, the use of nonlocality makes many DI tasks possible, such as, DI quantum key distribution (QKD), DI randomness certification etc [78–85]. In general, the benefit of CV-QKD over discrete variable QKD manifests in the higher efficiency and key rate [86]. Recently, long distance CV QKD has been achieved for as much as 80km [87]. In the CV scenario, measurement device independent (MDI) QKD has been recently introduced [88]. The advantage of MDI protocols over the standard quantum cases is that the trust in the measurement devices is not needed for the former one. But MDI protocols need a trustworthy quantum state preparation device which is not required in corresponding DI protocols. To further investigate various DI tasks in CV scenario, the notion of nonlocality is of vital importance. Since nonlocal correlations can provide cryptographic security not achievable within classical theory, and can be used to certify the presence of randomness and outperform classical communication at communication complexity problems, it is important to identify which nonlocal correlations are possible in a physical theory (more specifically, in quantum theory). Our study is thus significant in order to witness and rule out postquantum correlations in continuous outcome scenario.

Developing a systematic approach to study postquantum nonlocal correlations for continuous outcome scenario in multimode cases is thus quite important. Interestingly, we find that Robertson-Schrödinger (RS) uncertainty relation has a role to play in this regard. We construct a class of continuous outcome postquantum nonlocal correlations for generic m-mode scenario. While the nonlocality of the proposed class of correlations is certified through violation of CFRD inequalities, the postquantum nature is guaranteed by violation of the RS uncertainty relation.

Equipped with all the required tools described in the Preliminaries section, we now introduce continuous outcome postquantum nonlocal correlations for m-mode scenario. We start with an example in the 3-mode case.

2.2.1 3-mode Scenario

Consider the following 3-mode Bell behavior:

$$\xi_{111}^{\mathcal{A}_1\mathcal{A}_2\mathcal{A}_3} = \frac{1}{4}\left[\mathcal{N}_{(l,l,-l),\sigma} + \mathcal{N}_{(l,-l,l),\sigma} + \mathcal{N}_{(-l,l,l),\sigma} + \mathcal{N}_{(-l,-l,-l),\sigma})\right] \tag{2.14a}$$

$$\xi_{\text{rest}}^{\mathcal{A}_1\mathcal{A}_2\mathcal{A}_3} = \frac{1}{4}\left[\mathcal{N}_{(l,l,l),\sigma} + \mathcal{N}_{(l,-l,-l),\sigma} + \mathcal{N}_{(-l,l,-l),\sigma} + \mathcal{N}_{(-l,-l,l),\sigma}\right] \tag{2.14b}$$

where, rest $\in \{0,1\}^3 \setminus \{111\}$, with 0 and 1 denoting position and momentum measurements respectively. $\mathcal{N}_{\mathbf{a},\sigma}$ is the normal (Gaussian) probability measure defined through (2.6) with probability density centered around $\mathbf{a} := (a_1, a_2, a_3)$ with width σ, *i.e.*,

$$p_{\mathbf{a},\sigma}(\mathbf{a}') = \frac{1}{(\sigma\sqrt{2\pi})^3} \exp\left[-\sum_{i=1}^{3}(a_i - a_i')^2/(2\sigma^2)\right]$$

It is straightforward to see that the above behavior is indeed a no-signalling behavior.

Now we will derive the CFRD inequality as detailed in the Preliminaries. The CFRD inequality [36] for three modes is defined as $|\langle C_3\rangle|^2 \leq \left\langle |C_3|^2 \right\rangle$, where:

$$C_3 = \prod_{k=1}^{3}(X_0^k + \iota X_1^k) := \tilde{X}_3 + \iota\tilde{Y}_3 \tag{2.15}$$

Finally, we get the expression for 3-mode CFRD inequality as,

$$\left\langle \tilde{X}_3 \right\rangle^2 + \left\langle \tilde{Y}_3 \right\rangle^2 \leq \left\langle \prod_{k=1}^{3} \left(\left(X_0^k\right)^2 + \left(X_1^k\right)^2 \right) \right\rangle \tag{2.16}$$

Where k denotes the mode and X_0^k and X_1^k are the position and momentum observables respectively of the k-th mode.

Given a probability measure ξ with corresponding probability density p, the expectation $\langle \prod_k (X_{i_k}^k)^{n_k} \rangle$ can be calculated according to the following expression:

$$\left\langle \prod_k \left(X_{i_k}^k\right)^{n_k} \right\rangle := \int \prod_k \left(A_{i_k}^k\right)^{n_k} d\xi, \tag{2.17}$$

where $k \in \{1, 2, \cdots, m\}$ represents the mode, $i_k \in \{0, 1\}$ represents the measurement/observable, $n_k \in \{1, 2\}$.

For the 3-mode case, given the probability measure (2.14), we find:

$$\begin{aligned}
\left\langle \left(X_{i_1}^1\right)^2 \left(X_{i_2}^2\right)^2 \left(X_{i_3}^3\right)^2 \right\rangle &= \left(l^2 + \sigma^2\right)^3, \quad \forall i_1, i_2, i_3 = 0, 1; \\
\left\langle X_{i_1}^1 X_{i_2}^2 X_{i_3}^3 \right\rangle &= l^3, \quad \text{when } i_1 i_2 i_3 = 0; \\
\left\langle X_1^1 X_1^2 X_1^3 \right\rangle &= -l^3.
\end{aligned}$$

Using the above results, the CFRD expression (2.16) can be calculated for the correlation (2.14) and is seen to be,

$$5l^6 \leq 2\left(l^2 + \sigma^2\right)^3. \tag{2.18}$$

As can be seen below in Fig.2.1, for suitable choices of (l, σ), correlation (2.14) can violate inequality (2.18). This establishes nonlocality of those correlations. Naturally the question arises, whether such nonlocal correlations are quantum realizable or whether they are postquantum in nature. One way is to find the 2-mode marginal correlations and check whether the 2-mode marginals violate the 2-mode CFRD inequality. But in this case, the 2-mode marginals satisfy the corresponding CFRD inequality.

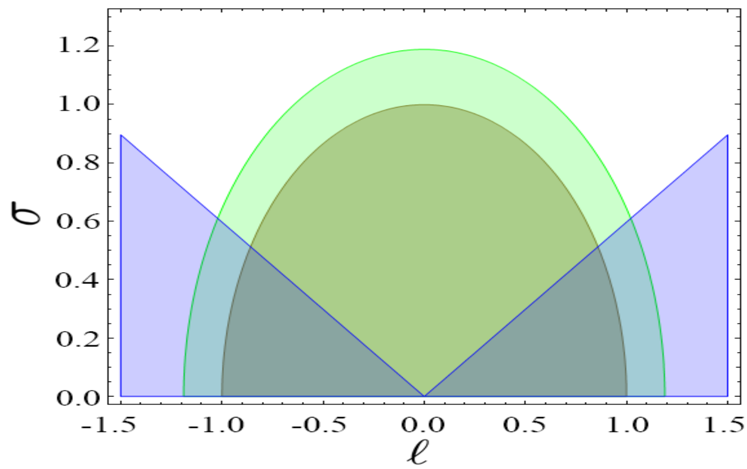

Figure 2.1: The blue region denotes the values of l and σ for which 3-mode CFRD inequality (2.18) is violated. The region bounded by the smaller green half-circle denotes the values of l and σ of (2.14) which violate the RS uncertainty relation with the product choice of joint probability distribution (ie $c = 0$). The region bounded by the larger green half-circle represents RS violation for non-product choice of single-mode joint distribution (here, we have considered $c = 1$). The overlap of blue region with the region bounded by the half-circles indicate 3-mode postquantum nonlocal correlations. Clearly, $c = 0$ corresponds to the minimum region violating the RS relation.

Hence, at this point we utilize the RS uncertainty relation which puts necessary conditions on a distribution to be quantum realizable: if the RS uncertainty relation is violated, then the given distribution cannot be quantum realizable.

Denoting the position and momentum observables for i^{th} mode as $(\hat{q}_i, \hat{p}_i)$, the vector $\vec{\alpha}$ for three modes can be written as:

$$\hat{\alpha} = (\hat{q}_1, \hat{p}_1, \hat{q}_2, \hat{p}_2, \hat{q}_3, \hat{p}_3)^T \equiv \hat{\alpha}_i \mid_{i=1,\cdots,6} \tag{2.19}$$

As explained in the Preliminaries section, the covariance matrix (CM) V is defined as,

$$V_{ij} = \frac{1}{2}\langle\{\Delta\hat{\alpha}_i, \Delta\hat{\alpha}_j\}\rangle \tag{2.20}$$

where, $i, j = \{1, 2...6\}$, $\Delta\hat{\alpha}_i = \hat{\alpha}_i - \langle\hat{\alpha}_i\rangle$ and $\{.,.\}$ is anti-commutator.

To calculate the CM from (2.14), we require the single-mode marginals $\xi^{\mathcal{A}_i}_{X_i}$ as well as the 2-mode marginals $\xi^{\mathcal{A}_i\mathcal{A}_j}_{X_iX_j}$ which can be readily calculated by integrating out the appropriate mode(s) from $\xi^{\mathcal{A}_1\mathcal{A}_2\mathcal{A}_3}_{X_1X_2X_3}$. They turn out to be,

$$\xi^{\mathcal{A}_i}_{X_i} = \tfrac{1}{2}\left[\mathcal{N}_{l,\sigma} + \mathcal{N}_{-l,\sigma}\right], \forall i = \{1, 2, 3\},\ X_i = \{0, 1\}, \tag{2.21}$$

$$\xi^{\mathcal{A}_i,\mathcal{A}_j}_{X_i,X_j} = \tfrac{1}{4}\left[\mathcal{N}_{(l,l),\sigma} + \mathcal{N}_{(l,-l),\sigma} + \mathcal{N}_{(-l,l),\sigma} + \mathcal{N}_{(-l,-l),\sigma}\right]. \tag{2.22}$$

where, $X_i, X_j = \{0, 1\}, \forall i, j = \{1, 2, 3\}; i \neq j$.

But calculation of CM also requires single-mode position-momentum joint distributions $\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)}$. While calculating terms like $\langle\hat{q}^i\hat{p}^i\rangle$, we require the position-momentum joint probability distributions $\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)}$ for i^{th} mode. We cannot derive such single-mode joint distribution from the probability measure (2.14) and so, we are forced to construct them by hand. Given the marginals $\xi^{\mathcal{A}_i}_{X_i=0}$ and $\xi^{\mathcal{A}_i}_{X_i=1}$, we can make a choice of $\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)}$ even though it is not unique.

First, we consider the (trivial) product choice $\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)} = \xi^{\mathcal{A}_i}_{X_i=0} \times \xi^{\mathcal{A}_i}_{X_i=1}$. In this case,

$\langle \hat{q}_i \hat{p}_i \rangle = \langle \hat{q}_i \rangle \langle \hat{p}_i \rangle = 0$ and the CM becomes,

$$\mathbf{V_p} = \bigoplus_{i=1}^{3} \begin{bmatrix} l^2 + \sigma^2 & 0 \\ 0 & l^2 + \sigma^2 \end{bmatrix}. \tag{2.23}$$

For the non-product choice, we will have $\langle \hat{q}_i \hat{p}_i \rangle = c$, where c is some non-zero real number. In this case CM becomes,

$$\mathbf{V_{np}} = \bigoplus_{i=1}^{3} \begin{bmatrix} l^2 + \sigma^2 & c \\ c & l^2 + \sigma^2 \end{bmatrix}. \tag{2.24}$$

A bona fide quantum CM must necessarily satisfy RS uncertainty relation,

$$\mathbf{V} + i\mathbf{\Omega} \geq 0 \tag{2.25}$$

where,

$$\mathbf{\Omega} = \bigoplus_{i=1}^{3} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{2.26}$$

For product and non-product choices respectively, the RS uncertainty relation will be violated if,

$$l^2 + \sigma^2 \quad < \quad 1, \qquad \text{(for product)} \tag{2.27}$$

$$l^2 + \sigma^2 \quad < \quad \sqrt{1 + c^2} \quad \text{(for non-product)}. \tag{2.28}$$

By comparing Eqs.(2.27)-(2.28), it is obvious that the region of (l, σ) violating RS uncertainty relation for product choice is strictly inscribed by the region of (l, σ) violating RS uncertainty relation for non-product choice.

Note that, given marginal probability distributions $\xi^{\mathcal{A}_i}_{X_i=0}$ and $\xi^{\mathcal{A}_i}_{X_i=1}$, the choice of joint distribution $\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)}$ is not unique. With the (trivial) product choice of joint distribution

$\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)} = \xi^{\mathcal{A}_i}_{X_i=0} \times \xi^{\mathcal{A}_i}_{X_i=1}$ we have $\langle \hat{q}_i \hat{p}_i \rangle = 0$, which in turn gives that the RS uncertainty relation will be violated if $l^2 + \sigma^2 < 1$ i.e. it describes a half-circle region on $l - \sigma$ plane.

In Fig.2.1, the overlapping region of blue curve and the inner half-circle violates both the CFRD inequality and the RS relation (calculated with product choice of distribution) and hence establishes postquantum nonlocality of those correlations. At this point, one can ask the question whether the values of l and σ lying outside the inner circle but within the blue region denote quantum realizable correlations. However, answering this question is not straightforward.

First of all, if we calculate CM with some non-product distribution $\xi^{\mathcal{A}_i}_{(X_i=0,X_i=1)} \neq \xi^{\mathcal{A}_i}_{X_i=0} \times \xi^{\mathcal{A}_i}_{X_i=1}$, we have $\langle \hat{q}^i \hat{p}^i \rangle = c$, with c being a real number, and consequently RS uncertainty relation will be violated if $l^2 + \sigma^2 < \sqrt{1 + c^2}$. Therefore, the area of postquantum region increases. It can be seen in Fig.2.1 as the larger green half-circle (for $c = 1$).

Even if one can specify the value of c, in general it will not be possible to guarantee quantumness of the correlations outside the green half-circle region since the RS uncertainty relation is a sufficient (& necessary) criterion for bona fide CM only in the case of Gaussian states. However, this calculation asserts the existence of postquantum nonlocal correlations independent of the fact that whether we take product or non-product form of joint position-momentum distribution for each of the modes.

2.2.2 m-mode Scenario

We now generalize the above 3-mode example to m number of modes. Consider, a vector $\mathbf{P}_i \in \mathbb{R}^m$ with first i number of elements being $-l$ and following $(m-i)$ number of elements being $+l$. Denote by $\mathcal{P}_i$ the set of all vectors obtained from $\mathbf{P}_i$ by permuting its elements. Consider now, an m-mode Bell behavior defined as,

$$\xi_{11\cdots 1}^{\mathcal{A}_0\mathcal{A}_1\cdots\mathcal{A}_m} = \frac{1}{2^{m-1}} \sum_{\substack{i\in\mathbb{N}_o \\ i\leq m}} \sum_{\mathbf{P}_i\in\mathcal{P}_i} \mathcal{N}_{\mathbf{P}_i,\sigma} \,, \tag{2.29a}$$

$$\xi_{\text{rest}}^{\mathcal{A}_0\mathcal{A}_1\cdots\mathcal{A}_m} = \frac{1}{2^{m-1}} \sum_{\substack{i\in\mathbb{N}_e \\ i\leq m}} \sum_{\mathbf{P}_i\in\mathcal{P}_i} \mathcal{N}_{\mathbf{P}_i,\sigma} \,. \tag{2.29b}$$

Here, $\mathbb{N}_o$ ($\mathbb{N}_e$) denotes the set of odd (even) integers, and $\mathcal{N}_{\mathbf{a},\sigma}$ is the normal (Gaussian) probability measure defined through (2.6) with probability density centered around $\mathbf{a} \equiv (a_1, \cdots, a_m)$ with widths σ, *i.e.*, $p_{\mathbf{a},\sigma}(\mathbf{a}') = 1/(\sigma\sqrt{2\pi})^m \exp\left[-(\sum_{i=1}^{m}(a_i - a_i')^2)/(2\sigma^2)\right]$.

In order to derive the m-mode CFRD inequality, we start by defining the following complex function of the local observables,

$$C_m = \prod_{k=1}^{m} \left(X_0^k + \iota X_1^k\right) := \tilde{X}_m + \iota\tilde{Y}_m \tag{2.30}$$

where, $\{X_0^k, X_1^k\}$ are of the k-th mode local observables. As explained previously, the CFRD inequality is defined as,

$$|\langle C_m\rangle|^2 \leq \left\langle |C_m|^2 \right\rangle \tag{2.31}$$

This can be simplified further to the following form,

$$\left\langle \tilde{X}_m \right\rangle^2 + \left\langle \tilde{Y}_m \right\rangle^2 \leq \left\langle \prod_{k=1}^{m} \left(\left(X_0^k\right)^2 + \left(X_1^k\right)^2 \right) \right\rangle, \tag{2.32}$$

Before calculating the exact form of the m-mode CFRD inequality, we calculate the following expectation values using the the correlation (2.29),

$$\left\langle X^1_{i_1} X^2_{i_2} \cdots X^m_{i_m} \right\rangle = l^m, \text{ if } \prod_{k=1}^{m} i_k = 0 \tag{2.33}$$

$$\left\langle X^1_1 X^2_1 \cdots X^m_1 \right\rangle = -l^m \tag{2.34}$$

$$\left\langle \left(X^1_{i_1}\right)^2 \left(X^2_{i_2}\right)^2 \cdots \left(X^m_{i_m}\right)^2 \right\rangle = \left(l^2 + \sigma^2\right)^m, \ \forall \quad i_1, \cdots, i_m \in \{0, 1\} \tag{2.35}$$

Thus, the RHS of (2.32) is readily seen as,

$$\left\langle \prod_{k=1}^{m} \left(\left(X^k_0\right)^2 + \left(X^k_1\right)^2 \right) \right\rangle = 2^m \left(l^2 + \sigma^2\right)^m. \tag{2.36}$$

Calculation of LHS of (2.32) requires us to know the number of terms with negative signatures in $\tilde{X}_m$ and $\tilde{Y}_m$ which we define as a_m and b_m respectively.

a_m and b_m have recursion relations which can be identified from the following expression,

$$\begin{aligned}
\tilde{X}_m + \iota \tilde{Y}_m &= \prod_{k=1}^{m} \left(X^k_0 + \iota X^k_1\right) \\
&= \prod_{k=1}^{m-1} \left(X^k_0 + \iota X^k_1\right) \left(X^m_0 + \iota X^m_1\right) \\
&= \left(\tilde{X}_{m-1} + \iota \tilde{Y}_{m-1}\right) \left(X^m_0 + \iota X^m_1\right) \\
&= \left(\tilde{X}_{m-1} X^m_0 - \tilde{Y}_{m-1} X^m_1\right) \\
&\qquad + \iota \left(\tilde{X}_{m-1} X^m_1 + \tilde{Y}_{m-1} X^m_0\right), \\
\Rightarrow \tilde{X}_m &= \left(\tilde{X}_{m-1} X^m_0 - \tilde{Y}_{m-1} X^m_1\right), \\
\& \quad \tilde{Y}_m &= \left(\tilde{X}_{m-1} X^m_1 + \tilde{Y}_{m-1} X^m_0\right).
\end{aligned}$$

Thus, we have the following coupled recursion relations,

$$a_m = 2^{m-2} + a_{m-1} - b_{m-1}, \tag{2.37}$$

$$b_m = a_{m-1} + b_{m-1}. \tag{2.38}$$

Closed form expressions for a_m and b_m can be found by solving the above coupled equations and they turn out to be,

$$a_m = \frac{1}{2}\left[2^{m-1} - 2^{m/2}\cos(\tfrac{m\pi}{4})\right], \tag{2.39}$$
$$b_m = \frac{1}{2}\left[2^{m-1} - 2^{m/2}\sin(\tfrac{m\pi}{4})\right]. \tag{2.40}$$

We also need to know the signature of the term $X_1^1 X_1^2 \cdots X_1^m$ as well as whether it is included in $\tilde{X}_m$ or $\tilde{Y}_m$. We notice that,

$$(-1)^{m/2} X_1^1 X_1^2 \cdots X_1^m \in \tilde{X}_m, \text{ if m is even,}$$
$$(-1)^{(m-1)/2} X_1^1 X_1^2 \cdots X_1^m \in \tilde{Y}_m, \text{ if m is odd.}$$

The required expectation values of $\tilde{X}_m$ and $\tilde{Y}_m$ are thus calculated. When m is even, we get:

$$\langle \tilde{X}_m \rangle = \left[2^{m-1} - 2a_m + (-1)^{\frac{m}{2}+1} 2\right] l^m,$$
$$\langle \tilde{Y}_m \rangle = \left[2^{m-1} - 2b_m\right] l^m \tag{2.41}$$

And when m is odd, we have,

$$\langle \tilde{X}_m \rangle = \left[2^{m-1} - 2a_m\right] l^m,$$
$$\langle \tilde{Y}_m \rangle = \left[2^{m-1} - 2b_m + (-1)^{\frac{m-1}{2}+1} 2\right] l^m \tag{2.42}$$

Finally, for the given m-mode correlation (2.29), the CFRD inequality – when m is even – is given by,

$$\left[\left(2^{m/2}\cos(\tfrac{m\pi}{4}) + (-1)^{\frac{m}{2}+1} 2\right)^2 + 2^m \sin^2(\tfrac{m\pi}{4})\right] l^{2m} \le 2^m \left(l^2 + \sigma^2\right)^m \tag{2.43}$$

And, when m is odd, it is given by,

$$\left[\left(2^{m/2}\sin(\tfrac{m\pi}{4}) + (-1)^{\frac{m-1}{2}+1}2\right)^2 + 2^m\cos^2(\tfrac{m\pi}{4})\right] l^{2m} \leq 2^m\left(l^2+\sigma^2\right)^m \tag{2.44}$$

In general, the violation of CFRD inequality is represented by the region between l-axis and two straight lines passing through the origin in the (l, σ) plane. Without loss of generality, the condition for violation of CFRD inequalities can be written as,

$$\alpha l^{2m} > \beta(l^2+\sigma^2)^m \tag{2.45}$$

where, α is the coefficient of l^{2m} in the LHS of the CFRD inequality and $\beta = 2^m$ is the coefficient of $(l^2+\sigma^2)^m$ in the RHS of the CFRD inequality. This is easily simplified to,

$$\sigma < \pm\tau_m l \tag{2.46}$$

where, the slope of the above straightlines is given by,

$$\pm\tau_m = \sqrt{\frac{\alpha^{1/m}}{2} - 1}$$

It is interesting to note that, for some values of m, the slope τ_m in (2.46) becomes imaginary. This means that there is no CFRD violation for those values of m for any (l, σ) by the corresponding m-mode correlations defined through (2.29).

For the calculation of the RS uncertainty relation, a similar approach to the 3-mode case is undertaken. As in the 3-mode case, for the m-mode case also we have single-mode and

2-mode marginals of the following forms,

$$
\begin{aligned}
\xi_{X_i}^{\mathcal{A}_i} &= \tfrac{1}{2}\left[\mathcal{N}_{l,\sigma}+\mathcal{N}_{-l,\sigma}\right], \forall i=\{1,\cdots,m\},\ X_i=\{0,1\} && (2.47)\\
\xi_{X_i,X_j}^{\mathcal{A}_i,\mathcal{A}_j} &= \tfrac{1}{4}\left[\mathcal{N}_{(l,l),\sigma}+\mathcal{N}_{(l,-l),\sigma}+\mathcal{N}_{(-l,l),\sigma}+\mathcal{N}_{(-l,-l),\sigma}\right] && (2.48)\\
&\qquad \forall\, i,j=\{1,\cdots,m\};\ \ i\neq j;\ \ X_i,X_j=\{0,1\}
\end{aligned}
$$

Following the same line of reasoning as in the 3-mode case, the product and non-product choices of single-mode position-momentum joint distributions give the below covariance matrices respectively:

$$
\mathbf{V_p}=\bigoplus_{i=1}^{m}\begin{bmatrix} l^2+\sigma^2 & 0\\ 0 & l^2+\sigma^2\end{bmatrix} \tag{2.49}
$$

and,

$$
\mathbf{V_{np}}=\bigoplus_{i=1}^{m}\begin{bmatrix} l^2+\sigma^2 & c\\ c & l^2+\sigma^2\end{bmatrix} \tag{2.50}
$$

Consequently, the RS uncertainty relation will be violated if,

$$
l^2+\sigma^2<1 \quad \text{(for product choice)} \tag{2.51}
$$

$$
l^2+\sigma^2<\sqrt{1+c^2} \quad \text{(for non-product choice)} \tag{2.52}
$$

respectively.

From the above equations we see that – the RS uncertainly relation – calculated with single-mode product and non-product joint distribution, will be violated by the probability measure (2.29) if $l^2+\sigma^2<1$ and $l^2+\sigma^2<\sqrt{1+c^2}$ respectively. Correspondingly, the values of l and σ that violate both the CFRD inequality and RS uncertainty relation gives the m-mode postquantum nonlocal correlations.

Fig. 2.2 below plots the CFRD and RS violations for different number of modes. It can be seen that for suitable choices of l and σ, m-mode probability measure (2.29) violates the corresponding CFRD inequality. It is interesting to note that violation of CFRD inequality is not guaranteed for any arbitrary m. For example, for $m = 7, 8, 9$, we do not have CFRD violations for the Bell behavior (2.29) .

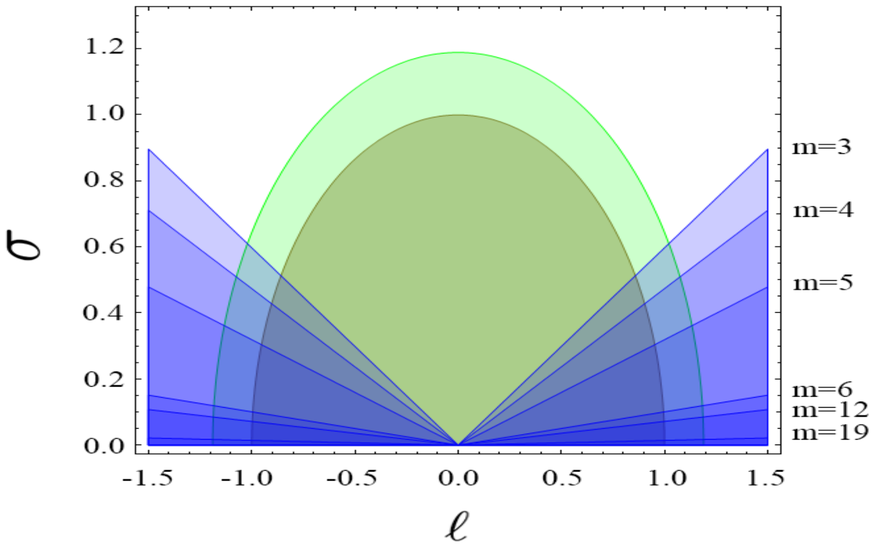

Figure 2.2: For different number of modes ($m = 3, 4, 5, 6, 12, 19$) the corresponding CFRD inequalities violation has been depicted by different shades of Blue regions as shown. The smaller and larger half-circular regions denote RS uncertainty violations for $c = 0$ and $c = 1$ as in Fig.2.1.

2.2.3 2-mode Scenario

So far, we have shown that the RS uncertainty relation plays a crucial role in certifying postquantumness for m-mode CV correlations, when $m \geq 3$. What will be the implication of our approach for 2-mode case? Is it still the case that RS uncertainty relation is necessary for certifying postquantumness?

Consider the 2-mode correlation introduced in Ref. [43]:

$$\xi_{00}^{\mathcal{A}_0\mathcal{A}_1} = \xi_{01}^{\mathcal{A}_0\mathcal{A}_1} = \xi_{10}^{\mathcal{A}_0\mathcal{A}_1} = \frac{1}{2}\left[\mathcal{N}_{(l,l),\sigma} + \mathcal{N}_{(-l,-l),\sigma}\right], \tag{2.53a}$$

$$\xi_{11}^{\mathcal{A}_0\mathcal{A}_1} = \frac{1}{2}\left[\mathcal{N}_{(l,-l),\sigma} + \mathcal{N}_{(-l,l),\sigma}\right]. \tag{2.53b}$$

In this case, the CFRD inequality turns out to be:

$$8l^4 \leq 4(l^2+\sigma^2)^2 \tag{2.54}$$

The calculation of CM is easily done as in the earlier cases. With product and non-product choices of single-mode position-momentum joint distribution the covariance matrix becomes,

$$\mathbf{V_p} = \begin{bmatrix} l^2+\sigma^2 & 0 & l^2 & l^2 \\ 0 & l^2+\sigma^2 & l^2 & -l^2 \\ l^2 & l^2 & l^2+\sigma^2 & 0 \\ l^2 & -l^2 & 0 & l^2+\sigma^2 \end{bmatrix} \tag{2.55}$$

$$\mathbf{V_{np}} = \begin{bmatrix} l^2+\sigma^2 & c & l^2 & l^2 \\ c & l^2+\sigma^2 & l^2 & -l^2 \\ l^2 & l^2 & l^2+\sigma^2 & c \\ l^2 & -l^2 & c & l^2+\sigma^2 \end{bmatrix} \tag{2.56}$$

Hence, the RS uncertainty relation $V + i\Omega \geq 0$ will be violated if,

$$(l^2+\sigma^2) < \sqrt{(1+2l^4)} \qquad \text{(for product)}, \tag{2.57}$$

$$(l^2+\sigma^2) < \sqrt{1+l^4+(l^2+c^2)^2} \quad \text{(for non-product)}. \tag{2.58}$$

From the above expressions, it is evident that any such correlation violating CFRD inequality also violates RS uncertainty relation. Therefore, the postquantumness of these

2-mode correlations can be asserted solely by the CFRD inequality without referring to RS uncertainty relation. This is unsurprising since it was already shown by Salles et. al. [51] that in 2-mode scenario there are no quantum violations of the CFRD inequality.

The regions of RS and CFRD violations for the 2-mode scenario are plotted in Fig. 2.3 below where it can be seen that the region of overlap is precisely the region of CFRD violation.

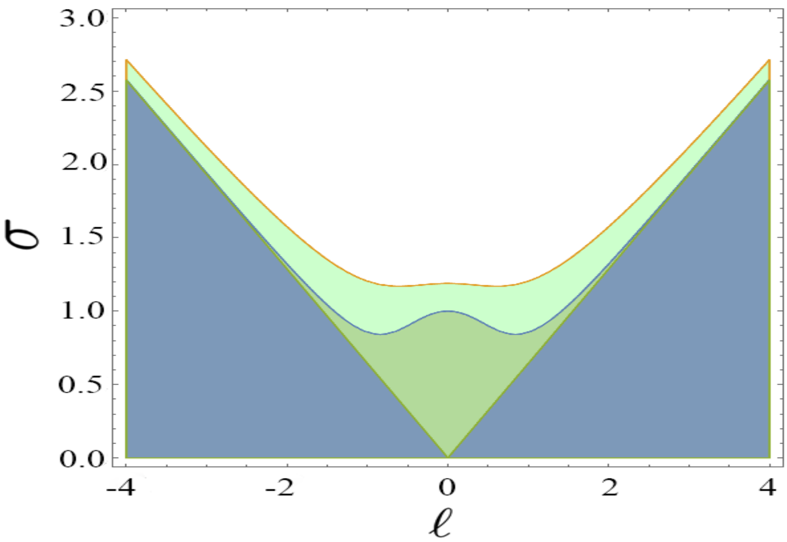

Figure 2.3: Blue region denotes violation of CFRD inequality. Dark and light green regions correspond to violation of RS uncertainty relation for product and non-product (with $c = 1$) choices of single mode position-momentum joint distribution.

2.3 Discussion

The usefulness of Robertson-Schrödinger uncertainty relation in detecting multimode entanglement has already been demonstrated in [89]. On the other hand, the work by Oppenheim and Wehner [67] is also worthy of mention in the context of the present work. In the $2-2-2$ scenario, they have shown that quantum mechanics cannot be more nonlocal with measurements that respect the uncertainty principle in *fine-grained* form. To the best of our knowledge, in the continuous outcome scenario the role of the uncertainty principle to certify post-quantumness has been explored for the very first time in the work presented in this chapter. The results obtained here could be further tightened if a similar analysis could be done with fine-grained uncertainty relations in the continuous variable paradigm.

2.4 Chapter Summary

In this chapter, we have presented a study of continuous variable nonlocal correlations that are stronger than quantum correlations. We have developed an approach to identify postquantum nonlocal correlations arising from continuous variable measurements in m-mode scenario. We have shown that the Robertson-Schrödinger uncertainty relation has a key role to play as a witness for postquantumness. The continuous variable Bell-type CFRD inequalities are used for establishing the nonlocal feature of correlations.

Chapter 3

Thermalization of Two-Level Quantum Systems

3.1 Preliminaries

3.1.1 Thermalizing maps for a qubit: Pin Map

Thermalization is the equilibriation process in which the equilibrium state of the system is the Gibbs thermal state corresponding to the temperature of the environment (for example, a heat bath). In other words, the system acquires thermal equilibrium.

Given the time-evolved state of the system $\rho_s(t)$ and the system Hamiltonian H, thermalization can be mathematically expressed as the following limit,

$$\lim_{t\to\infty} \rho_s(t) = e^{-H/k_B T} \equiv \rho_{th} \tag{3.1}$$

where, k_B is the Boltzmann constant and T is the temperature of the heat bath.

We look for the most general way a qubit can lead to thermalization – a qubit channel – a completely positive trace-preserving map $\mathcal{N} : \mathcal{L}(\mathbb{C}^2) \to \mathcal{L}(\mathbb{C}^2)$ such that $\mathcal{N}(\rho) = \rho_{th} =$

diag$(p, 1-p)$ for all single-qubit states ρ with $0 \leq p \leq 1$. Such a map is called a *pin map*. Here, $\mathcal{L}(\mathbb{C}^2)$ is the set of all bounded linear operators $A : \mathbb{C}^2 \to \mathbb{C}^2$.

The matrix representation for the pin map is given by:

$$\mathcal{N} = \begin{bmatrix} p & 0 & 0 & p \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1-p & 0 & 0 & 1-p \end{bmatrix}. \tag{3.2}$$

The Kraus operators for the pin map $\mathcal{N}$ are:

$$K_{00} = \begin{bmatrix} \sqrt{p} & 0 \\ 0 & 0 \end{bmatrix}, \quad K_{01} = \begin{bmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{bmatrix},$$

$$K_{10} = \begin{bmatrix} 0 & 0 \\ \sqrt{1-p} & 0 \end{bmatrix}, \quad K_{11} = \begin{bmatrix} 0 & 0 \\ 0 & \sqrt{1-p} \end{bmatrix}. \tag{3.3}$$

Thermalization can be described through several ways, one of which being Markovian master equations describing system interactions with a thermal bath. Therefore we will consider one such master equation – the quantum optical master equation – which will be detailed below.

3.1.2 Quantum Optical Master Equation

It would have been useful to have a dynamical version of the pin map, whose Kraus operators are given in equation (3.3). This would then give rise to a master equation corresponding to pin map, and thereby, for thermalization.

In the absence of such a general dynamical version, we now look at the quantum optical master equation to come up with one possible dynamical version of the Kraus operators in equation (3.3).

We choose the following Markovian master equation (quantum optical master equation) which corresponds to a qubit interacting with a bosonic thermal bath under Markovian conditions.

$$\begin{aligned} \frac{d\rho(t)}{dt} &= \gamma_0(N+1)\Big(\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho(t)\}\Big) \\ &+ \gamma_0 N\Big(\sigma_+\rho(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho(t)\}\Big) \end{aligned} \tag{3.4}$$

Here, $N = (\exp\frac{E(\omega)}{k_B T} - 1)^{-1}$ is the Planck distribution, k_B is the Boltzmann constant, T is temperature of the heat bath and $E(\omega) = \hbar\omega$ is the energy of the system at frequency ω. γ_0 is the spontaneous emission rate of the bath, and $\gamma = \gamma_0(2N+1)$ is the total emission rate (including thermally induced emission and absorption processes).

Here, the free evolution part of the dynamics is neglected since the point of interest is in the dissipative dynamics. For more details and derivation of the quantum optical master equation, refer to [37].

The master equation can be readily solved by choosing the initial system qubit state to be $\rho(0) = \frac{1}{2}(\mathbb{I} + \bar{r}(0).\bar{\sigma})$, where $\bar{r}(0) = (r_1(0), r_2(0), r_3(0))$ is the initial Bloch vector, and choosing the time-evolved state to be $\rho(t) = \frac{1}{2}(\mathbb{I}+\bar{r}(t).\bar{\sigma})$ where $\bar{r}(t) = (r_1(t), r_2(t), r_3(t))$. Solving, we find,

$$\begin{aligned} r_1(t) &= r_1(0)e^{-\gamma t/2}, \\ r_2(t) &= r_2(0)e^{-\gamma t/2}, \\ r_3(t) &= (r_3(0) + g)e^{-\gamma t} - g. \end{aligned} \tag{3.5}$$

Here, $g = \gamma_0/\gamma = (2N+1)^{-1}$. Hence, $g \in [0,1]$. g gives us a measure of the temperature T. It can be easily seen that higher the value of g, lower the temperature and vice versa. Specifically, $g = 0$ for $T = \infty$ and $g = 1$ for $T = 0$. The steady state solution for the system (i.e. in the limit $t \longrightarrow \infty$) is a thermal state as expected, and corresponds to the Bloch vector $(0, 0, -g)$. Explicitly,

$$\rho_{th} = \text{diag}(\frac{1-g}{2}, \frac{1+g}{2}). \tag{3.6}$$

3.1.3 Markovian Dynamics

In open quantum systems i.e. when there is interaction between the system and the environment, information exchange between them is an essential feature of the dynamics [37]. If there is no information flow from the environment to the system, then such a dynamics is called Markovian i.e. it has no memory. If there is information flow from the environment, then it has a memory-effect on the system and such dynamics are known as non-Markovian.

Originally, Markovianity in quantum regime was defined as the *semigroup* property of dynamical maps. A dynamical map Λ_t has semigroup property if we can write,

$$\Lambda_{t+s} = \Lambda_t \Lambda_s, \tag{3.7}$$

for all $t, s \geq 0$.

The master equation governing such a map in d-dimensions was derived by the pioneering work of Gorini, Kossakowski and Sudarshan (GKS) [90] and also, by Lindblad [91]. It is given by,

$$\frac{d\rho}{dt} = -i[H, \rho] + \frac{1}{2}\sum_j \left([V_j, \rho V_j^\dagger] + [V_j\rho, V_j^\dagger]\right) \tag{3.8}$$

Equation (3.8) is often called the Lindlad (or, the GKLS) form of master equation. A brief review can be found in Ref. [92].

In Ref. [93], Rivas, Huelga and Plenio generalized the idea of semigroup to define Markovianity in terms of *completely positive* (CP) divisibility. A dynamical map Λ_t is called CP divisible if it can be expressed as,

$$\Lambda_t = V_{t,s}\,\Lambda_s, \tag{3.9}$$

for any $t > s$, where $V_{t,s}$ is completely positive $\forall t > s$. $V_{t,s}$ can be seen as the intermediate evolution from s to t, and it is uniquely defined only when Λ_t is invertible i.e. $V_{t,s} = \Lambda_t \Lambda_s^{-1}$.

In this thesis, we will be using this CP divisibility defnition of Markovianity. It is also known that the master equation for a CP divisible dynamical map is of the GKLS form with but time dependent coefficients [94, 95]. And we can immediately see that the quantum optical master equation considered previously in (3.4) is one such example.

3.1.4 Parametrization of Affine Transformation

Affine transformation refers to the description of a qubit channel action in terms of the transformation of the Bloch vector of the qubit state [7, 38]. Any single-qubit channel can be written as an affine transformation, which is of the form:

$$r_i(t) = \sum_{j=0}^{3} M_{ij} r_j(0) + C_i \tag{3.10}$$

where, $\bar{r}(0) = (r_1(0), r_2(0), r_3(0))$ is the initial Bloch vector, $\bar{r}(t) = (r_1(t), r_2(t), r_3(t))$ is the time evolved Block vector (i.e. after channel action), $\{M_{ij}\}$ is a 3×3 matrix and $\{C_i\}$ is a column matrix.

In Ref. [38], G. Narang and Arvind used a single-qubit mixed state ancilla to parametrize the affine transformation of a single-qubit channel. We use their technique to simulate a dynamical process for qubit thermalization. To do so, we consider a single-qubit mixed state ancilla of the form,

$$\rho_e = (1-\lambda)\frac{\mathbb{I}}{2} + \lambda|\phi\rangle\langle\phi|. \tag{3.11}$$

where $\lambda \in [0,1]$, $\frac{\mathbb{I}}{2}$ is the maximally mixed state and $|\phi\rangle$ is a general pure state given by,

$$|\phi\rangle = \cos\left(\frac{\xi}{2}\right)|0\rangle + e^{-i\eta}\sin\left(\frac{\xi}{2}\right)|1\rangle.$$

If ρ_e plays the role of a bath state of a single-qubit system then evolution through the *most general* two-qubit unitary U (upto a freedom of local unitary actions), given in equation (3.12) below, will result in the following affine transformation for the system qubit, as given in equations (3.13) and (3.14) below. Apart from η, ξ, λ, three more parameters α, β, δ are required to completely identify the channel. Thus, the class of single-qubit channels which can be simulated by a single-qubit mixed state ancilla is a six parameter family $(\alpha, \beta, \delta, \eta, \xi, \lambda)$ of affine transformations:

$$U = \begin{bmatrix} \cos\frac{\alpha+\delta}{2} & 0 & 0 & i\sin\frac{\alpha+\delta}{2} \\ 0 & e^{-i\beta}\cos\frac{\alpha-\delta}{2} & ie^{-i\beta}\sin\frac{\alpha-\delta}{2} & 0 \\ 0 & ie^{-i\beta}\sin\frac{\alpha-\delta}{2} & e^{-i\beta}\cos\frac{\alpha-\delta}{2} & 0 \\ i\sin\frac{\alpha+\delta}{2} & 0 & 0 & \cos\frac{\alpha+\delta}{2} \end{bmatrix} \tag{3.12}$$

$$M = \begin{bmatrix} \cos\delta\cos\beta & \lambda\cos\delta\sin\beta\cos\xi & -\lambda\sin\delta\cos\beta\sin\eta\sin\xi \\ -\lambda\cos\alpha\sin\beta\cos\xi & \cos\alpha\cos\beta & \lambda\sin\alpha\cos\beta\cos\eta\sin\xi \\ -\lambda\cos\alpha\sin\delta\sin\eta\sin\xi & -\lambda\sin\alpha\cos\delta\sin\xi\cos\eta & \cos\alpha\cos\delta \end{bmatrix} \tag{3.13}$$

$$C = \begin{bmatrix} -\lambda\sin\delta\sin\beta\sin\xi\cos\eta \\ -\lambda\sin\alpha\sin\beta\sin\xi\sin\eta \\ -\lambda\sin\alpha\sin\delta\cos\xi \end{bmatrix}. \tag{3.14}$$

One may notice a slight discrepancy with our closed form expressions of M and C given in equations (3.13) and (3.14)) and those given by equations (11) and (12) in [38]. This is because there seems to be slight error in the latter's calculation. The explicit details of our calculation involved in parametrizing the M and C matrices are detailed below.

The form of U, given in equation (3.12), can be re-written after a simple basis change in the following way,

$$\begin{aligned} U = & K_0(\mathbb{I}^{(s)} \otimes \mathbb{I}^{(e)}) + K_1(\sigma_1^{(s)} \otimes \sigma_1^{(e)}) \\ & + K_2(\sigma_2^{(s)} \otimes \sigma_2^{(e)}) + K_3(\sigma_3^{(s)} \otimes \sigma_3^{(e)}) \end{aligned} \tag{3.15}$$

where,

$$\begin{aligned} K_0 &= \frac{1}{2}\left(\cos\frac{\alpha+\delta}{2} + e^{-i\beta}\cos\frac{\alpha-\delta}{2}\right), \\ K_1 &= \frac{i}{2}\left(\sin\frac{\alpha+\delta}{2} + e^{-i\beta}\sin\frac{\alpha-\delta}{2}\right), \\ K_2 &= \frac{-i}{2}\left(\sin\frac{\alpha+\delta}{2} - e^{-i\beta}\sin\frac{\alpha-\delta}{2}\right), \\ K_3 &= \frac{1}{2}\left(\cos\frac{\alpha+\delta}{2} - e^{-i\beta}\cos\frac{\alpha-\delta}{2}\right). \end{aligned} \tag{3.16}$$

Now recalling the form of the mixed state ancilla ρ_e from equation (3.11) and using an arbitrary initial state for the system qubit $\rho_s = \frac{1}{2}(\mathbb{I} + \bar{r}.\bar{\sigma})$, we can define the composite initial state,

$$\rho_{se}^{initial} = \rho_s \otimes \rho_e. \tag{3.17}$$

To find the final time-evolved state of the system qubit, we apply the unitary and then trace out the environment,

$$\rho_s^{final} = \mathrm{Tr}_e\left[U\rho_{se}^{initial}(U)^\dagger\right]. \tag{3.18}$$

Now we can find out the components of ρ_s^{final} in the basis $\{\sigma_1^{(s)}, \sigma_2^{(s)}, \sigma_3^{(s)}\}$ by computing $\mathrm{Tr}[\sigma_i^{(s)}\rho_s^{final}]$. Thereby, we can read out the elements of M and C. For example, consider

$i = 3$, we get:

$$\mathrm{Tr}[\sigma_3^{(s)} \rho_s^{final}] = M_{31} n_1 + M_{32} n_2 + M_{33} n_3 + C_3. \tag{3.19}$$

Finally, after somewhat lengthy calculations we arrive at the parametrized matrice forms M and C given above.

It is also important to note here that by using the ancilla qubit, we are only simulating the dynamics of the system qubit leading to the infinite time thermalization. More specifically, we do not have the ancilla state remaining static, as is the case for the bosonic bath. The ancilla qubit does in fact change its state.

3.1.5 Derivation of Qubit Master Equation

In Ref. [96], Pang et. al. gives a technique to derive the master equation for qubit dynamics given the time-evolved state $\rho_s(t)$ and initial state $\rho_s(0)$. First, we express $\rho_s(0)$ and $\rho_s(t)$ as vectors in the operator space of the system which has basis $\{\mathbb{I}, \sigma_1, \sigma_2, \sigma_3\}$. The density matrix of the system can be represented by a 4×1 vector, and a superoperator on the system can be represented by a 4×4 matrix.

In this representation, $\boldsymbol{v}_0 = \frac{1}{2}[1, x, y, z]^T$ is the vector form of the initial arbitrary density matrix of the system qubit and most general vector form of the system qubit at time t is,

$$\boldsymbol{v}_t = \frac{1}{2}[1, a_0 + a_1 x + a_2 y + a_3 z, b_0 + b_1 x + b_2 y + b_3 z, c_0 + c_1 x + c_2 y + c_3 z]^T = Q_t \boldsymbol{v}_0 \tag{3.20}$$

where, Q_t is the matrix representation of the system qubit evolution from the initial time to the time t,

$$Q_t = \begin{pmatrix} 1 & 0 & 0 & 0 \\ a_0 & a_1 & a_2 & a_3 \\ b_0 & b_1 & b_2 & b_3 \\ c_0 & c_1 & c_2 & c_3 \end{pmatrix}. \tag{3.21}$$

To proceed further, Q_t should necessarily be invertible (atleast for finite t). Thus, we can find that,

$$\partial_t \boldsymbol{v}_t = \dot{Q}_t \boldsymbol{v}_0 = \dot{Q}_t Q_t^{-1} \boldsymbol{v}_t. \tag{3.22}$$

Therefore, we see that $\dot{Q}_t Q_t^{-1}$ is the matrix representation of the linear transformation corresponding to the time derivative of the system density matrix.

Now we can find the superoperator corresponding to $\dot{Q}_t Q_t^{-1}$. In order to do this, we need to know the matrix representations s_{ij} for the basis of the superoperator $\sigma_i[\cdot]\sigma_j$. These representations are straightforward to find and are given in equation (S15) in [97]. They are given below for easy reference:

$$s_{00} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad s_{01} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}, \quad s_{02} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -i \\ 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},$$

$$s_{03} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad s_{10} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad s_{11} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$s_{12} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad s_{13} = \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \\ -i & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad s_{20} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \\ 1 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix},$$

$$s_{21} = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \quad s_{22} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad s_{23} = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$s_{30} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad s_{31} = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \\ i & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad s_{32} = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$
$$s_{33} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.23}$$

Decomposing $\dot{Q}_t Q_t^{-1}$ into the matrix representation, we get,

$$\dot{Q}_t Q_t^{-1} = \sum_{i,j=0}^{3} a_{ij} s_{ij} \tag{3.24}$$

Now by de-vectorizing, the master equation can be obtained in terms of the density operator.

$$\partial_t \rho = \sum_{i,j=0}^{3} a_{ij}\ \sigma_i \rho \sigma_j \tag{3.25}$$

3.2 Thermalization of a Qubit

The study of evolution of open systems towards equilibrium has always been a challenging problem in statistical mechanics. The difficulty lies in prescribing a form of interaction between the system and the environment at the microscopic level that will give rise to equilibration. It has been evaded by proposing the so called *H-theorem* which states that a system attains equilibrium when the entropy function is maximized over the accessible states of the system.

Although this has proved to be a very efficient way to calculate and work with equilibrium states, the heart of the problem remains unsolved. We look at this thermodynamic problem from a quantum mechanical perspective. Quantum thermodynamics has received a lot of attention in the recent past [98, 99]. The concepts and laws of thermodynamics are presumably valid only in the macroscopic regime. To see how the laws and definitions of thermodynamic quantities viz heat, work, etc behave in the microscopic regime is one of the main objectives of quantum thermodynamics.

There has been a number of works [100–104] where the problem of equilibration is looked at from a quantum mechanical perspective. For example, Linden et. al. [105] looked into the problem of the smallest possible quantum refrigerator. In the process, they considered a two-qubit system as a refrigerator in which one qubit acts as the system to be cooled while the other works as the coil of the refrigerator by extracting heat from the body (to be cooled), and releasing it to the environment. The two-qubit refrigerator is derived from the equilibrium (steady) state solution of a three-qubit master equation which the authors provided phenomenologically. This motivated us to see if, instead of following this phenomenological approach, a microscopic description for the thermalization process (equilibration to a thermal state) is possible through a thermalizing Hamiltonian. Such a simulation of the thermalization process can serve at least two purposes: (i) simulating a natural thermalization process in lab, and (ii) comparing different time scales (e.g., time scales for thermalization versus interaction time scales of different constituents of the system) without assuming a priori their ordering.

To completely characterize the joint Hamiltonian of the system and environment that results in equilibration of the system, is a formidable task. So, instead we ask the following question: whether for a given thermalization process of a system, there exists an ancilla in a specific state and a joint Hamiltonian of system-ancilla that gives rise to the exact same process of equilibration on the system. In this chapter, we provide an affirmative answer to this question in the case of the quantum optical master equation.

We work out a *thermalizing Hamiltonian* H_{th} for the quantum optical master equation [37] which gives rise to thermal equilibration of a qubit. We find that a single-qubit ancilla initialized in a thermal state is sufficient for such a dynamics to be mimicked.

Our next aim is to look for such simulations of the thermalization process which evolves under the action of non-Markovian dynamics. We analyze such situations further by considering a general form of thermalizing Hamiltonian of which the quantum optical master equation dynamics is a special case. We work out the necessary and sufficient conditions for Markovianity of the system dynamics given a form of the simulating interaction Hamiltonian. Note that not every non-Markovian dynamics gives rise to equilibration of the system, and thereby, thermalization. Our approach here provides one possible way of generating a thermalizing non-Markovian dynamics through the prescription of a simulating Hamiltonian. It is worth mentioning here that, as there are a number of definitions of Markovianity in the quantum mechanical scenario [93, 95, 106, 107], we adhere to the completely positive (CP) divisibility definition [93, 95] and use the characterization of Wolf et. al. [94] for finding out the aforementioned conditions.

An interesting model of thermalization was proposed by V. Scarani et. al. [108]. Another model of thermalization (for spin-$\frac{1}{2}$ systems) has been developed by Kleinbolting and Klesse [109]. In these works, they used the swap operation between system and bath to give rise to thermalization. But a drawback of these methods is that the system is fully thermalized after a *finite* time interval, which would imply that the thermalizing map is a function of only the temperature to which the system will thermalize and the time interval taken to reach it. This proposition seems to be unrealistic as this does not take into account the intricacies of the system, environment or the correlations shared between them that might affect the process of thermalization.

In [110–112], M. J. de Oliveira has shown another novel approach to thermalization for systems in contact with an environment (typically, heat reservoirs). In [110], a quantum Focker-Planck-Kramers (FPK) equation is derived via canonical quantization of the classical FPK equation to account for quantum dissipation of systems interacting with environment. The dissipation term is chosen such that the system equilibriates to the Gibbs thermal state i.e. system thermalizes. In [111, 112], the quantum FPK equation is further exploited to study heat transport properties in harmonic oscillator chains and bosonic systems. Although our approach to thermalization also begins with solving a master equation, it differs from de Oliveira's in that our aim is to derive simulating Hamiltonians for thermalization and thereby study generic features of thermalization in open quantum systems.

3.3 Thermalizing Hamiltonian

We derive a joint Hamiltonian between the system and an ancilla, which will give rise to the thermalization of the system. This system-ancilla Hamiltonian – henceforth called as thermalizing Hamiltonian H_{th} – will give rise to a unitary process where the system (two levels of the atom) will equilibriate to a (constant) thermal state with temperature corresponding to the heat bath.

To calculate the thermalizing Hamiltonian H_{th}, we consider the quantum optical master equation. We find the affine transformation on the Bloch vector of the system qubit that will give rise to the same evolution. Using the solution of the quantum optical master equation given previously in equation (3.1.2), we can find the corresponding affine transformation as:

$$M = \begin{bmatrix} e^{-\gamma t/2} & 0 & 0 \\ 0 & e^{-\gamma t/2} & 0 \\ 0 & 0 & e^{-\gamma t} \end{bmatrix} \tag{3.26}$$

$$C = \begin{bmatrix} 0 \\ 0 \\ g(e^{-\gamma t} - 1) \end{bmatrix}. \tag{3.27}$$

Here, we notice that this affine transformation is a special kind of generalized amplitude damping channel. Amplitude damping channels describe the effect of energy dissipation to environment at finite temperature [7].

The affine transformation for a generalized amplitude damping channel is given by:

$$M_{GAD} = \begin{bmatrix} \sqrt{1-B} & 0 & 0 \\ 0 & \sqrt{1-B} & 0 \\ 0 & 0 & 1-B \end{bmatrix}, \tag{3.28}$$

$$C_{GAD} = \begin{bmatrix} 0 \\ 0 \\ B(2p-1) \end{bmatrix}. \tag{3.29}$$

where, B, $p \in [0, 1]$ are two positive parameters. We can see that our thermalization process is a generalized amplitude damping channel with the parameter $p < \frac{1}{2}$.

We now refer to the result by Narang and Arvind [38], where it was shown that it is enough for certain qubit channels to have a single-qubit mixed state ancilla to simulate the action of the channel as a sub-system dynamics of a system-ancilla unitary evolution. It may be noted here that Terhal et. al. [113] have shown that certain single-qubit channels can only be simulated through qutrit mixed state environments. Incidentally, our affine transformation fits into the criterion for single-qubit ancilla as in [38], and we find a two-qubit Hamiltonian that simulates the dynamics of the system qubit as in the quantum optical master equation.

Now, we compare the parametrized forms of M and C matrices given earlier in equations (3.13) and (3.14) with the affine transformation corresponding to our soution of the quantum optical master equation i.e. equations (3.26) and (3.27) respectively. Thus, we can get a joint unitary giving rise to thermalization.

One can check that such a unitary does indeed lead to thermalization in the infinite time limit. Equivalently, this can also be seen by calculating the Kraus operators for the system qubit from the joint unitary operator and then applying the infinite time limit,

$$\lim_{t\to\infty} \rho_s(t) = \rho_{th}$$

Now, the thermalizing Hamiltonian (H_{th}) is calculated from the unitary time-evolution operator and the details of the derivation are given below.

To find the thermalizing Hamiltonian, we first need to find the values of the parameters that match with our particular affine transformation. For this, we compare the affine transformation for the quantum optical case in equations (3.26) and (3.27) with the parametrized matrices in equations (3.13) and (3.14) respectively. It can be easily seen that there exist, two sets of parameters that will satisfy. We will consider one of them for illustration:

$$\lambda = g, \cos\alpha = \cos\delta = e^{\frac{-\gamma t}{2}}, \cos\beta = \pm 1 = \cos\xi, \tag{3.30}$$

and η can be arbitrary. So finally, we get the mixed state ancilla as the following thermal state,

$$\rho_e = \frac{1+g}{2}|0\rangle\langle 0| + \frac{1-g}{2}|1\rangle\langle 1|. \tag{3.31}$$

Putting the values from equation (3.30) into the form of 2-qubit unitary given in equation (3.12), we get the unitary for the thermalization process. Note that we now have a time-dependent unitary of the form,

$$U(t,0) = \begin{bmatrix} e^{\frac{-\gamma t}{2}} & 0 & 0 & i\sqrt{1-e^{-\gamma t}} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i\sqrt{1-e^{-\gamma t}} & 0 & 0 & e^{\frac{-\gamma t}{2}} \end{bmatrix}. \tag{3.32}$$

We can now calculate H_{th} easily as follows. We know,

$$U(t_2, t_1) = \exp\Big(-i\int_{t_1}^{t_2} H(s)ds\Big), \text{ and}$$

$$\begin{aligned} U(t+\Delta t, t) &= \exp\left(-i\int_{t}^{t+\Delta t} H(s)ds\right) \\ &\approx \mathbb{I} - i\Delta t H(t) \end{aligned}$$

Using the semi-group property of $U(t)$ (which holds good for small time interval Δt even if H is time-dependent) we get,

$$\begin{aligned} U(t+\Delta t, 0) &= U(t+\Delta t, t)U(t, 0) \\ \Rightarrow U(t+\Delta t, t) &= U(t+\Delta t, 0)U^{\dagger}(t, 0) \\ &= \Big(U(t,0) + \Delta t\frac{dU(t,0)}{dt} + \cdots\Big)U^{\dagger}(t,0) \\ &\approx \mathbb{I} + \Delta t\frac{dU(t,0)}{dt}U^{\dagger}(t,0) \end{aligned}$$

Comparing with the RHS of the previous equation, we get:

$$H_{th}(t) = i\left(\frac{dU(t,0)}{dt}\right)U^{\dagger}(t,0)$$

Thus, we get:

$$H_{th}(t) = \frac{\pm\gamma e^{\frac{-\gamma t}{2}}}{2\sqrt{1-e^{-\gamma t}}}\Big(|00\rangle\langle 11| + |11\rangle\langle 00|\Big) \tag{3.33}$$

Without loss of generality, we choose the positive sign in our work.

Following exactly the same recipe for the second set of parameters, we get the second type of H_{th} as,

$$H_{th}(t) = \frac{\pm\gamma e^{\frac{-\gamma t}{2}}}{2\sqrt{1-e^{-\gamma t}}}\Big(|01\rangle\langle 10| + |10\rangle\langle 01|\Big)$$

But here, it is important to note that this Hamiltonian does not lead to the same thermal state as before. In the previous case, we get the thermalizing Hamiltonian corresponding to the Bloch vector $(0, 0, -g)$ which matches with the steady state of the quantum optical master equation. But in the second Hamiltonian, we get thermal state with the Bloch vector $(0, 0, g)$. Thus, we discard that set of parameters and concentrate only on the first set (3.30).

We re-write H_{th} in the following form,

$$H_{th}(t) = f(t)\Big(|\phi^+\rangle\langle\phi^+| - |\phi^-\rangle\langle\phi^-|\Big), \tag{3.34}$$

where,

$$f(t) = \frac{\gamma e^{-\gamma t/2}}{2\sqrt{1-e^{-\gamma t}}}, \tag{3.35}$$

$$|\phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle). \tag{3.36}$$

The most general two-qubit time-dependent Hamiltonian which gives rise to the affine transformation (3.26,3.27) by acting on the tensor product of the arbitrary intitial state of the system qubit and the initial state of the ancilla qubit being ρ_{th} (given in equation (3.6)), is of the form given in equation (3.34) above.

3.4 On Markovianity of Dynamics for Thermalization

Consider a 2-qubit Hamiltonian of the form,

$$H(t) = f(t)(|\phi^+\rangle\langle\phi^+| - |\phi^-\rangle\langle\phi^-|) \tag{3.37}$$

where, $|\phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$. Now, we can ask what the conditions on $f(t)$ such that the system will thermalize in the infinite time limit. Moreover, we can ask when the evolution of the system follows Markovian dynamics.

The main reason behind the search for generic properties of $f(t)$ in the above equation is to look for a generic Hamiltonian (involving qubit ancilla) method for thermalization which does not necssarily follow from the optical master equation - in the latter case, the system is known to thermalize in the infinite time limit.

We can also rewrite eq.(3.37) in the Pauli basis as,

$$H(t) = f(t)(\sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y).$$

This represents a kind of spin exchange interaction similar to the double-quantum Hamiltonian used in NMR experiments [114]. In particular, $f(t)$ can be interpreted as a time-dependent coupling strength between the spins. Such Hamiltonians can in principle be realized in lab.

3.4.1 Thermalization

Given an arbitrary initial state for the system (say, ρ_s^i) and an initial thermal state for the ancilla (say, $\rho_e^i = \frac{1}{2}\mathrm{diag}(1+g, 1-g)$), we can derive the condition on a generic $f(t)$ such that the system will thermalize in the infinite time limit i.e. by imposing the following constraint,

$$\lim_{t\to\infty} \mathrm{Tr}_e\left[U(t,0)(\rho_s^i \otimes \rho_e^i)U(t,0)^\dagger\right] = \mathrm{diag}(\frac{1-g}{2}, \frac{1+g}{2}) \tag{3.38}$$

where $U(t,0) = \exp\left(-i\int_0^t H(\tau)d\tau\right)$ with $H(\tau)$ defined above in (3.37) and the RHS is as we saw in (3.6).

This condition for thermalization is finally found to be,

$$\lim_{t\to\infty} F(t) = (2n+1)\frac{\pi}{2} \tag{3.39}$$

where, n is any integer and,

$$F(t) = \int_0^t f(\tau)d\tau \tag{3.40}$$

Thus, (3.39) gives us a necessary and sufficient condition for thermalization to occur given a 2-qubit Hamiltonian of the form (3.37).

3.4.2 Markovianity of System Evolution

Another interesting question we can raise is about the nature of the system evolution under such a Hamiltonian - will it be Markovian always? To answer this we refer to [94] in which the Wolf et.al. have produced necessary and sufficient conditions for a given master equation $\dot{\rho} = L_t[\rho]$ to be Markovian (CP divisible) in nature. These conditions are:

- L_t must be hermiticity preserving.
- $L_t^*(\mathbb{I}) = 0$, and
- $\omega_c L_t^\Gamma \omega_c \geqslant 0$,

for all times t, where L_t^* and L_t^Γ are the adjoint map and Choi map of L_t respectively. $\omega_c = \mathbb{I} - |\omega\rangle\langle\omega|$ is the projector onto the orthogonal complement of the maximally entangled state $|\omega\rangle = \sum_i \frac{1}{\sqrt{2}} |i, i\rangle$. Given a dynamical map of the form Λ_t such that $\rho_t = \Lambda_t \rho_0$ where ρ_0 and ρ_t are the initial and time-evolved states respectively, we have $L_t = \dot{\Lambda}_t \Lambda_t^{-1}$ (provided, the inverse of Λ_t exists). In our case, the inverse does exist. If Λ_t^{-1} doesnt exist, then one can follow the prescription given in Ref. [115].

It can be seen that the first two conditions will always be satisfied for our particular case. Imposing the third condition, we obtain the following necessary and sufficient constraints on the time dependence of the Hamiltonian for ensuring Markovianity of the dynamical map,

$$0 \leqslant F(t) \leqslant \frac{\pi}{2}, \ \forall t \tag{3.41}$$

$$\frac{d}{dt}F(t) \geqslant 0, \ \forall t \tag{3.42}$$

Note that alternatively, we can have a monotonically decreasing $F(t)$ bounded between $[-\frac{\pi}{2}, 0]$ if we choose $-f(t)$ in our Hamiltonian (3.37).

We may now think of a functional form of $f(t)$ which satisfies the thermalization condition but violates the markovianity conditions - namely that $F(t)$ be monotonic and bounded. A simple example for such a non-Markovian thermalizing form is,

$$F(t) = \frac{\sin(20t)}{1+10t} + (1-e^{-t})\frac{\pi}{2} \tag{3.43}$$

FIG. 3.1 plots the original $F(t)$ from (3.40) (black curve) and the one given in (3.43) (red curve).

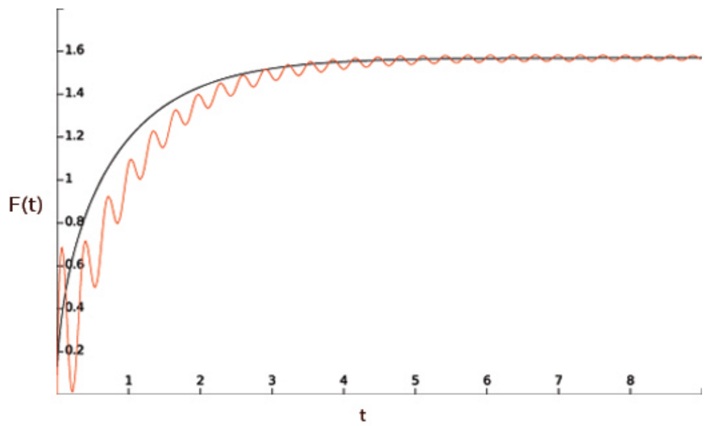

Figure 3.1: Red line is the $F(t)$ corresponding to non-Markovian thermalizing Hamiltonian while black corresponds to that of our original Markovian thermalizing form. Note that both converge to $\frac{\pi}{2}$ asymptotically and hence signify thermalization.

3.5 Lindblad-type Master Equation

In the preceding sections, we have derived a specific form of thermalizing Hamiltonian from the quantum optical master equation and then we generalized it by identifying conditions for the dynamics to be Markovian. We now derive the master equation that refers to the system dynamics for thermalization under our specific form of Hamiltonian given by equation (3.37). We will follow the derivation procedure given by [96] and described previously in the Preliminaries.

We consider a Hamiltonian of the form (3.37), with fixed initial state of ancilla qubit as $\sigma_e(0) = \frac{1}{2}(\mathbb{I} + g\sigma_3)$ (i.e. a thermal state with temperature defined through g as previously explained) and an arbitrary initial state of system qubit $\rho_s(0) = \frac{1}{2}(\mathbb{I} + \bar{r}.\bar{\sigma})$ with $\bar{r} = (x, y, z)^{\mathrm{T}}$. The time evolved state of the system under the action of such a Hamiltonian can be calculated as,

$$\rho_s(t) = \mathrm{Tr}_e\Big[U(t,0)\rho_s(0) \otimes \sigma_e(0)(U(t,0))^{\dagger}\Big]. \tag{3.44}$$

where, $U(t,0) = \exp\left(-i\int_0^t H(\tau)d\tau\right)$.

In the vector notation, $\boldsymbol{v}_0 = \frac{1}{2}[1, x, y, z]^{\mathrm{T}}$ is the vector form of the initial arbitrary density matrix of the system qubit and the vector form of the time-evolved system qubit at time t is,

$$\boldsymbol{v}_t = \frac{1}{2}[1, C_t x, C_t y, C_t^2 z + gS_t^2]^T = Q_t \boldsymbol{v}_0 \tag{3.45}$$

where, $C_t \equiv \cos(F(t)), S_t \equiv \sin(F(t))$ and Q_t is the matrix representation of the system qubit evolution from the initial time to the time t,

$$Q_t = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & C_t & 0 & 0 \\ 0 & 0 & C_t & 0 \\ gS_t^2 & 0 & 0 & C_t^2 \end{pmatrix}. \tag{3.46}$$

It can be seen that Q_t is invertible for finite t. Thus, using equation (3.22) we know,

$$\partial_t \boldsymbol{v}_t = \dot{Q}_t Q_t^{-1} \boldsymbol{v}_t. \tag{3.47}$$

Hence, we see that $\dot{Q}_t Q_t^{-1}$ is the matrix representation of the linear transformation corresponding to the time derivative of the system density matrix, and we have:

$$\dot{Q}_t Q_t^{-1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \alpha_t & 0 & 0 \\ 0 & 0 & \alpha_t & 0 \\ \beta_t & 0 & 0 & 2\alpha_t \end{pmatrix}. \tag{3.48}$$

where,

$$\alpha_t = -f(t)\tan(F(t))$$
$$\beta_t = 2gf(t)\tan(F(t))$$

Now we find the superoperator corresponding to $\dot{Q}_t Q_t^{-1}$ using the basis s_{ij} given in (3.23). Decomposing $\dot{Q}_t Q_t^{-1}$ into the matrix representation, we get,

$$\dot{Q}_t Q_t^{-1} = \sum_{i,j=0}^{3} a_{ij} s_{ij} \tag{3.49}$$

In our particular case, the non-zero components a_{ij} turns out to be, $a_{00} = 4\alpha_t$, $a_{03} = a_{30} = \beta_t$, $a_{11} = a_{22} = -2\alpha_t$ and $a_{21} = -a12 = i\beta_t$.

Now by de-vectorizing, the master equation can be found in terms of density operator. Thus, we get:

$$\partial_t \rho(t) = 4\alpha_t \rho - 2\alpha_t(\sigma_1\rho\sigma_1 + \sigma_2\rho\sigma_2) + i\beta_t(\sigma_2\rho\sigma_1 - \sigma_1\rho\sigma_2) + \beta_t\{\rho, \sigma_3\} \tag{3.50}$$

Using the fact that $\sigma_\pm = \sigma_1 \pm i\sigma_2$, the above equation can easily be recast into the Lindblad-type master equation as below,

$$\begin{aligned}\frac{d\rho(t)}{dt} &= \gamma_1(t)\Big(\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho(t)\}\Big) \\ &\quad + \gamma_2(t)\Big(\sigma_+\rho(t)\sigma_- \frac{1}{2}\{\sigma_-\sigma_+, \rho(t)\}\Big)\end{aligned} \tag{3.51}$$

where,

$$\gamma_1(t) = (1+g)f(t)\tan[F(t)]$$

$$\gamma_2(t) = (1-g)f(t)\tan[F(t)]$$

Here, $F(t) = \int_0^t f(\tau)d\tau$ and g is the parameter referring to the bath temperature used in defining the initial ancilla state as $\sigma_e(0) = \frac{1}{2}(\mathbb{I} + g\sigma_3)$.

The above form of master equation is immediately reminiscent of the Lindblad (Markovian) form [90–92] that we have used at the beginning in equation (3.4). Hence, we have a master equation that is of the Lindblad type, but with time-dependent coefficients $\gamma_1(t)$ and $\gamma_2(t)$. It has been shown that the negativity of these decoherence rates represent non-Markovianity [97].

Simply put, if the decoherence rates – $\gamma_1(t)$ and $\gamma_2(t)$ – remain non-negative for all time, then the master equation represents a Markovian evolution. On the other hand, if for some time interval, it becomes negative, the dynamics is necessarily non-Markovian in its nature.

Thus, we have derived a class of master equations that can describe both Markovian as well as non-Markovian thermalization depending on the choice of $f(t)$ in the Hamiltonian.

For example, consider the non-Markovian $F(t)$ we have defined in equation (3.43). The corresponding $f(t)$ is calculated by taking the time derivative of $F(t)$,

$$f(t) = \frac{\pi}{2}e^{-t} + \frac{20\cos(20t)}{1+10t} - \frac{10\sin(20t)}{(1+10t)^2}$$

Using the above form, we can derive the master equation governing such a dynamics. It can be checked that the coefficients $\gamma_1(t)$ and $\gamma_2(t)$ will not be non-negative for all time in this case. Thus, it is seen to signify the non-Markovian nature of the dynamics.

In order to get some practical estimate for the “infinite time limit" to the thermalization associated with the non-Markovian qubit dynamics corresponding to the above choice of the pre-factor $f(t)$ of the two-qubit interaction Hamiltonian, it may be useful to start from a known version of a non-Markovian dynamics in the form of the equation we derive. Thereby, we can try to find out the corresponding form of the aforesaid pre-factor. This will, in turn, help us to understand the asymptotic behavior of this pre-factor in terms of the system parmeters.

It can also be seen that when we consider the $f(t)$ we originally derived given by equation (3.35), we recover the quantum optical master equation (3.4) with $\gamma_1(t)$ and $\gamma_2(t)$ reducing to the appropriate time-independent, positive coefficients.

3.6 Discussion

In the work detailed in this chapter, we have primarily considered a Markovian model of thermalization (quantum optical master equation). But, there exist non-Markovian models as well. Those models need not necessarily be simulatable through a single-qubit ancilla (mixed or pure). For example, if we consider the case of post-Markovian master equations as in [116, 117], we find that a single-qubit ancilla is insufficient to simulate the thermalization processes described therein.

In principle, the method we have employed can be used for finding simulating Hamiltonians in higher (finite) dimensions as well. It is non-trivial because the parametrization of unitary operators for higher dimensions aren't readily available as was the case for 2-qubit unitaries. Nevertheless, in the case of infinite dimensional systems (eg: quantum harmonic oscillators), covariance matrices can be employed to proceed in this direction. As a future project, it would be interesting to study simulating thermalizing Hamiltonians for single mode harmonic oscillator.

3.7 Chapter Summary

In this chapter, we have presented a study of thermalization of a two-level quantum system interacting with a thermal reservoir. We have derived a 2-qubit simulating Hamiltonian for the Markovian thermalization process described by the quantum optical master equation. Further, we considered the general form of such a Hamiltonian and studied conditions for exhibiting thermalization and Markovianity. We found that it is indeed possible for us to have non-Markovian thermalization processes even for the specific kind of Hamiltonian we have described in this chapter. We also derived a Lindblad-type master equation for system dynamics arising out of the Hamiltonian described in our work. We confirmed that it is possible to find the signature of non-Markovian dynamics based on the negativity of decoherence rates in the master equation.

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Thesis Highlight

Name of the Student: Prathik Cherian J
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Thesis Title: Beyond quantum nonlocality in continuous variable systems and thermalization of a qubit.
Discipline: Physical Sciences **Sub-Area of Discipline: Quantum Information**
Date of viva voce: 18/06/2020

The advent of quantum theory in the twentieth century, forever altered the way we understand the world around us. Quantum information theory is an attempt to both understand and use the properties of quantum theory such as nonlocality. One of the most important fields of study in quantum information theory is that of quantum correlations. This is largely an exercise in characterization and quantification of various types of quantum correlations. Broadly, one may look at quantum correlations in terms of kinematic and dynamic correlations. Kinematic correlations are those correlations that do not change in time (for example, measurement statistics obtained from spatially separated parties/observers) whereas dynamic correlations are those that continuously evolve in time (for example, the correlation between an open quantum system and its environment that evolves due to the system-environment interaction). We focus on both of these categories through the two parts of the thesis.

In the first part, we endeavor to study kinematic (continuous outcome) correlations that are nonlocal and beyond quantum theory (i.e. postquantum). In particular, we are interested in understanding how we can establish both nonlocality and postquantumness of multimode systems when continuous outcome correlations are considered. We develop a systematic approach to study postquantum nonlocal correlations for continuous outcome paradigm in multi-mode systems. We find that Robertson-Schrödinger (RS) uncertainty relation has a key role to play in this regard. We construct a class of continuous outcome postquantum nonlocal correlations for a generic m-mode scenario. While the nonlocality of the proposed class of correlations is certified through violation of Cavalcanti-Foster-Reid-Drummond (CFRD) inequalities, postquantum nature is guaranteed by the violation of RS uncertainty relation. This study can be of importance to uncover and understand the foundational principles of quantum theory.

In the second part, we study the dynamics of correlations between a two-level quantum system and its environment. In particular, we are interested in those open system dynamics which result in the thermalization of the system. The study of evolution of open systems towards equilibrium has always been a challenging problem in Statistical Mechanics. The difficulty lies in prescribing a form of interaction between the system and the environment at the microscopic level that will give rise to equilibration. We consider the quantum optical master equation which describes such a system-environment description. We find that by using an ancilla qubit in the appropriate thermal state, a two-qubit Hamiltonian can be used to successfully simulate the reduced system dynamics. For such Hamiltonians, we further study the classification of them being Markovian or non-Markovian. We also give examples of non-Markovian Hamiltonians that achieve thermalization. Finally, we derive a class of Lindblad-type master equations that can describe either Markovian or non-Markovian processes. Overall, this work can lead us to understand the process of thermalization better and thus, enhance our understanding of a major area in quantum thermodynamics.